A Computational Workbench Environment
For Virtual Power Plant Simulation

Final Report

Reporting Period Start Date: October 1, 2000
Reporting Period End Date: September 30, 2004

Mike Bockelie, REI
Dave Swensen, REI
Martin Denison, REI
Adel Sarofim, REI
Connie Senior, REI

December 22, 2004

DOE Cooperative Agreement No: DE-FC26-00NT41047

Reaction Engineering International
77 West 200 South, Suite 210
Salt Lake City, UT 84101

Disclaimer

“This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.”

Abstract

In this report is described the work effort to develop and demonstrate a software framework to support advanced process simulations to evaluate the performance of advanced power systems. Integrated into the framework are a broad range of models, analysis tools, and visualization methods that can be used for the plant evaluation. The framework provides a tightly integrated problem-solving environment, with plug-and-play functionality, and includes a hierarchy of models, ranging from fast running process models to detailed reacting CFD models. The framework places no inherent limitations on the type of physics that can be modeled, numerical techniques, or programming languages used to implement the equipment models, or the type or amount of data that can be exchanged between models. Tools are provided to analyze simulation results at multiple levels of detail, ranging from simple tabular outputs to advanced solution visualization methods. All models and tools communicate in a seamless manner. The framework can be coupled to other software frameworks that provide different modeling capabilities.

Three software frameworks were developed during the course of the project. The first framework focused on simulating the performance of the DOE Low Emissions Boiler System Proof of Concept facility, an advanced pulverized-coal combustion-based power plant. The second framework targeted simulating the performance of an Integrated coal Gasification Combined Cycle - Fuel Cell Turbine (IGCC-FCT) plant configuration. The coal gasifier models included both CFD and process models for the commercially dominant systems. Interfacing models to the framework was performed using VES-Open, and tests were performed to demonstrate interfacing CAPE-Open compliant models to the framework. The IGCC-FCT framework was subsequently extended to support Virtual Engineering concepts in which plant configurations can be constructed and interrogated in a three-dimensional, user-centered, interactive, immersive environment. The Virtual Engineering Framework (VEF), in effect a prototype framework, was developed through close collaboration with NETL supported research teams from Iowa State University Virtual Reality Applications Center (ISU-VRAC) and Carnegie Mellon University (CMU). The VEF is open source, compatible across systems ranging from inexpensive desktop PCs to large-scale, immersive facilities and provides support for heterogeneous distributed computing of plant simulations. The ability to compute plant economics through an interface that coupled the CMU IECM tool to the VEF was demonstrated, and the ability to couple the VEF to Aspen Plus, a commercial flowsheet modeling tool, was demonstrated. Models were interfaced to the framework using VES-Open. Tests were performed for interfacing CAPE-Open-compliant models to the framework. Where available, the developed models and plant simulations have been benchmarked against data from the open literature. The VEF has been installed at NETL.

The VEF provides simulation capabilities not available in commercial simulation tools. It provides DOE engineers, scientists, and decision makers with a flexible and extensible simulation system that can be used to reduce the time, technical risk, and cost to develop the next generation of advanced, coal-fired power systems that will have low emissions and high efficiency. Furthermore, the VEF provides a common simulation system that NETL can use to help manage Advanced Power Systems Research projects, including both combustion- and gasification-based technologies.

Table of Contents

Disclaimer	i
Abstract	ii
Table of Contents	iii
List of Figures	v
List of Tables	x
Acronyms and Abbreviations	xii
Executive Summary	1
1 Experimental Methods	3
1.1 Project Overview	3
1.1.1 Project Objectives	4
1.1.2 Relationship of the Year 1-4 Work Efforts	4
1.1.3 Project Team	8
1.1.4 Technology Transfer and Collaborations	9
1.1.5 Deliverables	11
1.1.6 Value to DOE	11
1.1.7 Technical Spin-offs	12
1.2 Framework Software	17
1.2.1 History of Development/Evolution of the Framework	17
1.2.2 SCIRun Frameworks	18
1.2.3 VE-Suite Framework	26
1.3 Framework Models	37
1.3.1 Models for LEBS-POC Framework	38
1.3.2 Models for IGCC-FCT and VEF Frameworks	49
2 Results and Discussion	134
2.1 Example Calculations – LEBS-POC Framework	134
2.1.1 LEBS-POC Steady-State Demonstration	134
2.1.2 LEBS-POC Transient Demonstration	136
2.2 Example Calculations – IGCC-FCT Framework and VEF	138
2.2.1 Process Engineering Entrained Flow Gasifier	139
2.2.2 CFD Entrained Flow Gasifier	156
2.2.3 Comparison of Process and CFD Entrained Flow Gasifier Model	174
2.2.4 Example Calculation: Soot and Tar Models for CFD Entrained Flow Gasifier	176
2.2.5 Impact of Coal Gasification Kinetics on CFD Gasifier Model Results	180
2.2.6 IGCC-FCT Simulations for Vision 21 Reference Configuration and Parametrics	182
2.2.7 VEF Simulation of Vision 21 Reference Configuration	195
2.2.8 Impact on Plant Efficiency of CGCU for Hg Removal	199
2.2.9 Demonstration of Coupling the VEF to the IECM Framework	201
2.2.10 Demonstration of Coupling the VEF to Aspen Plus	206
2.2.11 Demonstration of Using VES-Open for Advanced Data Passing	207
2.2.12 Time-Dependent CFD Simulation of Entrained Flow Gasifier	209
3 Conclusion	222

Reference	224
Appendix A – Component Software Issues for Advanced Power Plant Simulation and Engineering – Findings and Recommendations	232
Appendix B – VES-Open – IDL used in Virtual Engineering Framework.....	242
Appendix C – Virtual Engineering Framework User Guide.....	248
Appendix D – REI Reacting CFD Model Capabilities.....	334
Appendix E – RECOM Reacting CFD Model Capabilities	336
Appendix F – Entrained Flow Gasifier – Slagging Wall Model	339
Appendix G – Entrained Flow Gasifier – <i>PREKIN</i> – A Preprocessor for Modeling Coal Gasification Kinetics	351
Appendix H – Entrained Flow Gasifier – Soot and Tar Models	406
Appendix I – Modeling of Gas Turbine Combustors	413

List of Figures

Figure 1.1.1. Schematic showing REI, CMU, ISU roles for coordinated efforts	6
Figure 1.1.2. Example of 2D and 3D UI used for prototype VEF	7
Figure 1.1.3. Software Framework to support problem-solving environment for generating and validating reduced chemical kinetic mechanisms	13
Figure 1.1.4. Example of framework capabilities for modeling chemical weapons incinerators.	14
Figure 1.2.1. LEBS framework.....	19
Figure 1.2.2. Summary table.....	22
Figure 1.2.3. Graphical front end for the Global coal Database.....	24
Figure 1.2.4. Network display windows	25
Figure 1.2.5. Existing VEF software design.....	26
Figure 1.2.6. Advanced Power Simulation Framework Design	27
Figure 1.2.7. Details of the UI Design.....	28
Figure 1.2.8. Details of the Computational Engine Design.....	31
Figure 1.2.9. Interaction of Framework and Component Models	33
Figure 1.2.10. Accessing help menus within framework	35
Figure 1.3.1. Schematic of LEBS-POC system.....	38
Figure 1.3.2. UI for prototype LEBS-POC framework	39
Figure 1.3.3. For furnace CFD module, shown are examples of (a) input dialog boxes for specifying coal composition and air-fuel distribution and (b) Summary Data output and XY plots of the mean gas temperature in the upflow section of the the furnace	40
Figure 1.3.4. For upper furnace module, shown are example steamside circuit (left) and steam properties output from steamside model.....	43
Figure 1.3.5. For SCR module, (A) example input dialog box, (B) output dialog box and (C) 1D plot of predicted NO _x reduction along axis of SCR unit.....	44
Figure 1.3.6. For air heater module, shown are the input dialog window and Port Interrogation window when applied to the exit port for the preheated air	45
Figure 1.3.7. For baghouse module, shown are windows for input dialog box, summary output and 1D plot of time-dependent pressure drop including a cleaning event.	46
Figure 1.3.8. For ESP module, shown are windows for input dialog box and summary output..	47
Figure 1.3.9. Stack module's summary	48
Figure 1.3.10. Vision 21 reference configuration.....	49
Figure 1.3.11. Mass and energy balance sheet provided by DOE for Vision 21 reference configuration.....	51
Figure 1.3.12. Gasifier CFD models.....	54
Figure 1.3.13. Input UI and summary table output for entrained flow gasifier.....	58
Figure 1.3.14. Schematic for the one-stage entrained flow engineering process model	63
Figure 1.3.15. Schematic for the two-stage entrained flow engineering process model	64
Figure 1.3.16. Configuring gasifier process model for burnout calculations	65
Figure 1.3.17. Example inputs for flows for gasifier process model.....	65
Figure 1.3.18. Example output for engineering process gasifier model	66
Figure 1.3.19. Comparison of calculated and measured pressure drops across the riser in a circulating fluidized bed	69
Figure 1.3.20. Comparison of model predictions with design syngas composition	71

Figure 1.3.21. Predicted pressure drop and temperature profile in the PSDF	73
Figure 1.3.22. Predicted gas velocity in the PSDF	73
Figure 1.3.23. Predicted pressure drop and temperature profile in the transport reactor gasifier for a proposed 300 MW TRIG plant.....	75
Figure 1.3.24. Predicted gas velocity in the transport reactor gasifier for a proposed 300 MW TRIG plant.....	75
Figure 1.3.25. Defining a profile for transport reactor gasifier	76
Figure 1.3.26. Defining feed for transport reactor gasifier	77
Figure 1.3.27. Additional inputs for transport reactor gasifier	77
Figure 1.3.28. ASU model inputs	79
Figure 1.3.29. ASU output oxygen product stream	80
Figure 1.3.30. ASU energy balance output window.....	80
Figure 1.3.31. Recuperator module UI	82
Figure 1.3.32. Input panel and summary data for cyclone model	83
Figure 1.3.33. Elements of WGCU system	84
Figure 1.3.34. Input panel and summary data for chlorine bed guard model	86
Figure 1.3.35. Input panel and summary data for bulk desulfurizer model.....	89
Figure 1.3.36. Input panel and summary data for sulfur polisher model.....	90
Figure 1.3.37. Input panel and summary data for AGR model	93
Figure 1.3.38. Input panel and summary data for Carbon Bed model.....	96
Figure 1.3.39. Water gas shift equilibrium conversion for several initial compositions.....	98
Figure 1.3.40. Catalytic membrane reactor configuration.....	99
Figure 1.3.41. Schematic of staged-membrane reactor system	101
Figure 1.3.42. Predicted temperature profile	105
Figure 1.3.43. Predicted gas composition profiles.....	105
Figure 1.3.44. Predicted CO conversion and pressure driving force.....	105
Figure 1.3.45. Input panel and summary data for water gas shift membrane reactor model.....	106
Figure 1.3.46. Schematic of SOFC unit.....	109
Figure 1.3.47. Input panel and summary data for lumped parameter SOFC model	110
Figure 1.3.48. Input panel and summary data for 1D SOFC model	111
Figure 1.3.49. SOFC tail gas composition.....	113
Figure 1.3.50. Results of PFR tests for the high-pressure SOFC tail gas at two initial temperatures.....	114
Figure 1.3.51. PSR simulations of the high-pressure SOFC exhaust gas and a stoichiometric ethane-air flame for comparison.	115
Figure 1.3.52. Dump combustor parametric tests, based on Figure 1.3.53 conditions, with 99% fuel conversion	116
Figure 1.3.53. Input panel and summary data for dump combustor model.....	117
Figure 1.3.54. Processes in a single monolith channel	119
Figure 1.3.55. Input panel and summary data for catalytic combustor model	123
Figure 1.3.56. Input panel and summary data for compressor/expander model.....	124
Figure 1.3.57. Input panel for kinetic reactor model	128
Figure 1.3.58. Input panel and summary data for steam turbine model	129
Figure 1.3.59. Input panels for Gas Source module	130
Figure 1.3.60. Input panel for Gas Separator module.....	130
Figure 1.3.61. Input panel for Gas Splitter module	131

Figure 1.3.62. Input panel for Gas Feedback module.....	131
Figure 1.3.63. Input and output panels for Gas Heat Exchanger module.....	132
Figure 1.3.64. Input panel for Water Source module	132
Figure 1.3.65. Input and output panels for Water Pump module.....	132
Figure 1.3.66. Input panel for Condenser module	133
Figure 1.3.67. Input panel for Evaporation Cooler module.....	133
Figure 2.1.1. Gas temperature field (left) and particle trajectories (right) in lower section of LEBS-POC furnace.....	135
Figure 2.1.2. Furnace exit temperature as a function of time for transient turn-down to 50% load	137
Figure 2.1.3. Gas temperature field at three instances of time for transient simulation	137
Figure 2.2.1. Effect of H ₂ O/coal (daf) and O ₂ /coal (daf) on gasifier exit temperature (K).....	151
Figure 2.2.2. Effect of H ₂ O/coal and O ₂ /coal (daf) on cold-gas efficiency (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed)	151
Figure 2.2.3. Effect of H ₂ O/coal (daf) and O ₂ /coal (daf) on CO mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed)	152
Figure 2.2.4. Effect of H ₂ O/coal (daf) and O ₂ /coal (daf) on CO ₂ mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed)	152
Figure 2.2.5. Effect of H ₂ O/coal (daf) and O ₂ /coal (daf) on H ₂ mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed)	153
Figure 2.2.6. Effect of H ₂ O/coal (daf) and O ₂ /coal (daf) on H ₂ O mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed)	153
Figure 2.2.7. Effect of steam/coal (daf) and O ₂ /coal (daf) on gasifier exit temperature (K) (single-stage gasifier, 30 atm, Illinois #6 coal, dry feed)	154
Figure 2.2.8. Effect of steam/coal (daf) and O ₂ /coal (daf) on cold-gas efficiency (% HHV) (single-stage gasifier, 30 atm, Illinois #6 coal, dry feed)	154
Figure 2.2.9. Effect of O ₂ /coal (daf) on cold-gas efficiency for different coal (single-stage gasifier, 30 atm, dry feed, steam/coal (daf) = 0.10)	155
Figure 2.2.10. Schematic of single stage up fired gasifier and of process conditions	156
Figure 2.2.11. Comparisons of flowing slag model results	159
Figure 2.2.12. Slag model results displayed as 2D plots	160
Figure 2.2.13. Shown are gas temperature, axial velocity and H ₂ and CO concentration (mole fraction) for single stage, dry feed, upflow gasifier	161
Figure 2.2.14. Volatile mass fraction and char mass fraction for coal with initial diameter of 137 microns for single stage, dry feed, upflow gasifier.	161
Figure 2.2.15. Schematic of two-stage upflow configuration and process conditions	162
Figure 2.2.16. Predicted gas temperature and axial velocity at selected elevations for two-stage, slurry-feed, upflow gasifier	163
Figure 2.2.17. Shown are predicted major gas species (vol. %) at selected elevations for two stage, slurry feed, upflow gasifier	164
Figure 2.2.18. Shown are coal volatile mass fraction, char mass fraction and water droplets for selected particle and droplet sizes for two stage, slurry feed, upflow gasifier	164
Figure 2.2.19. Plots of predicted gas temperature, major species concentration, cold gas efficiency and carbon conversion versus axial position for two stage, slurry feed, upflow gasifier	165
Figure 2.2.20. Shown are the predicted molten (liquid) slag thickness, solid slag thickness	

and surface temperature from the flowing slag model for a two stage, slurry feed, upflow gasifier	166
Figure 2.2.21. One-stage, slurry-feed downflow gasifier and process conditions.....	169
Figure 2.2.22. Shown for the one stage, slurry feed downflow gasifier are the predicted gas temperature and axial velocity at selected elevations.....	170
Figure 2.2.23. Shown are the predicted major gas species concentration (vol.%) at selected elevations for single stage, slurry feed, downflow gasifier	171
Figure 2.2.24. Shown for the one stage, slurry feed, downflow gasifier firing Illinois #6 are the gas temperature, CO and H ₂ species concentrations at selected planes	173
Figure 2.2.25. Shown for the one stage, slurry feed, downflow gasifier firing Petcoke are the gas temperature, CO and H ₂ species concentrations at selected planes	173
Figure 2.2.26 Gas temperature and velocity distribution comparisons between the soot correlation model and the soot and tar model	177
Figure 2.2.27. Comparison of oxygen distribution between the soot correlation model and the soot and tar model	177
Figure 2.2.28. Comparison of CO and H ₂ distributions between the soot correlation model and the soot and tar model	178
Figure 2.2.29. Comparison of soot volume fraction distribution between the soot correlation model and the soot and tar model. Tar mass fraction from soot and tar model	178
Figure 2.2.30. Net Wall Radiative Heat Flux Comparison between Soot Correlation and the Soot and Tar Model	179
Figure 2.2.31 Comparison of gas temperature and oxygen distribution for using kinetics from [Lupa and Kliesch, 1979]	181
Figure 2.2.32. UI for IGCC-FCT representation of Vision 21 reference configuration	183
Figure 2.2.33. Predicted plant efficiency for Vision 21 reference configuration	185
Figure 2.2.34. Predicted net power generated by main components in Vision 21 reference configuration	186
Figure 2.2.35. Example plot from IGCC-FCT framework of changes in user selected variable (gas temperature) through the Vision 21 reference plant configuration	187
Figure 2.2.36. Example plot from IGCC-FCT framework for changes in user selected variable through the Vision 21 reference plant configuration	188
Figure 2.2.37. Comparison of net power generation for the baseline network and three other configurations	189
Figure 2.2.38. Comparison of net plant power generation for different fuels	190
Figure 2.2.39. Comparison of power generation for dry and slurry feeds for the one-stage downflow and two-stage upflow gasifier.	191
Figure 2.2.40. Predicted plant efficiency trends for parametric variations of the Vision 21 reference configuration	192
Figure 2.2.41. Predicted plant power generation trends for parametric variations of the Vision 21 reference configuration	193
Figure 2.2.42. UI for the VE-Suite based VEF operating on a 2D screen. Shown is the Vision 21 reference configuration	196
Figure 2.2.43 Gasifier summary information in SCIRun and VE-Suite based VEF	198
Figure 2.2.44. WGPU configuration with three possible locations of the carbon bed Hg removal unit	200
Figure 2.2.45. Framework UI	202

Figure 2.2.46. Framework UI connection and execution pull down menus	203
Figure 2.2.47. Framework UI pre-configured networks	203
Figure 2.2.48. Virtual Reality pre-configured networks representation	204
Figure 2.2.49. Sample Framework UI GUI	204
Figure 2.2.50. Framework Plant Results	205
Figure 2.2.51. Framework Port Data Results	205
Figure 2.2.52. REI Gasifier model	206
Figure 2.2.53. Three CFD models connected in series	207
Figure 2.2.54. Profile data being passed between the CFD models	208
Figure 2.2.55. Interacting with coupled CFD models in virtual engineering space	208
Figure 2.2.56. Two-stage industrial gasifier configuration and geometry model	209
Figure 2.2.57. Average profiles of major species concentrations over gasifier height.	209
Figure 2.2.58. Profiles of average and peak temperature over gasifier height.	209
Figure 2.2.59. Results of inner, near wall, and mean CO concentrations (t=0.2s).	214
Figure 2.2.60. Results of inner, near wall, and mean temperature (t=0.2s).	214
Figure 2.2.61 Results of inner, near wall, and mean CO concentrations (t=0.3s).	215
Figure 2.2.62. Results of inner, near wall, and mean temperature (t=0.3s).	215
Figure 2.2.63. Results of inner, near wall, and mean CO concentrations (t=0.4s).	216
Figure 2.2.64. Results of inner, near wall, and mean temperature (t=0.4s).	216
Figure 2.2.65. Results of inner, near wall, and mean CO concentrations (t=0.5s).	217
Figure 2.2.66. Results of inner, near wall, and mean temperature (t=0.5s).	217
Figure 2.2.67. Results of inner, near wall, and mean CO-concentrations (t=0.6s).	218
Figure 2.2.68. Results of inner, near wall, and mean temperature (t=0.6s).	218
Figure 2.2.69. Results of inner, near wall, and mean CO concentrations (t=0.8s).	219
Figure 2.2.70. Results of inner, near wall, and mean temperature (t=0.8s).	219
Figure 2.2.71. Results of inner, near wall, and mean CO concentrations (t=1.0s).	220
Figure 2.2.72. Results of inner, near wall, and mean temperature (t=1.0s).	220
Figure 2.2.73. Results of inner, near wall, and mean CO-concentrations (t=2.0s).	221
Figure 2.2.74. Results of inner, near wall, and mean temperature (t=2.0s).	221

List of Tables

Table 1.3.1. Provided Operating Conditions For Vision 21 Energyplex	50
Table 1.3.2. Illinois Coal #6 Description.....	50
Table 1.3.3. Kinetic Rate Expressions Used In <i>AIOLOS</i> Model	60
Table 1.3.4. PSDF Operating Conditions Used For Benchmarking.....	70
Table 1.3.5. Operating Conditions Used For Benchmarking Transport Reactor Gasifier.....	72
Table 1.3.6. Comparison Of Syngas Composition Predicted By Transport Reactor Gasifier Model With Measured Values For The PSDF.....	72
Table 1.3.7. Comparison Of Predicted And Design Syngas Composition For 300 MW TRIG Plant.....	74
Table 1.3.8. ASU Types And Their Capacities	78
Table 1.3.9. Sulfur Removal Requirements For Syngas Applications	85
Table 1.3.10. Summary Of Default Values For Gas Clean Up Units.....	85
Table 1.3.11. Gasifier Product Composition	99
Table 1.3.12. Sample Simulation Inputs And Results	104
Table 1.3.13 Detailed Surface Mechanism For Reaction Of H ₂ And CO On Platinum	121
Table 2.1.1. Comparison Of Predicted Values For Baseline Firing Conditions And For Turning Off The OFA And Coal Return.	135
Table 2.2.1. Comparison Of Process Gasifier Model With Reported Data For Tampa Electric Gasifier	139
Table 2.2.2. Comparison Of Process (0D) Model Results With Reported Data For Wabash River Gasifier	140
Table 2.2.3. Comparison Of Process (0D) Model Results With Design Data [Black & Veatch, 1994]	141
Table 2.2.4. Syngas Composition After Cooling To 500 K	142
Table 2.2.5. Operating Conditions And Fuel Properties For The Cool Water Gasifier	143
Table 2.2.6. Comparison Of Process (0D) Model Results With Reported Cool Water Gasifier Data.	144
Table 2.2.7. Operating Conditions For The Shell Gasifiers	145
Table 2.2.8. Model Predictions In Comparison With Reported Data	145
Table 2.2.9. Effect Of Heat Extraction On Gas Composition, Exit Temperature, And Cold Gas Efficiency (Carbon Conversion Maintained Constant).	146
Table 2.2.10. Effect Of Pressure On Gasifier Performance For A Fixed Carbon Conversion. .	147
Table 2.2.11. Effect Of Slurry Concentration On Gasifier Performance For A Fixed Carbon Conversion.	148
Table 2.2.12. Effect Of Carbon Conversion On Gasifier Performance.	148
Table 2.2.13. Temperatures Of Critical Viscosity For Different Coals.	150
Table 2.2.14 Comparison Of Predicted Values For Single Stage, Dry Feed Upflow Gasifier. .	158
Table 2.2.15. Two-Stage Gasifier Comparison	167
Table 2.2.16. Two Stage Gasifier Performance For Firing Illinois #6 Versus Petcoke.	168
Table 2.2.17. Predicted Exit Values For One Stage, Slurry Fed, Downflow Gasifier.	172
Table 2.2.18. One Stage, Slurry Fed, Downflow Gasifier Comparison Of Firing Illinois #6 Versus Petcoke.	174
Table 2.2.19. Results Based On The Process Model.	175
Table 2.2.20. CFD Simulation Results (Same Operating Conditions As In Table 2.2.19).	176

Table 2.2.21. Exit Temperature And Composition Comparison Between Soot Correlation And The Soot And Tar Model.	179
Table 2.2.22. Global Gasification Kinetic Parameters.	180
Table 2.2.23. Fuel Properties For IGCC-FCT Simulations	184
Table 2.2.24. Entrained Flow Gasifier Conditions For IGCC-FCT Simulations	184
Table 2.2.25. Comparison Of Predicted Values For SCIRun Based IGCC-FCT Framework And VE-Suite Based VEF For Vision 21 Reference Configuration.	197
Table 2.2.26. Comparison Of Predicted Power Values For SCIRun Based IGCC-FCT Framework And VE-Suite Based VEF For Vision 21 Reference Configuration.	197
Table 2.2.27. Comparison Of Overall Plant Performance For The SCIRun Based IGCC-FCT Framework (Left) And VE-Suite Based VEF Framework (Right) For The Vision 21 Reference Configuration	199
Table 2.2.28 Predicted Plant Efficiencies.....	201
Table 2.2.29 Fuel Properties Of Illinois Coal #6	210
Table 2.2.30 Two-Stage Gasifier Exit Conditions Predicted By <i>AIOLOS</i> And <i>GLACIER</i>	211
Table 2.2.31 Time Marching Arrangement For The Two-Stage Gasifier Start-Up Scenario	212

Acronyms and Abbreviations

AGR	Acid Gas Removal
ASU	Air Separation Unit
BTU	British Thermal Unit
CAPE-Open	Component Architecture for Process Engineering Open Standard
CA	Component Architecture
CCA	Common Component Architecture
CCSD	Center for Coal Sustainable Development (Australia)
CFB	Circulating Fluidized Bed
CFD	Computational Fluid Dynamics
CGB	Chlorine Guard Bed
CGCU	Cold Gas Clean Up
CGE	Cold Gas Efficiency
CMU	Carnegie Mellon University
COM	Component Object Model
CORBA	Common Object Request Broker Architecture
CPD	Chemical Percolation Devolatilization
CSIRO	Commonwealth Scientific and Industrial Research Organization
DCOM	DistributedCOM
DLL	Dynamic Linking Library
DLN	Dry Low-NO _x
DOE	Department of Energy
EDC	Eddy Dissipation Concept
EPA	US Environmental Protection Agency
EPRI	Electric Power Research Institute
FutureGen	DOE FutureGen Program
GE	General Electric
GT	Gas Fired Combustion Turbine
GUI	Graphical User Interface
HHV	Higher Heating Value
HPC	High Performance Computing
IDL	Interface Definition Language
IEA	International Energy Agency
IECM	Integrated Environmental Control Model
IGCC	Integrated coal Gasification Combined Cycle
IGCC-FCT	IGCC with a FCT power block
ISU	Iowa State University
ISU-VRAC	Iowa State University Virtual Reality Applications Center
IVD	Institute of Process Engineering and Power Plant Technology
KBR	Kellog Brown Root
LEBS-POC	DOE Low Emissions Boiler System Proof of Concept
L-GPL	Library General Public License

MWe	Megawatt Electric
NETL	National Energy Technology Laboratory
NFCRC	National Fuel Center Research Center
NSF	National Science Foundation
ODE	Ordinary Differential Equation
OMG	Object Management Group
PFR	Plug Flow Reactor
PSDF	Process Simulation Development Facility
PSM	Power Systems Manufacturing
PSR	Perfectly Stirred Reactors
RECOM	Reaction and Combustion Modeling Services
REKS	Reaction Engineering Kinetics Solver
SCFM	Standard Cubic Feet per Minute
SCI	Scientific and Computational Imaging
SIDL	Scientific Interface Definition Language
SOFC	Solid Oxide Fuel Cell
SVN	Subversion open source versioning software
TAO	The ACE ORB
TPD	Tons Per Day
UI	User Interface
V21	DOE Vision 21 Program
VEF	Virtual Engineering Framework
VES-Open	VE-Suite-Open
VE-Suite	Virtual Engineering Suite
VR	Virtual Reality
WGPU	Warm Gas Clean Up
0D	Zero-Dimensional
1D	One-Dimensional
2D	Two-Dimensional
3D	Three-Dimensional

Executive Summary

The work conducted in this project received funding from the Department of Energy under Cooperative Agreement No: DE-FC26-00NT41047. The period of performance for the project spanned four years, from October 1, 2000 to September 30, 2004.

Computer simulation will play an important role in developing and deploying the next generation of Advanced Power Generation Systems. To reduce the time, cost and technical risk of evaluating the different possible near zero-emission, multi-product energyplex plant configurations will require assessment tools with modeling capabilities that go far beyond the tools traditionally used. Furthermore, it will be important that the plant configurations be able to assess the use of opportunity fuels. In particular, the use of coal as a primary fuel will be needed. Coal is an abundant, inexpensive, and secure source of fuel within the USA.

In this project, Reaction Engineering International (REI) has successfully developed and demonstrated an advanced process workbench, or *software framework*, for integrating a broad range of models, analysis tools, and visualization methods for evaluating the performance of Advanced Power Generation Systems. The framework provides a tightly integrated problem-solving environment, with plug and play functionality, and includes a hierarchy of models, ranging from fast running process models to detailed reacting Computational Fluid Dynamics (CFD) models. The framework places no inherent limitations on the type of physics that can be modeled, numerical techniques or programming languages used to implement the equipment models, or the type or amount of data that can be exchanged between models. Tools are provided to analyze simulation results at multiple levels of detail, ranging from simple tabular outputs to advanced visualization methods commonly used in CFD analysis. By design, the framework provides seamless communication between all models and tools.

The focus and capabilities of the framework have evolved during the course of the project.

- Initial efforts focused on creating a framework for simulating the DOE Low Emissions Boiler System Proof of Concept (LEBS-POC) facility, an advanced pulverized-coal combustion-based power plant.
- Subsequent efforts focused on developing a framework to simulate an Integrated coal Gasification Combined Cycle - Fuel Cell Turbine (IGCC-FCT) plant configuration. This work effort involved developing models for coal gasifiers and numerous pieces of downstream equipment. The coal gasifier models included in the framework include CFD and process models with state-of-the-art capabilities for the commercially dominant systems. Interfacing models to the framework was identified as an important feature of the framework; proof-of-concept tests were conducted for using CAPE-Open, and software support was provided for using VES-Open to interface models to the framework.
- Through funding from a budget revision, the IGCC-FCT framework was extended to support Virtual Engineering concepts in which plant configurations can be constructed and interrogated in a three-dimensional (3D), user-centered, interactive, immersive environment. The Virtual Engineering Framework (VEF) was developed in close collaboration with NETL supported research teams from Iowa State University Virtual Reality Applications Center (ISU) and Carnegie Mellon University (CMU). The VEF is

open source, compatible across systems ranging from inexpensive desktop PCs to large-scale, immersive facilities, and provides support for heterogeneous distributed computing of plant simulations. The ability to compute plant economics through an interface that coupled the CMU IECM tool to the VEF was demonstrated. Likewise, the ability to couple the VEF to Aspen Plus, a commercial flowsheet modeling, was also demonstrated. Software support is included for interfacing models to the framework with VES-Open. CAPE-Open-compliant models can be interfaced to the framework by using VES-Open.

Throughout the course of the project, evaluations and comparisons to available data have been performed for individual equipment components and of overall plant performance to build confidence in the developed models and analysis capability.

The project has been quite successful. The frameworks provide simulation capabilities not available in currently available commercial tools. The functionality and capabilities provided by the frameworks, as well as model validation results, have been highlighted through participation at NETL-sponsored technical conferences focused on coal utilization and gasification, NETL program workshops and NETL program reviews, and project-specific meetings held between REI and NETL personnel. The software frameworks, including the component models, have been installed at NETL and training provided to NETL personnel. Results from the simulations performed during this project have been used in discussions with personnel from the gasification industry to provide guidance and suggestions on equipment design and operational improvements. Likewise, the results of this project have been used in discussions with electric utility personnel and fuel suppliers to the utility industry for IGCC issues. In addition to advanced power systems, REI has successfully reused software elements and lessons learned from the frameworks created in this project to develop frameworks for addressing problems in other industries and other applications. Discussions with a potential commercialization partner for the framework are in progress.

NETL will benefit in several ways from the software frameworks and plant performance modeling capability developed in this project. The frameworks represent an important next step toward the ultimate goal for simulation for the NETL Advanced Research program - a fully integrated environment for performing dynamic plant simulation and engineering, which DOE has targeted to achieve by 2010. The frameworks also provide DOE with a mechanism to enable and foster collaborations amongst a broad range of Vision 21 and other virtual power plant researchers from universities, industry, or DOE, whether US based or International. Last, other DOE programs focused on advanced power generation systems can benefit from the developed software frameworks. With little effort, the VEF can be extended to support Ultra Super Critical (USC) boiler development or the proposed FutureGen initiative that would encompass hydrogen production and CO₂ capture and sequestration in addition to gasification.

As per the DOE reporting instructions, the remainder of this report is organized as follows:

- Chapter 1 - Experimental Methods, which includes sections describing an overview of the program, the software infrastructure, and model development efforts;
- Chapter 2 - Results and Discussion, which highlights usage of the framework and models to perform simulations; and
- Chapter 3 - Conclusions.

In addition, several appendices are attached that provide additional details on specific topics.

Chapter 1 - Experimental Methods

Within this chapter we present discussions on the main tasks addressed in developing the frameworks. The discussion is organized as follows:

- project overview;
- software infrastructure used for the frameworks; and
- models included in the frameworks.

In this report, emphasis is placed on the development of the IGCC-FCT and Virtual Engineering (VEF) frameworks. The LEBS POC was in effect a “stepping stone” to the later frameworks and thus is not described to the same level of detail.

1.1 Project Overview

The US Department of Energy (DOE) National Energy Technology Laboratory (NETL) is facilitating the development of future zero-emissions, high-efficiency *polygeneration* plants. These plant concepts could potentially include co-production, from fossil fuels and opportunity fuels, of a broad mix of power, heat, transportation fuels, and chemical products using a broad range of plant sizes and configurations. For many of the proposed concepts, Integrated coal Gasification Combined Cycle (IGCC) technology is a key technology within the plant. Virtual simulation will play an important role in the evaluation of different plant configurations under consideration. New assessment tools with advanced simulation capabilities are needed to reduce the time, cost, and technical risk to develop, deploy, and bring on-line these advanced plants [DOE,1999], [Stiegel, 2001], [Holt, 2004], [Boras, 2004]. As discussed at DOE-sponsored meetings (e.g., DOE Vision 21 held at Iowa State University (ISU) in November, 2002), the simulation tools must be extensible and flexible software environments that can support a broad range of plant engineering analyses.

To address this need, Reaction Engineering International (REI) has developed advanced process simulation workbenches that provide a software *framework* for integrating the hierarchy of models and visualization tools for performing simulations of polygeneration plants. By design, the framework supports the use of Computational Fluid Dynamic (CFD) and reactor (mass/energy balance) models. Likewise, the frameworks provide a user-friendly environment with snap-and-build functionality and a broad range of visualization and analysis capabilities for interrogating simulation results of individual components and overall plant simulations. The capabilities of the frameworks evolved during the course of the project. Our initial effort focused on developing a prototype framework for a conventional pulverized-coal combustion plant, the DOE Low Emissions Boiler System Proof-of-Concept (LEBS-POC) facility. Subsequent efforts focused on creating a framework to simulate an Integrated coal Gasification Combined Cycle Fuel Cell Turbine (IGCC-FCT) plant. During the final year of the project, through coordinated efforts with DOE-NETL funded projects at Carnegie Mellon University (CMU) and Iowa State University (ISU), REI developed a prototype framework that uses Virtual Engineering concepts. The Virtual Engineering Framework (VEF) allows simulations to be constructed and interrogated within a 3D, user-centered, interactive, immersive environment. The VEF utilizes the VE-Suite software developed at ISU and thus is open source and is compatible across systems ranging from PCs to large-scale, immersive facilities. A proof-of-concept coupling was implemented between the VEF and a second simulation framework, the *Vision 21 Planner* developed at CMU, which provided access to a library of fast running, reduced-order models for

plant components and models for plant economics. Likewise, a proof-of-concept testing was performed for coupling the framework to flowsheet tools, such as Aspen Plus. Models can be interfaced to the framework using VES-Open, and CAPE-Open-compliant models can also be interfaced to the framework through using VES-Open.

In the following, provided in order are summaries of the:

- project objectives;
- relationship of the work efforts for the three frameworks developed during the course of the project;
- project team members;
- technology transfer efforts;
- software delivered to NETL;
- value of the project to DOE; and
- technical spinoffs .

1.1.1 Project Objectives

The objective of this project was to develop and demonstrate a software framework that contains a hierarchy of models that can be used to perform simulations and visualize results for evaluating individual component models as well as overall plant performance. During the course of the project, the role and requirements for simulation within the DOE Vision 21 program evolved significantly. In response to these changes, REI adjusted its development efforts so that the final work product would better meet DOE's needs and objectives. Compared to currently available commercial tools, the VEF (the final work product of the project) provides a substantial increase in flexibility, ease of use, model selection, solution interrogation and simulation sophistication.

1.1.2 Relationship of the Year 1 – 4 Work Efforts

The work conducted in this project received funding through a targeted solicitation by NETL to develop modeling capabilities in support of the DOE Vision 21 program. The original period of performance for the project spanned three years, from October 1, 2000 to September 30, 2003. As the end of the original three year effort was drawing to a close, a natural and in-scope enhancement to the final product of the original three year effort became evident. REI requested and was granted a budget revision that allowed for 12 months of continued effort which resulted in the final work product, a prototype VEF.

Over the course of the four year project, three frameworks were developed. Each framework was an evolutionary step from the previous and made extensive use of the lessons learned from the previous work effort.

LEBS-POC framework

The Year One effort focused on developing a prototype framework for the LEBS-POC design, which is based on pulverized-coal combustion technology. The framework included a hierarchy of models for the system. The LEBS POC is a system that REI is familiar with due to having previously provided modeling support to the DOE-funded program. Thus, the LEBS POC provided an opportunity to quickly evaluate software design issues for the framework. The prototype framework used a CFD model for the radiant furnace box (a down-fired, slagging, J-shaped unit). Mass/energy balance process models were implemented to simulate steam

generation, the air preheater, NO_x reduction with a Selective Catalytic Reduction (SCR) unit and particulate removal using a baghouse or an Electric Static Precipitator (ESP). The framework was constructed using the SCIRun software system. SCIRun is a continuously evolving product of the Scientific and Computational Imaging (SCI) Institute of the University of Utah Computer Science Department [<http://www.sci.utah.edu>]. The SCI institute is headed by Prof. Chris Johnson, a recognized authority in the development of problem-solving environments for multiphysics applications. From inception, SCIRun was designed in an object-oriented manner with the intent of supporting interdisciplinary projects in which High-Performance Computing (HPC) models are needed. The framework was exercised through simulations of different firing conditions [Bockelie et al, 2001abc, 2002a,b].

IGCC-FCT framework

The Year Two and Year Three efforts developed a more advanced SCIRun-based framework environment for simulating an Integrated coal Gasification Combined Cycle-based (IGCC) Vision 21 energypex configuration. The Year two effort focused primarily on software enhancement, model development, and model implementation. The Year Three effort focused on continued development of the framework environment and application of the framework to Vision 21 plant configurations. Based on a request to DOE, REI was provided a reference IGCC plant configuration that used a hybrid power block based on a Fuel Cell – Turbine combination (IGCC-FCT). Models were developed for entrained flow and transport reactor coal gasifiers, gas clean up, heat exchanger equipment (with kinetics for water gas shift reactions), “balance of plant” equipment, and a hybrid power block that contains a solid oxide fuel cell (SOFC), turbine and fuel cell tail gas combustors (simple dump combustor or catalytic combustor). Models for shift reactors to concentrate and/or separate gas streams, such as for CO₂ capture, are also available. Both CFD and reactor (mass/energy balance) models are included. Within this effort, several improvements to the SCIRun software system were implemented to better support low-cost virtual reality visualization of CFD model results, remote computing of computationally intensive models and advanced model interfaces that don’t limit the quantity of data to be passed between models. The framework provided a user-friendly environment with plug-and-play functionality, a broad range of visualization and analysis capabilities for interrogating simulation results of individual components and overall plant simulations [Bockelie, 2002-2004]. Models are interfaced to the framework using VES-Open [<http://www.vrac.iastate.edu/~kmbryden/vesuite/vesopen.htm>], an open-source interface available within VE-Suite, which was jointly developed by REI and researchers at the ISU Virtual Reality Applications Center. The framework supports heterogeneous distributed computing, allowing models to be executed on remote computing resources (e.g., single computers or clusters accessible via a network). Last, the framework includes a web-based help system with HTML pages containing documentation of the models and their use.

Virtual Engineering Framework (VEF)

Within the Year Four effort, REI coordinated its efforts closely with NETL-funded projects at the ISU Virtual Reality Applications Center (ISU, Program Manager = Prof. Mark Bryden) and CMU (CMU, Program Manager = Prof. Ed Rubin) that are developing tools to support simulations and evaluations of advanced power generation systems (see Figure 1.1.1).

Figure 1.1.1. Schematic showing REI, CMU, ISU roles for coordinated efforts.

The coordinated effort resulted in a prototype VEF that utilizes Virtual Engineering Suite (VESuite), an open-source library of tools from ISU that enables the engineering analysis and design process to take place in a virtual environment and provides support for a broad range of advanced computing capabilities. The VEF provides support to construct and interrogate plant configurations with a snap-and-build approach in a 3D, user-centered, interactive, immersive environment (see Figure 1.1.2).

By design, the VEF is open source, compatible across systems ranging from inexpensive desktop PCs (using “3D glasses”) to large-scale, immersive facilities, and provides support for heterogeneous distributed computing of models contained in the plant configuration. To support analysis of plant economics, the framework was interfaced to a second framework – the CMU Integrated Environmental Control Model (IECM) financial planner, which provides access to a library of fast running, reduced-order models for plant components and models for plant economics (note: the VEF and IECM coupling was implemented as proof of concept only). The VEF contains the models needed to simulate an IGCC-FCT plant. The VEF supports the VES-Open model interfacing protocol, and CAPE-Open-compliant models can be interfaced to the framework using VES-Open. A simple coupling of the VEF to Aspen Plus, a commercially available flowsheet modeling tool, was implemented for proof-of-concept testing; this capability allows leveraging the many Aspen Plus flowsheets for plant configurations that have been developed by NETL researchers or NETL-funded projects. The VEF was intended as a prototype framework, and thus only the critical models and capabilities provided by the IGCC-FCT were ported to the VEF.

The VEF was demonstrated in a joint podium presentation at the Clearwater Conference 2004 [Rubin et al., 2004] using a passive-stereo virtual-reality (single) wall, a Linux cluster and a Windows-based tablet-PC. Individualized demonstrations of the VEF were conducted at the REI conference exhibit booth, which was coordinated with the NETL exhibit space to allow use of the single-wall visualization system, some of which also highlighted using VEF on inexpensive,

desktop PC equipment (containing stereo graphics). Additional demonstrations of the VEF are planned for the SuperComputing 2004 conference to be held in November, 2004 [Swensen, 2004]. The VEF has been installed at NETL.

Figure 1.1.2. Example of 2D and 3D UI used for prototype VEF.

1.1.3 Project Team

Project team members from REI included experienced combustion scientists and applications engineers that focused on developing the equipment models, and computer scientists and software engineers that focused on developing the software framework. The senior personnel from REI involved with the project included:

- Dr. Mike Bockelie (REI, Executive Vice President) was the Project Manager;
- Prof. Adel Sarofim (REI, Sr. Technical Advisor and University of Utah), an authority in industrial combustion and heat transfer, provided guidance on the development, benchmarking and proper use of many equipment models;
- Dr. Martin Denison (REI, Sr. Engineer) was lead engineer for developing the reacting CFD and process models used in the frameworks;
- Dr. Connie Senior (REI, Manager, Engineering Processes), an expert in air toxics issues, guided the effort on gas clean up and Hg capture; and
- Mr. Dave Swensen (REI, Manager, Computational Technologies) was the principal architect of the software frameworks and leads the software development and integration team.

The REI senior personnel were assisted by members of the REI Technical Staff as needed.

REI was assisted by several personnel through the course of the project.

- Mr. Neville Holt, Manager for Advanced Coal Generation Technology and Generation Development at the Electric Power Research Institute (EPRI) and head of the Gasification Users Association, an industry-based consortium of gasifier operators, is an internationally recognized expert in IGCC systems. Mr. Holt provided guidance on trends in the gasification industry, selection of simulations of industrial interest, and guidance on whether simulation results were in agreement with the accepted industry knowledge base.
- Prof. Chris Johnson and Dr. Steve Parker, University of Utah Scientific Computing and Imaging Institute and Visual Influence, Inc., provided guidance on the development of software frameworks, use of component architectures for interfacing models and analysis tools to frameworks, and the use of SCIRun.
- Prof. Terry Wall, Prof. John Stubington, Dr. David Harris and Dr. John Patterson of the Center for Coal Sustainable Development (CCSD) in Australia provided guidance, kinetics data and submodels relevant to coal gasification.
- Dr. Bene Risio, President, Reaction and Combustion Modeling Services (RECOM), provided CFD modeling for time-dependent and selected steady-state simulations. In addition, through RECOM, Prof. Klaus Hein, of the Institute of Process Engineering and Power Plant Technology (IVD) at the University of Stuttgart, provided guidance on coal gasifier issues.
- Prof. Leon Glicksman, Massachusetts Institute of Technology, provided guidance on fluidized bed modeling.
- Dr. Steve Freedman, consultant, provided guidance on direct-fired combustion turbines.
- In the last year of the project, REI worked closely with collaborators Prof. Ed Rubin and Mr. Mike Berkenpas (CMU) and Prof. Mark Bryden and Mr. Doug McCorkle (ISU). The coordinated effort resulted in the development of a prototype software framework based on Virtual Engineering methods (VEF) that used software elements from ISU and CMU.

1.1.4 Technology Transfer and Collaborations

The improved simulation capability provided by the LEBS-POC, IGCC-FCT, and VEF frameworks have been reported in the open literature at technical conferences and in NETL meetings. Presentations have been provided that

- focused on the models and the improved plant performance modeling capability provided by the developed frameworks [Bockelie et al., 2001-2005], [Denison et al., 2003], [Rubin et al., 2004], [Sarofim et al., 2004] and
- focused on the details of the software infrastructure on which the frameworks are built [Swensen et al., 2002-2005].

To enhance technology transfer to NETL, presentations have been provided at NETL-sponsored Program Reviews [Bockelie et al., 2001c] and NETL-sponsored Workshops [Bockelie et al., 2002e] and in project briefings held at NETL between REI and NETL personnel.

Demonstrations to highlight the capabilities of the developed frameworks, in particular the VEF, have been provided at the Clearwater Conference 2004 in a joint presentation within a technical session [Rubin et al., 2004] and in one-on-one demonstrations within REI's exhibit booth which was coordinated with a NETL exhibit booth. Demonstrations were also provided at the SuperComputing 2004 conference held in Pittsburgh [Swensen et al., 2004].

Discussions (seminars) have been provided to a US-based coal company and to electric utility research organizations from countries along the Pacific Rim that are interested in learning more about IGCC, advanced power plant concepts, practical issues on commercially available coal gasifiers, and how virtual simulation can assist them in technology development and/or selection.

Academic and Industrial Collaborations

REI and NETL have benefited from the collaborations REI instigated during the course of this project. In the collaborative efforts, each organization has covered their own costs associated with the collaborations. The collaborative efforts were summarized within the Technical Progress Reports provided to NETL on a quarterly basis. The following briefly summarizes the collaborative efforts:

- **Iowa State University Virtual Reality Applications Center (ISU-VRAC).** This effort has been facilitated through Prof. Bryden, who has been involved in the REI Vision 21 project from inception. The initial collaborative effort focused on REI and ISU technical staffs exchanging information and improved source code for software elements within the ISU VE-Suite software package. Within this effort, REI provided ISU with "alpha" versions of the IGCC-FCT framework for their own use, primarily testing of ISU visualization software and REI models. In Year 4 of this project, the REI technical staff worked closely with ISU to develop the VEF within VE-Suite.
- **Carnegie Mellon University (CMU).** Initially, this effort focused on REI and CMU technical staffs exchanging information on gasifier operation and modeling issues. In Year 4 of this project, the REI technical staff worked closely with CMU to implement a coupling between the VEF and the Vision 21 Planner tool, a framework that includes fast running process models developed using response surface methods applied to mass/energy balance models for IGCC systems, and includes financial models that can provide fast estimates for plant economics. In addition, during Year 4, the REI and CMU personnel exchanged information on gasifier model results for selected cases.

- **Collaborative Research Center for Coal and Sustainable Development (CCSD)** in Australia. The CCSD collaborated in REI's development of the flowing slag model used in the entrained flow gasifier model contained in the IGCC-FCT framework and VEF, general issues on coal gasification kinetics and specifically on intrinsic kinetics for char gasification. In return, REI provided the CCSD with an alpha version of the IGCC-FCT framework for testing (de-bugging) and use on CCSD-funded projects. This collaborative effort was performed through a Memo of Understanding (MOU) between REI and the CCSD.
- **NETL Researchers.** During the course of the project REI has collaborated with several NETL researchers to highlight to them how the work being performed by REI can benefit their own projects at NETL.
- **Fluent-AspenTech-Alstom Vision 21 project team.** A series of pre-competitive discussions have been held via conference call and at conferences/workshops with project team members from Fluent (Morgantown, WV; Lebanon, NH), AspenTech, and Alstom within the Fluent led Vision 21 team. The discussions focused on software issues, such as component architectures, model integration, and model interfacing.
- **National Fuel Center Research Center (NFCRC).** REI provided members of the NFCRC Vision 21 project team performing plant configuration analysis with gasifier modeling results for different process conditions.
- **Enertechnix.** REI provided Enertechnix with reacting CFD data sets from simulations performed with the REI two-stage entrained flow gasifier. Enertechnix is a leading provider of novel, gas temperature sensors for industrial combustion systems. Enertechnix has provided acoustic sensors for on-line gas temperature measurements in recovery boilers used in the pulp and paper industry and PC-fired electric utility boilers. Through NETL funding (DE-FC26-03NT41617), Enertechnix is developing an acoustic-based gas temperature sensor for use in coal gasifiers, with the intention of field testing the sensor in the E-Gas gasifier at the Wabash River plant. This collaborative effort was performed under a MOU between REI and Enertechnix.
- **DOE Albany Research Center (DOE ALRC).** REI exchanged information on the impact of gasifier operating conditions, particularly coal ash content, on flowing slag on gasifier walls with Dr. Cindy Dogan and her colleagues at the DOE-ALRC that are working on improving refractory used in entrained flow gasifiers.
- **UK Virtual Power Plant Project.** REI attended a NETL-organized workshop to discuss with UK-funded personnel potential collaborations with a project being funded by the British government to develop a power plant simulation tool to address conventional pulverized-coal power plants. The information exchange focused on procedures for component model benchmarking, software security, and the use of component architecture software methods for interfacing models to the simulator (framework).
- **Power Systems Manufacturing (PSM).** PSM is a leading "aftermarket" vendor of low NO_x combustors used in direct-fired stationary combustion turbines used in the power generation industry. Through a MOU agreement, REI, RECOM, and PSM collaborated on modeling for an industrially relevant design of an ultra-low NO_x combustor.
- **AspenTech.** AspenTech is a leading provider of commercial flowsheet software packages for performing processing modeling of industrial plants. Through a MOU, REI and Aspen collaborated on demonstrating a simple coupling between the VEF and the AspenPlus process modeling software package.

1.1.5 Deliverables

The contractually required (quarterly) Technical Progress Reports, Topical Reports, Financial Reports and Final Technical Report (this document) have been delivered to NETL. The IGCC-FCT and VEF software frameworks have been installed at NETL (Morgantown), and NETL personnel have been trained on the use of the frameworks. Note that the software modifications required to perform the proof-of-concept demonstrations for coupling the VEF to the IECM and Aspen Plus frameworks were not included in the deliverables to NETL. Likewise, to interface CAPE-Open-compliant models to the VEF installed at NETL will require the use of VES-Open. Further details about the non-included software pieces can be obtained from REI upon request.

1.1.6 Value to DOE

Over the last four years, the role and requirements for simulation within the Vision 21 program have evolved significantly. This somewhat “fluid” situation has been highlighted in DOE-sponsored meetings.

The Virtual Engineering-based framework (VEF) will provide a useful next step in the evolution of simulation capability. It will fulfill several NETL technical objectives for advanced power plant engineering simulation, including the use of:

- a hierarchy of CFD and reduced-order models;
- distributed computing and platform independence;
- 3D, immersive environments to interactively build plant configurations and simulations;
- improved *steady-state simulation*; and
- a software platform that is an important next step for NETL toward its stated goal of developing advanced, dynamic plant simulation capability by 2010.

The VEF will enable researchers to better understand the interactions of different equipment components and identify weaknesses and processes needing improvement, thereby allowing more efficient, less expensive plants to be developed and brought on-line faster and in a more cost-effective manner.

From a broader perspective, the VEF will be a valuable asset for NETL and industry to assist in decision-making, design, operation, and trouble-shooting of advanced power system plants, including IGCC-based plants with carbon capture and hydrogen production such as FutureGen [FutureGen, 2004]. With little additional effort, the framework could be enhanced to support DOE programs focused on combustion-based options for increasing plant efficiency and reducing greenhouse gas emissions, such as Super Critical and Ultra Super Critical boilers and oxy-fuel combustion. Last, the VE framework would be a valuable tool to help NETL manage Power Systems Advanced Research projects and highlight programmatic progress to NETL funding sources/stakeholders.

1.1.7 Technical Spin-offs

In the original solicitation for the DOE Vision 21 program, technical spin-offs in which the modeling tools and techniques developed/demonstrated within the DOE project were reused for other applications, were a part of the proposal consideration. REI has a track record of commercializing technologies and modeling capabilities developed under federal funding by applying such capabilities to address problems of interest to industry [<http://www.reaction-eng.com>].

Highlighted below are selected spin-offs from the software framework developed in this DOE-funded project. The selected spin-offs include software frameworks to:

- create reduced chemical kinetic mechanisms used in reacting CFD simulations;
- simulate the performance of chemical weapons incinerators;
- simulate the performance of laboratory and commercial incinerators when processing office materials contaminated by chemical or biological agent; and
- simulate the effect of blasts from landmines or roadside explosions on vehicles.

A Problem-Solving Environment for Creating Reduced Chemical Kinetic Mechanisms

National Science Foundation (NSF) SBIR Phase I, II, IIB, DMI-0091593,

completed: April, 2004

http://www.reaction-eng.com/r_and_d/advanced_carm_wb.html

Through funding from the NSF, REI developed a software framework, or problem-solving environment, that provides the ability to rapidly generate and validate reduced chemical kinetic mechanisms for use in reacting CFD simulations of industrial combustion systems [Montgomery et al., 2003], [Swensen et al., 2005]. The framework includes models of idealized combustion reactors (Perfectly Stirred Reactors (PSR), Plug Flow Reactors (PFR)), the CARM software for generating reduced chemical kinetic mechanisms [Chen, 1997], tools to create a matrix of parametric test cases, tools to access detailed chemical mechanisms located on the internet, and visualization and plotting tools for evaluating results. The framework was developed with assistance from Visual Influence and was originally SCIRun-based, but was eventually re-implemented as a custom built C++ application. Features of the framework include:

- intuitive graphical user interfaces (GUIs) to allow interacting with model setup, execution, and controlling visualization of all levels of models;
- extensive model bridging – all data exchange between models and tools performed in a seamless manner that hides the details from the user;
- distributed computing (ability to run models on distributed computational resources);
- platform independence and use of mixed-language models;
- application built using open-source GUI (Tcl/Tk);
- optimization methods (genetic algorithms, steepest gradient) included to automate the process and increase accuracy. GUIs are provided to support user-defined objective function within the optimization algorithm; and
- the reduced mechanism is output in a format that allows direct inclusion into commercial CFD codes (e.g., FLUENT) through use of a User-Defined Function.

A schematic of the framework is illustrated in Figure 1.1.3.

The framework has been used by REI to develop reduced chemical kinetic mechanisms for a variety of applications that involve reacting CFD simulations, including:

- NO_x and SO_x emissions from coal-fired industrial combustion systems (e.g., coal-fired utility boilers, cement kilns) and NO_x emissions from gas-fired chemical process furnaces (e.g., ethylene cracking furnaces);
- NO_x emissions from stationary gas turbines that use ultra-low NO_x combustors;
- thermal destruction of nerve agent and mustard blister agent within chemical weapons incinerators used by the US Army; and
- pollutant emissions (NO_x, soot) from military jet engines that operate on JP8 fuel.

Figure 1.1.3. Software Framework to support problem-solving environment for generating and validating reduced chemical kinetic mechanisms.

Engineering Design Software for Military Incinerators

Army SBIR Phase I, I Option, II, II Plus, DAAD19-01-C-0050, completed Sept., 2004.

http://www.reaction-eng.com/r_and_d/advanced_army_wb.html

Through funding from a US Army SBIR, REI developed a software framework to simulate the performance of US Army baseline Chemical Weapons Incineration facilities. The framework integrates a range of models, from *time-dependent* process models to detailed CFD models, which the user can use to create, execute, and interrogate a simulation. Note that two of the three incinerator trains at the plants have inherently time-dependent operation and thus the models are designed to capture this time-dependent behavior. The framework was originally SCIRun based, but was subsequently converted to be a custom C++ application. Agent destruction is computed using chemical kinetic models developed within the project using computational chemistry methods; the agent destruction models were developed under the guidance and review of an advisory panel of experts from the fields of chemical kinetics and chemical weapons demilitarization. Simulations can be performed for a broad range of operating conditions, including baseline operation and “what if” upset scenarios, for different munitions, storage containers, and chemical agents. Figure 1.1.4 illustrates aspects of the framework.

The incinerator framework has many of the capabilities and features as per the IGCC-FCT and VEF frameworks developed for the DOE:

- intuitive open-source GUI (TCL/TK) to allow the user to easily configure, execute, and control simulations;
- hierarchy of models:
 - tight coupling of models; no limitation imposed on physics or numerical methods;
 - simulation of time-dependent furnace processes;
- simulation results can be analyzed at multiple levels of detail;
 - 3D visualization of CFD results (VTK)
- extensive model interfacing – all data exchange between models and tools performed in seamless manner that hides the details from the user;
- platform-independent software and mixed-language support for models; and
- heterogeneous distributed computing of models.

This project was awarded a prestigious *US Army SBIR Phase II Quality Award for 2004*. The Quality Awards Program recognizes small businesses for exceptional performance that exemplifies the SBIR Program goal of bringing innovative technologies and products to the marketplace. The capabilities of the framework have been used to provide the Army and Army

Figure 1.1.4. Example of framework capabilities for modeling chemical weapons incinerators. contractors evaluations of plant operation that have resulted in substantial cost savings to the Army, including:

- analysis of an agent release event that occurred in the Discharge Air Lock (DAL) of a Metal Parts Furnace (MPF). REI's analysis was a critical link in *negotiations with regulators* to modify the clearance criteria for processed materials. The ruling allowed the plant to resume full operation, resulting in significant cost savings to the Army.
- an assessment of the fate of phosphorus from organophosphorus (nerve) agent from a baseline incineration plant preparing to start operation. The analysis was used by plant personnel in *negotiations with regulators* to explain expected phosphorus emissions for

processing nerve agent, as opposed to phosphorus emissions that occur when processing organometallic phosphorus during surrogate trial burns, thereby reducing the schedule to start plant operation.

- an evaluation of processing undrained mustard projectiles in a MPF. The analysis results will be used in *negotiations with regulators* to modify incinerator operation. The improved processing would result in reducing the schedule for plant operation.
- an evaluation of processing drained ton containers of mustard agent that contain solidified (undrainable) agent.
- an evaluation of the possible capture of mercury in the incinerator Pollution Abatement System (quench tower, scrubbers, etc.) when processing mercury-contaminated mustard agent.
- an assessment to troubleshoot slagging problems encountered when processing micronized charcoal in a specially designed solid fuel burner.

A chemical weapons incineration plant costs approximately \$300,000/day to operate. Hence, even small improvements in processing time can have a significant benefit. REI is actively discussing with non-incineration plant operators the possibility of extending the models in the framework to include equipment that uses indirect heating to thermally process agent-contaminated materials.

Modeling Support for Incineration of Building Materials

EPA National Center for Homeland Security Research and Development, 4C-R010-NASX, in progress - to be completed April, 2005.

Software elements, equipment models, and models to predict the thermal destruction of chemical warfare agent included in the Army incinerator framework described above are being leveraged to deliver a framework to the EPA that they will use in developing contingency plans for the thermal treatment in commercial incinerators of office building materials (e.g., rugs, wall paneling, wallboard) contaminated with chemical or biological agent due to a terrorist attack on an office building. The incinerator models will be pre-configured to operating units (rotary kiln hazardous waste incinerators, med-path hazardous waste incinerators) as determined by the EPA [Denison et al., 2005].

Simulation of Blast Events

US Army SBIR Phase I, 10 56 HZV-05-C-0115
in progress - to be completed October, 2005.

In this recently awarded project, REI is developing a software framework to support advanced simulations to analyze blast damage to civilian and military (armored) vehicles due to encountering land mines or roadside explosions. The framework will contain a hierarchy of models ranging from simple correlations to sophisticated 3D, time-dependent simulations that include container dynamics, explosions and blast-wave propagation. The advanced simulations will require intimate coupling of nonlinear finite-element analysis codes with state-of-the-art multi-point (Lagrangian) CFD-based tools that are used to perform explosion- and container-dynamics computations. The framework for blast-event simulation will leverage software

elements, software development methods, and lessons learned from creating the framework for advance power system simulations. For the blast simulation, the use of advanced visualization methods and interfacing the models in a manner that does not place limits on the type or quantity of data transferred between models and/or solution data analysis tools will be crucial.

1.2 Framework Software

Within this section we present software implementation details including development history, major framework features, and the various software components and user-interaction environments. The discussion is organized as follows:

- History of Development/Evolution of the Framework
- SCIRun Frameworks
 - SCIRun Overview
 - LEBS Framework
 - SCIRun Framework Enhancements
- VE-Suite Framework
 - VE-Suite Framework Overview
 - VE-Suite Software Design and Implementation Details
 - User Interface
 - Computational Engine
 - Visualization Engine and VES-Open Interface
 - Software Management and Documentation
 - Coupling of VEF to CMU IECM and Aspen Plus

1.2.1 History of Development/Evolution of the Framework

Over the course of the project, the core framework software evolved to make use of state-of-the-art software technologies. The first framework, which was used to simulate the LEBS facility, was implemented using the SCIRun computational framework. At that point in time, SCIRun was the logical choice for implementing a modular simulation framework. SCIRun was platform independent, had good visualization capabilities (via OpenDX coupling), and had a flexible and extensible architecture for incorporating new component models.

As the project moved toward modeling an IGCC-FCT plant, SCIRun was still the logical choice for the implementation. The general development approach remained basically the same as that used for the LEBS framework with the exception of visualization, which was accomplished using the more flexible VTK libraries. The SCIRun-based IGCC-FCT framework proved to be a success based on the target functional specification.

Following the completion of the IGCC-FCT framework, REI was awarded a budget revision that included collaboration with teams from ISU and CMU. At this point in time, the teams created a new, state-of-the-art functional specification based on a detailed review of future project requirements. Capabilities included in this new specification are a componentized software design, distributed computing, and immersive virtual engineering. Although SCIRun was a logical choice for the previous framework implementations, this new functional specification's requirements were beyond the scope of SCIRun's capabilities.

At this point, it was decided that a new framework would be created using the latest open source packages along with capabilities from the REI, ISU, and CMU teams. The result was the VE-Suite framework, which features platform independence, componentized software design, distributed computing, plug-and-play model extensibility, and immersive virtual engineering.

1.2.2 SCIRun Frameworks

SCIRun Overview

SCIRun is a scientific programming environment that allows the interactive construction, debugging and steering of large-scale, 3D scientific computations [Johnson, 1999], [Parker, 1998]. By design, SCIRun provides a high-level control over parameters in an efficient and intuitive way through GUIs and scientific visualization. SCIRun can be thought of as a *computational framework* in which an engineer can design and modify simulations interactively via a dataflow programming model. It enables engineers to interactively modify geometric models, boundary conditions, and physical and numerical model parameters. It provides the means for fully interactive control of the design, computation, and visualization phases of a simulation. SCIRun does not impose any inherent limitations on the type of computational model that can be used or the programming language used to create the model. In addition, SCIRun contains the flexibility to “bridge” the SCIRun system to other software packages to provide enhanced functionality or capability.

Visual Dataflow Programming Model

SCIRun makes use of a visual dataflow programming model to connect various computational models and to route data to auxiliary modules for visualization and interrogation of results. The user of the framework creates these connections in a plug-and-play manner by simply dragging the mouse between the outputs of one component to the input or inputs of other components. The dataflow paradigm naturally matches a physical process flow diagram.

Computer-Platform Flexibility

During the design of SCIRun, careful consideration was given to computer-platform flexibility. In particular, notoriously platform-dependent elements such as threading and GUIs were either abstracted or implemented using platform-flexible packages. As a result of this effort, SCIRun, and modules developed for it, can easily be used on a large number of Unix and Linux-based computer platforms.

Extensibility

SCIRun was designed to be highly extensible. This capability exists as a result of its widespread use of object-oriented programming concepts and methods. As a result, additional computational components can easily be added, and SCIRun itself can be modified to provide additional capabilities. In addition, a SCIRun developer can leverage the large number of existing modules and dataflow types, which have already been created. This results in significant code reuse and a corresponding reduction in development effort.

Bridging Capabilities

As a result of SCIRun’s extensibility features, it is possible to create software bridges to nearly any external software package. Currently, we use a software bridge to couple the OpenDX visualization software with SCIRun. Future bridges may include a link to 3DStudioMax, which would allow the comprehensive framework models to share a common database of geometric information of plant components.

High-Performance Computing (HPC) Emphasis

From inception, SCIRun has targeted HPC applications. This emphasis is reflected in its heavily multithreaded architecture and attention to performance details such as efficient dataflow handling mechanisms and state-of-the-art algorithms.

LEBS Framework

The LEBS-POC is a nominally 90 MW, down-fired unit. It contains four low NO_x burners in a staggered arrangement in a U-shaped, wet bottom boiler and has provisions for OFA and reburning. The LEBS-POC plant configuration, as represented in the framework, is shown in Figure 1.2.1. The framework uses a CFD model for the radiant furnace box. Reactor models have been implemented to simulate steam generation, the air preheater, NO_x reduction with a SCR unit and particulate removal. Modules for a baghouse and an ESP have been provided for modeling particulate removal.

Figure 1.2.1. LEBS Framework

LEBS Framework Model Integration

Model integration for the LEBS framework was accomplished using C++ wrapper classes, which encapsulate the model of interest. The wrappers perform several functions, including abstracting model inputs and outputs, providing execution controls, and providing SCIRun-to-model communication mechanisms. The instantiation of the resulting wrapper class yields a SCIRun-compliant module, which is capable of being composed as part of a dataflow network program.

While using the aforementioned mechanism of model integration was the natural choice for the LEBS Framework, it does have shortcomings as a final solution. The most significant issue is that of interoperability of the wrapped models. This method generates modules which will only

function within the SCIRun system. It is not possible to move these modules to other frameworks or to use modules developed for other frameworks inside SCIRun. In addition, the method places limits on model programming languages and provides no inherent parallelism.

IGCC-FCT Framework Model Integration

For the IGCC-FCT framework, support was added for a more sophisticated model integration approach based on component architecture methods for software integration. Infrastructure was added to support two different component architecture standards: CCA and CORBA. CCA (Common Component Architecture) was created to address the need for a component architecture for high-performance computing [<http://www.acl.lanl.gov/cca-forum/>]. The creation of the CCA forum, which oversees the development of the CCA standard, was inspired by the DOE2000 initiative. The specification created by this group provides the benefits of the standard business-oriented component architectures (interoperability, language independence, parallel capabilities), while addressing the issues of high-performance computing such as parallel communication channels between components and other elements required for dealing with extremely large data sets. CORBA (Common Object Request Broker Architecture) is a widely used, business-oriented component architecture standard developed by the Object Management Group (OMG). The OMG is an open-membership, not-for-profit consortium that produces and maintains computer industry specifications for interoperable enterprise applications. Membership includes virtually every large company in the computer industry, and hundreds of smaller ones. While lacking in the high-performance features of the CCA, the wide user base of CORBA makes it a logical choice for small- to medium-sized computational models.

One of the key advantages of using component architectures with standard interfaces is interoperability. For this framework, the standard interfaces being used were: 1) CAPE-OPEN for CORBA and 2) VES-open for CCA. CAPE-Open [<http://www.colan.org>] is a set of standards created to facilitate the use of COM and CORBA component software for process engineering problems. This standard has been well received by the process engineering community. By enabling support for CAPE-compliant components, we gained access to a potentially large number of process engineering models. VES-Open is a set of standards developed by REI specifically to address the need for interoperability of computational models developed for the Vision 21 program.

Prototype component-based models using both the CAPE and VES-Open interfaces were implemented and tested in the framework. These componentized models were used in combination with models that were integrated using the traditional C++ wrapping approach.

SCIRun Framework Enhancements

In the following sections, we provide a brief description of the enhancements made to the core SCIRun framework capabilities for the IGCC-FCT Framework.

Port Interrogation

Port Interrogation provides the user with a mechanism, or tool, to display all of the data contained within the gas and solids stream data structure that is passed between different framework modules through the data pipes. With this tool, the user can view detailed information about the composition, temperature, etc. for the gas and solids at any point within the module

network. The Port Interrogation can be performed for any module by placing the cursor over the desired data port and performing a right mouse click.

System Summary Information

As larger networks in SCIRun were executed, it became apparent that while detailed information at the module level is useful and necessary, this information was tedious to access when one is concerned with details of the overall system. To address this issue we incorporated functionality into SCIRun which adds a system-wide summary table. The table is accessible from each individual module in a network and is used to display high-level summary information. This new capability allowed the user to quickly see summary information from all modules in one window while still allowing the user to interrogate individual modules for more detailed data. An example of the Network Summary window is shown in Figure 1.2.2.

Network Summary	
Options	
ASU Compressor	
Power (MW)	-4.17
ASU	
Energy Requirement (MW)	-0.3573
Cyclone	
Particle Flowrate (kg/sec)	3.24
Particle flow collected (%)	73.31
Particle flow NOT collected (%)	26.69
Mass Mean diameter (microns)	69.84
Std Dev (NO UNITS)	2.32
Pressure Drop (kPa)	19.47
Cyclone cut diameter (micron)	42.17
Chlorine Bed	
Temperature Out (K)	668.308
Pressure Drop (psi)	10.000
HCL Reduction Efficiency (%)	99.88
Bed Desulfurizer	
Temperature Out (K)	668.308
Pressure Drop (psi)	5.000
H2S Reduction Efficiency (%)	99.98
COS Reduction Efficiency (%)	99.67
Expander	
Power (MW)	9.02
Fuel Cell - A	
Anode Temperature (K)	1098.34
Power Output (MW)	180.59
Fuel Cell - B	
Anode Temperature (K)	1241.74
Power Output (MW)	125.83
Gas Turbine Air Compressors	
Power (MW)	-128.69
Gas Turbine - High Pressure	
Power (MW)	126.96
Gas Turbine - Low Pressure	
Power (MW)	136.73
Steam Turbine - High Pressure	
Power (MW)	34.76
Steam Turbine - Low Pressure	
Power (MW)	56.79

Figure1.2.2. Summary table.

Overall Plant Efficiency

The software elements designed to create the system-wide summary table described above were extended to allow the framework to calculate overall plant efficiency.

Enhanced Model Execution Scheduler

The core SCIRun software infrastructure of the framework was modified to include a custom execution scheduler (the algorithm which determines which models to execute) that can handle more sophisticated module interconnections, including feedback loops.

This scheduler modification was necessary to address the material “loops” in Vision21 reference configurations. The original scheduler worked entirely within a pure dataflow paradigm and thus did not provide sufficient control over the sequence of models to be executed. In a pure dataflow network, data is provided to the upper most models and as these models complete their execution, the resulting data “flows” to downstream models. This scheme of execution makes the use of feedback loops (data from downstream models as inputs to upstream models) or iteration loops (hold execution in a section of a network until a user-specified variable converges) very difficult without significant code rewrite.

The scheduler employs a directed Painter’s algorithm to determine status of the network in combination with several graph analysis algorithms to determine execution order. The new scheduler correctly analyzes and schedules the operations to be performed within a network with single, multiple, or even deeply nested loops. In addition, the scheduler is now “aware” of the status of individual network models or entire network sections. This allows much greater user control of network execution, and naturally provides for “global” network variables (such as pressure drop through an entire furnace train) and enhanced error handling.

Coal Database

A coal database was added to the framework. This database is global in nature, making it accessible to any module that requires it. This database contains several default coals and their properties including ultimate and proximate analyses and ash composition. With the use of a graphical front end (Figure 1.2.3), a user is able to quickly retrieve, edit, and save new or existing coals. Figure 1.2.3 shows how this database is used within the framework.

Figure 1.2.3. Graphical front end for the Global coal database.

Expanded Network Display

Responding to the requests of framework users at the CCSD, REI developed a simplified but much improved network display window. Displaying of a network in the core SCIRun package takes the form of either a very small or a very large depiction, both of which can be seen in the SCIRun framework window (Figure 1.2.4 - left image). The small network allows the user to grasp the general configuration of the plant, but conveys no detail to the user. The large network provides a high level of detail on a small section of the plant. This larger view is useful, but makes comprehension of the overall plant schematic difficult. REI's network display window (also shown in Figure 1.2.4) attempts to solve these shortcomings. Features of the display are: 1) unwanted levels of detail are stripped away; 2) zoom in/out capability (aiding the user in visualizing plant configuration); and 3) the ability to save the display as a postscript file for sharing, viewing later, or importation into reports.

Figure 1.2.4. Network display windows.

Software Management and Documentation

The software design for the SCIRun-based frameworks was performed according to accepted industry standard procedures. The development team followed standard practices of creating functional specifications, and conducted design reviews to ensure interoperability among the various software components. Source-code control was accomplished using the CVS open-source versioning software.

Documentation for the SCIRun-based frameworks was accomplished by implementing a help system that uses HyperHelp, an iTCL html viewer, to display hypertext help files for each module. The Help content includes: instructions on usage of the module; a description of the module ports; a picture of the module UI; and a description of the fields in the UI. To access help for a given module, the user simply uses the mouse to right-click on the module and selects the “Help” item from the pop-up menu. Because the module documentation is created using HTML, the online help system is easy to create and maintain using the plethora of tools available for web development.

1.2.3 VE-Suite Framework

VE-Suite Framework Overview

During GFY2004, REI coordinated its efforts with NETL-funded projects at ISU (Program Manager - Prof. Mark Bryden) and CMU (Program Manager - Prof. Ed Rubin) to develop a Virtual Engineering framework (VEF). The VEF utilizes Virtual Engineering Suite (VE-Suite), an open source library of tools from ISU that enables the engineering analysis and design process to take place in a virtual environment and provides support for a broad range of advanced computing capabilities. The VEF provides capabilities above and beyond those available in the SCIRun-based frameworks. It supports the construction and interrogation of plant configurations with a snap-and-build approach in a 3D, user-centered, interactive, immersive environment (see Figure 1.2.5). By design, the VEF is open source, compatible across systems ranging from inexpensive desktop PCs (using “3D glasses”) to large-scale immersive facilities, and provides support for heterogeneous distributed computing of models contained in the plant configuration. For plant economics, the framework has been interfaced to a second framework – the CMU IECM financial planner, which provides access to a library of fast running, reduced-order models for plant components and models for plant economics. The VEF contains the full complement of models to simulate an IGCC-FCT plant.

Figure 1.2.5. Existing VEF software design.

The VEF leverages emerging simulation software methods from the field of computational sciences [Swensen et al., 2004-2005]. Specifically, rather than being a single monolithic application, VEF uses a *computational engine* to schedule, monitor, and control operations for a simulation executing in the framework, and a *visualization engine* (developed at ISU) is used to perform 3D renderings of plant equipment and dials/consoles (to report simulation summary results such as efficiency, net power generation, cost of electricity) and common CFD solution interrogation tools (see Figure 1.2.5). The 3D, immersive interface allows for limited manipulation of simulation parameters. Most user interaction with the framework is performed through a 2D UI operating on a handheld (tablet, PDA), laptop, or desktop computer. The 2D UI is platform (operating system) independent, allows accessing the framework and simulations remotely, and interacts with the framework in a detached mode; hence, using the 2D UI, an

engineer can access the framework remotely through the internet, modify parameters in an executing simulation, and exit the framework, and the simulation will continue to execute.

A hierarchy of simulation outputs and analysis tools are provided to review and interrogate simulation results at both the plant or component model level. At the highest level, overall plant engineering performance (e.g., plant efficiency, net electricity produced) and plant economics (e.g., cost of electricity) can be reviewed. At the component model level, model outputs can be viewed in tabular form (unit operation summary values) and all of the data contained within the stream data structures that are passed between different modules through the data pipes can be displayed using the port interrogation tools. CFD model outputs can be viewed using conventional CFD viewing techniques or in 3D space using virtual reality methods.

VE-Suite Software Design and Implementation Details

Figure 1.2.6 shows a high-level schematic of the software design. As seen in this figure, the key elements of the design are the UI, Computational Engine, Visualization Engine, and component models. Note that the various software elements all exist as independent CORBA components with standardized Interface Definition Language (IDL) implementations (VES-Open denoted with “C” in a circle). The use of component architecture design techniques has numerous advantages for this application including platform independence, location transparency, and reuse of component models.

Figure 1.2.6. Advanced Power Simulation Framework Design.

The following sections will detail the design of each of these elements and describe how they contribute to the overall framework functionality.

User Interface

To achieve the goals outlined for this project, a powerful and flexible UI was a necessity. The design goals for the UI were:

- multi-platform support;
- detachable/location transparency;
- extensibility; and
- unified control.

Figure 1.2.7 illustrates the internal construction of the UI and its interaction with other major software components. This figure provides a level of detail beyond that given in Figure 1.2.6.

Figure 1.2.7. Details of the UI Design

Multi-Platform Support: The UI makes use of platform-independent libraries to enable the software to run on a wide range of computer hardware and operating systems. These platforms range from Unix workstations to Pocket PC's and PDA's. This functionality is ideal for the virtual engineering-based system being developed since users will frequently make use of handheld computing devices inside of immersive environments (e.g. cave-like systems at ISU-VRAC, NETL).

In order to provide complete platform independence, it was necessary to choose two open-source libraries. The first library is for the UI functionality and the second is for the component architecture. Details of these library choices are given in the following sections.

- 1) *UI Library*: After reviewing a number of different UI packages, we chose wxWidgets [www.wxwidgets.org]. The wxWidgets is one of the best cross-platform GUI packages available. It is well maintained, has a large user base, and has ports for Windows, Unix/X11, Unix/Motif, OS2, Mac, and GTK. It also has an alpha version of a Windows CE port, which is under active development. This ensures that the UI will run on all major platforms and even on Pocket PC-based PDA's (limited functionality now). wxWidgets' license essentially is the L-GPL (Library General Public License), with an exception stating that derived works in binary form may be distributed on the users own terms. These characteristics make wxWidgets an excellent choice for this project.
- 2) *Component Architecture Library*: Given that CORBA was chosen as the component architecture, it was necessary to choose an open-source CORBA implementation. It should be noted that CORBA is used not just in the UI code, but is used throughout the various framework components to provide efficient, platform-independent, and distributed communication.

In choosing a CORBA implementation, there were two main points to be considered. First, the library must be an open-source library and under active development. Second, the library must support multiple operating systems. With these guidelines, two libraries, omniORB (omniORB.sourceforge.net) and TAO (The ACE ORB) [www.cs.wustl.edu/~schmidt/TAO.html], were selected for comparison and trial use with simple simulations. Both of these libraries are respected in the simulation community as solid implementations of the CORBA specification. They both support multiple operating systems and satisfied the initial requirements for the Computational Engine and the Visualization Engine.

Since both of the libraries were comparable, further criteria were used to select TAO for use in the framework. The main advantage influencing the decision was that TAO has a real-time interface that will allow better synchronization with the Computational Engine when dynamic and large simulations are run. The TAO library also supports the WinCE platform which will allow support of PocketPC PDAs.

Detachable/Location Transparency: The UI exists independently from the Computational Engine. This functionality allows the UI to be attached and detached from an active simulation from any compatible computer on the network. As an example, this would allow a user to build and start a simulation and then detach from the Computational Engine. The user could then go to a different location, re-attach to the simulation and regain monitoring and control functions.

To accomplish this functionality we have defined a CORBA IDL interface (VES-Open - see Appendix B) between the UI and the Computational Engine. This CORBA interface provides all the necessary communication mechanisms between these components. The communication link is bidirectional and handles items such as model parameters passed to the Computational Engine and receives items such as execution status and results from the Computational Engine.

Another advantage of this design is the ability for multiple UIs to be attached to the same Computational Engine, allowing multiple users to monitor a simulation from different locations.

A locking mechanism will be used so that only one UI (controller) can change the design and inputs of the simulation.

Extensibility: The UI is able to dynamically discover, identify, and load UI elements for new component models. This capability will keep the level of difficulty involved in integrating new component models to a minimum and require no modifications to the core interface when new models are added.

The dynamic discovery and load capability was accomplished by loading user-developed module UIs from dynamic linking library (DLL in windows) or shared library (Shared in Linux/Unix). A plug-in base C++ class defining this UI-module interface will be provided to all module developers. Developers can inherit from this class to create their own module UI and then compile the resulting code into a DLL/Shared library. The framework's UI code will recognize the new module and load it into the user-module library. By this mechanism, the core UI can plug in the third-party module-specific UI directly from binaries.

Unified Control: Another design goal was unified control for all user interaction. This ensures that the user is not burdened with moving between different UIs to perform operations. Thus, there will be a single UI with the ability to: 1) construct, specify, execute, and monitor simulations; and 2) provide complete control of the 3D VR environment.

To provide this functionality, the UI was designed to communicate via CORBA to not only the Computational Engine, but also to the ISU Visualization Engine (see Figure 1.2.6). As was discussed for the UI to Computational Engine link, the use of CORBA with an appropriate IDL provides a flexible, detachable, and platform-independent communication mechanism for this link.

Computational Engine

The Computational Engine is the core of the framework. Its duties are to construct, coordinate, schedule, and monitor plant simulation runs. It must be capable of running a simulation containing a multitude of different types of models, each accepting and generating a myriad of datatypes. Given the unlimited number of simulation scenarios available for the user to create, the Computational Engine design was focused on a single goal: the successful and accurate plant simulation of a user-supplied configuration. To this end, the Computational Engine is able to analyze a plant configuration, determine execution order, marshal system resources to create model instances, and coordinate the flow of data through the entire simulation framework. Tasks that require specific knowledge about a datatype or model are relegated to either a detachable UI or to a specific model, thus keeping the Computational Engine generalized at a high level.

Figure 1.2.8 illustrates the internal construction of the Computational Engine and its interaction with other major software components. This figure provides a level of detail beyond that given in Figure 1.2.6.

Figure 1.2.8. Details of the Computational Engine Design.

Important functions that the Computational Engine controls can be broken down into several pieces for explanation: plant configuration, data handling, error handling, relationship to detachable UI, scheduling, resource allocation, and relationship to models and logging. Each of these is described in detail below.

Plant Configuration: The configuration of the plant, provided by a detachable UI, is the primary data structure used by the Computational Engine. Nearly all algorithms utilized, such as proper dataflow, scheduling, and resource allocation depend on this topology.

Data Handling: Since there are an unlimited number of possible models capable of being integrated into the framework (with each model having a different input/output set), it is vital that the Computational Engine access only generalized datatypes. To address this requirement, we have designed the CORBA IDL interfaces between the Computational Engine and the component models to use mapped string blocks in combination with common dimensions of array data.

Error Handling: With the Computational Engine being the centralized power behind a simulation run, all errors that occur while performing this task (whether originating within its own structure or on an attached model) must be properly handled within the context of this overriding structure. Thus, the Computational Engine has sophisticated error handling routines and messaging facilities to alert attached users. To fit into the detached-UI paradigm, any errors that occur on an attached UI will be handled locally.

Relationship to Detachable UI: The Computational Engine is a CORBA server, into which a detachable-UI client can connect (see IDL in Appendix A). This detachable UI is where the user is able to create a plant configuration, set model inputs, start and stop execution of simulation,

and view simulation results. Once a client-server connection is made, the engine is able to send results, messages, updates, and communications from other attached UIs in real-time. The Computational Engine does not require a connection to a UI during a simulation run. Users can connect/disconnect at will to configure, modify, or monitor the simulation of a given plant configuration.

Scheduling: The Computational Engine utilizes advanced scheduling algorithms developed earlier in this program. The scheduler, at a minimum, is capable of handling single and embedded feedback loops, iterative solves, and eventually, transient simulation runs.

Relationship to Models: The Computational Engine, with its CORBA interface, is able to connect to the various component models available for a simulation. Information passed through this connection will include inputs (user supplied and stream data), outputs, results, and general messages. The importance of the CORBA interface being used for this purpose is discussed in detail in the *Component Models* section below.

Logging: The Computational Engine will be equipped with a full suite of logging capabilities. Data ranging from schedule information to model results will be logged into a database. This information will be archived for later retrieval.

Visualization Engine

The Visualization Engine provides the core functionality for the virtual engineering aspect of the framework. It is based on VE-Xplorer which is a portion of the VE-Suite software developed by Prof. Mark Bryden's research group at ISU. VE-Xplorer enables the engineering analysis and design process to take place in a virtual environment. For maximum graphical performance on multiple operating systems, it is built upon VRJuggler [www.vrjuggler.org], OpenGL Performer [www.sgi.com], and Kitware's Visualization ToolKit [VTK, www.vtk.org]. This visual interface, controlled by the UI and the Computational Engine, is a graphical representation of the simulation under review.

The Visualization Engine is being generalized to load data not only from comprehensive models, but also from other engineering sources, including results generated from the CMU Vision 21 planner software and other generalized datasets (e.g., experimental data from a test rig). The engine is also being modified to make use of the high-level CORBA-interface specifications used throughout the software framework. This interface allows the Visualization Engine to communicate with the component models, Computational Engine, and the UI directly.

Component Model Interfacing - VES-Open Interface

Component models are mathematical representations of individual plant components which are used by the framework to construct an overall simulation. The key to making the simulation framework extensible is to provide a mechanism by which component models can be easily integrated without the need for extensive software development tasks.

To address these needs, we adopted the relatively modern idea of component architecture design. CORBA (the component architecture) is used along with a standard model interface definition (implemented as an IDL) to create componentized computational models. These models can be

used interchangeably with any framework which supports the standardized IDL, are location transparent (run on any network accessible machine), are platform independent (Linux, Windows, etc.), are programming-language flexible, and can be distributed in binary form.

The interface to the CORBA-based component models is designed to allow the models to be autonomous, accepting inputs and stream data from the Computational Engine, running the encapsulated model, and generating outputs and modified stream data. Figure 1.2.9 illustrates the interaction of the framework with component models on a single computational resource.

Figure 1.2.9. Interaction of Framework and Component Models.

It is important to note that the CORBA interface between the Computational Engine and the component models is the standardized model interface supported by the framework for model integration. The interface defined for this project (see Appendix A) is analogous to that of the CAPE-Open specification used by chemical process simulation tools. This newly developed model interface will be able to support CAPE components through wrapping and function mapping. When compared to CAPE, the new interface specification more closely meets the needs of the current simulation framework in a number of ways:

- simplification – the new model interface specification eliminates the more obscure and infrequently used features of CAPE, making it more accessible to potential model developers;
- generalization – the new interface removes the specificity of chemical process to provide a more generic structure; and
- enhanced data passing – the new interface provides facilities for passing data beyond the level of simple scalars to downstream models (a CAPE-Open limitation).

In addition to providing a mechanism to interface with individual computational models, the VES-Open interface also provides capabilities to integrate other frameworks in their entirety into

VE-Suite. A prototype of this capability was demonstrated by creating a VE-Suite component model that encapsulated the Aspen Plus Process Engineering Framework. Such framework-to-framework coupling provides a “best of both worlds” scenario and significantly enhances the capabilities of VE-Suite.

Appendix B contains a listing of the VES-Open IDL interface code. Appendix A is a white paper which discusses the issue of component architectures and their applicability to various scientific computing roles.

Software Management and Documentation

All software design for the VE-Suite framework was performed according to accepted industry standard procedures. The software development team followed standard practices of creating functional and detailed design specifications, and conducted design reviews to ensure interoperability among the various software components. VE-Suite was and still is being maintained at ISU with the Subversion (SVN) open-source versioning software. SVN allows the code to be viewed and administered over the internet, thus allowing the entire team seamless access for the common development effort. In addition to SVN, the open source packages Bugzilla, WebSVN, and TortoiseSVN were used to increase the robustness and accessibility of the VE-Suite code base.

Online Documentation: To enhance usability, the framework is equipped with extensive documentation. Written in HTML, the web-based documentation outlines the use of the VEF to setup/configure simulation networks and interpret results. In addition, detailed documentation for each of the current modules is provided. The documentation has been designed to enable users to use the software with minimal help from REI.

The documentation is divided into five sections:

- The first section is intended as a basic instruction on the framework interface. Its purpose is to give an overall view of some basic software components.
- Section two provides information regarding simulation networks and its components. This is included to clearly instruct the user on effective use of the many items and ideas such as module layout, ports, and connectors. Step-by-step illustrated instructions guide the user through the construction of a module network by connecting multiple modules in series and configuring individual module inputs.
- The third section explains how to commence a simulation and some basic, built-in features for results investigation.
- Section four details how the user views simulation results. A myriad of investigations are possible, including viewing: module results (summary tables), stream data contained in module connections, and network-wide results (such as plant power generated and costs). Instructions are also provided for using VE-Xplorer visualization tools.
- The last section documents the design and capabilities of each individual computational module. Each module's documentation typically contains a brief description of unit operation followed by an explanation of how the module was designed to emulate that given process. The text includes descriptions of any assumptions made in creating the module and proper context and usage within a network. Detailed instruction outlines use of each module's UIs, and visual process schematics are also provided for most modules.

The framework documentation is available independent of the framework interface. Strategically linked pages with tiered explanations allow users to use the documentation to quickly and efficiently locate necessary information. In addition, the help system can be invoked via the main windows *help* menu item or by jumping directly to a particular modules help page by placing the cursor over a module icon and pressing the right mouse button and selecting the module's *help* option (see Figure 1.2.10).

Figure 1.2.10. Accessing help menus within framework.

Integration of the CMU IECM Model

To access the capabilities of the IECM model from within the VEF, a controller component was implemented which encapsulates and interacts with the IECM core computational driver. The framework computational engine interacts with the IECM controller via the standardized IDL interface (VES-Open), just as is the case with individual component models. Currently, the core IECM driver does not allow individual component models to be accessed independently of one another. Instead, the IECM controller executes the IECM total system models and extracts desired results. CMU is currently factoring the IECM core into individual models so that it more closely matches the design required by the framework.

The implementation of the IECM controller component provides the framework with complete access to system-wide IECM modeling capabilities. A subset of the IECM user-input parameters have been exposed in framework GUI plugins, although the complete set of parameters could be made accessible with additional GUI changes if desired. System model execution can be controlled, and the framework also provides capabilities to visualize the IECM plant configuration in 3D VR space. To conduct this test, AspenTech provided REI with a temporary license to an evaluation copy of Aspen Plus.

Coupling of the VEF and IECM was demonstrated in a joint technical presentation [Rubin et al., 2004] and in one-on-one demonstrations at the Clearwater Conference 2004.

Aspen Plus Coupling

To maximize the capabilities of the advanced simulation framework, special attention was given in the software design to ensure that coupling to other simulation packages was not only feasible, but practical as well. As a proof-of-concept test, REI software engineers created a simple coupling to the Aspen Plus process simulation software. Aspen Plus has a wide variety of component models, and thus represented an ideal test case for framework-to-framework coupling.

The coupling component made use of the Aspen Plus ActiveX Automation Server for controlling Aspen with software commands from C++. The simple prototype was used to set stream attributes, execute the flow sheet, and to retrieve simulation results. While the coupling component was not generalized, it did illustrate the ability of the framework to make use of Aspen for future upgrades in capabilities.

1.3 Framework Models

The software frameworks developed in this project consist of equipment models and software infrastructure, which provides the software support to control the execution of the models and the communication of data between models. The provided equipment models include mass/energy balance models, 1D models that allow for variation of properties along the main axis of the equipment, and reacting, 3D CFD models for selected pieces of equipment. Where possible, the models have been benchmarked against available data. The framework software has been designed to not impose inherent limitations on the:

- type of model that can be included in the framework;
- physics or chemistry included in the model;
- numeric schemes used to solve the governing equations contained in the model;
- programming language used to implement the model; or
- quantity/type of data that can be passed between models or between models and analysis tools.

In this section are provided details on the component models included in the

- LEBS-POC framework and the
- IGCC-FCT and VEF frameworks.

Note that the VEF which uses Virtual Engineering concepts includes the models developed for IGCC-FCT systems, as well as models for investigating advanced power generation systems that include hydrogen production and CO₂ capture such as Futuregen. For simplicity, the models for the combustion- and gasification-based frameworks are described separately.

1.3.1 Models For LEBS-POC Framework

The LEBS-POC is a nominally 90 MWe, down-fired unit. It contains four low NO_x burners in a staggered arrangement in a U-shaped, wet bottom boiler and has provisions for overfire air (OFA) and coal reburning. A schematic of the LEBS-POC system is shown in Figure 1.3.1, and in Figure 1.3.2 is the LEBS-POC configuration as represented in the framework. For this prototype framework, a CFD model is used for the radiant furnace box. Reactor models have been implemented to simulate steam generation, the air preheater, NO_x reduction with a SCR unit, and particulate removal. Modules for a baghouse and an ESP have been provided for modeling particulate removal.

Figure 1.3.1. Schematic of LEBS-POC system.

For the firebox, two CFD modules have been implemented. One module is based on *GLACIER*, a comprehensive two-phase CFD based combustion code. *GLACIER* has been used by REI to model a variety of utility boiler configurations [<http://www.reaction-eng.com>]. At present, *GLACIER* is limited to performing steady-state simulations. A module has also been implemented for *AIOLOS*, a comprehensive CFD combustion code developed at the University of Stuttgart that can be used for performing steady or unsteady simulations of coal-fired utility boilers.

Figure 1.3.2. UI for prototype LEBS-POC framework.

Below are described the modules (or models) that have been implemented. For each module, the functionality, model inputs, and model outputs are described. It should be noted that for each module included in the framework there is an on-line help panel that contains a short description of the model and basic instructions for running the module (see Figure 1.2.10).

GLACIER POC Furnace Module (Steady State)

The *GLACIER* CFD code is a comprehensive CFD modeling code that can be used to model a broad range of turbulent reacting flows. It is capable of modeling two-phase fuels for either gas-particle or gas-liquid applications. For establishing the basic combustion flowfield, full equilibrium chemistry is employed. To compute NO_x and other trace species, finite-rate chemistry effects can be included in a post-processor mode. Turbulence chemistry coupling is accomplished using PDF methods. An important aspect of *GLACIER* is the tight coupling used between the dominant physics for utility boiler applications: turbulent fluid mechanics, radiation heat transfer, chemical reactions, and particle/droplet dynamics. Further information on *GLACIER* is contained in Appendix D and available at <http://www.reaction-eng.com/combustion.htm>.

The UI for this module is illustrated in Figure 1.3.3a. It includes the inputs that control fuel, air, and recirculating flue gas flows, temperatures, and coal properties. Outputs are available in: tabular format for summary data for predicted performance; XY plots to show axial variations of averaged values; and 3D field data formats for use with standard and virtual reality-based CFD visualization techniques (see Figure 1.3.3b).

Coal Type:

Ultimate (Wt.%)		Proximate (Wt.%)		Size Data		Miscellaneous	
C	59.98	H ₂ O	9.43	% thru 50	99.2	Cake Ca (w%)	9.0
H	3.78	VM	34.34	% thru 200	73.5	Ash Ca (w%)	5.0
O	7.38	Ash	13.74			Dustcake pH	12.0
N	1.15	FC	42.50			T Softening (K)	1364
S	4.51					T Fluid (K)	1451
Ash	13.74						

Heating Value
HHV (BTU/lb)

Burner System

Primary Air		Coal		Secondary Air		Tertiary Air	
Temperature (K)	355.4	Temperature (K)	355.4	Temperature (K)	583.2	Temperature (K)	583.2
Flowrate (kg/s)	17.42	Flowrate (kg/s)	9.68	Flowrate (kg/s)	20.03	Flowrate (kg/s)	40.07

Re-Burn System

Primary Air		Coal		Flue Gas Recirculation	
Temperature (K)	355.4	Temperature (K)	355.4	Temperature (K)	669.3
Flowrate (kg/s)	1.94	Flowrate (kg/s)	1.08	Flowrate (kg/s)	5.22

OverFire Air System

Overfire Air	
Temperature (K)	583.2
Flowrate (kg/s)	15.29

Figure 1.3.3a. For furnace CFD module, shown are example input dialog boxes for specifying coal composition (left) and air-fuel distribution (right).

Figure 1.3.3b. For furnace CFD module, shown are example summary data output (left) and XY Plots of the mean gas temperature in the upflow section of the furnace (right).

AIOLOS POC Furnace Module (Transient/Steady State):

The *AIOLOS* CFD code is a comprehensive CFD modeling code that can be used to model a broad range of turbulent reacting flows. It can be used to model two-phase fuel applications, using either Eulerian-Eulerian or Eulerian-Lagrangian methods. *AIOLOS* employs an EDC technique for turbulence chemistry coupling. It can employ multi-domain grids and perform time-dependent coal combustion simulations using either implicit or explicit time stepping. It can be used on virtually any level of hardware or operating system. *AIOLOS* is parallel-capable on both SMP and distributed architectures. It can be executed on single or dual cpu PCs/workstations, PC clusters, and has been tuned for use on supercomputers. Further information on *AIOLOS* is available in Appendix E and can be found on the web at: http://www.ivd.uni-stuttgart.de/english/aiolos_e_fh.html. The *AIOLOS* model of the LEBS-POC was fully integrated into the framework and used the same UI as for the *GLACIER* model for inputting data. However, the strength of *AIOLOS* is in transient simulations and operation on supercomputers; hence, this model was typically run in standalone mode on a supercomputer rather than being executed within the control of the framework. Note that the reacting, 3D CFD simulations of the LEBS boiler for transient operations were very time consuming, requiring days of supercomputer time.

Upper Furnace Module

A simple model has been implemented to compute the steamside and CO burnout in the upper, or convective pass, of the furnace. For the steamside model, the steam flow rate and exit steam conditions are computed from thermodynamic steam calculations coupled with an integrated heat transfer rate to the steam from the CFD model for the POC boiler. The model is based on a tube bank heat exchanger model, with correlations taken from [B&W, 1992]. Included in the model is a stream property code. The module was tested by comparing predicted values versus design data for the LEBS-POC.

The provided module is configured specifically for the LEBS-POC furnace and thus contains a fairly limited UI (see Figure 1.3.4). Components available within the UI for building a heat transfer network include:

- Cavity - which calculates heat transfer from the gas in the boiler to the boiler walls; model parameters include boiler depth and width;
- Steam Drum - which calculates steam flow rate needed to produce saturation at outlet; model parameters include total heat to walls;
- Water Walls – which calculates heat transfer to water walls; calculations are performed with the tube bank model;
- Tube Banks – which calculates heat transfer across a bank of tubes; model is used for high/low temperature superheaters, waterwalls, and economizers; model parameters include tube arrangement, configuration, number of assemblies, rows, SI, St, tube inner/outer diameters, tube length, gas pass depth/width, and fin effectiveness; note that radiation properties of the tubes are treated as a continuum model; see Figure 1.3.6;
- Atempurator – which calculates water conditions following attemperating spray; model parameters include spay mass flowrate and spray pressure; and
- Superheater - which calculates heat transfer to superheater panels; calculations are performed with the tube bank model.

The default values provided with the module in the prototype workbench are for the LEBS-POC facility. All of the remaining input items for this module (e.g., furnace flue gas flow properties) are obtained directly from the output of the CFD model of the furnace. Note that this module has two exit ports. One port is for the flue gas leaving the furnace convective pass. Applying a Port Interrogation tool to this port allows the user to view detailed information about the predicted composition of the flue gas at the exit of the economizer. A second port is used for the steam exiting the boiler – this is the steam that would be sent to the steam turbine. By clicking on the steam port, the steam properties (e.g., flow rate, temperature, pressure) can be viewed.

Figure 1.3.4. For upper furnace module, shown are example steamside circuit (left) and steam properties output from steamside model (right; note that quality = 1 implies that pure steam is being sent to the turbine).

SCR Module

The purpose of the SCR is to reduce NO_x emissions in the boiler flue gas. Ammonia is injected into the flue gas immediately upstream of the SCR. Within the SCR, the ammonia-enriched flue gas then passes through an array of catalysts that induce catalytic reactions that in turn reduce the NO_x in the flue gas. A plug flow SCR model has been developed based on the microkinetic mechanism of Dumesic et al. (1996) (also known as the Topsoe mechanism) for NO_x reduction with vanadia/titania catalysts. This is a common SCR catalyst used by utilities and is the catalyst planned for use in the LEBS-POC facility. The model was verified through comparisons of predicted values and values presented in [Dumesic et al., 1993].

The UI for the SCR model includes the following inputs: NH₃/NO ratio of ammonia injection, ammonia cost, maximum allowable ammonia slip, number of computational cells, heat loss from the SCR, and pressure drop. Other inputs required by the model, such as gas flow rate and composition, are obtained from the gas data passed from upstream modules (see Figure 1.3.5). For outputs, the UI contains a summary data dialog box that lists the predicted NO_x reduction, ammonia slip, and annual ammonia costs, and a XY plot that illustrates the predicted NO_x destruction along the axis of the SCR unit (see Figure 1.3.5). The module will flash a warning message if the predicted ammonia slip exceeds the prescribed maximum level.

uiLebs_components_scr_0

Number of cells :	100
Catalyst (kg):	5364.0
NH ₃ /NO ratio :	0.8925
Pressure drop (Pa):	0
Heat loss (W):	10000
Maximum allowable NH ₃ (ppm):	5
NH ₃ cost (\$/ton):	210.52
Vector output name :	

Execute

(A)

sumLebs_components_scr_0

Description	Value
NO Reduction	89.25%
NO in (mol fraction)	0.000558
NO out (mol fraction)	5.9948e-05
Slip (ppm)	3.3079e-24
Annual NH ₃ Cost	\$161,148.85

(B)

(C)

Figure 1.3.5. For SCR module, (A) example input dialog box, (B) output dialog box and (C) 1D plot of predicted NO_x reduction along axis of SCR unit.

Air Heater Module

The air preheater is a heat exchanger that uses hot effluent gas from the furnace to heat the secondary and tertiary combustion air and OFA. The air heater module was created by reusing the tube bank heat transfer model developed for the steamside module.

The UI for this module includes a dialog box to prescribe the properties of the incoming external (cold) air (see Figure 1.3.6). Note that the properties for the (hot) furnace flue gas are extracted from the flue gas properties in the framework dataflow network. This module has two exit ports. One port is for the flue gas leaving the air heater and the second port is for the preheated air that is sent to the boiler. Applying a Port Interrogation tool to the flue gas exit port allows the user to view detailed information about the predicted composition of the flue gas. Likewise, applying a Port Interrogation tool to the preheated air exit port allows the user to view detailed information about the preheated air exiting the air heater device (see Figure 1.3.6).

Tube Bank Configuration

File

Number of Assemblies	100
Number of Rows	45
Heat Exchange Area (sq m)	7452.23
Tube Long Pitch-SI (m)	0.1016
Tube Cross Pitch-St (m)	0.1016
Tube Inner Diameter (m)	0.04623
Tube Outer Diameter (m)	0.0508
Tube Length (m)	15.25
Gas Pass Depth (m)	6.096
Gas Pass Width (m)	8.9154

Arrangement

- Parallel Flow
- Counter Flow
- Combination Flow

Tube Configuration

- Inline
- Staggered

Int. Pressure Drop (Pa) 996.9

Ext. Pressure Drop (Pa) 373.8

Include Radiation ☐

Finned tubes ☐

Fin Effectiveness 0

Execute

gas_out_1_Labs_components_airheater_0

Gas Average

Temperature (K):	598.17
Pressure (Pa):	101325
Gas Flowrate (kg/s):	75.4
Density (kg/m ³):	0.50803
Pressure Drop Accum (Pa):	0

Particle Average

Coal Calcium (wt%) :	0
Ash Calcium (wt%) :	0
Ash pH :	0
Mean Particle Size :	0
Particle Size Variance :	0
Particle Loading :	0
Particle Temperature (K):	0

Gas / Particles / Favorites

Specie	Mole Fraction
H2O	0.0181
N2	0.789
NO	0.000558
O2	0.0778

Figure 1.3.6. For air heater module, shown are the input dialog window (left) and port interrogation window (right) when applied to the exit port for the preheated air.

Baghouse Module

A baghouse is a device that uses fabric filters to remove particulates from effluent coal combustion gases. A simple 0D (reactor) model has been implemented that computes capture efficiency and pressure drop based on the amount of trapped solids. The pressure drop calculations are important to establish fan requirements. The baghouse model used here is based on a model originally developed by Southern Research Institute [Pontius et al., 1992].

The UI includes inputs for the number of filter compartments and their arrangements and cleaning frequency and method (see Figure 1.3.7). Ash properties pertinent to dust-cake buildup in the baghouse are input with the coal properties in the furnace UI (i.e., the UI for *GLACIER* and *AIOLOS*). All other flue gas properties required by the model are obtained directly from the gas data output from the upstream module. The output for the model consists of the time-averaged pressure drop across the baghouse (see Figure 1.3.7).

uiLebs_components_Baghouse_0

Duct Configuration: Parallel

Compartments

Number of Compartments	12
Number of Bags	150
Bag Length (ft)	30
Bag Diameter (in)	12

Duct Resistance (in.WC/(acfm)²)

Hopper Constant	5e-10
Outlet Poppet Constant	5e-10
Inlet Manifold	0
Outlet Manifold	0

Fabric Type: 75% EST

Cleaning Method: Reverse gas

Cleaning initiated on

Pressure (in.WC)	5.2
Time (min)	60

Reverse gas

Air-to-Cloth (ft/min)	2
-----------------------	---

Clean Timing Durations in minutes

First null period	0.5
Cleaning	1.5
Second null period	1
Time between cleans	4

Compartment Data

Compartment number: 7

Send

Execute

Baghouse	
Description	Value
Avg Flange Pressure Drop (Pa)	1.2E+04
Avg Tubesheet Pressure Drop (Pa)	5.1E+03

Figure 1.3.7. For baghouse module, shown are windows for input dialog box (left), summary output (lower right), and 1D plot of time-dependent pressure drop including a cleaning event (upper right).

ESP Module

An Electro-Static Precipitator (ESP) is a device for removing dust particles from a gas stream. Within the ESP, an electro-static charge is induced on the particles, causing the particles to be deposited onto a plate with an opposite charge. The model implemented here is a process engineering model based on work originally performed by Southern Research Institute and subsequently enhanced by Clean Air Engineering; funding for both projects was provided by the US EPA. The model calculates the voltage-current characteristics and electric potential, electric field, and space charge density distributions on a 2D grid. These fields are in turn used to predict the particulate removal efficiency. The resistivity of the particulates is a key input in determining charge accumulation.

The UI includes (see Figure 1.3.8) inputs for the precipitator geometry, voltage-current relationships, ash dielectric constant, and particle layer resistivity. Ash particle size distribution is input based on the coal size distribution in the furnace (note: coal size distribution is available from the inputs for the furnace CFD model) and a predetermined size reduction factor for the ash from an ash formation model developed under DOE funding [Bool et al., 1995]. All other properties of the flue gas that are required by the model are obtained directly from the gas data output from the upstream module. The output for the model consists of removal efficiency as a function of particle size and the ash particle concentration of the outlet stream (see Figure 1.3.8).

Figure 1.3.8. For ESP module, shown are windows for input dialog box (left) and summary output (right).

Stack Module

For completeness, the LEBS-POC framework includes a stack module. At present, the stack module does not contain any models or perform any calculations. However, models could be included to predict items such as aerosol formation, stack opacity, or particulate dispersion in the local environment. In the current configuration, the stack module provides a simple summary output dialog (see Figure 1.3.9) that provides gross properties of the flue gas exiting the stack (e.g., CO₂, CO, NO, particulates). Alternatively, using the Port Interrogation data viewer, the user can obtain detailed information about the predicted conditions of the flue gas at the stack (see Section 1.2.2 for example of data available with the Port Interrogation tool).

Stack	
Description	Value
CO dry (PPM)	0
O2 dry (VOL_%)	2
NO dry (PPM)	38
NH3 dry (PPM)	1
NO @3% O2 (PPM)	36
<hr/>	
CO dry (VOL_%)	3.0E-06
<hr/>	
CO (TONS/YR)	0.1
NO (TONS/YR)	127.0
NH3 (TONS/YR)	1.1

Figure 1.3.9. Stack module's summary.

1.3.2 Models For IGCC-FCT and VEF Frameworks

In the original Vision 21 Roadmap [DOE, 1999] there was no preferred plant configuration or fuel type. Thus it has been important to develop models for equipment that will be common to different potential configurations. In the last couple years, due to the high cost of natural gas, research interests have focused on plants based on IGCC technology. Although more expensive to develop than a natural gas-combined cycle plant, coal is an abundant, secure, inexpensive and stably priced source of fuel. In addition, it provides the possibility to co-fire other opportunity fuels, such as petcoke, biomass, or refuse-based fuels.

Illustrated in Figure 1.3.10 is the Vision 21 energyplex configuration that the DOE Vision 21 Program Manager suggested be used by this project to demonstrate the capabilities of developed framework environments. This configuration consists of an entrained flow gasifier, gas clean up system, gas turbines, heat recovery steam generator, steam turbine and SOFCs. As described below, a combination of CFD and reactor models will be used to simulate the performance of this configuration. A reacting, 3D CFD model is used for the entrained flow gasifier, a 0D process model is also provided for the gasifier, and simpler models are used for the remainder of the equipment and processes.

Figure 1.3.10. Vision 21 reference configuration.

Listed in Tables 1.3.1-1.3.2 are the gross conditions for the configuration that were originally provided by DOE. Shown in Figure 1.3.11 is a mass and energy balance sheet obtained from DOE that provides more detailed information about the targeted Vision 21 configuration. A comparison of Figures 1.3.10 and 1.3.11 shows some discrepancies. Where information is

missing, REI has used data available in the literature, combined with engineering judgment, to develop the required information to create the needed models.

Table 1.3.1. Provided Operating Conditions for Vision 21 Energyplex.

Gasifier (18 atm)	Two-stage, up-fired
Coal Input to Gasifier (lb/hr)	256,142
Coal Type	Illinois #6
Thermal Input (MW)	875.8
HP SOFC dc/ac	189.4/182.8
LP SOFC dc/ac	121.4/117.2
Gas Turbine, MW	133.7
Steam Turbine, MW	118.0
Fuel Expander, MW	9.6
Gross Power	561.3
Auxiliary Power, MW	40.4
Net Power, MW	520.9
Efficiency, % HHV	59.5

Table 1.3.2. Illinois Coal #6 Description.

Proximate Analysis	As-Received (wt%)
Moisture	11.12
Ash	9.70
Volatile Matter	34.99
Fixed Carbon	44.19
TOTAL	100.00
HHV (Btu/lb)	11666
Ultimate Analysis	As-Received (wt%)
Moisture	11.12
Carbon	63.75
Hydrogen	4.50
Nitrogen	1.25
Sulfur	2.80
Ash	9.70
Oxygen (by difference)	6.88
TOTAL	100.00

Figure 1.3.11. Mass and energy balance sheet provided by DOE for Vision 21 reference configuration.

In the following are provided, in order, descriptions of the models available for use in the IGCC-FCT framework and VEF. These include:

- Coal Gasifiers (entrained flow , transport reactor);
- Heat Exchangers (syngas cooler, HRSG, recuperator);
- Air Separation Unit (ASU);
- Gas Clean Up (cyclone, chlorine guard, bulk desulfurizer, sulfur polisher, mercury capture, Acid Gas Removal, carbon bed);
- Gas Turbine Equipment (turbine, compressors, expanders, combustors);
- Solid Oxide Fuel Cells (SOFC) and SOFC Exhaust Gas Combustors (dump, catalytic);
- Membrane-Based Gas Separation Units (water gas shift membrane reactor);
- Balance of Plant (Water Mixer, Water Splitter, Water Pump, Water Heat Exchanger, Condensor, Evaporation Cooler); and
- Idealized kinetic reactors (Perfectly Stirred Reactor (PSR), Plug Flow Reactors (PFR)).

Where feasible, multiple choices for model types are provided. The reactor models include simple algebraic models and mass/energy balance models; reaction kinetics is included where needed. The IGCC-FCT framework included “virtual sensors” that monitored component model calculations and thus could be used to indicate equipment (or model) operation problems; due to budget constraints, the virtual sensor feature was not implemented into the VEF.

The majority of the equipment components are modeled using 0D or 1D process engineering models. In general, the models were developed using information from standard engineering reference manuals, textbooks, handbooks and other information available in the open literature. Several of the models were created by reusing models developed earlier in the project for the LEBS-POC framework; this is particularly true for the heat exchanger models.

In addition to the above, a simple coupling between the VEF and two additional plant modeling frameworks has been demonstrated. A coupling to the Aspen Plus flowsheet modeling tool was implemented and demonstrated [Swensen et al., 2004] to allow accessing the many models available within Aspen Plus as well as Aspen Plus flowsheets for advanced power plant configurations developed by other researchers. A coupling between the VEF and the CMU IECM Vision 21 Planner framework was also implemented that provided access to the plant economics models available within IECM. The coupling of the VEF and IECM tools was demonstrated at the Clearwater Conference 2004 [Rubin et al., 2004]. Further details on the models in IECM and Aspen Plus are available at <http://www.epp.cmu.edu/research/iecmdoc.html> and <http://www.aspentech.com>, respectively. For further details on the coupling of the VEF to the Aspen Plus and IECM tools used in this project, see Section 1.2.3 of this report.

As discussed in Section 1.2, a hierarchy of simulation outputs and analysis tools are provided to review and interrogate simulation results at both the plant or component model level. At the highest level, overall plant results can be viewed in tabular format (tables of values) or in bar charts (note: bar chart capability not implemented in the VEF). At the component model level, model outputs can be viewed in tabular form (summary values) and 1D plots (to review bulk values along the main axis of a device; note: 1D plot capability is not implemented in the VEF). For CFD models, outputs can be viewed using the usual (conventional) 3D CFD viewing techniques. In addition, for CFD results, advanced visualization tools from ISU are included that allow displaying simulation results using virtual reality methods on systems ranging from

inexpensive desktop PCs (using “3D glasses”) to large-scale, immersive environments. The software interfaces between the component models and the framework are performed with component architecture methods; particular care has been used to allow flexibility in the quantity and type of data that can be passed between models and/or the framework (for further details see Component Model Interfacing in Section 1.2.3 and Appendices A and B).

Included in the IGCC-FCT and VEF frameworks are web-based (html) help pages that provide quick reference information about the models and their use.

Entrained Flow Gasifiers - Overview

The coal gasifier is one of the most important systems in an IGCC cycle because it converts a solid fossil fuel into more environmentally attractive hydrocarbon fuel or feedstock. Our modeling efforts focused on two “generic”, cylindrical, gasifier configurations: single stage, down fired and two stage, upflow with multiple feed inlets that can be opposed or tangentially fired (see Figure 1.3.12). Either model can use a slurry feed or a dry feed. These systems are representative of the dominant, commercially available gasifier systems [Holt, 2001].

- The single-stage gasifier configuration contains a single fuel injector located along the gasifier centerline. However, configurations with multiple injectors or an up-fired orientation could also be studied. Examples of a commercial-sized single-stage, down-fired gasifier would be those used at the Polk Power Station, Eastman Chemical plant or the gasifier test facility at the Freiberg R&D center in Germany.
- The two-stage gasifier consists of two sections connected by a diffuser. Each section can have two or four feed injectors. The first stage is assumed to be a slagging combustor used to separate the ash from the slag and to provide hot gases to the second stage. For both classes of gasifiers hot mineral matter is deposited on the wall as slag. Proper slagging behavior is important for protecting the refractory-lined walls of the gasifier from the harsh environment within the gasifier. Examples of commercial-sized two-stage gasifiers are the opposed fired used at the Wabash River power plant and the air-blown, tangentially fired systems being developed in Japan.

As described below, both CFD and engineering process models have been developed to predict the performance of the gasifiers. The CFD models provide detailed information about the flowfield, slagging behavior, etc. but require long runtimes. The process models run quickly and thus can be used for scoping studies and for investigating optimal process conditions prior to running the CFD models.

Although our focus is on oxygen-blown, slurry-feed, pressurized systems, the same modeling tools can be used to model air-blown, dry-feed or atmospheric systems. The gasifier model development efforts were guided through collaborations with Mr. Neville Holt (EPRI), Prof. Terry Wall and his colleagues at the CCSD in Australia, and Prof. Klaus Hein from the IVD at the University of Stuttgart, Germany.

Figure 1.3.12. Gasifier CFD models.

GLACIER CFD Entrained Flow Gasifier Module (Steady State)

The *GLACIER* CFD code is a comprehensive two-phase, reacting CFD-based code that can be used to model a broad range of steady-state turbulent reacting flows. It is capable of modeling two-phase fuels for either gas-particle or gas-liquid applications. For establishing the basic combustion flowfield, full equilibrium chemistry is employed. To compute pollutant emissions, vaporized metals, and other trace species, finite-rate chemistry effects can be included in a post-processor mode. Turbulence-chemistry coupling is accomplished using PDF methods. An important aspect of *GLACIER* is the tight coupling used between the dominant physics for utility boiler applications: turbulent fluid mechanics, radiation heat transfer, chemical reactions, and particle/droplet dynamics. As noted below, the gasifier model accounts for the effects of

- slagging walls in the gasifier;
- high-pressure coal kinetics; and
- soot and tar formation within the gasifier.

Further information on the general capabilities of *GLACIER* is contained in Appendix D and is available at http://www.reaction-eng.com/modeling_tools/glacier.html.

Slagging Wall Submodel

Slagging of hot mineral matter on the walls of an entrained flow coal gasifier is important for good gasifier operation and thus is included within our comprehensive gasifier model. The slagging wall model is based on work previously funded by the DOE in combination with research work performed by researchers at the CCSD in Australia that have developed submodels for coal gasifier applications. The model uses information from the gas flowfield in the gasifier (e.g., gas composition, gas temperature, incident heat transfer, and particle deposition rate) to predict the slag properties (e.g., slag flow, slag thickness, frozen slag thickness) and heat transfer through the walls of the gasifier (for an assumed refractory resistance and external ambient temperature). The model is sufficiently general to include the effects of using a cooling jacket/system on the outside of the gasifier. The critical viscosity for the flowing slag is computed using a correlation from the literature that utilizes the ash composition (wt% of SiO_2 , Al_2O_3 , Fe_2O_3 , CaO , MgO) and numerical parameters based on experimental data. A detailed description of the model, implementation into a CFD-based gasifier model, and example calculations are contained in Appendix F as well as in the open literature [Bockelie et al., 2002c], [Bockelie et al., 2002d], [Bockelie et al., 2003b].

High-Pressure Coal Gasification Kinetics

The gasification kinetics used in a coal gasifier model will impact the ability of the model to accurately predict carbon conversion, a key parameter for gasifier performance. Of particular concern is the change in gasification kinetic rates with the operating pressure within the gasifier. Commercial gasifiers used for power generation are typically operated at about 30 bar, and thus kinetics developed for these units are interchangeable. However, if the syngas is to be used for chemical production, or if carbon sequestration processes are to be used, then the gasifier is typically operated at a much higher pressure (e.g., 60-80 bar). For either situation, for engineering purposes, the minor variations in pressure within the gasifier can be ignored.

There is extensive literature on the kinetics of devolatilization and gasification. However, much of it is directed at the early moving bed and fluidized bed gasifiers and therefore is not directly

relevant to entrained flow gasifiers, which involve higher temperatures and shorter residence times than packed and fluidized bed gasifiers. The literature on entrained flow gasification is limited; furthermore, some of the gasification kinetics at high pressures have been carried out on char samples generated at atmospheric pressure or slow heating conditions and therefore are not representative of chars present in entrained flow gasifiers.

In our model we use the best available data for gasification kinetics. As such, we draw extensively on an ongoing effort on gasification kinetics being carried out in Australia under the directions of Dr. David Harris at the CSIRO and Prof. Terry Wall at the University of Newcastle. The Australian data constitute one of the best sources of information and we have ready access to the information through a MOU between REI and the CCSO. Provided below is a brief overview of the models that have been used for devolatilization and char kinetics. A more detailed discussion can be found in [Bockelie et al., 2002b] and in Appendix G (see section entitled Literature Survey & Assessment of Kinetics Database).

- Devolatilization: Thermal decomposition kinetics is fast at entrained gasification temperatures and is not a strong function of pressure. Volatile yields are suppressed because volatile transport out of coal particles is inhibited as the pressure is increased. Many models have been developed for devolatilization, which give the rate, volatile yield, and composition of the products. The three most widely used are those developed by Solomon and co-workers (1988, 1992), Niksa and Kerstein (1991), and Fletcher and Pugmire (1990). The models yield relatively comparable results. We have chosen the Chemical Percolation Devolatilization (CPD) model of Fletcher and Pugmire to provide information of importance to gasification, such as tar yields because it is in the public domain. CPD also provides the effect of pressure on volatile yields, although it tends to under-predict this value. Future studies at the CCSO involving entrained flow gasification will hopefully resolve these issues. Within the CFD model, the kinetics for devolatilization are modeled using the two-step reaction model [Kobayashi et al., 1977]; however, the input parameters for the model are modified to allow for the above described pressure dependence on volatile yield.
- Kinetics of char gasification: Having the correct gasification kinetics is critical for any gasifier model. Kinetics are needed to size the gasifier/combustor and determine the char combustion efficiency and possible char recycle requirements. The three reactants of importance are O_2 , H_2O , and CO_2 , with the possible addition of H_2 that can contribute to the formation of CH_4 at high pressures. The kinetics are determined by three resistances, that of external diffusion of the gas-phase reactants to the particle surface and diffusion of the reactants from the surface, diffusion through the porous structure of the char, and reaction at the internal (mostly) and external char surface. Our models use the *apparent* kinetic rates (based on the external surface area of the char):

$$R_s = k_i P_{si}^{n_i} e^{-E_i/RT} \quad (1.3.1)$$

where the rate constant k_i , activation energy E_i , and reaction order n_i include the complexity of the internal diffusion and therefore may vary with extent of reaction, and the exponent n_i includes the effects of partial pressures P_{si} of other species at the particle surface and therefore also applies only over a limited range of pressures and gas concentrations. The actual rate is obtained with allowance for resistances for chemical kinetics and mass transfer. Rate coefficients are taken from the literature for O_2 , H_2O , and

CO₂ with preference given to studies for high temperature and pressure. Although there can be wide differences in rates at low temperatures, the actual rates are within a factor of two at high temperatures (2500 K). In our models, we use default values based on studies by Lupa and Kliesch (1979) and updated values based on studies by the CCSD in Australia. Correlations to estimate the actual rate should include the impact of coal type and pressure on the volatile yields and char structure and kinetic parameters. In addition, volatile yields and n_i decrease with increasing pressure.

To simplify generating the kinetic rates used by our coal gasifier modeling tools, as well as the models used by many other researchers, as part of this project REI has developed a preprocessor (*PREKIN*) that uses as input intrinsic coal gasification rates and information that are valid across a broad range of pressures and conditions to rigorously calculate the apparent kinetic rates (i.e., global kinetic rates) that are limited to use for the operating pressure of a particular unit. See Appendix G for a discussion of the submodels contained in *PREKIN* and its use.

Soot and Tar Generation

Soot formation due to the reducing conditions within the gasifier plays an important role in radiative heat transfer in gasifiers. Likewise, tar formation imposes a limit on the oxygen-carbon ratios that can be used to operate a gasifier. The initial versions of our gasifier model calculated local soot concentrations from a correlation and ignored tar formation. In the last year of the project, REI implemented into the gasifier model soot and tar models from the open literature. The soot model is based on work by Brown and Fletcher (1998). This model is comprised of three transport equations for tar mass fraction, soot mass fraction, and soot number density. Coal-derived soot is assumed to form only from tar, which we calculate from Lagrangian particle-phase equations that use the CPD model to determine devolatilization rates and tar yields. The CPD model describes the devolatilization behavior of a rapidly heated coal based on the chemical structure measured by ¹³C NMR. REI had previously implemented the soot and tar models into REI's combustion modeling tools used for utility boiler coal combustion (not gasification) simulation tools [Shim et al., 2003]. Hence, the effort to integrate the improved soot and tar models into our coal gasification models was incremental. Further details on the soot and tar models are available in Appendix H and in [Bockelie et al., 2004].

Model Input / Output

Illustrated in Figure 1.3.13 is a data input panel for the entrained flow gasifier model. With this panel the user can specify the injector properties. The same panel is used for either a one-stage or two-stage gasifier by selecting the appropriate radio button at the top of the panel. Note that for the two-stage gasifier, each level of injectors (three) can be set to different values. Required fields include steam flowrate as well as slurry properties, including temperature, flowrate, and wt% coal. The recycled char is an externally computed value specified by the user to represent the % char returning to the gasifier (typically from a feedback loop running through a cyclone unit). Information on the "Misc" panel includes particle size distribution information (e.g., % through 50 mesh and 200 mesh) and coal type. Using a pull-down menu, the user can select fuels from a database of pre-defined coals (e.g., Illinois #6, Pittsburgh #8, Wyodak, Petcoke, etc.). Fuel properties contained in the database include the fuel ultimate and proximate analysis, higher heating value (HHV), and ash composition.

Outputs from the gasifier CFD model include summary data information presented in tabular form (see Figure 1.3.13) as well as detailed flowfield information that can be viewed using conventional 3D CFD viewing techniques (e.g., planes, contours, iso-surfaces, flowfield vectors, particle trajectories, wall properties; see Figure 1.3.12) or viewed using advanced CFD visualization tools from ISU that allow displaying simulation results using virtual reality methods on systems ranging from inexpensive desktop PCs (using “3D glasses”) to large-scale, immersive environments.

For future reference, when comparing gasifier performance we typically focus on characteristics of the syngas generated. The principle items of interest are the carbon conversion (i.e., % of carbon from the solid fuel converted to carbon in the syngas) and the syngas temperature, composition, higher heating value (HHV, in BTU or BTU/SCF) and cold-gas efficiency (CGE) which is defined as in [Benyon et al., 2000]:

$$CGE = (\dot{M}_{syngas} * HHV_{syngas}) / (\dot{M}_{fuel} * HHV_{fuel}) \quad (1.3.2)$$

where $\dot{M}_{fuel}$ and $\dot{M}_{syngas}$ are the mass flow rate of the fuel and syngas, respectively, and HHV_{fuel} and HHV_{syngas} are the higher heating value of the fuel and syngas, respectively.

Figure 1.3.13. Input UI (left) and summary output table (right) for entrained flow gasifier.

AIOLOS CFD Entrained Flow Gasifier Module (Transient/Steady-State):

The *AIOLOS* CFD code is a comprehensive CFD modeling code developed at the University of Stuttgart that can be used to model a broad range of steady or transient turbulent reacting flows. It can be used to model two-phase fuel applications, using either Eulerian-Eulerian or Eulerian-Lagrangian methods. *AIOLOS* employs an EDC technique for turbulence-chemistry coupling. It can employ multi-domain grids and perform time-dependent coal combustion simulations using either implicit or explicit time stepping. It can be used on virtually any level of hardware or operating systems. *AIOLOS* is parallel-capable on both SMP and distributed architectures. It can be executed on single or dual CPU PCs/workstations and PC clusters and has been tuned for use on supercomputers. Further information on *AIOLOS* can be found on the web at: http://www.ivd.uni-stuttgart.de/english/aiolos_e_fh.html. For modeling entrained flow gasifiers, submodels that approximate coal kinetics under gasification conditions are used (see below). As with the LEBS-POC simulations, gasifier simulations performed using *AIOLOS* were run in a standalone mode to allow RECOM to execute the simulations at the supercomputer center at the University of Stuttgart. The *AIOLOS* simulations were targeted toward unsteady simulations for gasifier startup and shutdown.

The following paragraphs briefly describe the kinetic model of gasification chemistry implemented into *AIOLOS*, the treatment of turbulence-chemistry interaction in *AIOLOS*, and the verification of the correct implementation of the chemistry model.

Kinetic Model of Coal Gasification

The modeling of coal gasification is based on the assumption that the conversion of coal can be divided into three steps. These steps are drying (in case of a wet fuel like biomass or brown coal) and pyrolysis, heterogeneous char reactions, and combustion of volatiles. During pyrolysis the coal decomposes to volatile matter and char. The heterogeneous char reactions consider the reactions of char with the gas-phase species. For the coal gasification, these species are mainly oxygen, steam, and carbon dioxide. The third step contains all reactions of the gas-phase species. The reaction scheme of the gasification model used in this project is described below by the following reactions.

a) Drying and pyrolysis

b) Heterogeneous reactions:

c) Homogenous reactions:

These reactions determine the composition of the gas produced and the residual char content depending on the following parameters: total pressure p , temperature T , composition of the fuel (proximate analysis), and the gasification agent (air, oxygen, steam or CO_2) used.

While the residual char content is mainly determined by the heterogeneous reactions, the composition of the produced gas is a function of the very slow homogeneous reactions. This is due to the typically long residence times in gasifiers. Therefore, a reliable gasification model has to consider both sets of reactions. All reactions except {G3} and {G4} are forward reactions. The reaction pathways {G3} and {G4} are considered in the forward and backward directions, which is essential for the accurate prediction of the gas composition. The underlying kinetic rate expressions are summarized in Table 1.3.3.

Table 1.3.3. Kinetic Rate Expressions Used in *AIOLOS* Model.

Reac	Kinetic rate	$k_{0,i}$	E_i/R	src
{E1}	$\frac{dw_{FB}}{dt} = -k_{0,F1} \cdot \exp\left(-\frac{E_{F1}}{RT_S}\right) \cdot w_{FB}$	$5.13 \cdot 10^6 \text{ s}^{-1}$	$1.06 \cdot 10^4 \text{ K}$	[Chan,1985]
{E2}	$\frac{dw_{TB}}{dt} = -k_{0,F2} \cdot \exp\left(-\frac{E_{F2}}{RT_S}\right) \cdot w_{TB}$	$1.14 \cdot 10^5 \text{ s}^{-1}$	$8.9 \cdot 10^3 \text{ K}$	[Norman,1997]
{F1}	$\frac{dw_C}{dt} = -k_{0,F3} \cdot \exp\left(-\frac{E_{F3}}{RT_S}\right) \cdot a_P \cdot w_C \cdot p_{O_2}^*$	$2.08 \cdot 10^2$ ($\text{kg/m}^2 \cdot \text{s} \cdot \text{bar}$)	$9.55 \cdot 10^3 \text{ K}$	[Norman,1997]
{F2}	$\frac{dw_C}{dt} = -k_{0,F4} \cdot \exp\left(-\frac{E_{F4}}{RT_S}\right) \cdot a_P \cdot w_C \cdot p_{H_2O}^*$	$2.47 \cdot 10^3$ ($\text{kg/m}^2 \cdot \text{s} \cdot \text{bar}$)	$2.10 \cdot 10^4 \text{ K}$	[Norman,1997]
{F3}	$\frac{dw_C}{dt} = -k_{0,F5} \cdot \exp\left(-\frac{E_{F5}}{RT_S}\right) \cdot a_P \cdot w_C \cdot p_{CO_2}^*$	$2.47 \cdot 10^3$ ($\text{kg/m}^2 \cdot \text{s} \cdot \text{bar}$)	$2.10 \cdot 10^4 \text{ K}$	[Norman,1997]
{G1}	$\frac{dc_{C_m H_n}}{dt} = -k_{0,G1} \cdot T^{0.5} \cdot \exp\left(-\frac{E_{G1}}{RT_G}\right) \cdot c_{C_m H_n} \cdot c_{O_2}$	$2.33 \cdot 10^{11}$ $\text{m}^3/(\text{kmol} \cdot \text{s} \cdot \text{K}^{0.5})$	$2.01 \cdot 10^4 \text{ K}$	[Jones,1988]
{G2}	$\frac{dc_{C_m H_n}}{dt} = -k_{0,G2} \cdot \exp\left(-\frac{E_{G2}}{RT_G}\right) \cdot c_{C_m H_n} \cdot c_{H_2O}$	$3.0 \cdot 10^8 \text{ m}^3/(\text{kmol} \cdot \text{s})$	$1.51 \cdot 10^4 \text{ K}$	[Zimont,1969]
{G3+}	$\frac{dc_{CO}}{dt} = -k_{0,G3} \cdot \exp\left(-\frac{E_{G3}}{RT_G}\right) \cdot c_{CO} \cdot c_{H_2O}$	$2.75 \cdot 10^9$ $\text{m}^3/(\text{kmol} \cdot \text{s})$	$1.01 \cdot 10^4 \text{ K}$	[Zimont,1969]
{G3-}	$\frac{dc_{CO_2}}{dt} = -\frac{k_{0,G3}}{K_{G3}} \cdot \exp\left(-\frac{E_{G3}}{RT_G}\right) \cdot c_{CO_2} \cdot c_{H_2}$	$2.75 \cdot 10^9$ $\text{m}^3/(\text{kmol} \cdot \text{s})$	$1.01 \cdot 10^4 \text{ K}$	[Zimont,1969]
{G4+}	$\frac{dc_{H_2}}{dt} = -\frac{k_{0,G4}}{T_G} \cdot \exp\left(-\frac{E_{G4}}{RT_G}\right) \cdot \frac{c_{O_2}^{2.25} \cdot c_{H_2}^{0.5}}{c_{H_2O}}$	$2.5 \cdot 10^{17}$ $\text{m}^{2.25} \cdot \text{K}/(\text{kmol}^{0.75} \cdot \text{s})$	$2.01 \cdot 10^4 \text{ K}$	[Zimont,1969]
{G4-}	$\frac{dc_{H_2O}}{dt} = -\frac{k_{0,G4}}{T_G \cdot K_{G4}} \cdot \exp\left(-\frac{E_{G4}}{RT_G}\right) \cdot \frac{c_{O_2}^{1.75}}{c_{H_2}^{0.5}}$	$2.5 \cdot 10^{17}$ $\text{m}^{2.25} \cdot \text{K}/(\text{kmol}^{0.75} \cdot \text{s})$	$2.01 \cdot 10^4 \text{ K}$	[Zimont,1969]
{G5}	$\frac{dc_{CO}}{dt} = -k_{0,G5} \cdot \exp\left(-\frac{E_{G5}}{RT}\right) \cdot c_{CO} \cdot c_{O_2}^{0.5} \cdot c_{H_2O}^{0.5}$	$1.3 \cdot 10^{11} \text{ m}^3/(\text{kmol} \cdot \text{s})$	$1.51 \cdot 10^4 \text{ K}$	[Howard, 1972]

The quantities in this table are defined as:

- w_j is the concentration of the species j in $\text{kg}_j/\text{kg}_{\text{gas}}$;
- p_j^* is the partial pressure of component j at the particle surface (value is lower than partial pressure in the gas phase due to effects of boundary layer diffusion);
- c_j is the concentration of species j in kmol/m^3 ;
- $k_{0,i}$ and E_i are the prefactor and the activation energy of reaction i ; and
- a_p is the specific particle surface in m^2/kg .

The reactions {G3} and {G4} are evaluated as forward and backward reactions. The corresponding equilibrium constants K_{G3} and K_{G4} are calculated according to [Mueller,1998]:

$$K_{G3} = \frac{c_{\text{CO}_2} \cdot c_{\text{H}_2}}{c_{\text{CO}} \cdot c_{\text{H}_2\text{O}}} = \exp[4708524 - 1758711(\ln T_G) + 2195011(\ln T_G)^2 - 0.9192934(\ln T_G)^3] \quad (1.3.3)$$

$$K_{G4} = \frac{c_{\text{H}_2\text{O}}}{c_{\text{H}_2} \cdot c_{\text{O}_2}^{0.5}} = \exp\left(-6.9793 + \frac{30261.7}{T_G}\right) \text{ in } \text{m}^{1.5}/\text{kmol}^{0.5} \quad (1.3.4)$$

The reaction scheme should be able to predict the gasification process at any pressure level. The heterogeneous reactions consider the partial pressure directly in the corresponding equation. The effect of pressure in the homogeneous reactions is indirectly taken into account by using the unit of kmol/m^3 for the concentrations. So each concentration linearly scales with pressure. Nevertheless, it should be noted that the pressure dependence in the heterogeneous reactions is only linear, while in the homogeneous reactions, the pressure dependence is quadratic.

Heterogeneous Char Reactions

The previously described heterogeneous reaction rates ($k_{0,F1} - k_{0,F3}$) only consider the chemical reaction rate per surface area of the char particles. The effective reaction rate for char reactions is a combination of the chemical reaction rate k_S and the diffusion rate k_D . So in general, the total reduction of char mass can be expressed as:

$$\frac{dw_{\text{Char}}}{dt} = -k_{\text{Char}} \cdot a_p \cdot w_{\text{Char}} \quad (1.3.5)$$

where k_{Char} is the effective reaction rate which can be computed by the following equation:

$$k_{\text{Char}} = \frac{p_j^*}{\frac{1}{k_S} + \frac{1}{k_D}} \quad (1.3.6)$$

The chemical reaction rate for each char reaction can now be expressed by the following Arrhenius equation with the frequency factor $k_{0,i}$ and the activation energy E_i/R given in Table 1.3.3:

$$k_S = k_{0,i} \cdot e^{-(E_i/RT)} \quad (1.3.7)$$

For spherical particles the diffusion rate can be calculated by

$$k_D = \frac{24 \cdot Sh \cdot D_j}{R \cdot d \cdot T_{GS}} \cdot 10^5 \quad (1.3.8)$$

Sh is the Sherwood number and can be set to 2 for spherical particles, D_j is the diffusion coefficient for species j, d is the diameter of the particle, and T_{GS} is the boundary layer temperature, which can be assumed to be the mean temperature between the particle temperature and the surrounding gas temperature.

The Eddy Dissipation Concept (EDC)

The turbulence-chemistry interaction is modeled using the Eddy Dissipation Concept [Magnusson, 1989] which is a general concept for treating the interaction between turbulence and chemistry in flames. In the EDC the total space is subdivided into a reaction space, the fine structures and the surrounding fluid. All homogeneous reactions are assumed to take place only within these fine structures which can locally be treated as a well-stirred reactor transferring mass and energy only to the surrounding fluid. The mean residence time τ_D of fluid within the fine structures is modeled by:

$$\tau_D = 0.41 \cdot \left(\frac{\nu}{\varepsilon} \right)^{0.5} \quad (1.3.9)$$

with the dissipation of turbulent kinetic energy ε and the kinematic viscosity ν . The mass fraction γ^* occupied by the fine structures is modeled by:

$$\gamma^* = \left[2.13 \cdot \left(\frac{\nu \cdot \varepsilon}{k^2} \right)^{0.25} \right]^2 \quad (1.3.10)$$

The reaction rates of all species are calculated on a mass balance for the fine structure reactor. Denoting quantities in the fine structures with an asterisk, the conservation equation of a species j can be written as:

$$\frac{\rho^*}{\tau \cdot (1 - \gamma^*)} \cdot (w_j^* - w_j) = M_j \cdot \omega_j^* \quad (1.3.11)$$

in which w_j is the mean mass fraction of species j, w_j^* is the mass fraction of species j within the fine structure, M_j is the molecular weight of species j, and ω_j^* denotes the fine structure chemical reaction rate for species j. The mean chemical reaction rate of the species j (ω_j) can then be determined from the chemical reaction rate in the fine structures ω_j^* and the mass fraction of the fine structures γ^* . The presented homogeneous reactions G1 – G5 are modeled as EDC equations and only take place in the fine structures.

Entrained Flow Gasifier - Process Engineering Model

The CFD gasifier model requires significant computational time to arrive at a steady-state solution. Hence, a simpler model that can be used for faster calculations either within the energyplex framework or as a preprocessor to optimize operating inputs before running the CFD model was developed. The model can be used to optimize gasifier efficiency while providing indicators for proper slag flow.

The engineering process gasifier (0D) model consists of two submodels: an equilibrium zonal equilibrium submodel with heat transfer and a coal burnout submodel. The heat transfer submodel accounts for heat transfer to the ash contained in the solid fuel, and heat transfer to walls to account for backside cooling (including heat extraction); the wall heat submodel only required the wall resistance and backside temperature (e.g., steam temperature) to be specified. The zonal submodel calculates the equilibrium exit gas concentration and temperature given a prescribed heat transfer through the walls. An ash viscosity submodel from the CFD gasifier slag model is used to calculate a representative ash viscosity and critical viscosity temperature.

The fuel burnout and char recycle are required inputs to the zonal submodel obtained from the burnout submodel, while the gas and radiation temperatures are the required inputs into the burnout submodel obtained from the zonal submodel. A schematic of the model for a one- and two-stage gasifier are illustrated in Figures 1.3.14 and 1.3.15, respectively.

Figure 1.3.14. Schematic for the one-stage entrained flow engineering process model.

Figure 1.3.15. Schematic for the two-stage entrained flow engineering process model.

In the one-stage gasifier, particle burnout can be entered by the user or computed. In preliminary versions of the process engineering model, the particle burnout was computed with CBK8, a model developed at Brown University which includes intrinsic oxidation of coal in lean pulverized combustion [Sun and Hurt, 2000]. However, CBK8 was not sufficiently flexible to support two-stage gasifiers or fuel staging. Hence, CBK8 was replaced with the heterogeneous particle reaction model used within *GLACIER* to provide the desired flexibility. If the geometry is specified by the user, the burnout is calculated by the burnout submodel. If the desired burnout is specified by the user, the burnout submodel is used to determine the residence time and the geometry needed to produce the input burnout.

For the two-stage gasifier, the particle burnout is computed by coupling two one-stage gasifier models, with the outlet of the first acting as an inlet for the second, along with additional inlet flows representing the staged fuel and transport fluid (see Figure 1.3.15). Two-stage gasifiers are operated with the first stage serving as a combustion stage, which provides the heat needed to drive endothermic gasification reactions in the reducing second stage. The first stage is operated closer to stoichiometric, while the remaining feedstock fuel is introduced in the second stage with very little or no oxidant. The particle burnout model was extended, from its original form, to allow for incomplete burnout of the fuel in the first stage of the gasifier. This allows modeling of staged fuel injection in the two-stage model. As highlighted in Figure 1.3.15, iterations proceed in the first stage between the particle burnout, equilibrium, and heat transfer models until the exit temperature is converged. The same iterations for the second stage then follow, except that any unburned particles from the first stage are also integrated in the second stage.

The process engineering model includes a coal gasification kinetics model to account for high-pressure kinetics effects, a flowing slag indicator, and soot and tar models that are based on the corresponding models as used in the *GLACIER* CFD entrained flow model.

For the two-stage gasifier, the model can account for the effects of syngas being recycled to the second stage (i.e., to temper the outlet syngas stream). Likewise, for both gasifier types the impact of recycled char, which is fed back from the cyclone and injected with the coal or slurry, can be included in the calculations.

Illustrated in Figure 1.3.16 and Figure 1.3.17 are the UI for the gasifier process model. Note that the user can specify geometry information, process conditions, select coal type from a database of coals, and prescribe coal grind (particle size distribution). If desired, the model can be used in design mode in which the carbon conversion (particle burnout) is specified and the equivalent gasifier geometry (diameter, height) is computed to account for wall heat transfer and residence time needed to provide the specified fuel conversion. The UI for the “Flows” tab for the process model (Figure 1.3.17) is identical to that used for the CFD-based entrained flow gasifier model (i.e., Figure 1.3.13).

Gasifier0D

Flows | Misc

Geometry Specified

☒ Specify Geometry

Dimensions

Diameter (m) 2.2

Length (m) 5.5

1st Stage 1

2nd Stage 1

Rwall (m²K/W)

1st Stage 1

2nd Stage 1

Burnout Specified

Burnout (%) 98

Heatloss (%) 0

1st Stage 0

2nd Stage 0

☒ Design Mode

L/D 3

Emis

1st Stage 0.75

2nd Stage 0.75

Misc

Backside Temp (K) 300

Slag Efficiency (%) 50

Pressure Drop (Pa) 502042

Coal Info

Coal Type Illinois_#6

Size percent thru 50 99.2

Size percent thru 200 90

OK Cancel

Figure1.3.16. Configuring gasifier process model for burnout calculations.

Gasifier

Flows | Misc

☐ One-stage Gasifier0D ☒ Two-stage Gasifier0D

slurry oxidant steam

Fuel Injectors - level 1

Steam

Temperature (K) 0

Flowrate (kg/s) 0

Slurry

Temperature (K) 422

Flowrate (kg/s) 17.18

Coal (%) 74.26

Re-Cycled Char (%) 0

Fuel Injectors - level 2

Steam

Temperature (K) 0

Flowrate (kg/s) 0

Slurry

Temperature (K) 422

Flowrate (kg/s) 17.18

Coal (%) 74.26

Re-Cycled Char (%) 0

Fuel Injectors - level 3

Steam

Temperature (K) 0

Flowrate (kg/s) 0

Slurry

Temperature (K) 422

Flowrate (kg/s) 9.10

Coal (%) 74.26

Re-Cycled Char (%) 0

OK Cancel

Figure1.3.17. Example inputs for flows for gasifier process model. Input panel is same as per CFD model.

Output from the process engineering entrained flow gasifier model is summarized in tabular form in a summary table. An example is illustrated in Figure 1.3.18.

Description	Value
+++++	
1st Stage Wall Heat Transfer (	0.00e+000
2nd Stage Wall Heat Transfer (	0.00e+000
Burnout (%)	98.00
Cold gas efficiency (% (HHV))	83.93
Cold gas efficiency (% (LHV))	79.79
HHV (BTU/lb)	5023.06
LHV (BTU/lb)	4571.53
Output Temperature (K)	1470.28
Slag Critical Viscosity Temper	1627.59
Slag Flow (kg/sec)	1.57
Slag Surface Temperature (K)	2121.25
Slag Viscosity (Pa-s)	7.03e-001
Thermal Input (MW)	8.76e+002
Thermal Output (MW)	7.35e+002

Figure 1.3.18. Example output for engineering process gasifier model.

Transport Reactor Gasifier Model

A transport reactor is an alternative gasifier concept that could potentially be used in an advanced power generation plant. The transport reactor is in effect a circulating fluidized bed (CFB) with a fast solids recirculation rate and a high gas velocity in the riser. An example of a transport reactor gasifier is the KBR coal gasifier being used at the DOE Wilsonville Process Simulation Development Facility (PSDF). The CFD tools being used in this project to simulate the flowfield of entrained flow gasifiers are not appropriate for modeling a transport reactor due to the dense particle loading encountered in the transport reactor. Hence, a different modeling tool is required. The transport reactor gasifier model developed by REI uses a traditional 1D, core-annulus engineering model originally developed for CFB combustors, which has been modified for gasifier applications.

The model provides elevation profiles for the computed

- gas flowfield: temperature, velocity, and species (concentrations);
- wall conditions: temperature, heat flux;
- solids: carbon conversion, particle size for the coal, char, limestone, sand (inert)

and overall (summary) estimates for

- cold-gas efficiency;
- syngas: species, temperature, particle loading; and
- solids/particles: size distribution, carbon conversion.

The model can be used to help evaluate the impact on carbon conversion, syngas, particle size, and refractory due to operational changes, such as

- fuel change: coal, char-recycle, petcoke, waste, biomass;
- feed rates and ratios for fuel:limestone;
- oxidizer: air, oxygen blown/enriched, preheat;
- FGR;
- solids: grind, drying, preheat; and
- design changes (e.g., vessel diameter, height).

The model was used in the IGCC-FCT framework to perform example calculations. However, due to budget constraints, this model was not ported to the VEF. Implementation of the transport reactor gasifier model into the VEF would be a straightforward process.

Model Description

The transport reactor gasifier model is based on a computer model originally developed in Europe with funding from the International Energy Agency (IEA) that was designed to simulate coal combustion in an atmospheric or pressurized CFB. The model uses a 1-½ dimensional steady-state model (core-annulus model) based on energy balance and species mass balance equations. The model includes submodels for the riser, cyclone, return leg, and the solids flow control valve. The model describes the reactor hydrodynamic behavior, reactions involved with coal combustion, emissions and sulfur dioxide removal, heat transfer, including gas and solid flows, development of coal/char particle size distribution during combustion, coal conversion, and homogeneous and catalytic gas reactions. Reduction of sulfur dioxide using limestone/dolomite was also taken into account. The model predicts coal conversion, cyclone

efficiency, temperature profile in the furnace and emissions of CO, CO₂, NO, N₂O and SO₂ from the furnace. Detailed information regarding the basic model is available in [Hannes, 1993].

In the model, the dense bed height is calculated iteratively based on an assumed pressure drop across the riser. In the original model, the pressure drop was an input. REI enhanced the original model formulation so that the riser pressure drop is predicted once the solids circulation rate is known. Here, the solids volume fraction in the dilute zone of the riser is assumed to be [Kunii and Levenspiel, 1991]

$$\varepsilon_p = \varepsilon_{p,\infty} + (\varepsilon_{p,d} - \varepsilon_{p,\infty})e^{-az} . \quad (1.3.12)$$

At the exit of the riser, the solids fraction is

$$\varepsilon_{p,\text{exit}} = \frac{G_p}{\rho_p(u_o - u_t)} . \quad (1.3.13)$$

Thus,

$$H_{\text{dilute}} = \frac{1}{a} \ln \left(\frac{\varepsilon_{p,d} - \varepsilon_{p,\infty}}{\varepsilon_{p,\text{exit}} - \varepsilon_{p,\infty}} \right) \quad (1.3.14)$$

and

$$H_d = H_{\text{riser}} - H_{\text{dilute}} . \quad (1.3.15)$$

The riser pressure drop can then be calculated directly as

$$\Delta P_{\text{riser}} = \rho_p g \{ \varepsilon_{p,d} H_d + \int_0^{H_{\text{dilute}}} [\varepsilon_{p,\infty} + (\varepsilon_{p,d} - \varepsilon_{p,\infty})e^{-az}] dz \} . \quad (1.3.16)$$

To benchmark the above model, calculations were conducted to simulate the pressure drop along the riser height in a circulating fluidized bed and to compare model predictions with experimental data [Monazam et al., 2001] measured along the riser in a circulating fluidized bed consisting of a riser 0.3048 m in diameter and 17.0 m in height. In the experiment, air was used as the fluidizing media and PVC particles were employed as the solid phase. The superficial air velocity in the riser was 6.4 m/s and the particle circulation rate was 26 kg/m²·s. Predicted and measured values are compared in Figure 1.3.19. It can be seen that the model predictions are in reasonable agreement with the measurements. Both the experimental data and the model predictions clearly indicate a dense, bubbling bed at the bottom of the riser and a dilute regime at the top of the riser.

Figure 1.3.19. Comparison of calculated and measured pressure drops across the riser in a circulating fluidized bed: PVC particles, $u_g = 6.4$ m/s and $G_p = 26$ kg/m²·s.

The original model was targeted for simulating coal combustion. Hence, REI implemented coal gasification kinetics into the model. The kinetics implemented were taken from MFIX [Guenther et al., 2002]. In a coal combustion system the sulfur from the coal oxidizes to form SO_2 that oxidizes further to form SO_3 and then reacts with calcium oxide, resulting from calcinations of limestone or dolomite, to form gypsum (CaSO_4). In contrast, in a coal gasification system sulfur is present in the form of hydrogen sulfide. Under the gasifier conditions, in the presence of limestone or dolomite, hydrogen sulfide reacts with CaCO_3 forming calcium sulfide that can be easily removed from the fluidized bed. The model was modified to include this process.

The initial version of the transport gasifier model was benchmarked against available information for the PSDF transport reactor at Wilsonville, Alabama. For these simulations it was assumed that the reactor had a riser 62 ft in height, a mixing zone 20 ft in height, and that the riser cross-sectional area was about 1.5 to 3 ft². Table 1.3.4 summarizes the ranges of reported operating conditions of the gasifier [Davis et al., 2002]. Note that precise operating conditions and corresponding syngas conditions were not available in the open literature when the simulations were performed. For the baseline simulations, for each operating variable the calculations were performed at the midpoint of the range shown in Table 1.3.4.

Table 1.3.4. PSDF Operating Conditions Used For Benchmarking.

Fuel type	Powder River Basin, Alabama Calumet Bituminous
Fuel particle size, μm	200 - 350
Fuel feed rate, pph	2700 - 5000
Sorbent type	Ohio Bucyrus limestone
Sorbent particle size, μm	10 - 30
Sorbent feed rate, pph	0 - 200
Reactor temperature, $^{\circ}\text{F}$	1670 - 1825
Reactor pressure, psig	140 - 240
Riser gas velocity, fps	40 - 60
Riser mass flux, $\text{lb/ft}^2\text{ s}$	150 - 700
Air/coal mass ratio	2.5 - 3.5
Steam/coal mass ratio	0.0 - 1.0

Figure 1.3.20 illustrates a comparison of the design conditions and the values predicted by the model (denoted as REI). It can be seen that the model predictions are in good agreement with the design syngas composition except for methane concentration. Note that the model predicts a carbon conversion of 99.8%, and carbon conversion higher than 95% has been reported for this system [Leonard et al., 2002]. The model under-predicts the methane concentration because the coal devolatilization model used assumes that volatiles are a mixture of CO, H₂S, NH₃ and NO or H₂. Methane formation is expected during coal devolatilization. To verify this hypothesis, a computer code, CPD, developed by Prof. Fletcher at BYU, was used to calculate volatile composition and release rate. These computations were combined with an in-house software package (Modlink), which calculates gas composition under homogeneous reaction conditions, to calculate the composition of final product syngas by assuming volatiles are well mixed with coal off-gas and air from the inlet for a given carbon conversion. The results, referred to as CPD+Modlink, are also presented in Figure 1.3.20. It is clear that methane concentration is consistent with the design data. To further benchmark the model, operating conditions were changed in the simulations to span the ranges shown in Table 1.3.4. The minimums and the maximums of gas species concentrations from these simulations are also plotted in Figure 1.3.20. It can be seen that the design syngas composition is bounded between the minimums and the maximums of the gas species concentrations. Overall, the transport reactor model provides a reasonable estimate of the performance of the PSDF gasifier.

Figure 1.3.20. Comparison of model predictions with design syngas composition.

Based on the above benchmarking exercise, several model enhancements to improve the predictive ability and robustness of the model were implemented:

- 1) A mixing zone was added to the riser section of the gasifier in the structure of the model. This allows a better description of the introduction of the fuel, the limestone and the recirculating material, and the reactions taking place in the mixing zone of the gasifier.
- 2) Calculation of the gas velocity has been refined to account for the gas generated through the heterogeneous reactions.
- 3) Calculation of particle temperature has been modified so that particle temperature is calculated based on bed temperature, which is calculated from the energy balance.
- 4) Heat transfer to water walls has been removed since the gasifier is refractory lined.

The improved Transport Reactor Gasifier model was used to simulate another test case of coal gasification in the Wilsonville PSDF transport reactor for which more specific reactor conditions have been reported [PSDF, 2002]. The operating conditions for the benchmarking study are shown in Table 1.3.5. Note that the riser and mixing zone geometry was estimated based on the reported riser gas velocity and other information in the literature.

The simulated syngas composition compared to reported measured data is shown in Table 1.3.6. It can be seen that the predictions are in reasonably good agreement with the measured data. However, the predicted methane concentration is lower than the reported concentration. As explained above, this is due to the coal devolatilization model which assumes that no methane is formed during coal devolatilization. The model could be improved by using a better devolatilization submodel in the overall reactor model. Above it was shown that by using a combination of CPD and Modlink, better prediction of methane concentration in the syngas can

be achieved. Also shown in Table 1.3.6 are the lower heating value of syngas and the cold-gas efficiency of the gasifier. Again, the predictions are in reasonable agreement with measurements.

Table 1.3.5. Operating Conditions Used For Benchmarking Transport Reactor Gasifier Model.

		Wilsonville	300 MW
Riser:	Diameter	10 in	4 ft
	Height, ft	62	65
Mixing zone:	Diameter	16 in	6.5 ft
	Height, ft	20	25
Fuel type		PRB	PRB
Fuel size, μm		272	350
Fuel feed rate, lb/hr		5110	245000
Sorbent particle size, μm		20	60
Sorbent feed rate, lb/hr		175	8000
Reactor pressure, psia		242	385
Reactor temperature, $^{\circ}\text{F}$		1743	1800
Riser gas velocity, ft/s		40	54
Solids circulation rate, lb/(ft ² ·s)		300	600
Air flow rate, lb/hr		14866	708907

Table 1.3.6. Comparison of Syngas Composition Predicted by Transport Reactor Gasifier Model with Measured Values for the PSDF.

	Predictions	Experimental
H ₂ O	6.0	9.1
CO	20.2	17.9
H ₂	10.1	9.7
CO ₂	6.6	8.9
CH ₄	0.07	1.3
N ₂	57.1	53.1
LHV, Btu/SCF	92	96
CGE (LHV), %	61.0	62.8

The pressure drop profile and the temperature profile from the model calculations are presented in Figure 1.3.21. It is shown that the reactor has a lower dense bed and a lean zone in the riser. The temperature profile is quite flat with only about 20°C difference from the top to the bottom of the reactor. The riser temperature is very similar to the reported operating temperature of the riser. The core temperature is slightly higher than that of the annular region because the gas flow rate in the core is higher, carrying up more energy from the lower section of the gasifier where coal combustion takes place. The velocity profile in the gasifier is shown in Figure 1.3.22, along with the operating range of the riser gas velocity. Due to the difference in bed cross-sectional area, the mixing zone has a lower velocity than the riser. In the model calculations, it is found that volatile and char combustion processes occur in the lower dense bed region as oxygen is consumed.

Figure 1.3.21. Predicted pressure drop and temperature profile in the PSDF.

Figure 1.3.22. Predicted gas velocity in the PSDF.

300 MW IGCC Power Plant

Southern Company conducted an engineering study for a commercial plant design that would use a nominal 300 MW, air-blown Transport Reactor Integrated Gasification (TRIG) combined cycle based on a General Electric (GE) 7FA gas turbine [Leonard et. al., 2002]. Although very little design information is reported in the paper [Leonard et. al., 2002], the reported information was used to test the model for simulating a commercial-scale gasifier.

The operating conditions of the plant are given above in Table 1.3.5. The syngas composition from the model predictions is compared with the design conditions as shown in Table 1.3.7. It can be seen that the agreement is reasonable. Again, methane concentration prediction requires a better devolatilization model. The predicted lower heating value (LHV) of the syngas and cold-gas efficiency (CGE) of the gasifier are lower than the design syngas LHV and CGE primarily due to under-prediction of methane concentration in the model.

Table 1.3.7. Comparison of Predicted and Design Syngas Composition for 300 MW TRIG Plant.

	Predictions	Design
H ₂ O	7.1	4.7
CO	20.8	20.0
H ₂	11.3	10.3
CO ₂	6.5	7.5
CH ₄	0.24	2.1
N ₂	54.0	55.3
LHV, Btu/SCF	99	110
CGE (LHV), %	65.0	73.0

The predicted pressure drop and temperature profiles are shown in Figure 1.3.23. Note that the riser temperature is very close to the design operating temperature of the riser. Due to the somewhat taller gasifier in this commercial plant, the overall pressure drop is slightly higher than that in the PSDF. However, the temperature profile remains fairly flat. The gas velocity profile is shown in Figure 1.3.24 and the mixing zone has a lower velocity than the riser. The wide range of the design operating gas velocity of the riser is also shown in the figure.

Figure 1.3.23. Predicted pressure drop and temperature profile in the transport reactor gasifier for a proposed 300 MW TRIG plant.

Figure 1.3.24. Predicted gas velocity in the transport reactor gasifier for a proposed 300 MW TRIG plant.

UI (IGCC-FCT only)

In the IGCC-FCT framework, the UI for the transport gasifier included three panels:

- The panel labeled “Geometry” contains a tool to create the profile of the reactor to be modeled, inflow and outflow locations, and cyclone geometries (Figure 1.3.25). The riser geometry of the gasifier can be specified by dragging a currently selected point after pressing the *Lock* icon (changing to *Unlock*). The number of cyclones and cyclone geometry can also be specified by entering data in the spaces on the right-hand side of the window. Inlet locations of coal feed and limestone feed should also be provided. Locations of returning streams from the return leg and external heat exchangers can also be specified. Recycled flue gas can be specified as a percentage of recycle flue gas flow rate and air flow rate. The number of computational cells between a currently selected point and a point above the selected point can be specified here;
- The panel labeled “Feed” contains input dialog boxes that are used to define the feed rates and coal properties (which can be retrieved from the coal database provided with the framework), particle size distribution for the coal, limestone, and inert material (Figure 1.3.26). Particle density and sphericity for different materials can be specified here; and
- The panel labeled “Misc” is for entering other process information (Figure 1.3.27). The flow rate and temperature of the recycled flue gas can be specified. Re-entered particle temperature and riser wall temperature are also specified here. Coal combustion and limestone- H_2S reaction kinetics are required and should be provided here; default values can be used. Solids recirculation rate in the riser is important in the model and is used to calculate pressure drop in the riser and is input here as one of the operating conditions.

Figure 1.3.25. Defining a profile for transport reactor gasifier.

Feed Mass Flows (kg/s)

Coal	0.485
Lime	0.0126
Inert (Sand)	0.401

Particle Properties

	Coal	Lime	Bed	Char
Density (kg/m ³)	1400.0	2600.0	2600.0	800.0
Sphericity	0.710	0.710	0.710	0.710

Coal Analysis

Reset Coal: **Pittsburg_#8**

Coal:

Ultimate (Wt.%)		Proximate (Wt.%)	
C	72.11	H ₂ O	20.93
H	4.73	VM	46.11
O	15.38	Ash	6.61
N	0.84	FC	47.28
S	0.33		
CL	0.0		
Ash	6.61		

Size Distribution (%)

Size(um)	Coal (%)	Lime (%)	Inert (%)
1000.0	0.0	0.0	0.0
710.0	0.0	0.0	0.0
500.0	0.0	0.0	0.0
355.0	0.0	0.0	0.0
250.0	0.0	0.0	0.0
180.0	0.0	0.0	0.0
125.0	0.0	0.0	0.0
90.0	0.0	0.0	0.0
63.0	0.0	0.0	0.0
45.0	0.0	0.0	0.0
20.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0

Figure 1.3.26. Defining feed for transport reactor gasifier.

Flue Gas Recycle

Flow (Nm³/sec)

Temperature (K)

Temperatures (K)

Re-entered Particles

Wall

Combustion

k₀ (kg/m²sPa)

E₀/R_g (K)

D (m/s)

SO₂

BET surface(m²/g)

Max conversion (-)

k_s (ms/s)

XCaCO₃ (-)

Solids circulating rate (kg/m²s) G_s

Working directory

Figure 1.3.27. Additional inputs for transport reactor gasifier.

Air Separation Unit (ASU)

For the high efficiency, low cost power generation plants of interest in advanced power generation plants, such as Vision 21 plant configurations, air separation units (ASUs) are employed to provide high purity oxygen for reaction and combustion. Using oxygen rather than air has the primary advantages of 1) reducing the gas volumetric flow rate, which reduces equipment sizes, hence capital costs, and 2) the overall thermal efficiency is increased due to the higher temperatures associated with pure oxygen combustion/reaction.

Several industrial processes exist for producing enriched oxygen streams, including membrane separation, pressure-swing adsorption, and cryogenic distillation. Table 1.3.8 gives typical ranges of operation for air separation units [Seader, 1998]. A 500 MWe plant requires processing of around 9000 tpd of air, and cryogenic distillation is the only feasible option. Hence, the ASU model assumes cryogenic distillation.

Table 1.3.8. ASU Types and Their Capacities.

ASU Type	Air Processed (tons/day)
Cryogenic Distillation	> 100
Pressure-Swing Adsorption	20 – 50
Membrane Separation	< 10

Cryogenic distillation involves the separation of liquid/vapor mixtures based on differences in the vapor pressure of the various components. The ASU distillation column(s) typically operates in the range of 8-20 bar and at temperatures of around -170°C . Air is first compressed and then passed through a molecular sieve bed to filter out any water, CO_2 , or hydrocarbons that would freeze at the low operating temperatures. The air is then cooled in a heat exchanger prior to flowing into the distillation column, where approximately 95% purity oxygen and >99% purity nitrogen streams are obtained. These products are cold and generally provide refrigeration to cool the incoming air stream in the above-mentioned heat exchanger, with the product streams exiting the unit at near ambient temperature. If desired, the high-pressure streams could be expanded through turbines to produce work. The primary energy requirements of the ASU are for gas compression.

The ASU model developed for this project is a zero-order process engineering model that acts as a component separator and computes material and energy balances across the unit. The model combines the primary air heat exchanger, distillation column, molecular sieves, and any turbines. All gas compression is done externally with the compressor and heat exchanger models developed. The user inputs are the temperature and pressure of the oxygen and nitrogen product streams as well as the oxygen purity in the oxygen-rich stream as shown in Figure 1.3.28. The energy requirements for the unit are computed as the difference in enthalpy between the product and inlet air streams. The following assumptions are made regarding the material balance.

- All of the oxygen entering the unit with the air stream is assumed to exit with the oxygen-product stream. The % oxygen in the nitrogen stream is typically between 0.1 and 1%, so little error is introduced [Allam, 1992]. Without this assumption, the user would be forced to iterate on the air supply to achieve the desired oxygen product flow rate for a given oxygen impurity in the nitrogen stream.
- The inlet argon is assumed to partition 75% to the oxygen stream and 25% to the nitrogen stream. This assumption is based on the relative vapor pressure of argon with respect to nitrogen and oxygen: $(P_{N_2} - P_{Ar}) / (P_{N_2} - P_{O_2}) = (\text{fraction of total argon in the oxygen stream})$. For a 95% purity oxygen stream, argon is 3.4% and nitrogen 1.6%, which agrees with literature values [Woodward, 1990].
- All water, CO₂, and any hydrocarbons in the incoming air stream are removed to account for the molecular sieve. However, the species are retained in the energy balance where they are assumed to exit at ambient temperature and pressure.

Figure 1.3.28. ASU model inputs.

The model checks the consistency of the data entered by the user. The nitrogen and oxygen product streams will not be liquids for IGCC applications. The model checks the user specification of composition, temperature, and pressure to ensure vapor-phase effluents. Figure 1.3.29 shows the oxygen product output stream properties of the ASU. These outputs include the temperature, pressure, and composition as well as the density and flow rate of the oxygen-rich stream to be fed to the gasifier. Although particle properties are shown in the general output module, the particle flow rate will be zero for the ASU. Figure 1.3.30 shows the energy requirement of the ASU as output. This value is the difference in enthalpy between the inlet and outlet gas. The primary energy requirements of the unit are in gas compression, which is done in compressor modules outside the unit. Note that the energy requirement can be negative, indicating an energy surplus. As the high-temperature, high-pressure inlet air is cooled in the unit, and the exit pressure is reduced, power is sometimes obtained in actual units by gas expansion through a turbine.

Figure 1.3.29. ASU output oxygen product stream.

Figure 1.3.30. ASU energy balance output window.

Syngas Cooler

The syngas cooler is the heat exchanger located immediately downstream of the gasifier that increases the overall thermal efficiency of the energyplex. The process engineering (0D) model used is the steam heat exchanger model originally developed for the LEBS-POC framework (see Section 1.3.1). The steam properties were upgraded from the original model to use correlations based on the ASME 67 steam tables [McClintock and Silvestri, 1970]. The improved steam properties module expands the range of temperature and pressure data and includes entropy needed for the steam turbine thermodynamic calculations. The syngas cooler's UI inputs are set to size the syngas cooler consistent with the 118 MWe steam turbine generator output contained in the Vision 21 reference configuration shown in Figure 1.3.10.

Heat Recovery Steam Generator (HRSG)

The HRSG is a heat exchanger located downstream of the syngas cooler and downstream of the hybrid power block exhaust. Use of the HRSG increases the overall thermal efficiency of the energypex. The process engineering (0D) model used is the steam heat exchanger model originally developed for the LEBS-POC framework (see Section 1.3.1). The steam properties were upgraded from the original model to use correlations based on the ASME 67 steam tables [McClintock and Silvestri, 1970]. The improved steam properties module expands the range of temperature and pressure data and includes entropy needed for the steam turbine thermodynamic calculations. The HRSG's UI inputs are set to size the HRSG consistent with the 118 MWe steam turbine generator output contained in the Vision 21 reference configuration shown in Figure 1.3.10.

Recuperator

A recuperator is a gas-to-gas heat exchanger. In the Vision 21 reference plant configuration a recuperator is used to preheat the compressed air being fed to the high-pressure SOFC. The model was developed as a process engineering (0D) model and is based on the process engineering air preheat heat exchanger model developed for the LEBS-POC framework. As per the other heat exchanger models, the recuperator model has been sized for the specified gas temperatures of the Vision 21 reference configuration shown in Figure 1.3.10. By accessing the UI, the equipment can be re-sized (see Figure 1.3.31). The Internal Pressure Drop and External Pressure Drop fields allow the user to specify desired pressure drops for the two gas streams. The Internal Pressure Drop field corresponds to the change in pressure for the gas stream that is heated by the recuperator whereas the External Pressure Drop field corresponds with the change in pressure of the hot gas stream as it flows through the recuperator. The user can also toggle whether the unit uses finned tubes and (when toggled) the fin effectiveness of those tubes.

The image shows a software dialog box titled "Recuperator". It contains several input fields and checkboxes for configuring a recuperator. The "Arrangement" is set to "Counter Flow" and "Tube Configuration" is set to "Inline". The "Number of Tubes (Long)" is 64, "Number of Tubes (Cross)" is 28, "Tube Long Pitch-Sl (m)" is 0.127, "Tube Cross Pitch-St (m)" is 0.0826, "Tube Inner Diameter (m)" is 0.03, "Tube Outer Diameter (m)" is 0.045, "Tube Length (m)" is 10, "Internal Pressure Drop (Pa)" is 0, and "External Pressure Drop (Pa)" is 0. The "Finned Tubes" checkbox is checked, and the "Fin Effectiveness" is 0.7. At the bottom are "OK" and "Cancel" buttons.

Parameter	Value
Arrangement	Counter Flow
Tube Configuration	Inline
Number of Tubes (Long)	64
Number of Tubes (Cross)	28
Tube Long Pitch-Sl (m)	0.127
Tube Cross Pitch-St (m)	0.0826
Tube Inner Diameter (m)	0.03
Tube Outer Diameter (m)	0.045
Tube Length (m)	10
Internal Pressure Drop (Pa)	0
External Pressure Drop (Pa)	0
Finned Tubes	☒
Fin Effectiveness	0.7

Figure 1.3.31. Recuperator module UI.

SCR

The data provided by DOE did not include an SCR. Our current SCR model developed for the LEBS-POC is based on Vanadia/Titania catalysts, which would require placement of the SCR midway in the HRSG for the optimum temperatures. This model was not ported from the SCIRun-based framework to the VEF.

Gas Clean Up Equipment - Overview

Early in this project the focus was on implementing models to simulate warm gas clean up (WGPU) systems. However, several presentations at the Gasification Technologies Conference have highlighted concern over mercury removal from the syngas. At present, the only practical approach is to use a conventional or cold gas clean up (CGCU) system. Hence, models to simulate the impact on plant operation and efficiency of using a CGCU system were implemented.

In the following are described the process engineering models used to simulate the performance of gas clean up equipment. Included are models for:

- particulate removal with a cyclone separator;
- warm gas clean up; and
- cold gas clean up.

Cyclone Separator

In the DOE Vision 21 reference configuration the cyclone is located immediately downstream of the gasifier and serves the purpose of eliminating particulate matter from the syngas before it reaches the gas clean up system. A process engineering (0D) model was developed based on mathematical correlations to calculate pressure drop and particulate removal efficiency as a function of particle diameter provided in [De Nevers, 2000]. Model inputs supplied by the incoming gas stream (from the framework) include the particle mass flow rate, density and size distribution, gas density and viscosity, and mass flow rate. User inputs to the model define cyclone geometry parameters (cyclone diameter, particle turn count, and velocity heads). The model makes use of the thermodynamics database functionality discussed in previous sections. The model output (summary table) information includes the cyclone cut diameter (in μm), the gas velocity entering the cyclone chamber, the mass mean diameter (in μm) of the particles, the total particle flow rate (kg/s), the % particle flow collected (removed), the % particle flow passed (not removed), pressure drop across the module, and the standard deviation for the mean diameter calculation.

Summary Data	
Description	Value

Cyclone cut diame	41.39
Inlet gas velocit	40.79
Mass Mean diamete	60.50
Particle Flowrate	0.65
Particle flow col	68.51
Particle flow pas	31.49
Pressure Drop (kP	21.39
Std Dev (microns)	8.09

Figure 1.3.32. Input panel (left) and summary data (right) for cyclone model.

Warm and Hot Gas Clean Up

The current generation of gasification systems relies heavily on so-called CGCU systems, which remove particles, acid gases and other trace contaminants at the low temperatures characteristic of conventional power plants and chemical process industry scrubbers. However, DOE has recognized that there is a significant benefit associated with hot gas clean up for gasification systems because of the higher system efficiencies that result when the syngas does not have to be cooled down and reheated before and after the gas clean up process. Several large DOE-funded programs have been undertaken to develop hot gas desulfurization systems and hot gas particulate removal systems that would operate at temperatures on the order of 1000°F. Recently, DOE has promoted the use of lower temperatures (500-900°F) for the gas clean up systems, under the umbrella of WGCU systems. Warm gas clean up does not differ in principle from hot gas clean up, except that at the lower temperatures new sorbents must be utilized for desulfurization.

The Vision 21 reference configuration (Figure 1.3.10 and 1.3.11) originally was to use hot gas clean up. However, based on advice from the DOE, we have targeted our modeling efforts toward warm gas clean up. There is little, if any, operating experience for full-scale equipment in either temperature regime. Hence, the gas clean up system is modeled with a sequence of simple, process engineering models. The equipment and process components are appropriate for both hot and warm gas clean up processes. The equipment components in the train include:

- chlorine bed guard for HCl removal;
- transport reactor bulk desulfurizer; and
- sulfur polisher for removal of H_2S , and COS.

Figure 1.3.33 shows the elements of the WGPU system.

Figure 1.3.33. Elements of warm gas clean up system.

For these models, the user must specify the removal efficiency (%) and temperature change (loss) across each component. Due to the lack of full-scale operating experience with WGPU systems and incomplete sorbent properties, kinetics, etc., the acid gas species are simply removed from the units by allowing the user to specify either removal efficiencies, or exit concentrations in ppm. We have implicitly assumed that HCl, H_2S , and COS are the main pollutants that need to be removed. The gas temperature is expected to change across each of the units due to heat losses to the environment, and to a lesser extent, heats of reaction as the acidic gaseous species are adsorbed. These temperature changes are expected to be small compared to the overall gas temperature and represent a tiny fraction of the overall plant power output. The pressure drop across the components can be calculated or specified by the user. Note that the pressure drop across this equipment is used in the calculations for overall plant efficiency due to the high cost of power for gas compression. To compute the pressure drop requires several input values for each piece of equipment. The performance of sorbents used for the gas clean up is not included in the models. Default values are provided for all model inputs.

The default values provided for temperature changes and pressure drop have been estimated using a combination of information from the DOE Vision 21 reference configurations (Figures 1.3.9-1.3.10) and process flow sheet data from a DOE-NETL funded analysis of various cold and hot gas clean up systems for an IGCC plant with a Texaco-style gasifier [Shelton and Lyons, 2000]. The default values for acid gas species removals are taken from typical values expected for the given units as required for the downstream equipment, as listed in Table 1.3.9. Listed in Table 1.3.10 is a summary of the default values provided in our models.

Table 1.3.9. Sulfur Removal Requirements for Syngas Applications.

Application	Total Sulfur (H ₂ S + COS), ppmv	H ₂ S Alone, ppmv
Gas Turbine	<20	Not specified
Molten Carbonate Fuel Cell (MCFC)	0.5	Not specified
Phosphoric Acid Fuel Cell (PAFC)	<50	<20
Solid Oxide Fuel Cell (SOFC)	<0.1	Not specified
Chemical production	<0.06	

Table 1.3.10. Summary of Default Values for Gas Clean Up Units (values are estimated).

	Pressure Drop (psi)	Temperature Change (°F)	HCl Concentration (ppm)	H ₂ S Concentration (ppm)	COS Concentration (ppm)
Chlorine Bed	15	-5	1	---	---
Transport Reactor	10	10	---	10	1
Sulfur Polisher	5	0	---	0.1	0.01

The output of each gas clean up model includes the gas temperature, pressure, and acid gas species removal efficiency. The overall stream composition is also available.

In the following are provided further details about the specific models used for modeling warm and hot gas clean up. Note that for these systems it may be necessary to use a heat exchanger model in the system. If so, the heat exchanger is modeled using the heat exchanger model described within this report.

Chlorine Guard Bed

The chlorine guard bed (CGB) module is part of the warm (hot) gas clean up system designed to remove chlorine from the gas stream. Chlorine removal is required prior to desulfurization because chlorine tends to react with sulfur sorbents. A commercially available nahcolite sorbent operating at 1000°F has been proposed to remove chloride (and other halogens). The CGB module is intended to be placed after the syngas has been cooled to the appropriate temperature (about 1000°F), and before the desulfurization steps. It is assumed that a chlorine guard bed would be used for both warm and hot gas clean up, provided the appropriate sorbent is used.

The CGB model acts as a component separator. The user provides either a HCl removal efficiency or an exit HCl concentration (required to be below the inlet concentration). In addition, a temperature drop can be specified to account for heat losses (note: positive values represent an increase of temperature in the gas between inlet and outlet ports and the specified temperature change is in degrees Fahrenheit). Pressure drop across the unit can either be specified (in psi) or computed using required unit configurations specified by the user in the UI (see Figure 1.3.34). Default values are provided for the user inputs. The unit outputs are the exit gas state: temperature, pressure, and composition.

ChlorineBed

Temperature change (F)

HCL

☐ HCL efficiency (%)

☒ HCL ppm :

Pressure Drop

☒ Specify Pressure Drop (psi)

☐ Calculate Pressure Drop:

Bed diameter (m)

Bed depth (m)

Bed void fraction

Particle size (m)

Particle sphericity

OK Cancel

Result Dialog

Summary Data

Description	Value

HCL Reduction Eff	99.87
Pressure Drop (ps	10.00
Temperature Out (	639.90

OK

Figure 1.3.34. Input panel (left) and summary data (right) for chlorine bed guard model.

The CGB is a fixed bed. Thus, the pressure drop can be modeled using the Ergun equation [Kunii and Levenspiel, 1969]:

$$\frac{\Delta P}{L} = 150 \cdot \frac{(1 - \varepsilon)^2}{\varepsilon^3} \cdot \frac{\mu \cdot u_o}{(\phi \cdot d)^2} + 1.75 \cdot \frac{(1 - \varepsilon)}{\varepsilon^3} \cdot \frac{\rho \cdot u_o^2}{\phi \cdot d}, \quad (1.3.17)$$

where P is the pressure, L is the bed depth, ε is the bed void fraction, d is the sorbent particle diameter, ϕ is the particle sphericity, μ is the gas viscosity, ρ is the gas density, and u_o is the gas superficial velocity. To apply this equation, the user must specify the bed depth, particle diameter (computed as the diameter of a sphere of the same volume as the particle) and sphericity (the surface area of the sphere described above divided by the actual particle surface area), bed void fraction (defined as $1 - \text{sorbent volume} / \text{bed volume}$), and the bed diameter (to compute the gas superficial velocity). The gas viscosity and density are computed as a function of temperature and composition. A typical default value of 0.65 is provided for the particle sphericity. The bed void fraction depends on the packing particle size and shape and the method of packing. A plot of void fraction versus particle sphericity is given in [Kunii and Levenspiel, 1969]. The pressure drop is computed neglecting wall friction and static head losses, as these are expected to be much smaller than the pressure drop through the packed bed.

Bulk Desulfurizer

The bulk desulfurizer module is a part of the warm (hot) gas clean up unit designed for bulk removal of sulfur species from the gas stream. The primary sulfur species of concern are H_2S and COS , and the unit is designed to achieve exit concentrations of about 10 ppm H_2S and 1 ppm COS . Sulfur species must be removed because of emissions requirements and adverse interactions in downstream equipment such as poisoning of fuel cells and other catalytic units.

The bulk desulfurizer is based on a transport reactor that has been demonstrated for high-temperature operation. The reactor consists of a recirculating system in which the syngas flows cocurrently with sorbent in a riser section. A cyclone separates the cleaned syngas from the sorbent and the sorbent falls through a return leg, at the bottom of which it contacts incoming dirty syngas. A portion of the sorbent is removed in a return leg and sent to a regeneration riser. Off-gas from regeneration is processed to produce elemental sulfur or sulfuric acid using conventional technology. Regenerated sorbent is injected back into the riser section of the desulfurization reactor. The bulk desulfurizer is intended to be placed downstream of the chlorine guard bed and upstream of the sulfur polisher. A heat exchanger may be required upstream of the unit to achieve the desired operating temperature (~ 672 K for warm gas operation). The module is assumed to be of use in both hot and WGPU systems, provided a suitable sorbent is used.

The bulk desulfurizer module acts as a component separator. The user provides either a removal efficiency or a desired exit concentration for COS and H_2S (see Figure 1.3.35). A temperature change can be specified to account for heat effects (note: positive values represent an increase of temperature in the gas between inlet and outlet ports and the temperature change is measured in degrees Fahrenheit). Pressure drop across the unit can be specified or computed using specific module configuration details. Default values are provided for all required inputs. The module outputs are the reduction/removal efficiencies for both COS and H_2S , the pressure drop across the module (in psi), and the temperature of the exiting gas stream (in Kelvin). In addition, the exit gas composition is available.

The bulk desulfurizer operates with the sorbent particles carried cocurrently with the gas stream. The void fraction in these units is generally fairly large. The pressure drop is again correlated by the Ergun equation with additional terms to account for the static head pressure drop (pressure loss in suspending the solid particles) and the wall friction. The following equation is used [Wen and Galli, 1971]:

$$\frac{\Delta P}{L} = \frac{150 \cdot \mu \cdot (1 - \varepsilon)^2 \cdot (u_o / \varepsilon - u_p)}{(\varepsilon \cdot \phi \cdot d)^2} + \frac{1.75 \cdot (1 - \varepsilon) \cdot \rho \cdot (u_o / \varepsilon - u_p)^2}{\varepsilon \cdot \phi \cdot d} + (1 - \varepsilon) \cdot (\rho_s - \rho) \cdot g + \frac{\rho \cdot u_o^2 \cdot f}{2 \cdot D \cdot \varepsilon^2}, \quad (1.3.18)$$

where all variables are defined as per Equation (1.3.17), and ρ_s is the particle density, D is the unit diameter, u_p is the particle velocity, g is the gravitational acceleration, and f is the Fanning friction factor. In this equation, the first two terms account for the fluid/particle friction losses, the third term is the static head loss, and the last term is the wall friction loss. The wall friction

term ignores the effect of the particles. The fanning friction factor for rough pipes is used [Perry, 1997],

$$f = \left[-4 \cdot \log \left(\frac{0.27 \cdot \varepsilon}{D} + (7 / \text{Re})^{0.9} \right) \right]^{-2} \quad (1.3.19)$$

where Re is the Reynolds number and ε is the wall roughness taken as 0.05 mm. The user is required to specify the sorbent particle density or use a default value of 2 g/cm³. The mass throughput of sorbent is also required to compute the sorbent particle velocity from the following material balance equation where G is the solids mass flow rate:

$$u_p = \frac{4 \cdot G}{\pi \cdot D^2 \cdot \rho_s \cdot (1 - \varepsilon)} \quad (1.3.20)$$

After the module has executed, the Summary Data button provides summary information. The module outputs the reduction/removal efficiencies for both COS and H₂S, the pressure drop across the module (in psi), and the temperature of the exiting gas stream (in Kelvin).

The figure shows two windows from a software application. The left window is titled 'BulkDesulfurizer' and contains input fields for various parameters. The right window is titled 'Result Dialog' and displays the 'Summary Data' output.

BulkDesulfurizer Input Panel:

- Temperature change (F): 0
- H₂S section:
 - ☐ H₂S efficiency (%): 0
 - ☒ H₂S ppm: 1
- COS section:
 - ☐ COS efficiency (%): 0
 - ☒ COS ppm: 1
- Pressure Drop section:
 - ☒ Specify Pressure Drop (psi): 24
 - ☐ Calculate Pressure Drop:
 - Bed diameter (m): 0
 - Bed depth (m): 0
 - Bed void fraction: 0
 - Particle size (m): 0
 - Particle sphericity: 0.65
 - Particle density (kg/m³): 2000
 - Solids Mass Flow (kg/s): -1

Result Dialog Summary Data:

Description	Value

COS Reduction Eff	99.67
H ₂ S Reduction Eff	99.99
Pressure Drop (ps	24.00
Temperature Out (	639.90

Figure 1.3.35. Input panel (left) and summary data (right) for bulk desulfurizer model.

Sulfur Polisher Model

The sulfur polisher module is part of the warm (hot) gas clean up unit, designed to follow the bulk desulfurizer and achieve very high removal of sulfur species from the gas stream. The primary sulfur species of concern are H_2S and COS, and the unit is designed to achieve exit concentrations of about 0.1 ppm H_2S and 0.01 ppm COS. While the bulk desulfurizer can reduce sulfur emissions to levels acceptable for gas turbine operation, very high removal is required for downstream equipment such as fuel cells and other catalytic units, and a sulfur polisher is needed. The sulfur polisher module is based on a non-regenerable, fixed sorbent bed (typically ZnO), operating at a nominal temperature of 672 K. The unit is intended to be placed downstream of the bulk desulfurizer and is assumed to be of use in both hot and WGPU systems, provided a suitable sorbent is used.

The sulfur polisher module acts as a component separator. The user provides either a removal efficiency or an exit concentration for COS and H_2S (see Figure 1.3.36). A temperature change can be specified to account for heat effects. Pressure drop across the unit can be specified or modeled (computed). The sulfur polisher is modeled as a fixed bed unit and the computed pressure drop is computed using the Ergun equation [Kunii and Levenspiel, 1969], Equation 1.3.17; required inputs include the bed diameter, depth, void fraction, nominal particle size, and particle sphericity. The module outputs include the reduction/removal efficiencies for both COS and H_2S , the pressure drop across the module (in psi), and the temperature of the exiting gas stream (in Kelvin). In addition, the exit gas composition is available.

SulfurPolisher

Temperature change (F)

H₂S

☐ H₂S efficiency (%)

☒ H₂S ppm :

COS

☐ COS efficiency (%)

☒ COS ppm :

Pressure Drop

☒ Specify Pressure Drop (psi):

☐ Calculate Pressure Drop:

Bed diameter (m)

Bed depth (m)

Bed void fraction

Particle size (m)

Particle sphericity

OK Cancel

Result Dialog

Summary Data

Description	Value

COS Reduction Eff	0.00
H ₂ S Reduction Eff	0.04
Pressure Drop (ps)	5.00
Temperature Out (	639.90

OK

Figure 1.3.36. Input panel (left) and summary data (right) for sulfur polisher model.

Cold Gas Clean Up and Mercury Capture

The current generation of gasification systems relies heavily on CGCU systems to remove particles, acid gases, and other trace contaminants at the low temperatures (100-300°F) characteristic of conventional power plants and chemical process industry scrubbers. These systems are well established and are being used at the existing IGCC plants at Tampa Electric and Wabash River. CGCU has an adverse impact on the plant efficiency because the syngas must be cooled prior to the gas clean up process and then must be reheated prior to the next process at the plant. However, including models for CGCU allows investigating existing (conventional) IGCC plant configurations.

Including equipment models used in a CGCU system provides the capability to model mercury capture in the plant. This is an important capability because mercury has been identified as the air toxic substance of greatest concern among all the air toxics released from coal-fired power plants [Keating, 1997]. The EPA has proposed regulations for emissions of mercury from coal-fired electric utility steam generating units. The draft regulations were issued in January, 2004 and are currently being reviewed by the agency. Final regulations are to be issued by March 15, 2005. A US DOE study on major environmental aspects of gasification-based power generation technologies [Ratafia-Brown et al., 2002] revealed that approximately 60 to 70% of the mercury in the coal escaped in the flue gas of the Polk and Wabash River IGCC plants. A separate joint DOE/EPRI/LGTI study, also reported in [Ratafia-Brown et al., 2002], showed that mercury emissions at the Louisiana Gasification Technology Inc. (LGTI) project accounted for only 31% of the initial mercury input in the coal. Hence, further insight into the fate of the mercury through the gasification plant would be of use.

A study by Korens et al. (2002) on an alternative process for gas treating and sulfur removal for gasification contends that efficient and economical removal of mercury from syngas streams will require the use of activated carbon beds and syngas temperatures consistent with CGCU plants. The suppliers of activated carbon for mercury removal also recommend that to be effective, the carbon beds must be operated at temperatures ranging from 70°F to 150°F. Last, all gasification processes include an AGR unit, regardless of the downstream use of the syngas.

In the following, described are process engineering (0D) models for

- an acid gas removal (AGR) unit and
- a carbon bed absorber for mercury removal.

Both models are configured for use in a CGCU system.

Acid Gas Removal Model

A process engineering (0D) model is used to simulate the performance of the Acid Gas Removal (AGR) unit. For advanced power generation configurations that involve a SOFC, the primary purpose of the AGR is to remove the H_2S in the syngas down to less than 1ppm to avoid damaging the SOFC materials.

The solvents used in an AGR fall into two broad categories: physical and chemical solvents. The choice of solvent is usually dictated by the H_2S/CO_2 ratio in the syngas, the solvent's selectivity for H_2S over CO_2 , carbonyl sulfide removal, and whether total removal of CO_2 is desired. Physical solvents rely upon variations in the physical solubility of gases to effect separation. Examples are Selexol and Rectisol. Chemical solvents are usually amine-based and remove H_2S and CO_2 through an acid-base reaction path. One of four amine-based solvents is usually employed (MEA, DGA, TEA, and MDEA). In IGCC, selectivity of H_2S over CO_2 is important. Thus the best chemical solvent for this task is MDEA (Methyldiethanolamine). MDEA actually reacts with H_2S but only as a catalyst for hydrolysis of CO_2 [Kohl and Nielsen, 1997]. MDEA has the lowest capital cost in comparison with Selexol and Rectisol, which may also be selected for IGCC service. Rectisol is the costliest solvent but may be the best choice if complete removal of CO_2 is preferred. The AGR model is configured to only use MDEA.

Modeling the AGR unit provides information on the amine circulation rate required to meet the H_2S removal levels, the size of the absorption tower, and the number of stages required to effect the removal of H_2S . The key design equations used in the model are:

1) The amine circulation rate:

$$GPM = \frac{0.206 \cdot MM \cdot (H_2S + CO_2) \cdot MolWT}{ML \cdot WT} \quad (1.3.21)$$

where

GPM = amine circulation rate

MM = actual gas flow rate, million cubic ft/day

H_2S = Mol% of H_2S in gas mixture to be removed

CO_2 = Mol% of CO_2 in gas mixture to be removed

ML = Mol loading or (moles of acid gas) / (mol of syngas)

WT = Amine solution wt% circulated

2) Absorber bubbling gas velocity:

$$U_{al} = K \left(\frac{\rho_L - \rho_G}{\rho_G^{0.5}} \right)^{0.5} \quad (1.3.22)$$

where

K = 0.25 for valve trays, 0.20 for bubble cap trays

U_{al} = Allowable velocity of gas through bubbling area, ft/s

ρ_L = Density of amine solution, lb/ft³

ρ_G = Density of syngas at tray conditions, lb/ft³

3) Theoretical number of stages (see [Perry, Seventh Edition Chapter 14]):

$$N = \frac{\ln \left[(1 - A^{-1}) \left(\frac{y_1 - y_2^0}{y_2 - y_2^0} \right) + A^{-1} \right]}{\ln(A)} \quad (1.3.23)$$

where

N = Number of Stages

$A = L_m/mG_m$ is the Absorption factor

L_m = liquid molar flow rate/unit area (i.e. solvent entering at the top of tower)

G_m = Gas molar flow rate/unit area (i.e. syngas entering at bottom of tower)

m = slope of equilibrium curve

note: this analysis is valid only if the equilibrium curve is represented by $y_e = mx$

4) Absorption Factor

$$A = \frac{L_m}{mG_m} \quad (1.3.24)$$

where A , L_m , G_m and m are defined as above.

Model inputs for the AGR model are the tray type and solvent (MDEA) properties (molecular weight and density). The UI for entering model inputs for an example case is shown in Figure 1.3.37. The model outputs include the amine circulation rate, size of the absorption tower, number of stages required to effect the removal of H_2S , and CO_2 and H_2S concentrations at the exit of the unit. A complete description of the exhaust gas from the AGR can be obtained by using the port interrogation tool (see Section 1.2.2).

Figure 1.3.37. Input panel (left) and summary data (right) for AGR model.

Carbon Bed Model

A process engineering (0D) model is used to simulate mercury removal from the syngas within the CGCU stream. The use of carbon beds to remove mercury from syngas has been demonstrated at the Eastman Chemical plant in Kingsport, TN [Eastman Chemical Co, 2003].

Activated carbon, which can have internal surface area of the order of $10^6 \text{ m}^2/\text{kg}$ [Coulson et al., 1991], is effective in removing mercury from syngas streams. Calgon Carbon Corporation of Pittsburgh supplies two versions of sulfur-impregnated activated carbons in granular form in 4x10 US Mesh (HGR) and 4mm pellet as HGR-P. These carbons are made from bituminous coals. The sulfur in the carbon reacts with elemental mercury to form a stable mercuric sulfide compound (HgS). Calgon Product Bulletin [1994] states that adsorption systems using the HGR-type activated carbon can be designed to reduce mercury concentrations to below 0.001 ug/Nm^3 in the treated gas. The adsorptive capacity of these carbons can be as high as 20 wt%. NORIT Americas Inc., of Texas, supplies sulfur-impregnated activated carbon in the form of powder (DARCO FGD) and 3 or 4mm pellets (RBHG) made from lignite coal. Both suppliers report that in a properly designed carbon system, the mercury removal process is not affected by inlet mercury concentration or changing the operating pressure. However, increasing the gas temperature or moisture content of the gas stream would drastically affect mercury removal.

Design calculations of a fixed bed adsorber can be readily made from feed and product gas specifications, equilibrium data, and knowledge of the bed saturation at the break point under the desired operating conditions. A theoretical basis for design of fixed bed adsorbers is given by Brown et al. (1998), McCabe et al. (1985), and Coulson et al. (1991). However, for adsorption with chemical reaction, the interrelation of these variables is so complex that methods of design usually rely heavily on experimental and operating data of existing plants. The purpose of an adsorber design is to determine the dimensions of the vessel and the quantity of activated carbon required to achieve a specified mercury removal rate. The key equations used in the model are:

1) The minimum fluidization velocity:

$$U_{mf} = \text{Re}_{mf} \left(\frac{\mu}{d\rho} \right) \quad (1.3.25)$$

where

$$\text{Re}_{mf} = 25.7 \left\{ \sqrt{1 + (5.53E - 5)Ga} - 1 \right\}, \quad (1.3.26)$$

$$\text{Ga} = \frac{d^3 \rho (\rho_s - \rho) g}{\mu^2}, \quad (1.3.27)$$

and d is diameter, ρ_s and ρ are the densities of the solid and fluid, respectively, μ is viscosity, and g is gravitational acceleration.

- 2) The superficial velocity, U_0 , through the bed:

$$U_0 = 0.85U_{mf} \quad (1.3.28)$$

- 3) The adsorber dimensions (bed height and diameter):

Height, $H =$

$$H = U_0\tau \quad (1.3.29)$$

where τ is residence time and is taken as 20 sec to remove the mercury.

Cross-sectional area, $A =$

$$A = \frac{Q}{U_0} = \left(\frac{\dot{M}_{\text{syngas}}}{\rho_{\text{syngas}}} \right) \frac{1}{U_0} \quad (1.3.30)$$

where Q , $\dot{M}_{\text{syngas}}$, and ρ_{syngas} are the volumetric flow rate, mass flow rate, and density of the syngas, respectively.

The adsorber diameter, $D =$

$$D = \sqrt{\frac{4A}{\pi}}. \quad (1.3.31)$$

- 4) Pressure Drop:

$$\frac{\Delta P}{L} = \frac{150(1-e)^2}{e^3} \frac{\mu U_0}{d^2} + 1.75 \frac{(1-e)}{e^3} \rho \frac{U_0}{d} \quad (1.3.32)$$

where L is the length of the carbon bed, d is the carbon particle diameter, and e is the voidage [Kunii and Levenspiel, 1969].

Model UI

The UI for entering the carbon bed model inputs for an example case is shown in Figure 1.3.38. Inputs include operating parameters, carbon particle size and allowable pressure drop. Module calculations are governed by these parameters as well as by the properties of the input gas stream. The module outputs include the calculated absorber diameter, bed height, mercury leaving the adsorber (lbm/hr), minimum fluid velocity, number of adsorbers, pressure drop per meter, superficial velocity, and pressure drop across the bed (see Figure 1.3.38).

The figure displays two side-by-side windows from a software application. The left window, titled 'CarbonBed', is an input panel with a 'Parameters' section containing several text input fields. The right window, titled 'Result Dialog', displays a 'Summary Data' table with two columns: 'Description' and 'Value'.

CarbonBed Input Panel:

- Allowable Pressure Drop (psi/ft): 0.26
- Carbon Particle Diameter (mm): 3.38
- Bulk Density (kg/m³): 592.7
- Operating Temperature (K): 313
- Operating Pressure (psi): 255
- Carbon Replacement Time (years): 2
- Carbon Bed Porosity: 0.7
- Absorber Residence Time (sec): 20

Result Dialog Summary Data:

Description	Value
Adsorber Diameter (m)	5.67
Bed Height (m)	3.75
Hg Leaving Adsorber (lb/hr)	2.28e-004
Min. Fluidization Vel. (m/sec)	0.22
Number of Adsorbers (#)	1.00
Pressure Drop (Pa/m)	211.99
Superficial Velocity (m/sec)	0.19
Total Bed Pressure Drop (Pa)	796.02

Figure 1.3.38. Input panel (left) and summary data (right) for carbon bed model.

Water Gas Shift Membrane Reactor

A 1D, process engineering model for a membrane-based reactor unit is used to simulate the performance of a water gas shift converter. The membrane reactor converts the CO in clean syngas to hydrogen over a catalyst by permeation through a palladium-based membrane. In general, the reactor is placed downstream of the gas clean up units and prior to fuel cells, combustors, or other process equipment. The model assumes hydrogen permeation is slower than chemical reaction and chemical equilibrium is assumed throughout the reactor. A sweep gas is required to remove the hydrogen and is assumed to flow concurrently to the feed gas. The model can be run in two stages with intercooling in between to maintain catalyst operating temperatures and minimize membrane size and costs. The model allows calculation of CO conversion, H₂ recovery, sweep gas flow rate, and required heat transfer (for staged operation). The effects of reactor dimensions, number of parallel modules, membrane thickness, steam-to-CO ratio, and heat losses on the reactor performance can be tested. Alternately, the model can compute the required reactor length and sweep flow rate for a desired CO conversion.

Background

The conversion of the syngas product of coal gasification to hydrogen fuel via the water gas shift reaction (WGS):

The importance of this reaction lies in the ability to convert CO (along with steam) to H₂, which is valuable both as a fuel and as a chemical feedstock. In addition, as CO₂ sequestration becomes more important, the use of H₂ as a clean-burning fuel for fuel cell or combustion power generation is attractive. The WGS reaction converts CO to CO₂, which can be separated from hydrogen and subsequently sequestered.

A membrane reactor for WGS is a two-zone, catalytic fixed bed reactor with an integrated hydrogen selective membrane. Syngas enters and reacts on the feedside of the membrane, and hydrogen permeates to and is carried away by a sweep gas on the permeate side of the membrane. By selectively removing the hydrogen product, high reaction conversions are possible. A membrane reactor module would be positioned after gas clean up units and before fuel cells, combustors, or other equipment which would process the hydrogen product gas.

Reaction Characteristics

The WGS reaction occurs at high temperatures, is exothermic ($\Delta H_{\text{rxn}} = -41$ J/mole), and equilibrium limited. Thus conversion of CO to H₂ is favored at low temperatures. In order to achieve sufficient reaction rates at lower temperatures, however, the reaction is carried over a catalyst. Because the reaction is exothermic, the temperature rises with conversion. Conventional WGS reactors operate in two stages with intercooling in between. The first stage, where the bulk of the reaction occurs, operates over a (typically) promoted ferrochrome catalyst at a higher temperature of between 600-750 K. The second stage operates at a lower temperature with a CuZn-based catalyst (Ma and Lund, 2003), allowing higher H₂ yields.

Figure 1.3.39 shows the WGS equilibrium CO conversion as a function of temperature for several feed compositions. These curves give the theoretical maximum conversion of CO to

hydrogen in a conventional reactor (without membrane separation) for various initial compositions. The stoichiometric curve is with equimolar amounts of CO and H₂O in the feed and no other species initially. The H₂O:CO = 2 curve is the stoichiometric curve with twice the initial steam, again no products initially. As shown in the figure, higher conversions are possible at a given temperature when running excess steam. This is explained by the WGS equilibrium constant ($K(T)$) given by

$$K(T) = \frac{[H_2] \cdot [CO_2]}{[CO] \cdot [H_2O]}, \quad (1.3.34)$$

where [species] denotes the gas concentration of a species. Because the moles of product equal the moles of reactant, the concentration of each species can be replaced with mole fraction of each species, or moles of each species in the gas. As expected, at a given temperature (fixed K) the equilibrium curve shifts to higher CO conversion (H₂ production) when the initial steam is increased, to maintain the equilibrium constant given by Equation 1.3.34. Steam is often injected in order to increase equilibrium conversion, mitigate carbon deposition, and control temperature increases. If product species are present initially, the CO conversion decreases relative to the reactant-only condition. The syngas curve in Figure 1.3.39 is the CO conversion with a typical gasifier exhaust taken from a gasifier simulation, as given in Table 1.3.11. The maximum CO conversion is so low because the H₂O:CO ratio is less than 1 - H₂O acts as a limiting reagent. When steam is injected into this gas to give an H₂O:CO ratio of 1, the maximum conversion increases, but the conversion is generally less than the stoichiometric reactants-only curve because WGS products are present initially. Inert species have no effect on the WGS equilibrium, although reaction rates would be adversely affected by large amounts of inert or diluent species.

Figure 1.3.39. Water gas shift equilibrium conversion for several initial compositions.

Table 1.3.11. Gasifier Product Composition.

Species	Simulated Gasifier Product (Cleaned)
AR	0.87%
CO	42.83%
CO ₂	8.34%
H ₂	27.42%
H ₂ O	19.70%
N ₂	0.84%

In order to overcome the equilibrium constraints outlined above, an attractive alternative to conventional WGS reactors is to combine a catalytic reactor with a hydrogen selective membrane. The membrane simultaneously allows purification of the hydrogen product, and shifts the WGS reaction toward higher equilibrium conversion by continually removing hydrogen product from the gas stream. The equilibrium constraint is not removed, rather, the equilibrium conversion can be made complete. In addition, the operating temperature requirements are no longer dictated by chemical conversion, but only by material constraints such as catalyst operating temperature, membrane requirements, etc.

G. Marigliano et al. / Catalysis Today 67 (2001) 85–99

Figure 1.3.40. Catalytic membrane reactor configurations.

Membrane Reactor Configuration

For large-scale applications, parallel banks of concentric tubular arrangements are considered the best option to combine large membrane areas with construction requirements [Bracht et. al., 1997]. Figure 1.3.40 shows a schematic of a typical configuration in which catalyst pellets fill the reaction/feed side of the membrane, with a sweep/H₂ product gas flowing on the permeate side of the membrane reactor. The figure shows two possible arrangements with the reaction

occurring either in the annulus or in the circular pipe. The upper configuration seems to be more popular than that with reaction occurring in the inner tube, and this configuration is assumed in the model [Bracht et. al., 1997], [Devarajan et. al., 1991]. Marigliano et. al. (2001) found that the annular feed configuration gave higher conversions for the same reactor size.

Membrane Properties

The membrane of choice for hydrogen removal is a thin metal palladium or palladium alloy on a porous support. The porous support is required to provide mechanical strength given a relatively large pressure difference across the membrane. Other membrane materials consist of microporous ceramic membranes in which Knudsen diffusion occurs. These membranes are not as selective to hydrogen since the diffusion rate is inversely proportional to the square root of the species molecular weight. Palladium is 100% selective to hydrogen, the hydrogen being transported by a solution-diffusion mechanism. Solution diffusion is governed by a square root pressure driving force due to dissociation of H_2 to H atoms in the metal [Devarajan et. al., 1991]. The thickness of the palladium film is on the order of 10 microns. This thin layer is required to allow high hydrogen permeation, which is inversely proportional to the membrane thickness. The hydrogen permeation rate is given by

$$N_p = \frac{P_o \cdot \exp(-E_p / R \cdot T)}{l} \cdot (\sqrt{P_{H_2}^R} - \sqrt{P_{H_2}^P}), \quad (1.3.35)$$

where P_o is a pre-exponential factor, E_p is the permeation activation energy, l is the membrane thickness, P_{H_2} is the hydrogen partial pressure, and N_p is the hydrogen flux (moles/ $m^2 \cdot s$).

Palladium membranes are subject to deactivation by sulfur species, so it is important that the gas be cleaned prior to introduction into the membrane. Damle et. al. (1994) state that palladium is stable in a reducing hydrogen environment with H_2S levels < 100 ppm, which are much higher than levels exiting a WGPU zinc oxide sulfur polisher expected for Vision 21 gas cleaning. Edlund (1994) states that operational lifetimes greater than 2 years are expected with projected membrane module costs of \$275/ ft^2 . Pure palladium metal tends to become embrittled by hydrogen, thus a palladium alloy is typically employed.

Model Description

The membrane reactor (MR) model is a 1D, process engineering model that integrates the hydrogen flux across the catalyst over the length of the unit. The MR is divided into two zones, the feed or reaction zone and the product or permeation zone. Each zone is assumed to be in plug flow with no axial dispersion. A sweep gas (typically nitrogen and/or steam) is required to reduce the hydrogen product partial pressure. The feed and sweep gases flow concurrently with the feed gas flowing in the annulus and the permeate flowing in the inner tube.

The MR is assumed to be adiabatic with no heat transfer across the membrane between the two zones. A heat loss term from the reaction side to the environment is allowed however, and is specified as a fraction of the inlet gas sensible heat relative to 298 K. This heat loss is assumed uniform over the length of the reactor and is treated as a sink term in the energy equation to be solved.

The hydrogen permeation rate is assumed to be the limiting process; chemical reactions are assumed fast compared to hydrogen permeation. Thus, the feed gas is assumed to be in chemical equilibrium, and all catalytic reaction dependencies are ignored. This assumption has been used and validated in models in the literature [Damle et. al., 1994], [Devarajan et. al., 1991]. Only chemical equilibrium for the WGS reaction is assumed, all other species are assumed inert. This option simplifies the solution procedure and, more importantly, allows reasonable computation times. Full equilibrium among 23 species was tested, with totally unrealistic results, as expected at relatively low temperatures of 700 K. However, as catalysts are designed to increase reaction rates and be selective to the desired reaction, equilibrium limited to the WGS reaction is reasonable.

To allow further flexibility, the model is configured with an option to simulate the requirements of a staged operation in which the feed gas is first introduced to a preshift catalytic non-membrane reactor, cooled, and then fed to the membrane reactor. A schematic of this option is presented in Figure 1.3.41, taken from [Bracht et. al., 1997]. As equilibrium is assumed with the aid of a catalyst, the preshift reactor is simply modeled as an adiabatic equilibrium on the feed gas. The temperature of the gas is then dropped to a user-specified value as the gas is injected into the MR, with the required heat duty computed.

Figure 1.3.41. Schematic of staged-membrane reactor system.

For heat and mass transfer devices, countercurrent operation is more efficient than concurrent operation. The latter is assumed here because of computational convenience: countercurrent simulation requires iteration on the guessed permeate exit flow to achieve convergence of the known inlet sweep condition. The assumption is conservative in that any increase in required reactor size requirements will tend to balance any decrease in reactor size from the equilibrium assumption. Damle et. al. (1994) have shown that the error incurred is only a couple percent at the high feed-to-permeate pressure ratios required for high CO conversion and hydrogen recovery.

Model Equations

The following two ODEs are solved:

$$\frac{dn_{dp}}{dx} = \frac{A_m}{L} \cdot N_p, \quad (1.3.36)$$

$$\frac{dH}{dx} = -h_{H_2}(T) \cdot \frac{dn_{dp}}{dx} - \frac{Q_{loss}}{L}, \quad (1.3.37)$$

where n_{dp} is the moles of hydrogen transferred across the membrane, A_m is the membrane area, L is the reactor length, and N_p is the hydrogen molar flux given by Equation 1.3.35. In Equation 1.3.37, Q_{loss} is the heat loss to the environment based on the user's fractional heat loss specification, H is the feed gas enthalpy, and $h_{H_2}(T)$ is the molar enthalpy of hydrogen at the local temperature of the feed gas. The integration is performed numerically using a second order explicit predictor corrector method, and the adiabatic equilibrium is computed locally from the feed gas enthalpy and composition:

$$K(T) = \frac{n_{H_2} \cdot n_{CO_2}}{n_{CO} \cdot n_{H_2O}}, \quad (1.3.38)$$

$$n_{CO} = n_{CO}^o - \xi, \quad (1.3.39)$$

$$n_{H_2O} = n_{H_2O}^o - \xi, \quad (1.3.40)$$

$$n_{CO_2} = n_{CO_2}^o + \xi, \quad (1.3.41)$$

$$n_{H_2} = n_{H_2}^o + \xi - n_{dp}, \quad (1.3.42)$$

$$H = \sum_i h_i(T) \cdot n_i, \quad (1.3.43)$$

where ξ is the extent of reaction variable and n_i^o is the initial moles of species i . Equations 1.3.39-1.3.42 are substituted into Equation 1.3.38 and the nonlinear equations in Equation 1.3.38 and 1.3.43 are solved with Newton's method for ξ and T . The moles of all reaction species are then updated using Equations 1.3.39-1.3.42. The equilibrium constant was curvefit to thermodynamic data of the relation $K(T) = \exp(-\Delta G_{rxn}^o/RT)$ to yield:

$$K(T) = 91607 \cdot T^2 + 1680 \cdot T - 1.6097, \quad (T \text{ in Kelvin}) \quad (1.3.44)$$

The sweep gas composition is updated at each point as the hydrogen permeates. Because there is no heat transfer over the membrane, the sweep temperature is only computed at the exit using the sweep composition and enthalpy computed from an energy balance over the unit.

Model Capabilities

The membrane reactor model can be run in one of two modes.

- 1) Specification of the reactor dimensions and gas flow properties. The exiting gas streams are computed along with CO conversion, hydrogen recovery, superficial space velocity, and approximate unit footprint.
- 2) The second mode allows specification of a desired CO conversion, along with reactor dimensions. The required MR module length is output as a result, along with the required sweep flow rate.

The model allows evaluation of the effect of reactor dimensions, membrane thickness, steam to carbon monoxide ratio, as well as all gas exit properties on the required module dimensions and/or extent of reaction and hydrogen permeation.

Example Model Results

The following results were computed using the WGS membrane reactor. For this case, a preshift stage was included as shown in Figure 1.3.41. The input conditions and results are shown in Table 1.3.12. The inlet gas is that of Table 1.3.11, for a simulated gasifier product. The temperature and pressure of the inlet gas stream are taken from the Vision 21 reference flowsheet of Figure 1.3.10 and 1.3.11. The sweep gas temperature was arbitrarily set at 300 K. This temperature does not affect the calculations, but its value should be consistent with the tube size to give reasonable gas velocity. The sweep inlet velocity is shown in Table 1.3.12 and is proportional to the flow rate, temperature, and inverse pressure. The sweep pressure is set at 1 atm. This is the absolute (practical) minimum. The low sweep pressure allows a relatively high hydrogen concentration in the sweep gas. It is important to note that the membrane reactor only works so long as there is a hydrogen partial pressure driving force. Once the feedsides hydrogen pressure matches that of the sweep gas, the WGS reaction is limited by the equilibrium composition. The primary purpose of the sweep gas is to dilute the hydrogen enough to provide a sufficient driving force over the membrane, hence allowing high CO conversion. A feed-to-permeate pressure ratio of 15 atmospheres is typical [Bracht et. al., 1997].

Figures 1.3.42-1.3.44 show profiles of temperature, gas composition, and CO conversion and pressure driving force over the length of the membrane reactor. As expected, the temperature increases due to the exothermic reaction. In Figure 1.3.42, the mole fraction of CO actually increases slightly in the first half of the unit because the total moles is decreasing (due to hydrogen permeation) faster than the CO. Note that the temperature (and CO conversion) are shown to begin higher than the MR inlet values specified in Table 1.3.12. Since the WGS reaction is adiabatic and occurs catalytically, reactions should not occur during external heat exchange; the gas at the inlet to the MR is not at equilibrium at the specified MR inlet temperature of 565 K. The equilibrium gas at the preshift reactor exit (higher temperature) has a lower conversion than at the lower MR inlet temperature, so the conversion increases quickly in the MR from 50% to 72%.

For a specified CO conversion, the reactor length and sweep gas flow rate are not independent. High sweep flow rates give a higher pressure driving force at the outlet (minimizing reactor length for a given conversion), but gives a highly diluted hydrogen product. Conversely, a very small pressure driving force maximized hydrogen concentration in the sweep, but results in a very long reactor. The compromise lies in specifying a minimum pressure driving force, computed from the position of the bend in the CO conversion curve as the conversion levels off, as noted in the shape of the curves at the reactor exit in Figures 1.3.43-1.3.44.

Design characteristics for membrane reactors for IGCC applications are contained in [Bracht et. al., 1997]. The dimensions used in the present simulation are based on these values. The membrane tube diameter is given as 10.4 cm, with a tube length of 2 m. The total number of modules is 3300, giving a membrane area of 2176 m². The catalyst volume is given as 25.3 m³. These values assume a Knudsen diffusion membrane rather than a Pd membrane. These values compare reasonably well with the current values considering membrane differences and the unknown degree (if any) of conversion in the preshift reactor. The palladium membrane hydrogen flux depends exponentially on temperature. At the present reactor exit temperature,

the Pd membrane used has an H₂ flux approximately 2.4 times that of Knudsen diffusion membranes listed in [Bracht et. al., 1997].

Table 1.3.12. Sample Simulation Inputs and Results.

Inputs

Inlet Feed Gas Composition (vol % dry)	
CO	42.82%
H ₂ O	19.70%
H ₂	27.42%
CO ₂	8.34%
Other	1.72%
Temperature (K)	672
Pressure (atm)	15
Flow Rate (moles/s)	3312
Sweep Gas (N ₂)	
Temperature (K)	300
Pressure (atm)	1
<i>H₂O:CO ratio (inject steam)</i>	<i>1</i>
Module Shell Diameter (cm)	15
Module Membrane Diameter (cm)	10
Number of Modules	1280
Specified CO Conversion (%)	95%
Membrane Thickness (micron)	10
Specified MR Inlet Temperature (K)	565
Specified Heat Loss (%)	0

Results

H ₂ Recovery	96.14%
MR Length (m)	2.2
Total Membrane Area (sq. m)	925
Intermediate Heat Transfer (kW)	42,158
MR Footprint (sq. ft)	309
Preshift CO Conversion (%)	49.5%
Preshift Reactor Exit Temperature (K)	852
Sweep Gas Flow Rate (moles/s)	17416
H ₂ Concentration in Sweep (vol %)	11%
Inlet Sweep Velocity (m/s)	42.7

Figure 1.3.42. Predicted temperature profile.

Figure 1.3.43. Predicted gas composition profiles.

Figure 1.3.44. Predicted CO conversion and pressure driving force.

Model UI

The model can be used in evaluation mode or design mode (see Figure 1.3.45). Evaluation mode (shown) allows the user to input existing membrane geometries (diameter, thickness, and length), and the module will use these values to calculate the resultant CO conversion. (note: the provided model is configured *only* for the annular design shown in the upper portion of Figure 1.3.40). In design mode, the user specifies a desired CO conversion, and uses a user-specified diameter and thickness to determine the reactor length necessary to achieve the desired conversion. The steam is added simply by changing the composition and flow rate of the inlet

feed stream (not temperature). This option is intended as a design tool; if strict accounting of stream flows is required, the steam should be added to the feed stream via a gas mixer, prior to the WGS module, and the H₂O:CO specification should not be selected. An option is provided to simulate the requirements of a staged operation in which the feed gas is first introduced to a preshift catalytic non-membrane reactor, cooled, and then fed to the membrane reactor (a schematic of this option is shown in Figure 1.3.41). As equilibrium is assumed with the aid of a catalyst, the preshift reactor is simply modeled as an adiabatic equilibrium on the feed gas. The temperature of the gas is then dropped to the user-specified MR inlet temperature, with the required heat duty computed and displayed in the summary window (see Figure 1.3.45). An option is provided to specify the H₂O:CO ratio explicitly to evaluate the effect on the reactor operation.

The model outputs are shown in Figure 1.3.45 for an example case. The categories shown at left represent those displayed when both the preshift and H₂O:CO ratio options are toggled. The CO conversion is displayed as a fraction, as is the H₂ recovery, pre-membrane reactor CO conversion, and the sweep H₂ concentration. Also displayed are the catalyst space velocity, exit gas temperature, unit footprint (size), preshift heat duty (in MW), and the steam required (kg/s).

The figure consists of two side-by-side windows. The left window is titled 'MembraneReactor' and contains input fields for various parameters. The right window is titled 'Result Dialog' and displays a table of summary data.

MembraneReactor Input Panel:

- ☒ Evaluation Mode ☐ Design Mode
- Membrane Diameter (m): 0.1
- Membrane Thickness (m): 1e-005
- Reactor Length (m): 1.5
- Desired CO conversion: 0.9
- Number of Modules: 1200
- Shell Diameter (m): 0.15
- ☒ Allow Preshift Reactor
- M.R. inlet temp (K): 565
- ☒ Specify H₂O : CO
- H₂O : CO (ratio): 1
- Buttons: OK, Cancel

Result Dialog Summary Data:

Description	Value

CO Conversion (fr)	0.79
Catalyst Space Ve	2651.73
Exit Gas Temp (K)	621.17
Footprint (m ²)	27.00
H ₂ Recovery (frac)	0.32
Pre- MR CO Conver	0.64
Pre-Shift Heat Du	11.43
Steam Required (k	9.8819
Sweep H ₂ Concentr	0.41

Buttons: OK

Figure 1.3.45. Input panel (left) and summary data (right) for water gas shift membrane reactor model.

Error handling is provided in the module to output warning or error conditions resulting from incorrect inputs such as specification of a temperature increase between the preshift and membrane reactors, a shell diameter that is less than the membrane diameter, an $\text{H}_2\text{O}:\text{CO}$ ratio requiring steam removal from the feed, or an impossible desired CO conversion based on the available steam reactant.

It is important to note that the membrane reactor only works so long as there is a hydrogen partial pressure driving force. Once the feedside hydrogen pressure matches that of the sweep gas, the WGS reaction is limited by the equilibrium composition. The primary purpose of the sweep gas is to dilute the hydrogen enough to provide a sufficient driving force over the membrane, hence allowing high CO conversion. A feed-to-permeate pressure ratio of 15 atm is typical [Bracht et. al., 1997].

Power Generation Component Models - Overview

For plants based on IGCC technology there are a variety of systems and equipment that can be used for generating power. In this project we have focused on two technologies, each of which presents a different set of modeling challenges.

The power block configuration contained in the Vision 21 reference configuration (see Figures 1.3.10 and 1.3.11) is based on a hybrid scheme that combines the use of a fuel cell in combination with a simple turbine (compression, expansion) to extract work from the fuel cell tail gas. In such a system the fuel cell acts as the combustor for the simple turbine. The high efficiency of fuel cells make them attractive for advanced power plant configurations. For large-scale power generation the preferred fuel cell technology is a SOFC; this also is the fuel cell technology shown in the Vision 21 reference configuration.

- To allow investigating the performance of IGCC plant configurations that use hybrid power blocks, models to simulate the performance of a SOFC, SOFC tail gas oxidizer, and turbine compressor/expander equipment were developed and incorporated into the framework. Present generation SOFCs do not achieve 100% fuel conversion. The resulting low BTU tail (exhaust) gas must be further processed to achieve high plant efficiency. Hence, models are included for processing the SOFC tail gas using a dump combustor or a catalytic combustor. Simple (isentropic) expansion/compression models are used to simulate the turbine equipment that would be used to extract work from the SOFC effluent gas.

The existing IGCC plants, such as Polk Power and Wabash River, use direct-fired gas turbines to generate power. These systems use a combustion turbine for which the combustor has been modified to fire syngas (which is composed of CO and H₂) rather than natural gas (predominantly methane, or CH₄).

- Both equilibrium- and kinetics-based combustion models are provided for modeling the turbine combustor; the models to simulate the expansion and compression sections of the turbine described above are reused to calculate power generated.

Overall, the provided models allow engineers to investigate and identify operating parameters and conditions that could improve overall plant efficiency, such as fuel gas inlet temperature, residence time, gas velocity, adiabatic combustion temperature, and fuel/air ratio. Obtaining both complete fuel conversion and minimal pollutant emissions will be important for advanced power plant configurations to be accepted by industry.

In addition to the above, the framework also includes a model for a steam turbine. Regardless of the type of power block used, steam generated from the HRSG or other equipment can be passed through a steam turbine to further increase the plant efficiency.

In the following section are provided discussions for the different component models included in the framework related to power generation. Described are the models for:

- SOFC;
- SOFC tail gas combustors;
- turbine compressor/expander;
- the combustor of the combustion turbine; and
- a steam turbine.

Lumped Parameter Process Engineering SOFC Model

Based on a request to NETL, REI obtained a lumped parameter (0D) process engineering model for a SOFC (see Figure 1.3.46) that had been developed at NETL [Ruth and James, 2002]. The original model consisted of an Aspen Plus flowsheet, which used a combination of standard Aspen Plus calculation blocks for thermodynamics calculations and user-defined imbedded FORTRAN blocks for electrochemistry calculations. The Nernst equation and equations for activation, concentration, and ohmic losses are used to calculate fuel cell electrical output. Thermodynamics calculations were performed using a combination of Aspen RGIBBS (equilibrium) and HX (heat exchanger) blocks. An Aspen Plus calculator block was used to iterate the anode temperature until the thermodynamic output from the fuel cell matched the electrical output.

Figure 1.3.46. Schematic of SOFC unit.

The model obtained from NETL was ported to C++ and successfully integrated into the framework. The Aspen Plus functionality for looping, data handling, and thermodynamics was implemented using C++. Likewise, the imbedded FORTRAN blocks responsible for electrochemical calculations were ported to C++. For testing purposes, in the SCIRun-based IGCC-FCT framework, this model was implemented using CAPE-Open. This functionality was not carried over to the VEF.

Enhancements implemented to the original model included:

- use of coal-derived syngas that contains predominantly CO and H₂ as the SOFC fuel gas;
 - the model will only handle CO and H₂ coming into the anode as fuels. This is hardwired in both the thermal and electrical calculations. The cathode air stream, however, is not limited to just O₂ and N₂. The cathode composition is arbitrary - the code pulls off just enough O₂ to react with the CO and H₂ entering in the anode stream at the specified fuel utilization level.
- eliminated the internal reformer because the SOFC is now tuned for syngas firing;
- ability to operate the SOFC at elevated pressure (as per gasifier syngas stream); and
- more robust equation solvers used within the model.

The enhanced SOFC model was tested to ensure proper function. The inputs for the model include cell component thickness and electrical resistivity data, anode and cathode channel gas flow rates and compositions, and the exchange current density parameters (see Figure 1.3.47). The cell active area and the total number of cells required are also specified in the input dialog. The cell physical dimension dialog is straightforward. The resistivity of the cell component materials is a function of temperature and is evaluated in the same manner as [Gemmen et al., 2000] using $R = Ae^{(E/T)}$. The pre-exponential factor, A, and the exponential factor, E, for the anode, cathode, and electrolyte are defined in the dialog window. The outputs for the model in the summary window include fuel cell plant power output (MWe) and the temperature of the exiting gas stream (K).

The figure shows two windows from a software interface. The left window is titled 'SOFC' and contains input fields for construction, cell resistance, and cells. The right window is titled 'Result Dialog' and shows summary data.

SOFC Input Panel:

- Construction:**
 - Anode Thickness (cm): 0.15
 - Cathode Thickness (cm): 0.01
 - Electrolyte Thickness (cm): 0.001
 - Fuel Cell Pressure Drop (Pa): 27576
- Cell Resistance: $R = Ae^{(E/T)}$**
 - Anode, A: 0.00298
 - Anode, E: -1392
 - Cathode, A: 0.008144
 - Cathode, E: 600
 - Electrolyte, A: 0.00294
 - Electrolyte, E: 10350
- Cells:**
 - Area per unit cell (cm²): 305
 - Number of cells: 70000
- Fuel Utilization (%):** 85

Result Dialog Summary Data:

Description	Value

Anode Temperature	1129.19
Fuel Cell Power (	140.45

Figure 1.3.47. Input panel (left) and summary data (right) for lumped parameter SOFC model.

Process Engineering (1D) Fuel Cell Model

Based on a request to NETL, REI obtained a 1D process engineering model for a SOFC that was developed by researchers at NETL [Ruth and Gemmen, 2002]. The model provides a higher fidelity representation of the physics and chemistry involved with a SOFC than the lumped parameter model. The 1D model was developed using C++ and accounts for the energy transport in and out of a flow channel of a fuel cell, heat transfer to and from the walls, heat generation from the electrochemical reactions, and fuel cell power output. A finite-difference approach is used to solve integrated forms of the mass, momentum, and energy conservation equations along the main axis of the fuel cell. The model uses a dynamic simulation approach that is geared for performing the safety analysis of hybrid fuel cell turbine systems. The 1D model does require more cpu time to execute than does the lumped parameter model. The details of the model are available in the open literature [Bessette, 1994], [Gemmen et al., 2000], [Liese and Gemmen, 2002], [Liese et al., 2000] and thus not repeated here. REI modified the model to output values for steady-state operation.

The UI for the model allows the user to manipulate fuel cell characteristics and performance (see Figure 1.3.48). The user can input the fuel cell size and parameters pertaining to the cell resistance and general construction. Default values are provided. The model outputs are shown below.

SOFC1D

Working Directory:

Anode		Cathode	
Channel Height (m)	0.001	Channel Height (m)	0.003
Channel Width (m)	0.001	Channel Width (m)	0.001
Channel Spacing (m)	0.001	Channel Spacing (m)	0.001
Exg. Cur. Den. (Amp/m ²)	5	Exg. Cur. Den. 'b' Coeff	-13595
Trans. Coeff	1e+006	Exg. Cur. Den. 'm' Coeff	15
Electrode Thickness (m)	5e-005	Trans. 'B' Coeff	0.5
Pressure Drop (Pa)	3250	Trans. 'M' Coeff	0
		Electrode Thickness (m)	5e-005
		Pressure Drop (Pa)	431

Separator		Electrolyte	
Thickness (m)	0.002	Thickness (m)	0.00018
Heat Capacity (J/kg-K)	400	Res. PreExpon. (ohm-cm)	0.002838
Density (kg/m ³)	8000	Res. Expon. (K)	10300

Electrodes		Interconnect	
Fuel Res. PreExpon. (ohm-cm)	0.0014	Res. PreExpon. (ohm-cm)	0.5
Fuel Res. Expon. (K)	0	Res. Expon. (K)	0
Air Res. PreExpon. (ohm-cm)	0.0186		
Air Res. Expon. (K)	0		

Cells		Operational	
Number of Cells	1000	Stop Time (sec)	1000
Heat Capacity (J/kg-K)	800	Number of Axial Nodes	5
Density (kg/m ³)	1500	Load Resistance (ohm)	0.006
Axial Length (m)	1		
Axial Width (m)	1		

OK Cancel

Result Dialog

Summary Data

Description	Value
+++++	
Overall Q (MW)	40.30
Produced Power (MW)	32.40

OK

Figure 1.3.48. Input panel (left) and summary data (right) for 1D SOFC model.

SOFC Tail Gas Dump Combustor

A 1D model based on an idealized PFR that includes chemical kinetics is used to model the performance of a simple combustor. Including kinetics allows for a more accurate calculation of the combustion requirements to oxidize the low BTU tail gas that exhausts from the SOFC. As discussed above, a SOFC does not achieve complete fuel conversion. The remaining, unreacted fuel represents available energy that must be used in order to maintain high overall plant efficiency. Although the SOFC tail gas is quite dilute (i.e., low energy density), the composition and operating conditions of the gas is such that its combustion depends primarily on the residence time for combustion, and reaction occurs over a wide range of temperatures, with no apparent blowout condition.

The combustor model can be run in one of two modes:

- evaluation mode, in which the combustion volume is specified, and the fuel conversion and exit properties are computed; and
- design mode, in which the program computes the required volume for a user-specified degree of fuel conversion.

A heat loss and pressure drop over the unit can be specified. Outputs include heat loss and pressure drop (if any), combustor volume (for design mode), fuel conversion (for evaluation mode), and residence time. For modeling purposes, the combustor is placed in the equipment network immediately downstream of the SOFC.

In the following, we examine representative SOFC exhaust gas to determine its combustion requirements and describe the capabilities of the combustor model, example calculations performed with the model, and, last, the UI for the dump combustor model.

SOFC Exhaust Gas

The Vision 21 reference configuration (Figures 1.3.10 and 1.3.11) includes high and low pressure fuel cells operating at 14.7 and 3.3 atm, respectively. Illustrated in Figure 1.3.49 is the composition of the tail gas from the high-pressure SOFC; calculations have shown that the tail gas from the low-pressure SOFC is similar. Important characteristics of this gas are the temperature, pressure, energy density, and oxidizer content. Combustion stability and reaction rate is of primary concern in a dump combustor when processing a low BTU off-gas. Combustion rates generally increase with increasing pressure. Also note that the oxygen content is very high in the gas - the stoichiometric ratio for the high-pressure gas is 18. Thus, no air needs to be added to the gas. This results in an energy density of 4.8 Btu/scfm. In contrast, typical molten carbonate fuel cell exhaust contains 30-40 Btu/scfm (S.R. = 1) [Gemmen, 1998], and for comparison, methane contains about 80 Btu/scfm (S.R. = 1). Because the exhaust gas is so dilute, the adiabatic equilibrium temperature is only about 120 K higher than the inlet gas, so high combustion temperatures will not be achieved. Note the relatively high temperature of the gas, 850°C. At present, SOFCs operate at high temperatures (~900 °C). The values listed in Figure 1.3.49 for SOFC exhaust properties are typical of those found in the literature for operating temperature of >800°C and fuel and air utilizations of 85% and 25%, respectively, resulting in exhaust gases with stoichiometric ratios of about 15, [Campanari, 2001].

Figure 1.3.49. SOFC tail gas composition.

SOFC Tail Gas Combustion Characterization

The combustion characteristics of the SOFC tail gas of Figure 1.3.49 were characterized by running two idealized reactor models: PSR and PFR models. The PSR is a steady-state model of a perfect-mixing chamber in which the exiting reacting fluid composition is the same as the reactor composition. This type of model is useful for estimating combustion flames, in which large amounts of mixing and recirculation in the flame are expected, with reactants flowing into and out of the flame zone. A PFR, by contrast, describes the time evolution of a well-mixed, reacting fluid. Reacting flow in a pipe, with perfect radial mixing and zero axial mixing, is well characterized by a PFR.

Illustrated in Figure 1.3.50 are the fuel conversion versus time for adiabatic PFR simulations for the high-pressure SOFC tail gas of Figure 1.3.49. These calculations were performed using the GRImech 3.0 kinetic mechanism [Smith et al., http://www.me.berkeley.edu/gri_mech/]. Two temperatures are shown in the figure. The upper curve is at the lower range of exhaust temperatures (850°C) and shows complete conversion in approximately 0.1 seconds. The lower curve is for 427°C, much lower than a typical SOFC exhaust temperature, and shows that a high degree of conversion is possible even at low initial temperatures, provided the residence time for reaction is long enough (i.e., if the combustion volume is sufficiently large).

The gas composition (fuel, oxygen concentration) and conditions (temperature, pressure) that exist at the SOFC exit will result in very fast oxidation of the unreacted fuel in the tail gas. If there is good mixing conditions, the oxidation could possibly occur in the ductwork exiting the fuel cell. Hence, combustion of the SOFC exhaust gas is treated only minimally in the literature sources examined; typically, researchers have assumed the combustion occurs in a plenum as part of the SOFC device. The combustion plenum is intended to be a mixing chamber for the anode and cathode gases, providing sufficient residence time for complete combustion to occur.

Figure 1.3.50. Results of PFR tests for the high-pressure SOFC tail gas at two initial temperatures.

To evaluate the stability of exhaust gas combustion, preliminary PSR simulations were run on the high-pressure SOFC tail gas of Figure 1.3.49. Figure 1.3.51 shows the exit temperature as a function of residence time in the reactor (which is proportional to reactor volume) for the high-pressure exhaust, and for a stoichiometric ethane-air mixture. As the residence time decreases, the extent of reaction decreases and the fuel conversion (indicated by temperature) decreases. For typical combustion (ethane-air mixture), at low residence times, the reaction vessel is too small to support combustion, and the flame “blows out”. This is evident from the jump from ~ 1800 K to 300 K as the residence time decreases. For the exhaust gas, no such jump occurs. Reaction takes place for all residence times, and combustion proceeds in a flameless fashion.

Figure 1.3.51. PSR simulations of the high-pressure SOFC exhaust gas (left) and a stoichiometric ethane-air flame (right) for comparison.

The results of the PFR and PSR simulations indicate the SOFC exhaust gas is stable and reactive over a wide range of inlet temperatures and residence times. The primary issues for combustion are (1) mixing, and (2) sufficient residence time (or combustor volume).

Model Description

As described above, the combustion of the SOFC exhaust gas depends primarily on the residence time for combustion, and reaction occurs over a wide range of temperatures, with no apparent blowout condition. The dump combustor model provided in the framework is based on a PFR. The model is designed to provide the combustor volume required for a given fuel conversion, or the fuel conversion for a given volume. The PFR model used within the dump combustor model is based on the PFR option for the *kinetic reactor model* described below.

Example Calculations

Parametric cases were run with the dump combustor model for a wide range of inlet temperatures, pressures, and compositions. The baseline composition is that of Figure 1.3.49, and Figure 1.3.52 shows the results; all cases are for a specified 99% fuel conversion. At a given temperature, the required residence time decreases with increasing pressure, as expected. The dependence of residence time on pressure is fairly linear in the given range. The dependence of residence time on temperature is very nonlinear, with large increases in the required residence time at low temperatures. When the amount of oxygen and nitrogen in the exhaust gas is decreased to half the original value, the required residence time decreases from 0.14 to 0.036 s at 1100 K and from 7.8 s to 1.5 s at 900 K. This occurs because the O_2 and N_2 are in such large excesses that the effect of increasing their values is to dilute the system, resulting in lower fuel concentrations and combustion temperatures, resulting in reduced reaction rates. Note that 99% conversion was possible for all cases. Clearly, at low temperatures, the residence time is so high that a prohibitively large combustion chamber would be required. For these conditions an

alternate combustion process would be required. Options for combustion include preheating the inlet gas or use of catalytic combustion.

Temperature = 1100 K	
P (atm)	Residence Time (s)
14.7	0.145895
30	0.123962
60	0.0877269
90	0.0667489

Pressure = 14.7 atm	
Temp (K)	Residence Time (s)
1100	0.145895
1000	0.98721
900	7.76659
800	79.2054

Half the O ₂ and N ₂	
Pressure = 14.7 atm	
Temp (K)	Residence Time (s)
1100	0.036
900	1.5

Figure 1.3.52. Dump combustor parametric tests, based on Figure 1.3.49 conditions, with 99% fuel conversion.

Model UI

Illustrated in Figure 1.3.53 is the window for inputting model parameters, and an example model output. The model can be run in one of two modes:

- evaluation mode, in which the combustion volume is specified, and the fuel conversion and exit properties are computed; and
- design mode, in which the program computes the required volume for a user-specified degree of fuel conversion.

A heat loss and pressure drop over the unit can also be specified.

Outputs include heat loss and pressure drop (if any), combustor volume (for design mode), fuel conversion (for evaluation mode), and residence time (tau average). Full error handling is provided to alert the user of error or warning conditions and to enforce proper input specifications. For example, an error occurs if the equilibrium fuel conversion is below the specified fuel conversion.

Figure 1.3.53. Input panel (left) and summary data (right) for dump combustor model.

In general, the dump combustor would follow the SOFC module, and the outlet dump combustor gas stream (not shown) would be further processed, likely in a turbine for power production.

SOFC Tail Gas Catalytic Combustor

The SOFC tail gas catalytic combustor model is based on an idealized PFR that accounts for gas-phase chemical kinetic reactions and surface reactions for the catalyst material. The model is based on gas-phase and catalyst surface kinetics, geometry, and model results published in the open literature. The model attempts to balance the tradeoffs between providing a detailed description of the physical processes occurring versus the inherent complexity of the system.

From a practical perspective, catalytic combustors will only be needed when SOFC systems become available that can operate at a lower temperature than current commercial systems. As per the dump combustor, in the modeling framework the catalytic combustor should be located immediately downstream of the SOFC; however, in practical applications the catalytic combustor will probably be integrated into the SOFC.

In the following we provide additional background information on the potential need for a catalytic combustor to oxidize the SOFC tail gas, a description of the model, example calculations, and the model UI.

Background

In fuel cell applications, catalytic combustion offers an efficient means of recovering heat from the low heating value (LHV) fuel cell effluent streams that may otherwise be difficult to burn directly. This is particularly manifest in molten carbonate fuel cell systems where the cell discharges unreacted fuel at about 600°C. In these systems, the anode exhaust containing the unreacted fuel is mixed with air and then oxidized completely in a catalytic combustor [Ghezeli-Ayagh and Maru, 2002]. At present, SOFC systems operate at temperatures in the window of 800-1000°C because the oxygen ion conduction in yttria stabilized zirconia (YSZ) is best in this temperature window. However, with the current research emphasis on developing low temperature solid electrolytes for SOFC systems, the operating temperature window is likely to fall in the range 700-800°C where catalytic oxidation of the lean-fuel/air mixtures is an attractive option. In addition to the ability to burn lean-fuel/air mixtures completely [Tucci, 1982], catalytic combustors operate at low enough temperatures such that NO_x emissions are minimized [Kolaczowski, 1995].

Model Description

The catalytic combustor model will provide the user the ability to:

- identify operating parameters that influence efficiency, such as inlet temperature, gas velocity, combustion temperature, fuel/air ratio and pressure;
- identify flow rates that lead to blowout conditions (extinguishing of reaction); and
- predict light-off conditions (initiation of catalytic combustion).

Overall, the model provides a tool that can assist in guiding the development of concepts, design, scale-up, and operation strategies of hybrid Fuel Cell – Turbine systems.

In order to achieve these goals, the model is designed to account for detailed homogeneous and heterogeneous chemical kinetics along with heat and mass transfer within a single channel of a monolith reactor. Monolith reactors are preferred over other configurations because they provide

the best combination of high catalyst surface area and low-pressure drop. Thus, only monolith-type combustors are considered for this project.

Many levels of complexity exist in describing the processes that occur in a single channel of a monolith as well as in the monolith as a whole. A review of the literature [Bond et al., 1996], [Chou et al., 2000] revealed that the majority of existing models were limited to modeling heterogeneous reactions within a single channel of a monolith for combustion of methane. Figure 1.3.54 provides a schematic showing the processes occurring in a single monolith channel. These processes include bulk fluid flow, mass transfer of species to the catalyst surface, and within catalyst pores, adsorption and reaction of reactants, followed by desorption of product species. Gas-phase reactions occur in parallel with surface reactions, whose rates relative to the heterogeneous surface reactions depend upon the gas temperature and composition and may vary with position. Heat transfer effects include radiation, convection, and axial conduction along the channel walls.

Figure 1.3.54. Processes in a single monolith channel. Shown are: (1) fuel and air flow into the channel, (2) diffusion and surface reaction, (3) desorption of products, (4) gas-phase reactions, (5) conduction, (6) radiation, and (7) convection.

Models from the literature include 1D and 2D models with and without detailed gas chemistry. Most older models treated the catalytic reactions as a black box, or utilized global surface chemistry, as opposed to detailed surface mechanisms that have recently become available. Nearly all models reviewed neglected axial conduction and diffusion, assuming convective effects dominated. Radiation is also typically ignored.

The catalytic combustor model developed here is for a single monolith channel. In order to extend the single channel model to a full monolith for a plant-size combustor, the monolith is assumed to be adiabatic, with no temperature gradients, and of uniform inlet velocity and composition profile. Thus, all properties of the single channel, such as temperature and composition profiles, apply directly to the entire monolith. Nearly all computational models found in the literature make this assumption or treat the entire monolith with a simplified description of the complex interactions occurring in each channel. In reality, the characterization

of the monolith as a whole depends upon heat losses and gradients in the inlet velocity and composition profiles, resulting in different composition and temperature profiles along each individual channel. The only interaction between channels in a monolith is through conductive heat transfer. Due to the high cell density (typically 200 cells per square inch), modeling and coupling each cell in a monolith in order to obtain the overall performance is not feasible and would require excessive computation time.

The following assumptions are made for the channel model and are typical of those used in the literature:

- the fluid is assumed to be in plug flow, thus no axial diffusion of heat or mass transfer is accounted for; the model is 1D;
- steady-state operation is assumed;
- the gas-phase composition at the gas-surface interface is different than the bulk gas composition; the bulk and surface-gas compositions are coupled through species mass transfer correlations for channel flow; bulk gas and surface temperatures are treated likewise, by solution of an energy equation;
- radiative heat transfer is ignored;
- detailed homogeneous gas-phase kinetics are assumed; and
- detailed heterogeneous surface kinetics are accounted for.

The surface mechanism is taken from the literature for methane combustion on platinum [Chou, et al., 2000], which has shown good agreement with literature data. For methane combustion, palladium currently offers the highest activity, but hydrogen and CO are sufficiently reactive over platinum to warrant its use. In addition, detailed surface chemistry and thermodynamics are readily available for platinum, and most of the literature data assume a platinum catalyst. For these reasons, platinum is assumed for the catalytic combustor; other metals could be implemented in the future provided detailed (or global) chemical kinetics are available. Since methane is not expected to be present in any appreciable quantities, the mechanism is simplified to include only H₂ and CO chemistry. Table 1.3.13 lists the surface reactions considered. Units are cm-mole-s for the pre-exponential factor, and J/mole for the activation energy. The sticking coefficients are dimensionless. Detailed gas-phase chemistry is taken from GRI_{mech} 3.0 [Smith et al., http://www.me.berkeley.edu/gri_mech/]. In Table 1.3.13 the rate constant is computed as $k = A \cdot T^B \cdot \exp(-E_a/R \cdot T)$. The sticking coefficient is computed differently.

The catalytic combustor model was developed using REKS, REI's in-house chemical kinetics solver. Note that REKS was used to create the PFR and PSR models used in the kinetics reactor model (see below) and was used to create the PFR model that forms the basic model within the dump combustor model. REKS computes the time evolution of a reacting, homogeneous gas-phase mixture by solving a coupled, nonlinear, stiff set of ODEs describing species composition and temperature. REKS employs the open-source software CVODE, developed at Lawrence Livermore National Laboratory, to solve the system of ODEs. REKS can be run in several modes to solve the temporal or spatial evolution of the gas state in constant temperature, adiabatic, constant pressure, and constant volume modes. The catalytic combustor model modifies the adiabatic, constant pressure mode of operation to include source and sink terms for the species continuity and energy equations, thus accounting for the effects of heterogeneous surface reactions as well as heat and mass transfer to the catalyst surface.

Table 1.3.13 Detailed Surface Mechanism for Reaction of H₂ and CO on Platinum.

ADSORPTION	A	S	B	Ea
O ₂ + 2PT(S) => 2O(S)		0.003	0	0
CO + PT(S) => CO(S)		0.84	0	0
H ₂ + 2PT(S) => H(S) + H(S)		0.046	0	0
OH + PT(S) => OH(S)		1	0	0
H ₂ O + PT(S) => H ₂ O(S)		0.5	0	0
SURFACE REACTION				
H(S) + O(S) => OH(S) + PT(S)	1.00E+19		0	1.05E+04
OH(S) + PT(S) => H(S) + O(S)	1.00E+12		0	2.08E+04
H(S) + OH(S) => H ₂ O(S) + PT(S)	1.00E+21		0	6.25E+04
2OH(S) => H ₂ O(S) + O(S)	1.00E+20		0	5.13E+04
H ₂ O(S) + PT(S) => OH(S) + H(S)	1.80E+13		0	5.42E+04
C(S) + O(S) => CO(S) + PT(S)	5.00E+20		0	6.25E+04
CO(S) + PT(S) => C(S) + O(S)	1.00E+13		0	1.57E+05
CO(S) + O(S) => CO ₂ + 2PT(S)	4.00E+20		0	1.01E+05
DESORPTION				
2O(S) => O ₂ + 2PT(S)	1.00E+21		0	2.16E+05
CO(S) => CO + PT(S)	8.50E+12		0	1.53E+05
2H(S) => H ₂ + 2PT(S)	5.00E+20		0	6.74E+04
OH(S) => OH + PT(S)	1.50E+13		0	1.93E+05
H ₂ O(S) => H ₂ O + PT(S)	1.00E+13		0	4.50E+04

Model Equations

The following is a description of the equations to be solved by REKs and the surface program. The gas species compositions are defined by

$$\frac{dy_k}{dx} = \frac{\omega_{k,g} M_k A_{cs}}{m} + \frac{k_m \cdot P_w \cdot \rho}{m} (C_{k,s} - C_{k,b}), \quad (1.3.45)$$

where y_k is the mass fraction of species k , x is axial position, $\omega_{k,g}$ is the molar production rate of species k in the bulk gas phase due to homogeneous reaction, k_m is the mass transfer coefficient for species k , P_w and A_{cs} are the wetted perimeter of the channel and the channel cross sectional area, respectively, M is the molecular weight, ρ is density, m is mass flow rate, and $C_{k,s}$ and $C_{k,b}$ are the gas concentration of species k at the surface and in the bulk gas, respectively. Equation 1.3.45 is given for all gas-phase species in the system. The species molar production rate is computed as a function of temperature and bulk gas composition. The mass transfer coefficient is computed using species diffusivities and mass transfer correlations for flow in ducts.

The bulk species composition is computed from the following equation found by equating the rate of mass transfer of a species to the catalyst surface to the rate of surface reaction of that species, a requirement of the steady-state assumption:

$$k_m \cdot (C_{k,s} - C_{k,b}) = \omega_{k,s}, \quad (1.3.46)$$

where $\omega_{k,s}$ is the rate of production of gas species k at the surface per unit area of surface. $\omega_{k,s}$ depends upon the surface-site composition of the catalyst (e.g. adsorbed species), the gas surface composition, and the surface temperature.. The surface composition at any given location along a channel is in steady state; hence the composition is computed by solving the set of nonlinear algebraic equations given by

$$\omega_{j,s} = 0, \quad (1.3.47)$$

for each surface-site species j .

The bulk gas temperature is computed from the following equation:

$$m \cdot c_p \cdot \frac{dT_b}{dx} = \sum_k h_k \cdot \frac{dy_k}{dx} \cdot \frac{m}{M_k} + k_T \cdot P_w \cdot (T_s - T_b), \quad (1.3.48)$$

where c_p is the gas specific heat capacity, T_b and T_s are the bulk gas and surface temperatures, respectively, k_T is the heat transfer coefficient for channel flow, and h_k is the molar enthalpy. The first term on the right in Equation 1.3.48 is the heat release due to homogeneous chemical reaction and the enthalpy associated with species mass transfer (Equation 1.3.45), and the second term is the rate of convective heat transfer to the surface. The surface temperature is computed from the steady-state energy balance at the surface,

$$\sum_i h_i \cdot (\omega_{i,s} - k_m \cdot (C_{i,s} - C_{i,b})) = k_T \cdot (T_s - T_b), \quad (1.3.49)$$

where the summation is carried over all gas and surface-site species.

Model Algorithm

An iterative solution procedure is being implemented. Equations 1.3.45 and 1.3.48 are solved using REKs. At each step in the solution, the source terms (rightmost terms in both equations) are computed in a predictor-corrector manner as follows.

- 1) the surface-gas composition, surface-site composition, and surface temperature are estimated;
- 2) the surface-site species concentrations are computed by solving Equation 1.3.47; and
- 3) the gas surface species rates are then computed and substituted into Equation 1.3.46, and the surface-gas composition is updated, followed by the surface temperature from Equation 1.3.49.

This procedure is repeated to convergence of the surface-gas composition and surface temperature. To ensure robustness, the steady-state surface composition is computed in a time-accurate manner using CVODE (see above).

Model UI

This UI requires the user to first specify the method of module calculation (see Figure 1.3.55). If evaluation mode is selected (shown), this allows the user to input the length of the combustor and the hydraulic diameter of the channel; the model will then calculate the maximum possible conversion. When design mode is specified, the user inputs a desired conversion and the module

calculates the necessary combustor geometry to achieve that specified conversion. An additional input for both model uses is the inlet gas velocity to the combustor unit. Model outputs include the items noted above, the pressure drop across the system, and gas residence time within the system.

Figure 1.3.55. Input panel (left) and summary data (right) for catalytic combustor model.

Compressor / Expander

The compressor and expander components of the turbine used to extract work from the syngas flow are modeled with a process engineering (0D) model based on thermodynamic calculations. The same model is used for both components. The thermodynamic calculations involve the assumption of isentropic compression/expansion processes, coupled with user-supplied isentropic efficiencies. The thermodynamic properties needed for the models are obtained from the thermodynamics database that can be accessed as needed by any module in the framework.

The UI for these models is quite simple (see Figure 1.3.56). In addition to the isentropic efficiency, the user must specify the pressure change across the unit. Note that negative values decrease the pressure (i.e., model an expander) and positive values increase the pressure (i.e., model a compressor). Model inputs such as the gas composition, temperature, and pressure are obtained directly from the incoming syngas dataflow. Model outputs include the power requirements of the device. When used to model compressors, the resultant number will be negative and will represent the power required to compress the inlet gas. When the module is used to model expanders, the number will be positive and represents the power generated as a result of the pressure drop. The modifications to the gas stream passing through the device are transferred to downstream modules by the dataflow within the framework. Using other tools, the composition and properties of the syngas at the exit of the compressor or expander can be viewed.

Figure 1.3.56. Input panel (left) and summary data (right) for compressor/expander model.

Combustion Turbine Modeling - Overview

The gas turbine in an IGCC plant has to be tailored to allow for differences in mass flow rate, combustion temperature, gas emissivity, and composition of the syngas supplied to the turbine. The present generation of turbine combustors for burning syngas has been developed as a permutation of conventional (natural gas) fired combustors. If the use of hydrogen as a fuel becomes more prevalent, there are concerns that the radiative heat flux to the liner may lead to de-rating of the gas turbine. The changes in hardware are issues that the manufacturers are addressing.

Within the framework, options are provided for calculating the performance of a direct-fired combustion turbine that would be used for power generation within present IGCC plant configurations. The options include using

- full chemical equilibrium or
- idealized chemical kinetic calculations based on the PSR or PFR models available in the kinetic reactor model.

The combustion calculations provide an estimate of the combustor exhaust gas conditions (gas temperature and major and minor species concentrations). The simple (idealized) turbine compressor/expander models described above are used to calculate the power that can be generated from the exhaust gas of the combustor.

The models provided in the framework are fast running and provide a good first estimate of combustor performance. Thus, these models are appropriate to use when evaluating overall plant performance. However, it was important to study at a finer level of detail the issues associated with combustor operation, performance (emissions), and modeling. In particular, the emissions from the turbine need to be quantified to ensure that the IGCC plant meets the goals set by DOE. A particular challenge in developing a gas turbine model is that the turbines meet the ultra-low NO_x levels projected for the next generation plants.

For this purpose, REI and RECOM worked together to develop a CFD model of a combustor that would be representative of the type used in major manufacturer's mainframe gas turbines. A DLN (dry Low-NO_x) combustor rig for the GE Frame 7 machine was selected for this purpose. The model results were compared with data from a rig combustor operated by PSM of Jupiter, FL, the *only* after-market company with a viable DLN combustion system for the GE Frame 7 installed base. Another motivation for developing a combustor model, as discussed above, is that radiation to the liner may become a problem with hydrogen, leading to de-rating of the gas turbine. The CFD model developed for the combustor could be incorporated into REI's framework and used to assess issues of NO_x and CO emissions and heat transfer. The model could also be used as a basis to generate a reduced-order model for the combustor. The combustor modeling was performed under a MOU between REI, RECOM, and PSM.

In the following, we provide further details on the following:

- a chemical equilibrium reactor model for simulating the turbine combustor and
- a chemical kinetic reactor model for simulating the turbine combustor.

A description of the work effort and findings from the CFD combustor modeling study is provided in Appendix I.

Chemical Equilibrium Reactor

The equilibrium reactor module is a process engineering (0D) model that calculates full chemical equilibrium for the provided conditions. This model can be used to estimate the performance of the combustor in a direct-fired gas turbine. The model is implemented in a general manner and thus can be used for calculating equilibrium gas compositions in other devices as well. The equilibrium calculation is implemented as a member function within the thermodynamics class contained within the framework.

The supporting C++ code for equilibrium reactor is based on the chemical equilibrium capability included in REI's proprietary Reaction Engineering Kinetics Solver (REKS) software package described below. Briefly, chemical equilibrium is usually described by either equilibrium constants or direct minimization of the Gibbs free energy. The use of equilibrium constants is not well suited for calculation of complex chemical equilibrium. Therefore, the free energy minimization is used within REKS, which can handle a large number of species. An element potential method is used where the number of iteration equations solved is one more than the number of elements in the system. The approach of Gordon et al. (1994) is used.

Chemical Kinetic Reactor

The turbine combustor can be modeled using the PFR or PSR chemical kinetic models available in the kinetic reactor module. The kinetic reactor module provides a general purpose homogeneous gas-phase kinetics integration capability. Using this model, finite-rate chemistry effects on turbine combustor performance can be computed. Because the kinetic reactor uses PFR and PSR submodels, the kinetic reactor module can also be used to model devices other than the turbine combustors, such as computing the effect of finite-rate quench on the WGS reaction occurring in the gasifier syngas. The model can read a wide variety of chemical kinetic mechanism file formats, but is currently configured for GRI Mech 3.0 [http://www.me.berkeley.edu/gri_mech/].

The PFR and PSR modules make use of a second software package, REKS, a generalized package for performing kinetics calculations. REKS is a proprietary software package developed by REI (outside of DOE funding) specifically to address chemical kinetics issues for combustion problems with complex fuels. The governing equations for mass and energy conservation within the PFR and PSR modules are formulated as time-dependent ODEs, which are integrated through time using CVODE, a publicly available ODE integration package [<http://www.netlib.org>]. The initial value problem (IVP) is solved by CVODE by the backward differentiation formula (BDF). The BDF uses a fixed-leading-coefficient form. For stiff problems, a Newton iteration scheme is used in which at each iteration an underlying linear system must be solved. The option used in CVODE for solving the stiff linear systems involved in chemical kinetics is a direct method with dense treatment of the Jacobian. The error control mechanism in CVODE varies the step size and order in an attempt to take a minimum number of steps while satisfying the local error test. REKS is capable of using compounds containing six elements (many commercial and open-source reacting flow simulation packages are limited to using compounds with at most five elements).

For generality as well as problem initialization, REKS is also capable of performing full equilibrium calculations. Chemical equilibrium is usually described by either equilibrium constants or direct minimization of the Gibbs free energy. The use of equilibrium constants is not well suited for calculation of complex chemical equilibrium. Therefore, the free energy minimization is used within REKS, which can handle a large number of species. An element potential method is used where the number of iteration equations solved is one more than the number of elements in the system. The approach of [Gordon et al., 1994] is used.

Model UI

The UI for the kinetic reactor model is shown in Figure 1.3.57 for an example calculation. Note that in the PFR CONP (constant pressure) mode, the residence time is a required input; in this mode the temperature is integrated adiabatically or a heat loss may be specified. In the PFR TTIM mode a quench rate can be input (i.e., linear time-temperature profile). In the PSR mode, the residence time and volumetric heat loss are required inputs. For modeling a turbine combustor, it is suggested that the PSR mode be used. For modeling a SOFC tail gas combustor, the PFR TTIM model should be used.

The image shows a software dialog box titled "KineticReactor". It contains a "Case Type" section with three radio buttons: "PFR CONP" (which is selected), "PFR TTIM", and "PSR". Below this, there are three input fields: "Residence Time (s)" with the value "0.05", "Desired Conversion" with the value "1000", and "Fraction Heatloss" with the value "0". At the bottom of the dialog are "OK" and "Cancel" buttons.

Figure 1.3.57. Input panel for kinetic reactor model.

Steam Turbine

A simple process engineering (0D) model based on thermodynamic calculations using adiabatic efficiency is used to simulate performance of the steam turbine. The efficiency is applied to an isentropic expansion process using the ASME 67 steam properties. The UI allows the user to input adiabatic efficiency. The efficiency is applied to an isentropic expansion process using the ASME 67 steam properties module.

The UI for the model is quite simple (see Figure 1.3.58). The user can specify the isentropic efficiency (as a fraction) and the pressure drop across the unit. The output from the model is the power generated.

Figure 1.3.58. Input panel (left) and summary data (right) for steam turbine model.

Gas Source

The gas source module allows the user to fully specify the properties of a gas stream. The module carries only a single output which contains the generated data structure. The UI for the model (Figure 1.3.59) provides all inputs necessary to set gas conditions at the lone data output port.

Species	Composition	Mole Fraction
AR	AR	0.001
C(GR)	N2	0.789
C2H2	O2	0.21
C2H6		
CH		
CH4		
CO		
CO2		
COS		
H		
H2		

Constituent	Composition	Mass Fraction
ASH	ASH	0.0
CHAR	CHAR	0
COAL	COAL	0
WATER	WATER	0

Figure 1.3.59. Input panels for gas source module.

Gas Mixer

The gas mixer is a utility module for mixing gas streams. The module calculates the outlet composition and temperature based on the relative flow rates of the individual inlet streams. The mixture temperature is determined from the sum of the total enthalpy of the individual inlet streams. The higher pressure input stream is assumed throttled to the lower pressure input stream and therefore the pressure of the outlet mixture is calculated to be the lesser of the inlet pressures.

Gas Separator

The Gas Separator module is used to separate a species out from a mixed gas stream. Two gas streams are found at the output, one contains the concentrated target species, and the other is the main gas minus the separated species. The user, via the UI, determines which species is to be separated from the gas stream as well as the desired purity. The “Remaining” input is the percentage of the species that will remain in the non-pure stream (Figure 1.3.60).

Figure 1.3.60. Input panel for gas separator module.

Gas Splitter

The gas splitter module is used to split a single inlet gas stream into multiple outlet gas streams. The module simply redirects gas, and therefore only the flowrates of the outlet gases will differ from the inlet gas. Compositions and gas properties remain the same through the module. The UI specifies the number of desired outlet streams as well as the percentage of the inlet stream to be diverted into each outlet stream (Figure 1.3.61).

Figure 1.3.61. Input panel for gas splitter module.

Gas Feedback

The gas feedback module facilitates feedback loops, which may be found within a user-generated network configuration. A feedback loop occurs when an inlet to a given module is dependent on the same module's outlet. Network feedback is accomplished by executing a series of iterations until properties of the cycling gas between sequential iterations fall within certain user-specified parameters. Parameters within this module's UI (Figure 1.3.62) that are used to control the iterations, include: temperature, pressure, flowrate, composition, and a maximum number of allowable iterations.

Figure 1.3.62. Input panel for gas feedback module.

Gas Heat Exchanger

The gas heat exchanger module allows the user to heat or cool a gas stream to a desired temperature. The module calculates both the heat transfer necessary to bring the gas stream to the specified temperature, and also outputs the resultant temperature change between inlet and outlet streams. Inputs and outputs can be seen in (Figure 1.3.63).

Figure 1.3.63. Input and output panels for gas heat exchanger module.

Water Source

The water source module allows the user to fully specify the properties of a water stream. The module carries only a single output which contains the generated data structure. The UI (Figure 1.3.64) for the model provides the inputs: temperature (when Temperature/Pressure is selected), pressure, enthalpy (when Pressure/Enthalpy is selected), and flowrate. Either temperature or enthalpy is determined, using heat transfer correlations, depending on calculation type selected.

Figure 1.3.64. Input panel for water source module.

Water Pump

A water pump model has been added which calculates required power needed to achieve either a desired pressure change or outlet pressure (depending upon calculation type provided by user) based on an input isentropic efficiency of the pump. Inputs and outputs are illustrated in (Figure 1.3.65).

Figure 1.3.65. Input and output panels for water pump module.

Condenser

The condenser model is a process engineering (0D) heat exchanger model that involves heat transfer between two water streams. The first is superheated water vapor that is to be condensed to liquid, and the second is a liquid stream used for the cooling. The heat transfer correlations used are for condensation heat transfer on tube banks [Dhir and Lienhard, 1971]. Figure 1.3.66 contains the UI for this model.

Figure 1.3.66. Input panel for condenser module.

Evaporation Cooler

The process engineering (0D) evaporation cooler model is used to simulate a cooling tower for cooling the heated liquid water from the condenser via a direct contact heat exchange evaporation process. The ambient relative humidity and desired outlet water temperature are included as inputs. Model calculations range from the required air flow to evaporated water loss from the process. Inputs and outputs windows are shown in Figure 1.3.67.

Description	Value

Air flow required	2075.88
Evaporation rate	54.73

Figure 1.3.67. Input panel for evaporation cooler module.

Chapter 2 – Results and Discussion

Within this chapter we present results and discussions on example calculations performed with the frameworks and models. The discussion is organized as follows:

- LEBS-POC framework;
- IGCC-FCT framework; and
- VEF framework.

2.1 Example Calculations - LEBS-POC Framework

To demonstrate the functionality of the prototype framework for the LEBS-POC facility, simulations have been performed to study the impact of changes to the boiler firing conditions on the performance of other equipment located downstream of the boiler.

2.1.1 LEBS-POC Steady-State Demonstration:

For the test, the OFA and reburn ports in the upflow portion of the furnace have been turned off and the impact on the downstream equipment studied. Note that the air and fuel flows through the burners were correspondingly increased to maintain the same overall firing rate and furnace stoichiometry. The firing conditions correspond to 100% nominal load (86 MWe) firing Illinois #6 coal and a furnace stoichiometric ratio of 1.12 [Bockelie et al., 2001a-c], [Bockelie et al., 2002ab].

Table 2.1.1 illustrates the type of information that can be obtained. From the table it can be seen that the changed firing conditions result in reduced LOI, increased furnace exit gas temperature, and a slight increase in the steam flow rate and steam temperature. For both firing conditions, the flue gas temperature at the economizer exit is about the same.

The simulations also predict that the modified firing conditions increase the NO_x levels at the furnace exit. In both simulations, the SCR model was run in an iterative manner so that the ammonia flow rate was automatically adjusted to the desired NO_x level at the SCR exit (it is assumed that the NO_x and ammonia levels in the flue gas exiting the SCR do not change between the SCR and the stack). For these tests, the target NO_x level at the stack is the anticipated NO_x regulation limit of 0.15lb/mmBTU. From Table 2.1.1, it can be seen that the SCR operation can be modified to ensure that both firing configurations achieve the desired NO_x level at the stack. However, the modified firing condition requires more ammonia to be used in the SCR. Assuming an ammonia cost of \$200/ton, the increased ammonia usage results in ammonia costs increasing from \$30,000/year to \$54,000/year.

Illustrated in Figure 2.1.1 are representative plots of the gas temperature field and coal trajectory for coal injected through the low NO_x burners. In the gas temperature plots, the interaction of the flames can be seen from the “foot print” from the down-fired burners which persists until the combustion gases reach the slag screen located at the bottom of the J shape.

Simulations performed to investigate the impact of replacing the reburn coal with a biomass fuel (sawdust) provided similar results to that highlighted in Table 2.1.1. Sawdust is an opportunity fuel that could potentially reduce the cost of plant operation. Based on biomass cofiring studies, the use of sawdust could provide additional NO_x reductions but might require a redesign effort to optimize the injection of the reburn fuel into the furnace [Harding and Adams, 2000].

Table 2.1.1. Comparison of Predicted Values for Baseline Firing Conditions and for Turning Off the OFA and Coal Reburn.

	Baseline	OFA & Reburn OFF
Furnace Exit NO _x , ppm dry (lb/mmBTU)	200 (0.25)	257 (0.33)
Stack NO _x , ppm dry (lb/mmBTU)	119 (0.15)	119 (0.15)
Ammonia Slip, ppm dry	< 1	< 1
Ammonia Cost, \$/yr	\$30,000	\$54,000
Steam Flow Rate, kg/s	60	66
Steam Temperature, K	1019	1025
Heat Transfer to Water Walls, MW	68	76
LOI, %	2.6	1.6
Furnace Exit CO, ppm dry	11460	7492
Furnace Exit Temperature, K	1482	1572
Economizer Gas Outlet Temperature, K	674	679
Air Heater Outlet Air Temperature, K	598	606

Figure 2.1.1. Gas temperature field (left) and particle trajectories (right) in lower section of LEBS-POC furnace.

2.1.2 LEBS-POC Transient Demonstration

To demonstrate the transient capability of the *AIOLOS* reacting CFD model, a simulation for a 50% load turndown of the POC furnace has been performed. For this simulation, it is assumed that the unit is operating at 100% load, and then at time $t = 0$, the burner fuel and air flow rates are instantaneously turned down to 50% load. The integration of the solution through time was performed in a time-accurate mode. This simulation was performed by project team members at RECOM Services and the simulations were executed at the supercomputer center at the University of Stuttgart.

Figure 2.1.2 shows the transient response of furnace exit gas temperature. Note that the load change is also shown in the figure. The simulation involved a real-time integration of about 24 seconds. A unit of this size (90 MWe) responds quickly to the load reduction. The predicted exit temperature is seen to be approaching steady state at 24 seconds.

Illustrated in Figure 2.1.3 are three snapshots in time of the gas temperature field, at $t = 0$ sec, $t = 6$ sec, and $t = 24$ sec, respectively. The highest temperatures in the flame are seen to move closer to the burner plane as time progresses.

The computer runtime required for this simulation was quite large - 76 real-time hours on a single node (which contains 8 processors) of a Hitachi SR8000. The Hitachi is a hybrid supercomputer that distributes computations and memory across nodes. Within each node, the computations are performed in a SMP parallel mode across eight processors. Another high-performance computer was available for these computations - the NEC SX-5 vector machine. The single node of a Hitachi is comparable to a single processor of a NEC SX-5. Using 4 NEC SX-5 processors in parallel would reduce the real-time to perform this simulation by (approximately) a factor of 4; even with this reduction, the simulation runtime would be quite large.

It would not be practical to perform this type of simulation on a standard desktop workstation due to the long runtime required. Although *AIOLOS* is fully integrated into the framework, to perform this simulation *AIOLOS* was run in standalone mode on the supercomputer. One of the goals of this project was to implement into the framework environment the ability to perform cpu-intensive computations on remote computers connected via a network. As highlighted in this test, to have the framework execute models on remote computing resources, the issues are not so much technical but rather administrative – such as dealing with firewalls and other security measures used at supercomputer centers (note: REI demonstrated the ability for the SCIRun-based framework to access remote computing resources and control execution of the simulation through a test for remotely executing a relatively small model (i.e., the SCR model) using CORBA-based components. In addition, support for remote computing capabilities was significantly improved in the IGCC-FCT and VEF frameworks later in the project).

Figure 2.1.2. Furnace exit temperature as a function of time for transient turn-down to 50% load.

Figure 2.1.3. Gas temperature field at three instances of time for transient simulation.

2.2 Example Calculations – IGCC-FCT Framework and VEF

During the course of this project a large number of simulations have been performed for models of individual pieces of equipment and processes for the full Vision 21 reference configuration (Figures 1.3.10 and 11) and for one-off variations on the Vision 21 reference configuration. Test cases for the individual models were typically performed in standalone manner and the simulations focused on building confidence that the model reproduced known (or accepted) behavior as perceived by industry. Simulations for the full plant configuration typically focused on the impact of changes in equipment, process conditions, or equipment configuration on the overall plant performance (e.g., plant efficiency, net power generation). It must be noted that there is a general lack of well-documented (reliable) data for the performance of the individual component devices (processes) or overall IGCC plant.

In this section we present a selected subset of the available modeling results generated during the course of this project. Simulation results that highlight the models and the improved plant simulation capability have been reported in the open literature at a variety of technical conferences and NETL meetings [Bockelie et al., 2001-2004], [Denison et al., 2003], [Rubin et al., 2004], [Sarofim et al., 2004]. In addition, presentations have been provided to the DOE at NETL-sponsored Program Reviews [Bockelie et al., 2001c] and NETL-sponsored Workshops [Bockelie et al., 2002e] and in project briefings held at NETL between REI and NETL personnel.

In the following we have focused on simulation results that highlight the capability of the entrained flow gasifier model and the overall plant simulation. The entrained flow gasifier is a critical component to any IGCC-based plant and thus it has been provided special attention. Results are presented for selected simulations of the Vision 21 reference configuration. Although emphasis is placed on the VEF capability, some results for using the older SCIRun-based IGCC-FCT framework are also provided. Example calculations are presented in the following order:

- process engineering entrained flow gasifier model;
- CFD entrained flow gasifier model;
- comparison of process engineering and CFD entrained flow gasifier models;
- impact of improved soot and tar model on CFD entrained flow gasifier performance;
- impact of alternative gasification kinetics on CFD entrained flow gasifier performance;
- IGCC-FCT simulations for Vision 21 reference configuration;
- VEF simulation for Vision 21 reference configuration;
- VEF simulation for Vision 21 reference configuration with CGCU for mercury capture;
- VEF simulation with coupling to IECM;
- VEF simulation with coupling to Aspen Plus; and
- example of using VES-Open.

Last, we present an example transient 3D, reacting CFD simulation of the entrained flow gasifier for changing load.

2.2.1 Process Engineering Entrained Flow Gasifier

The process engineering (0D) entrained flow gasifier model has been benchmarked through comparisons of model predictions with reported gasifier performance for several gasifiers (e.g., Texaco-style, one-stage, slurry-feed, downflow gasifier; E-Gas-style, two-stage, slurry-feed, upflow gasifier; and Shell-style, one-stage, dry-feed, upflow gasifier) under different process conditions. Test results demonstrate that the predicted syngas composition, carbon conversion, gasifier exit temperature, and gasifier cold-gas efficiency from the process model are generally in good agreement with reported data. It can thus be concluded that the process model can reasonably predict the performance of different types of gasifiers and thus be used in evaluations of different plant configurations. Details are provided below.

Tampa Electric Gasifier

The Tampa Electric gasifier is an oxygen-blown, down-fired entrained flow gasifier. It processes approximately 2200 tons/day of Pittsburgh #8 coal in slurry of 60-70% solids. To benchmark the process model, the performance of this gasifier has been simulated. The comparison of the model results with the reported data is presented in Table 2.2.1 along with the process conditions. It can be seen that the predicted gasifier exit temperature is in the range of 2400 – 2600°F as expected for the one-stage Texaco gasifier, while the syngas composition is similar to that reported by Tampa Electric [USDOE, 2000].

Table 2.2.1. Comparison of Process Gasifier Model with Reported Data for Tampa Electric Gasifier.

	Tampa	0D model
Pressure, psia	400	400
Fuel, ton/day	2200	2200
Oxidant, ton/day	2171	2171
Coal, %	60-70	64.5
Slurry water, ton/day	-	1211
Mole fraction: N ₂	0.033	0.021
Ar	0.009	-
CO ₂	0.144	0.116
CO	0.427	0.519
H ₂	0.383	0.335
CH ₄	0.001	0.000
HHV, Btu/scf	~258	271
Exit temperature, K	1589 - 1700	1675

Wabash River Gasifier

The Wabash River gasifier is an E-Gas, oxygen-blown, upflow, two-stage gasifier operating at a pressure of 400 psia. It processes two different coals (Hawthorn coal and Miller Creek coal), a blend of the two, and petroleum coke. In the process (0D) model results, two fuels were used: a sub-bituminous coal and petroleum coke. Properties of these fuels can be found in a DOE report on the Wabash River Project [USDOE, 2002]. Table 2.2.2 compares the model predictions with the plant data. Notice that oxidant flow rate was not reported. In the simulations, the oxidant flow rate was adjusted so that the predicted gasifier exit temperature was close to 1900°F as reported for the two-stage gasifier. It is clear from the table that the model predicted syngas composition is similar to the plant data, though there are some discrepancies due primarily to unknown oxidant flow rate and coal concentration in the slurry for the case with petroleum coke. The predicted syngas thermal flows for both cases are in good agreement with the reported data.

Table 2.2.2. Comparison of Process (0D) Model Results with Reported Data for Wabash River Gasifier

	Typical coal		Petroleum coke	
	Wabash	0D model	Wabash	0D model
Pressure, psia	400	400	400	400
Fuel, ton/day	2450	2450	2000	2000
Oxidant, ton/day	-	1982	-	1747
Coal, %	60	60	-	50
Slurry water, ton/day	1633	1633	-	2000
Mole fraction: N ₂	0.019	0.022	0.019	0.016
Ar	0.006	-	0.006	-
CO ₂	0.158	0.216	0.154	0.180
CO	0.453	0.380	0.486	0.433
H ₂	0.344	0.373	0.332	0.362
CH ₄	0.019	0.000	~0.005	0.000
HHV, Btu/scf	272	239	268	252
Syngas, MBtu/hr	1690	1630	1690	1811
Exit temperature, K	1311	1388	1311	1396

Black & Veatch Study of Shell Gasifier

Calculations using the process model were also performed to simulate the performance of a Shell gasifier described in an engineering study performed by Black & Veatch under EPRI funding [Black & Veatch, 1994]. The gasifier used in the study is a dry-feed, oxygen-blown, Shell gasifier processing 2560 tons/day of Illinois #5 coal. The coal is pulverized and pre-dried to less than 2% moisture, and then transported to the gasifier burners by high-pressure N₂. Oxygen of 95% purity is supplied by the ASU to support the gasification reaction. Heat generated during gasification is extracted through an internal waterwall in the gasifier. The gasifier operates at a pressure of 24 barg. In the simulations, the oxidant flow rate was assumed to be 2053 tons/day based on the operating conditions for a similar Shell gasifier [Eurlings and Ploeg, 1999]. Carrier N₂ flow rate was adjusted so that N₂ concentration in the syngas was similar to what had been reported. Heat flux through the gasifier wall was 15.7 kW/m². Three cases have been simulated using different oxidant compositions:

- Case 1: 95% O₂, 5% N₂; Carrier N₂: 0.05 lb N₂/lb coal
- Case 2: 95% O₂, 3% Ar, 2% N₂; Carrier N₂: 0.06 lb N₂/lb coal
- Case 3: 95% O₂, 2% Ar, 3% N₂; Carrier N₂: 0.05 lb N₂/lb coal

Simulation results are summarized in Table 2.2.3. It can be seen from the table that the predicted cold-gas efficiency is the same as that provided in the project report [Black & Veatch, 1994]. Predicted CO concentration is in good agreement with the reported concentration. However, the model somewhat under-predicts H₂ concentration. Except Ar and N₂ concentrations, all gas species concentrations are very similar for all three cases.

Table 2.2.3. Comparison of Process (0D) Model Results with Design Data [Black & Veatch, 1994].

Case		1	2	3
	B&V	0D model	0D model	0D model
Exit Temperature, K	-	1742	1708	1723
Carbon Conversion, %	-	99.4	99.1	99.2
Mole Fraction: CO	0.6284	0.6186	0.6173	0.6199
H ₂	0.2837	0.2240	0.2264	0.2264
H ₂ O	0.0122	0.0530	0.0492	0.0506
CO ₂	0.0104	0.0410	0.0391	0.0397
CH ₄	0.00030	0.00003	0.00004	0.00004
H ₂ S	0.0106	0.0121	0.0121	0.0121
COS	0.0008	0.0012	0.0011	0.0012
Ar	0.0093	-	0.0105	0.0071
N ₂	0.0440	0.0497	0.0439	0.0426
LHV of Syngas, Btu/lb	5207.5	4533.1	4522.7	4546.2
HHV of Syngas, Btu/lb	5486.2	4777.4	4765.0	4790.2
HHV of Syngas, Btu/SCF	297.0	277.8	277.9	278.9
Cold-Gas Efficiency (LHV), %	79.5	79.3	79.5	79.5

The difference between the predicted syngas composition and the reported data may be due to the fact that the syngas composition in the second column of Table 2.2.3 is of the gas after the gasification product gas mixes with cool recycled gas. To examine the effect of cooling on the syngas composition, the product gas of Case 2 was passed through a PFR and cooled to 500 K at two cooling rates. The results are given in Table 2.2.4. It can be seen from the table that both CO and H₂ concentrations are closer to the reported data, though H₂ concentration is still somewhat lower.

Table 2.2.4. Syngas Composition After Cooling to 500 K.

Case		2	2	2
	B&V	0D model	3000 K/s	10000 K/s
Exit Temperature, K	-	1708	-	-
Carbon Conversion, %	-	99.1	-	-
Mole Fraction: CO	0.6284	0.6173	0.6230	0.6260
H ₂	0.2837	0.2264	0.2320	0.2300
H ₂ O	0.0122	0.0492	0.0471	0.0499
CO ₂	0.0104	0.0391	0.0424	0.0397
CH ₄	0.00030	0.00004	0.00004	0.00004
H ₂ S	0.0106	0.0121	-	-
COS	0.0008	0.0011	-	-
Ar	0.0093	0.0105	0.0106	0.0106
N ₂	0.0440	0.0439	0.0445	0.0445
LHV of Syngas, Btu/lb	5207.5	4522.7	4519.3	4523.9
HHV of Syngas, Btu/lb	5486.2	4765.0	4761.4	4766.5
HHV of Syngas, Btu/SCF	297.0	277.9	281.4	281.8
Cold-Gas Efficiency (LHV), %	79.5	79.5	-	-

Cool Water Gasifier

The EPRI-funded Cool Water coal gasification program used the Texaco coal gasification process to convert coal to clean fuel gas. The gasifier was designed to process up to 1000 tons of coal per day, using a slurry-feed system. The coal-water slurry was gasified with O₂ at a pressure of approximately 600 psig and a temperature between 2100°F and 2500°F. Several coals, including Illinois #6, Pittsburgh #8, and SUFCo and Lemington coals, were used in the system. A summary of the operating conditions and coal properties is shown in Table 2.2.5. Results from the process (0D) model simulations are given in Table 2.2.6. In the simulations the gasifier was assumed to be nearly adiabatic (wall heat transfer resistance was fixed at 1 m²·K/W).

Table 2.2.5. Operating Conditions and Fuel Properties for the Cool Water Gasifier.

Case	1	2	3	4	5	6
Coal Type	Illinois #6	Pitt.#8	SUFCo	SUFCo	SUFCo	Lemington
Dry coal feed rate, tons/day	1000	934	1000	1100	1000	1000
Dry, wt%, C	72.21	77.74	71.85	71.45	72.20	69.82
H	4.94	5.32	4.94	4.88	5.04	4.49
S	3.08	2.66	0.43	0.47	0.36	0.42
N	1.57	1.45	1.22	1.21	1.13	1.55
O	6.92	5.46	12.74	11.94	12.59	8.32
Ash	11.28	7.37	8.82	10.05	8.68	15.40
HHV, Btu/lb	12820	14100	12360	12443	12530	12232
as-recd, HHV, Btu/lb	11552	13438	11125	11321	11276	11114
Slurry Conc., wt%	63.4	59.3	60.6	61.7	59.7	62.9
Oxygen flow rate, kscfh	915	933	888	978	907	912
Oxygen purity, %	99.5	99.5	99.5	99.5	99.5	99.5

From Table 2.2.6, it is clear that the HHVs of syngas calculated based on predicted clean syngas composition are in good agreement with those from the reported syngas composition. The predicted syngas composition is in reasonable agreement with the reported data, especially for Cases 3, 4, and 5. Note that in all the cases, the predicted hydrogen sulfide (H₂S) and carbonyl sulfide (COS) concentrations are higher than the reported values; this is because the reported syngas composition is that after cleaning, while the simulated results are essentially the dry syngas, and all formed H₂S and COS during gasification remain in the gas.

Table 2.2.6. Comparison of Process (0D) Model Results with Reported Cool Water Gasifier Data.

Case	1		2		3	
	CW	0D model	CW	0D model	CW	0D model
Exit Temperature, K	-	1624	-	1731	-	1357
Carbon Conversion, %	96.5	96.5	96.4	96.4	98.5	98.5
Mole Fraction: CO	0.4488	0.4487	0.4427	0.4954	0.4297	0.4162
H ₂	0.3346	0.3427	0.3342	0.3347	0.3813	0.3721
CO ₂	0.1548	0.1897	0.1547	0.1546	0.1807	0.2025
CH ₄	0.00160	0.00005	0.00160	0.00002	0.00210	0.00177
Ar+N ₂	0.0102	0.0076	0.0066	0.0039	0.0062	0.0080
H ₂ S+COS	0.0003	0.0102	0.0003	0.0033	0.0000	0.0014
HHV of Syngas, Btu/SCF	266.0	264.1	267.3	263.2	259.4	252.8

Case	4		5		6	
	CW	0D model	CW	0D model	CW	0D model
Exit Temperature, K	-	1408	-	1445	-	1213
Carbon Conversion, %	98.1	98.1	96.2	96.2	98.0	98.0
Mole Fraction: CO	0.4366	0.4369	0.4277	0.4238	0.4420	0.3938
H ₂	0.3814	0.3672	0.3790	0.3624	0.3666	0.3536
CO ₂	0.1733	0.1884	0.1889	0.2063	0.1795	0.2211
CH ₄	0.00220	0.00089	0.00040	0.00039	0.00070	0.02241
Ar+N ₂	0.0063	0.0061	0.0040	0.0069	0.0093	0.0076
H ₂ S+COS	0.0000	0.0015	0.0000	0.0012	0.0000	0.0014
HHV of Syngas, Btu/SCF	261.7	266.6	256.4	260.6	257.9	259.4

Shell Gasifier

In [Eurlings and Ploeg, 1999] the performance of three Shell coal gasification processes at Harburg (Germany), Houston (Texas) and Demkolec (the Netherlands) are reported. Illinois #5 coal and Drayton coals were gasified in these facilities. Heat was extracted through a membrane wall in the gasifiers, which are dry-feed, single-stage, upflow reactors; pre-dried coals (about 2 % moisture) are transported to the gasifier by high-pressure N_2 . The operating conditions for these processes are given in Table 2.2.7. Note that coal properties are those after coal milling and drying. Carrier N_2 flow rates were not reported in [Eurlings and Ploeg, 1999]; in the calculations, these flow rates were adjusted so that the N_2 concentration in the syngas was the same as that reported in the paper. Table 2.2.8 shows comparison of the model predictions with the reported data. In the simulations, wall heat transfer rate was adjusted so that carbon conversion and syngas composition are similar to those reported in the paper. It can be seen that the predicted syngas composition is in very good agreement with the reported data; carbon conversion is also in good agreement with the reported carbon burnout. The predicted cold-gas efficiency is nearly identical to that given in the paper, especially for the last three cases.

Table 2.2.7. Operating Conditions for the Shell Gasifiers.

Case	1	2	3	4
Coal type	Illinois #5	Illinois #5	Drayton	Drayton
Pre-dried, moisture, wt%	2.2	2.1	1.5	2.0
ash, wt%	14.2	10.6	12.3	12.2
LHV, Btu/lb	11351	11781	11953	11910
Coal flow rate, kg/s	1.033	1.814	1.588	19.832
Oxidant flow rate, kg/s	0.868	1.524	1.477	17.453
Steam flow rate, kg/s	0.000	0.000	0.000	1.396
Carrier N_2 , kg/s	0.168	0.178	0.159	1.983
Gasifier pressure, barg	20	24	24	27

Table 2.2.8. Model Predictions in Comparison with Reported Data (Shell Gasifiers).

	Case 1		Case 2		Case 3		Case 4	
	Shell	OD model	Shell	OD model	Shell	OD model	Shell	OD model
Exit Temperature, K	-	1534	-	1652	-	1581	-	1713
Carbon Conversion, %	> 99	99.0	>98.5	98.7	-	99.3	>98	98.1
Mole Fraction (dry): CO	0.6270	0.6308	0.6410	0.6499	0.6530	0.6537	0.6340	0.6261
H ₂	0.2550	0.2577	0.2660	0.2667	0.2620	0.2659	0.2840	0.2899
CO ₂	0.0220	0.0078	0.0160	0.0054	0.0160	0.0123	0.0150	0.0188
N ₂	0.0880	0.0888	0.0650	0.0633	0.0650	0.0637	0.0620	0.0616
others	0.0080	0.0150	0.0120	0.0146	0.0040	0.0044	0.0050	0.0035
LHV of Syngas (dry), Btu/lb	4732.8	4832.5	4950.9	5050.1	4975.6	5036.2	5114.6	5121.3
HHV of Syngas (dry), Btu/lb	4954.9	5060.1	5186.8	5288.8	5206.8	5272.6	5372.3	5385.6
Cold-Gas Efficiency (LHV), %	75.5	79.5	77.2	77.3	78.0	78.7	78.6	79.4

Parametric Studies

The process model can be used to study the effects of a wide range of parameters, such as coal or other solid fuel composition, reactor volume, pressure, oxygen/carbon ratio, steam/carbon ratio, wall heat extraction, dry versus slurry feed, and feed preheat. Selected parametric studies have been conducted to show the importance of different parameters. The base case is for a gasifier operating at 30 atm, firing an Illinois #6 coal, a coal slurry feed with 65% slurry concentration, a slurry temperature of 298 K, a coal flow rate of 25.8 kg/s (about 2400 tpd), an oxidant (95% O₂, 5% N₂) flow rate of 13.9 kg/s (about 1345 tpd) and a temperature of 298 K, and a heat extraction rate of 100 kW/m². In running the parametric analysis, one choice is to vary the parameters keeping the gasifier volume fixed, which is what is expected for changing the process variables for an existing gasifier. However, for the present case the parameter variation was so large that it was decided to vary the volume to keep the carbon conversion efficiency constant, since so many of the observed changes were a consequence of the effect of the parameters on carbon-conversion efficiency.

The effect of the heat extraction on gasifier performance for the case of fixed-carbon conversion efficiency is seen in Table 2.2.9. The range of heat extraction rates was varied from adiabatic (0 kW/m²) to a value of 200 kW/m² (the high end of a membrane wall heat transfer rate). It can be seen that the extraction rates are a small fraction of the total heat input so that the changes in gas composition, gas heating value, and cold-gas efficiency are correspondingly small. The change in gas temperature of 60°C is large enough to affect the kinetics of gasification so that the impact on carbon-conversion efficiency could be significant, as will be shown later.

Table 2.2.9. Effect of Heat Extraction on Gas Composition, Exit Temperature, and Cold-Gas Efficiency (Carbon Conversion Maintained Constant).

Heat Extraction, kW/m ²	0	50	100	150	200
Exit Temperature, K	1683	1668	1653	1638	1623
Thermal Input, MW	700.6	700.6	700.6	700.6	700.6
Thermal Output, MW	526.7	526.6	526.4	526.3	526.2
Carbon Conversion, %	97.9	97.9	97.9	97.9	97.9
Mole Fraction: CO	0.3529	0.3519	0.3509	0.3499	0.3489
H ₂	0.2487	0.2497	0.2506	0.2516	0.2526
H ₂ O	0.2626	0.2616	0.2606	0.2596	0.2586
CO ₂	0.1118	0.1127	0.1137	0.1147	0.1157
CH ₄	0.00001	0.00001	0.00002	0.00002	0.00002
H ₂ S	0.00653	0.00654	0.00654	0.00654	0.00655
COS	0.00032	0.00032	0.00031	0.00031	0.00031
N ₂	0.0165	0.0165	0.0165	0.0165	0.0165
Syngas Flow Rate, kg/s	59.92	59.92	59.92	59.92	59.92
HHV of Syngas, MJ/kg	8.80	8.79	8.79	8.79	8.79
CGE (HHV), %	75.2	75.2	75.1	75.1	75.1

A similar result is seen on the impact of pressure in Table 2.2.10. The volume of the reactor was decreased as the pressure was increased to maintain a constant carbon-conversion efficiency. This results in a fraction of the energy input being lost to the wall, but since the heat loss does not significantly influence the gasifier performance, this is not significant. Furthermore, the major equilibrium reactions, such as the water gas shift, do not involve a volume change on reaction so that the effect of pressure on the gas-phase composition is negligibly small.

Table 2.2.10. Effect of Pressure on Gasifier Performance for a Fixed Carbon Conversion.

Pressure, atm	20	30	55	75	100
Exit Temperature, K	1653	1653	1653	1654	1654
Thermal Input, MW	700.6	700.6	700.6	700.6	700.6
Thermal Output, MW	526.4	526.4	526.4	526.4	526.3
Carbon Conversion, %	97.9	97.9	97.9	97.9	97.9
Mole Fraction: CO	0.3509	0.3509	0.3509	0.3509	0.3508
H ₂	0.2507	0.2506	0.2505	0.2504	0.2502
H ₂ O	0.2606	0.2606	0.2607	0.2607	0.2608
CO ₂	0.1137	0.1137	0.1137	0.1137	0.1138
CH ₄	0.00001	0.00002	0.00005	0.00010	0.00018
H ₂ S	0.00654	0.00654	0.00654	0.00654	0.00654
COS	0.00031	0.00031	0.00031	0.00032	0.00032
N ₂	0.0165	0.0165	0.0165	0.0165	0.0165
Syngas Flow Rate, kg/s	59.92	59.92	59.92	59.92	59.92
HHV of Syngas, MJ/kg	8.79	8.79	8.79	8.79	8.79
CGE (HHV), %	75.1	75.1	75.1	75.1	75.1

The effect of slurry concentration in Table 2.2.11 is dramatic. The impact of the water mass on the temperature in the gasifier is enormous. The variations provided here are unrealistic, but demonstrate that a decrease in gasifier exit temperature is accompanied by the increase in cold-gas efficiency related to the increase in water content.

The last parametric variation was that of carbon-conversion efficiency, varied here by changing the gasifier length, as shown in Table 2.2.12. Again, the range of parameters is not realistic, but makes the point of how sensitive the performance of the gasifier is to changing carbon conversion.

From these parametric studies it can be seen that the parameters of greatest importance are:

- the pressure because of the effect of gasifier volume;
- the slurry concentration because of the impact of moisture on temperature and the gasifier performance; and
- any parameter (furnace length, O₂ concentration, furnace temperature) that affects the carbon-conversion efficiency.

Because of the interdependence of the parameters, it's difficult to draw conclusions from varying one parameter at a time.

Table 2.2.11. Effect of Slurry Concentration on Gasifier Performance for a Fixed Carbon Conversion.

Slurry Concentration, %	30	48	65	83	100
H ₂ O Flow Rate, kg/s	60.244	27.971	13.903	5.288	0
Exit Temperature, K	895	1222	1653	2093	2475
Thermal Input, MW	700.6	700.6	700.6	700.6	700.6
Thermal Output, MW	559.3	546.5	526.4	511.9	503.6
Carbon Conversion, %	97.9	97.9	97.9	97.9	97.9
Mole Fraction: CO	0.0181	0.1946	0.3509	0.4832	0.5899
H ₂	0.1255	0.2700	0.2506	0.2379	0.2301
H ₂ O	0.5890	0.3430	0.2606	0.1764	0.1019
CO ₂	0.2014	0.1705	0.1137	0.0734	0.0432
CH ₄	0.05178	0.00289	0.00002	0.00000	0.00000
H ₂ S	0.00398	0.00531	0.00654	0.00758	0.00830
COS	0.00002	0.00012	0.00031	0.00057	0.00084
N ₂	0.0096	0.0130	0.0165	0.0198	0.0225
Syngas Flow Rate, kg/s	106.26	73.98	59.92	51.30	46.01
HHV of Syngas, MJ/kg	5.27	7.39	8.79	9.98	10.95
CGE (HHV), %	79.8	78.0	75.1	73.1	71.9

Table 2.2.12. Effect of Carbon Conversion on Gasifier Performance.

Gasifier Length, m	0.029	0.1	1.1	5.5	9.9
Exit Temperature, K	2642	2387	1862	1653	1596
Thermal Input, MW	700.6	700.6	700.6	700.6	700.6
Thermal Output, MW	68.3	247.5	447.9	526.4	541.1
Carbon Conversion, %	36.3	64.0	88.7	97.9	99.6
Mole Fraction: CO	0.0185	0.2146	0.3254	0.3509	0.3536
H ₂	0.0064	0.0989	0.2079	0.2506	0.2599
H ₂ O	0.6168	0.4797	0.3186	0.2606	0.2486
CO ₂	0.2730	0.1792	0.1235	0.1137	0.1138
CH ₄	0.00000	0.00000	0.00000	0.00002	0.00003
H ₂ S	0.00000	0.00102	0.00623	0.00654	0.00659
COS	0.00000	0.00009	0.00035	0.00031	0.00031
N ₂	0.0213	0.0195	0.0172	0.0165	0.0164
Syngas Flow Rate, kg/s	47.33	52.98	58.03	59.92	60.27
HHV of Syngas, MJ/kg	1.44	4.67	7.72	8.79	8.98
CGE (HHV), %	9.8	35.3	69.9	75.1	77.2

Selecting Operating Conditions

Most of the comparisons between model results and data performed during this project were conducted where the oxidant and steam flow rates were specified. The question remains of how such conditions are selected. The criteria that are generally proposed are that the gasifier should be operated at a sufficiently high temperature to maintain the slag flowing, the cold-gas efficiency be maximized, that the carbon conversion be high, and that the temperatures be moderated to protect the refractory.

The flowing characteristics of a slag is given by the critical viscosity for the slag, corresponding to the point at which the viscosity becomes non-Newtonian and corresponds to the point at which there is a change in slope of a plot of $\log(\text{viscosity})$ vs. $(1/T)$, and is of order 25 Pa·s. Correlations have been provided for the critical viscosity of ashes of different iron content by the CCSD [Patterson et al., 2001]. For slags with an iron content of less than 15%, temperature corresponding to the critical viscosity is given by:

$$T_{cv}(\text{K}) = 3452 - 519.2\alpha + 74.5\alpha^2 - 67.8\beta + 0.86\beta^2 \quad (2.2.1)$$

where $\alpha = \text{SiO}_2 / \text{Al}_2\text{O}_3$, $\beta = \text{Fe}_2\text{O}_3 + \text{CaO} + \text{MgO}$, and $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 + \text{CaO} + \text{MgO} = 100$, and where concentrations are expressed in wt%. The result of applying the correlation to a few of the coals above is given in Table 2.2.13. The ash composition was used to obtain T_{cv} here; in practice allowance should be made for the differences in composition between the slag and the carryover ash in making such calculations. It can be seen that the critical viscosity is low for the alkaline slags and high for high silica and alumina slags. In the following calculations, a maximum gasifier exit temperature of 1627 K was chosen to protect the refractories.

The optimization for O_2/fuel and $\text{H}_2\text{O}/\text{fuel}$ can be performed. The first set of calculations were for a slurry-feed gasifier with the baseline coal of the Illinois #6 coal considered above. The $\text{H}_2\text{O}/\text{coal}(\text{dry-ash-free})$ and $\text{O}_2/\text{coal}(\text{daf})$ were varied systematically for a fixed carbon-burnout efficiency of 98%, and the results on gasifier exit temperature, cold-gas efficiency, and the concentrations (mole %) of CO , CO_2 , H_2 , and H_2O are presented in Figures 2.2.1-2.2.6. Increasing $\text{O}_2/\text{coal}(\text{daf})$ at a fixed $\text{H}_2\text{O}/\text{coal}(\text{daf})$ or decreasing $\text{H}_2\text{O}/\text{coal}(\text{daf})$ at a fixed $\text{O}_2/\text{coal}(\text{daf})$ results in a systematic increase in temperatures as shown in Figure 2.2.1. The isotherm for 1627 K is highlighted to show the approximate demarcation between the slagging and nonslagging regimes. The operating conditions of interest are therefore to the right of the slagging line, although there clearly is an upper limit on O_2 content before refractory damage becomes an issue. There is a penalty in increasing $\text{H}_2\text{O}/\text{coal}$ since this increases the O_2/coal ratio needed to achieve slagging. The benefit of varying the water content at a fixed-oxygen content is seen in Figure 2.2.2. The changes in cold-gas efficiency with increasing water content are a trade-off between (1) the increase in the chemical energy in the CO and H_2 at the expense of the sensible enthalpy, and (2) the decrease in the syngas heating value as CO is converted to CO_2 (note: H_2 concentration remains approximately constant because of the increase in H_2O). This results in a peaking in the cold-gas efficiency (see Figure 2.2.2). We would wish to select values of $\text{O}_2/\text{coal}(\text{daf})$ and $\text{H}_2\text{O}/\text{coal}(\text{daf})$ that lie on the locus of maximum cold-gas efficiency that can be seen in Figure 2.2.3 but also can be in the slagging region. The conditions close to the knee of the slagging curve provide the desired high cold-gas efficiency and a slagging temperature. The optimum conditions therefore correspond to an $\text{O}_2/\text{coal}(\text{daf})$ of about 0.85 and an $\text{H}_2\text{O}/\text{coal}(\text{daf})$ of about 0.05. Also shown on Figure 2.2.3 are the operating conditions for the slurry-feed Tampa

Electric and Cool Water Gasifiers described earlier. The slurry-feed gasifiers operate with a $\text{H}_2\text{O}/\text{coal(daf)}$ concentration higher than the optimum because of the water in the slurry feed. In [Holt, 2001b], schemes are described in which advantages can be taken of both slurry feed (ease of pumping to a high pressure) and dry feed (lower O_2 consumption, higher cold-gas efficiency). In these schemes, the slurry is pumped to pressure, heated, the steam flashed so that it can bypass the gasifier, and the coal then fed dry. The advantages of such a scheme for reducing O_2 use and increasing cold-gas efficiency are clear from Figure 2.2.3, with the difference in operating conditions for the Tampa Electric Plant and those at the optimum point for a dry feed.

A set of calculations were also carried out for a dry feed with a systematic variation of the steam/coal(daf) and $\text{O}_2/\text{coal(daf)}$ ratios. The results for temperature, cold gas efficiencies, and the concentrations of CO , CO_2 , H_2 , and H_2O show similar trends as in Figures 2.2.1-2.2.6 and are therefore not reported here. Figure 2.2.1 shows the combination of O_2 and steam flows required to obtain slagging conditions. Figure 2.2.7 shows that the optimum cold-gas efficiency is, as before, in the non-slagging regime. The optimum conditions satisfying both the slagging constraint and yielding high cold gas efficiencies are, from Figure 2.2.8, an $\text{O}_2/\text{coal(daf)}$ around 0.85 and a steam/coal (daf) around 0.1. Also shown in Figure 2.2.8 are the operating conditions from data found in the literature for dry-feed gasifiers. It can be seen that they cluster around the optimum conditions but with a number of the points at higher $\text{O}_2/\text{coal(daf)}$ ratios. This can be explained to a large part by the variation in coal (or coke) compositions. The effect of $\text{O}_2/\text{coal(daf)}$ ratio on the cold-gas efficiency, for a fixed steam/coal(daf) is shown in Figure 2.2.9 to illustrate that the optimum varies widely, being governed by the O/C ratio in the fuel. In addition, the coals for which the operating conditions are summarized in Figure 2.2.8 have a range of temperatures for critical viscosity that also contributes to the spread of the data points.

The above examples illustrate how the contour plots of cold-gas efficiency together with the constraint of ash viscosity can be used to select operating conditions for gasifiers and provide input conditions for the more detailed process design optimization using CFD.

Table 2.2.13. Temperatures of Critical Viscosity for Different Coals.

wt, %	Illinois #5	Illinois #6	Pittsburgh #8	Drayton	Petcoke
SiO_2	53.82	57.75	47.44	53.02	39.13
Al_2O_3	18.62	22.92	25.28	29.33	9.94
Fe_2O_3	21.85	15.90	21.21	8.29	15.73
CaO	4.63	2.44	4.99	8.70	24.64
MgO	1.08	1.00	1.08	0.65	10.56
Total	100	100	100	100	100
α	2.89	2.52	1.88	1.81	3.94
β	27.56	19.33	27.27	17.64	50.93
$T_{\text{crit}}, \text{K}$	1358	1627	1530	1628	1339

wt, %	SUFCo	Lemington	Pike County	Falkirk Lignite	Freedom Lig
SiO_2	52.47	53.92	57.14	49.76	46.01
Al_2O_3	12.74	32.14	35.07	15.42	16.76
Fe_2O_3	8.36	5.77	5.30	5.42	8.78
CaO	22.33	7.63	1.88	18.67	21.14
MgO	4.11	0.54	0.61	10.72	7.31
Total	100	100	100	100	100
α	4.12	1.68	1.63	3.23	2.75
β	34.79	13.94	7.79	34.82	37.23
$T_{\text{crit}}, \text{K}$	1258	2012	2327	1233	1255

Figure 2.2.1. Effect of $\text{H}_2\text{O}/\text{coal}$ (daf) and O_2/coal (daf) on gasifier exit temperature (K) (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed). Solid line is locus for slagging condition.

Figure 2.2.2. Effect of $\text{H}_2\text{O}/\text{coal}$ and O_2/coal (daf) on cold-gas efficiency (% HHV) (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed).

Figure 2.2.3. Effect of $\text{H}_2\text{O}/\text{coal (daf)}$ and $\text{O}_2/\text{coal (daf)}$ on CO mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed).

Figure 2.2.4. Effect of $\text{H}_2\text{O}/\text{coal (daf)}$ and $\text{O}_2/\text{coal (daf)}$ on CO_2 mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed).

Figure 2.2.5. Effect of $\text{H}_2\text{O}/\text{coal}$ (daf) and O_2/coal (daf) on H_2 mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed).

Figure 2.2.6. Effect of $\text{H}_2\text{O}/\text{coal}$ (daf) and O_2/coal (daf) on H_2O mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal, slurry feed).

Figure 2.2.7. Effect of steam/coal (daf) and O_2 /coal (daf) on gasifier exit temperature (K) (single-stage gasifier, 30 atm, Illinois #6 coal, dry feed).

Figure 2.2.8. Effect of steam/coal (daf) and O_2 /coal (daf) on cold-gas efficiency (% CGE) single-stage gasifier, 30 atm, Illinois #6 coal, dry feed).

Figure 2.2.9. Effect of $O_2/coal$ (daf) on cold-gas efficiency for different coal (single-stage gasifier, 30 atm, dry feed, steam/coal (daf) = 0.10).

2.2.2 CFD Entrained Flow Gasifier

The steady-state, CFD entrained flow gasifier model has been benchmarked through comparisons of model predictions with reported performance for generic one- and two-stage gasifiers. The internal dimensions of commercial gasifier designs are proprietary information. Hence, the geometry of the gasifiers used in this study is based on a combination of publicly available information (e.g., conference papers, advertising literature, web pages, etc.) and engineering judgment. For comparing the predicted gasifier performance we focus on characteristics of the syngas generated, in addition to the basic flowfield features. The principle items of interest are the carbon conversion (i.e., % of carbon from the solid fuel converted to carbon in the syngas) and the syngas temperature, composition, higher heating value (HHV, BTU and BTU/SCF), and cold-gas efficiency (CGE).

The comparisons indicate that the models produce values that agree with the industry-accepted values. Hence, the CFD entrained flow gasifier model can be used in studies to investigate design and process changes to improve gasifier performance. Further details on the gasifier study are provided below.

Single Stage, Up Fired

Firing Conditions

- System Pressure = 26 atm.
- 2600 tpd Dried Bituminous Coal
 - 22% ash
- Dry Feed
 - N_2 : Coal (lb) = 0.075
- Oxidant (wt %)
 - 76% O_2
 - 11% H_2O
 - 10% N_2
 - 3% Ar
- O_2 : C (molar) = 0.46

Figure 2.2.10. Schematic of single-stage, up-fired gasifier and summary of process conditions.

Simulations have been performed for a single-stage upflow, dry-feed gasifier that uses a water jacket to cool the refractory. The configuration is representative of the gasifier being used at the IGCC plant at Puertellano, Spain. The geometry and process conditions for the gasifier are summarized in Figure 2.2.10. Detailed descriptions of the gasifier geometry and process conditions are available in [Seggiani, 1998] and [Benyon, 2002] and thus not repeated here. Our interest in this configuration is the availability of flowing slag model results that have been published by other researchers [Seggiani, 1998], [Benyon, 2002]. The comparisons are intended to build confidence in the predictive capability of the model developed in this project.

Gasifier Description

The gasifier is assumed to have a diameter of about 1.7 m and a L/D ratio slightly less than two (where L is the length of the constant diameter section). The firing system consists of four fuel injectors in a diametrically opposed pattern located near the bottom of the gasifier. It is assumed that no gas exits through the slag tap at the bottom of the reactor, and thus all flue gas must exit through the top opening. The gasifier employs a dry-feed system – N₂ is used for the solids transport gas. The fuel injectors are assumed to be simple “concentric pipes” through which all solids and gases enter the gasifier. As per Seggiani, we have assumed an inlet velocity for the solids of 8 m/s. The stoichiometry at the gasifier inlets is ~0.4.

The gasifier uses a water jacket to provide backside cooling to the refractory. The objective of the backside cooling is to create a “frozen” or “solid” slag layer on the hot-side refractory surface to protect the refractory from the corrosive nature of the molten slag.

Predicted Exit Conditions

Table 2.2.14 lists the gasifier performance in terms of syngas exit conditions for the simulations conducted by Seggiani, Benyon and this project (REI). Overall there is good agreement between the three models. Note that table entries in parentheses [] indicate values from the other researchers that we have estimated based on their published values. Similarly, table entries with a dash (-) indicate items for which data is not listed in the reports from the other studies. In the report by Seggiani, it is stated that the design conditions for this gasifier call for ~99% carbon conversion. It should be noted that the gasifier model used in our study has substantially more mesh resolution than used by the other researchers. The model developed by Seggiani was a 1D zonal model consisting of ~15 zones and the model by Benyon was a 3D CFD model that used ~10K cells to model a 90 degree section of the gasifier. The model used in this study contains ~400K cells. Likewise, there are notable differences in the gasification and combustion chemistry models and techniques used to model the coal particle dynamics and reactions. In general, REI has employed more sophisticated techniques to model the multiphase combustion/gasification problem. However, the slag flow models of Seggiani, Benyon, and this project are relatively similar.

Table 2.2.14. Comparison of Predicted Values for Single-Stage, Dry-Feed Upflow Gasifier.

Exit conditions	Seggiani	Benyon	REI
Gas temp, K	1803	[1650]	1790
CO (wt%)	76.5	70.9	76.8
CO ₂ (wt%)	3.2	10.0	6.0
H ₂ (wt%)	1.8	1.8	1.9
H ₂ O (wt%)	-	-	3.2
N ₂ (wt%)	-	-	10.1
Deposition (%)	-	-	4.7
Carbon conversion (%)	-	-	99.99
HHV, Btu/lb	[4431]	[4248]	4622
Cold-gas efficiency (%)	-	[91.5]	80.5

Predicted Flowing Slag Results

Illustrated in Figure 2.2.11 are plots that compare the slag model values predicted by Seggiani, Benyon and this project (REI). Plotted as a function of gasifier elevation is the local average value for:

- liquid (molten) slag thickness;
- frozen or solid slag thickness;
- slag surface temperature (i.e., surface temperature “seen” by the gas field);
- net heat flux to the liquid slag surface (wall heat flux), and
- near wall gas temperature.

Overall, the three models qualitatively predict the same trends and about the same magnitudes. The model results predict a liquid slag thickness of a few millimeters and a solid slag thickness that varies between 10-20 mm. (<1 inch). Anomalies in the slag properties can be seen at the fuel injector elevation (~2 m.) and near the slag tap (~0 m.). Based on the coal and flux material properties in [Seggiani, 1998], the critical viscosity should be about 1625 K, which the model predicts to be achieved, implying that a solid slag layer should exist. In addition, our slag model results indicate very high gas temperatures near the bottom of the gasifier, resulting in a high heat flux and thus potentially creating a situation where it is too hot for solid slag to exist on the bottom face of the gasifier.

Figure 2.2.11. Comparisons of flowing slag model results. Shown are the predicted slag surface temperature (top, left), liquid slag thickness (top, center), solid slag thickness (top, right), near wall gas temperature (bottom, left) and heat flux to the slag (top, right).

Illustrated in Figure 2.2.12 is a more detailed representation of our predicted flowing slag model results. Here, we have mapped the local values from the slag model to a 2D representation of the inner surface of the gasifier. The figure is created, in effect, by “painting” the inside surface of the gasifier with the predicted values and then plotted by projecting these values onto a flat, 2D plane. With this representation the local variations in the predicted values can be visualized. The color map for the different plots is included in Figure 2.2.12 (in general, dark blue is a low value and red is a high value). From the plots it can be seen that the predicted slag thickness, surface

temperature, and wall heat flux do not change significantly in the circumferential direction except for near the fuel injectors where a noticeable anomaly in values occurs.

Figure 2.2.12. Slag model results displayed as 2D plots. Shown are the predicted liquid slag thickness (left), solid slag thickness (center) and slag viscosity (right).

Predicted Flowfield

Illustrated in Figure 2.2.13 are the gas temperature, velocity, and concentration of major gas species within the gasifier. From the figure, the location of the four diametrically-opposed fuel injectors located near the bottom of the gasifier are readily apparent. Note that the bulk of the chemical reactions occur in a narrow band at the fuel injector elevation. As expected, the flowfield in the lower region of the gasifier is roughly symmetric in 90 degree sections.

Illustrated in Figure 2.2.14 are representative particle trajectories for this gasifier. Shown are particles with an initial diameter of $137\ \mu\text{m}$, one of the largest sizes used in the simulation. From the plot of the volatile mass fraction it can be seen that the volatiles are released quickly; even the large particles shown here release the volatiles very near the fuel injectors. From the plot of char mass fraction (and ash) it can be seen that it requires a much longer time to burn out the char particles. In addition, the char mass fraction plot highlights the relatively chaotic flow patterns within the gasifier that are a result of the four opposed-fired fuel injectors and upflow configuration.

Figure 2.2.13. Shown are gas temperature, axial velocity and H₂ and CO concentration (mole fraction) for single-stage, dry-feed, upflow gasifier.

Figure 2.2.14. Shown are volatile mass fraction and char mass fraction for coal with initial diameter of 137 μm for single-stage, dry-feed, upflow gasifier.

“Generic” Two-Stage Upflow

This section describes simulation results for our two-stage upflow gasifier and compares these results to reported values from a DOE-NETL study for a comparable gasifier under roughly similar process conditions. The objective is to build confidence in our CFD-based gasifier model.

Gasifier and Process Conditions

The process conditions and gross gasifier geometry used for these simulations are summarized in Figure 2.2.15. The shape of the two-stage gasifier is based on information contained in a series of articles by Chen et al. (1999, 2000) that describe modeling studies and scale-up for a pressurized, air-blown entrained flow gasifier designed to operate at 2000 tons/day of coal. Additional assumptions used to determine the size of the gasifier were that the gasifier should provide about a two second residence time for the gases (assuming idealized flow) and has a length to diameter ratio (L/D) of about ten. The two-stage gasifier contains three levels of symmetrically placed injectors. The fuel injectors are assumed to have a simple annular passage (concentric pipes) that does not produce a spray action. The bottom two levels of injectors are oriented as per a tangential-firing system to create a strong swirling flowfield that spirals upward along the axis of the gasifier. The upper-level injectors are oriented opposed to each other. The process conditions are based on the Vision 21 reference configuration. The system pressure for the gasifier is set at 18 atm. The slurry and oxidant temperatures are to be 422 K and 475 K, respectively. All of the oxidant and 78% of the coal is uniformly distributed amongst the fuel injectors in the first stage and the remaining coal is uniformly distributed across the injectors in the second stage. No oxidant is injected into the upper stage. The overall oxygen:carbon ($O_2:C$) mole ratio is ~ 0.40 , resulting in an overall stoichiometry of about 0.47 and a stoichiometry in the lower stage of about 0.60.

Firing Conditions

- System Pressure = 18 atm.
- 3000 tpd Illinois #6
 - 11% H_2O , 10% ash
- Slurry Feed: 74% solids (wt.)
- Slurry Distribution
 - 39%, 39%, 22%(upper)
- Oxidant (wt %)
 - 95% O_2 , 5% N_2
- $O_2 : C$ (molar) = 0.40
- Inlet Stoichiometry ~ 0.47

Figure 2.2.15. Schematic of two-stage upflow configuration and summary of process conditions.

Predicted Flowfield

Illustrated in Figures 2.2.16-2.2.18 are the gross flowfields for the two-stage gasifier for the prescribed operating conditions. To simplify plotting, only the bottom portion of the gasifier is included in the figure. Shown in Figures 2.2.16 and 2.2.17 are the predicted gas temperature, axial velocity, and major gas species concentration (volume %) at selected elevations. Illustrated in Figure 2.2.18 are representative coal particle trajectories colored by coal volatile content and coal char content. Also shown in Figure 2.2.18 are representative trajectories for water droplets from the slurry. From the figures one can see a strong swirling flow pattern in the gas flow and the particle trajectories in the lower section. This pattern is to be expected with a tangential-firing system used for the lower injectors. Looking at the flowfield immediately in front of the top level of injectors, the flow pattern changes due to these injectors being oriented opposed to each other. As illustrated by the fuel particle trajectories shown in Figure 2.2.18, the fuel injected into the first stage devolatilizes very quickly, but the fuel injected at the top injectors requires a slightly longer time to devolatilize. The char from fuel injected in the first stage almost completely gasifies prior to reaching the upper injectors. However, the char in the fuel particles from the upper injectors requires a very long time to fully gasify. From Figure 2.2.18 it can be seen that the water droplets evaporate very quickly.

Figure 2.2.16. Predicted gas temperature and axial velocity at selected elevations for two-stage, slurry-feed, upflow gasifier.

Figure 2.2.17. Shown are predicted major gas species (vol. %) at selected elevations for two-stage, slurry-feed, upflow gasifier.

Figure 2.2.18. Shown are coal volatile mass fraction, char mass fraction and water droplets for selected particle and droplet sizes for two-stage, slurry-feed, upflow gasifier.

Illustrated in Figure 2.2.19 are XY plots of the bulk gas temperature and major species concentration, cold-gas efficiency, and carbon conversion as a function of height in the gasifier. Note that the plots of carbon conversion and cold-gas efficiency are plotted using a normalized (nondimensional) axial length. The plots indicate little change in the major species concentrations (on average) for the region between the top of the second level of injectors to just below the upper injectors, at the 4 m elevation ($x/D \sim 2.5$). At the upper injectors, all of the values show a relatively sharp change for a short distance, after which the values asymptote to their final values. There is little if any change in moisture concentration after the 12 m elevation, implying that little gasification occurs above this level. The overall decrease in gas temperature above the upper injectors is due to the endothermic reactions associated with gasification.

Figure 2.2.19. Plotted as a function of axial position for the two-stage, slurry-feed, upflow gasifier are the predicted a) bulk gas temperature and major species concentration, b) cold-gas efficiency and c) carbon conversion.

Flowing Slag Model Results

Illustrated in Figure 2.2.20 are 2D plots showing the liquid (molten) slag thickness, solid slag thickness, and slag surface temperature. The location of the two lower level fuel injectors can be seen in the slag thickness plots as dark blue rectangles (in the lower half of the pictures) and as bright red regions in the slag surface temperature plot. The predicted slag thickness is quite high, ~50 mm and ~100 mm for liquid and frozen slag, respectively, in the “combustion” zone at the bottom of the gasifier. The model also predicts a high liquid and frozen slag thickness above the third level of injectors. A region of shallower slag occurs in the “transition” between the second and third level of fuel injectors. The change in slag thickness is reasonable. The slag surface temperature increases in this region, resulting in a lower slag viscosity making the slag flow into a thinner layer. Note that the model predicts no slagging activity in the upper half of the gasifier. In this region there is little ash deposition, and the predicted surface temperature is not high enough to maintain the slag flow.

Figure 2.2.20. Shown are the predicted molten (liquid) slag thickness (left), solid slag thickness (center) and surface temperature (right) from the flowing slag model for a two-stage, slurry-feed, upflow gasifier.

Predicted Exit Conditions

Shown in the Table 2.2.15 are the average values for the syngas quantity and composition at the gasifier exit. From the table it can be seen that for the baseline conditions the model predicts a high carbon conversion (over 96%), cold-gas efficiency of about 81%, and a syngas heating value of about 247 Btu/SCF. Listed in the table are values for the residence times of the gas and fuel particles. For the given conditions and reactor volume this results in a PFR residence time of about 1.8 seconds. For fuel particles, the model predicts an average residence time of slightly less than one second. The strong swirling flow pattern provides the means to provide a seemingly long fuel residence time. Also shown in the table are predicted LOI (carbon content) in the flyash escaping through the gasifier exit and in the slag on the walls.

Table 2.2.15. Two-Stage Gasifier Comparison.

	REI	DOE
Average Wall Temp., K	1705	-
Exit Temperature, K	1390	1300
Carbon Conversion, %	96.1	-
Exit LOI, %	19.7	-
Deposit LOI, %	47.9	-
Deposition, %	3.3	-
PFR Residence Time, s	1.797	-
Particle Residence Time, s	0.926	-
Mole Fraction: CO	42.5%	43.5%
H ₂	32.3%	32.5%
H ₂ O	13.8%	13.6%
CO ₂	8.7%	8.6%
H ₂ S	0.8%	-
COS	0.0%	-
N ₂	1.6%	0.9%
Exit Mass Flow, klb/hr	493	499
HHV of Syngas, Btu/lb	4899	0
HHV of Syngas, Btu/SCF	247	250
Cold-Gas Efficiency, %	80.9	-

Also shown in Table 2.2.15 are the results from a DOE-funded study that employed an ASPEN analysis for an IGCC plant with a two-stage gasifier for comparable operating conditions as used in this simulation (same coal, slurry and oxidant flow rate, higher gasifier pressure) [DOE-NETL, 2000b]. As noted in previous reports, altering the system pressure has had little effect on the gas composition predicted with our gasifier model. All REI values are reported at the exit of the gasifier. The listed DOE results for syngas temperature, mass flow, and heating value are assumed to be at (or near) the gasifier exit. The listed DOE gas composition is assumed to be the composition after the gas clean up process. Despite the inconsistencies, there is good agreement between the two simulations.

Firing Petcoke In a Shorter Gasifier

The simulations described above were performed assuming the gasifier had a L/D ratio of 11. Subsequently, it was determined that a L/D ratio of 6 would be of more interest from an industry perspective. In addition, the simulations reported above were performed for Illinois #6, but there are economic advantages to firing a gasifier with Petcoke. Hence, in the following we explore using a shorter gasifier and for firing Petcoke. In the following, a baseline simulation was performed using Illinois #6 using the same process conditions as used for the result in Table 2.2.14. However for firing Petcoke, the overall O₂:C mole ratio is assumed to be ~0.34, resulting in an overall stoichiometry of about 0.47 and a stoichiometry in the lower stage of about 0.60.

Listed in Table 2.2.16 are the gross gasifier exit values from the CFD simulation for firing Illinois #6 and Petcoke. Only minor differences in the gasifier performance are witnessed, most notably in the exit CO concentration and the predicted LOI for the unburned fuel exiting the gasifier and deposited on the walls. The predicted flowfields for firing Petcoke (for the assumed process conditions) result in flowfield patterns, gas temperature distribution, and major species concentrations that differ only slightly from those for firing Illinois #6 (see Figures 2.2.16-2.2.18) and thus are not repeated here. The similar flowfields are not surprising because the gasifier operating conditions for firing Petcoke were designed to provide a comparable gasifier temperature as for firing Illinois #6.

Table 2.2.16. Two-Stage Gasifier Performance for Firing Illinois #6 versus Petcoke.

	Illinois#6	Petcoke
Exit Temperature, K	1412	1406
Carbon Conversion, %	91.4	93.9
Exit LOI, %	34.2	76.7
Deposit LOI, %	47.9	96.4
Deposition, %	8.5	4.7
PFR Residence Time, s	0.83	0.83
Particle Residence Time, s	0.37	0.19
Mole Fraction: CO	43.3%	47.3%
H ₂	32.7%	31.4%
H ₂ O	13.3%	11.0%
CO ₂	8.1%	7.6%
H ₂ S	0.8%	1.2%
COS	0.0%	0.1%
N ₂	1.6%	1.3%
Exit Mass Flow, klb/hr	497	507
HHV of Syngas, Btu/lb	4988	5050
HHV of Syngas, Btu/SCF	248	257
Cold-Gas Efficiency, %	82.9	85.5

Process Conditions and Gasifier Geometry

Firing Conditions

- fuel injector model*

Figure 2.2.21. Schematic of one-stage, slurry-feed, downflow gasifier and process conditions.

Predicted Flowfield

Illustrated in Figures 2.2.22 and 2.2.23 are the single-stage gasifier gross flowfields for the prescribed firing conditions. Shown in Figure 2.2.24 are predicted gas temperature, axial velocity, and major gas species concentration (vol. %) at selected elevations. Also shown in Figure 2.2.25 are representative coal particle trajectories, colored by coal volatile content and char content and representative trajectories for water slurry droplets. Overall, the flowfield is similar to that of an immersed jet exhausting into a confined volume. There is a core of high-velocity, hot gas traveling down the center of the gasifier. Away from the centerline, there exists a slow-moving, much cooler reversed flow (i.e., recirculating flow) that travels back toward the injector end of the gasifier. From the particle trajectories it can be seen that the fuel enters the chamber and quickly devolatilizes. Likewise, the fuel initially contains no char, rapidly forms char, and then burns out (oxidizes) the char through the remainder of the chamber. From the water droplet plot it can be seen that a large portion of the water-slurry droplets evaporate quickly, but that some rogue droplets can exist until well into the gasifier.

Figure 2.2.22. Shown for the one-stage, slurry-feed downflow, gasifier are the predicted gas temperature (left) and axial velocity (center) at selected elevations. Also shown are the coal volatile mass fraction and char fraction (center) for representative coal particle trajectories and representative trajectories for water droplets (right) where the end of the droplet trajectory indicates the droplet has completely evaporated.

Figure 2.2.23. Shown are the predicted major gas species concentration (vol.%) at selected elevations for single-stage, slurry feed, downflow gasifier.

Shown in Table 2.2.17 are the average values for the syngas quantity and composition at the gasifier exit. For plant operations the syngas conditions are typically reported on a dry basis for measurements taken at a location downstream of the syngas clean up system. For simplicity, our results are reported on a wet basis at the model exit plane. From the table it can be seen that for these conditions the model predicts a high carbon conversion (over 94%), cold-gas efficiency of slightly more than 74%, and a syngas heating value of about 220 Btu/SCF.

Listed in Table 2.2.17 are some reference values for gas, solid, and droplet residence times. The PFR residence time provides a reference for the gas residence time and is computed from a single, volume-averaged gas density for the reactor and assuming a plug flow; for the given conditions and reactor volume this results in a PFR residence time of about 0.6 seconds. Due to the strong recirculating flow pattern within the gasifier chamber the PFR residence time is not representative of the real residence time. For fuel particles, the model predicts an average residence time of about 0.04 seconds. For particles, the residence time is defined as the time from when the particle enters the reactor until it impacts on a wall or exits the gasifier. Note that even if the particle “burns out”, we continue to track the remaining ash particles until the ash impacts the wall or exits the gasifier. Considering the high velocity flow passing down the center of the gasifier (see Figure 2.2.22), the short residence time of the particles is not unreasonable. For this case, the average residence time for slurry water droplets (i.e., the average time required for a water droplet to evaporate) is about one tenth that of the fuel particles.

Also shown in Table 2.2.17 are the results from a DOE-funded study that employed an ASPEN analysis for an IGCC plant with a single-stage gasifier for comparable operating conditions as used in this simulation (same coal, slurry flow rate, but higher gasifier pressure and oxidant flow rate) [DOE-NETL, 2000a]. As noted in previous reports, altering the system pressure has had little effect on the gas composition predicted with our gasifier model. All REI values are reported at the exit of the gasifier. The listed DOE results for syngas temperature, mass flow, and heating value are assumed to be at (or near) the gasifier exit. The listed DOE gas composition is assumed to be the composition after the gas clean up process. Despite the inconsistencies, there is reasonable agreement between the two simulations.

Table 2.2.17. Predicted Exit Values For One-Stage, Slurry-Feed, Downflow Gasifier.

	REI	DOE
Average Wall Temp., K	1853	-
Exit Temperature, K	1807	1650
Carbon Conversion, %	94.4	-
Exit LOI, %	33.7	-
Deposit LOI, %	25.1	-
Deposition, %	3.5	-
PFR Residence Time, s	0.683	-
Particle Residence Time, s	0.041	-
Water Droplet Res. Time, s	0.004	-
Mole Fraction: CO	41.7%	41.8%
H ₂	24.7%	30.8%
H ₂ O	21.3%	15.3%
CO ₂	9.6%	10.2%
H ₂ S	0.8%	0.0%
COS	0.0%	-
N ₂	1.8%	0.9%
Exit Mass Flow, klb/hr	542	524
HHV of Syngas, Btu/lb	4099	-
HHV of Syngas, Btu/SCF	220	240
Cold-Gas Efficiency, %	74.4	-

Firing Petcoke

Illustrated in Figures 2.2.24 and 2.2.25 are the gasifier gross flowfields for a single stage firing Illinois #6 and Petcoke, respectively. Shown in Figure 2.2.24 are the predicted gas temperature and CO and H₂ species concentration (volume %) at mid-plane of the gasifier. Figure 2.2.25 contains the same plots as Figure 2.2.24, but for firing Petcoke instead of Illinois #6. Comparing the flowfield for firing Illinois #6 versus that of firing Petcoke, the only noticeable difference is for the CO concentration. Listed in Table 2.2.18 is a comparison of average values for the one-stage gasifier simulations. Again, there are not significant differences.

Figure 2.2.24. Shown for the one-stage, slurry-feed, downflow gasifier firing Illinois #6 are the gas temperature and CO and H₂ species concentrations at selected planes.

Figure 2.2.25. Shown for the one-stage, slurry-feed, downflow gasifier firing Petcoke are the gas temperature, and CO and H₂ species concentrations at selected planes.

Table 2.2.18. One-Stage, Slurry-Feed, Downflow Gasifier Comparison of Firing Illinois #6 versus Petcoke.

	Illinois#6	Petcoke
Exit Temperature, K	1595	1669
Carbon Conversion, %	92.2	89.1
Exit LOI, %	22.4	79.6
Deposit LOI, %	53.1	97.9
Deposition, %	8.5	9.0
PFR Residence Time, s	0.80	0.78
Particle Residence Time, s	0.16	0.12
Mole Fraction: CO	43.4%	47.2%
H ₂	29.7%	28.0%
H ₂ O	16.3%	14.6%
CO ₂	8.1%	7.6%
H ₂ S	0.8%	1.1%
COS	0.0%	0.1%
N ₂	1.7%	1.4%
Exit Mass Flow, klb/hr	517	522
HHV of Syngas, Btu/lb	4671	4674
HHV of Syngas, Btu/SCF	241	246
Cold-Gas Efficiency, %	80.9	82.1

2.2.3 Comparison of Process and CFD Entrained Flow Gasifier Model

Comparisons have been performed between the process and CFD entrained flow gasifier model. Although the CFD model provides detailed information on the flowfield within the gasifier, it can require significant computational time. The process models are fast running and thus can be useful to guide the selection of gasifier conditions and gasifier type for a desired carbon conversion or other output requirements. The test case is for a one-stage, slurry-feed system operating at 30 atm, firing an Illinois #6 coal, a coal slurry feed with 65% slurry concentration, a slurry temperature of 298 K, a coal flow rate of 25.8 kg/s (about 2400 tpd), an oxidant (95% O₂, 5% N₂) flow rate of 13.9 kg/s (about 1345 tpd) and a temperature of 298 K, and a heat extraction rate of 100 kW/m². The purpose of the test is to provide confidence that the two models, which contain vastly different resolution of the physics within the gasifier, provide comparable predictions for carbon conversion and syngas composition.

Table 2.2.19 shows the process model results using three different gasifier lengths. For the tests the gasifier diameter is fixed, and by varying the length of the gasifier, different carbon conversions can be achieved due to changes in the residence time of coal particles. Also reported in the table are the net plant power output and the overall plant efficiency calculated using the REI Vision 21 framework. As expected, as carbon conversion increases, both the cold-gas efficiency and the overall plant efficiency increase. CFD simulations have also been performed using the same conditions as given in Table 2.2.19 and are summarized in Table 2.2.20.

Table 2.2.19. Results Based on the Process Model.

P, psia	400	400	400
Particle Size, μm	39.8	39.8	39.8
Slurry Temperature, K	298	298	298
Water Droplet Size, μm	25	25	25
Gasifier Diameter, m	1.00	1.00	1.00
Gasifier Length, m	1.175	1.742	3.000
Carbon Conversion, %	90.0	95.0	99.98
Exit Temperature, K	1869	1754	1652
Mole Fraction: CO	0.3903	0.4057	0.4200
H ₂	0.2297	0.2526	0.2744
H ₂ O	0.2508	0.2200	0.1908
CO ₂	0.1048	0.0976	0.0911
H ₂ S	0.0058	0.0059	0.0060
CH ₄	0.000002	0.000007	0.000029
COS	0.000351	0.000333	0.000318
HCl	0.000228	0.000231	0.000235
N ₂	0.0179	0.0175	0.0170
Syngas Flow Rate, kg/s	54.77	55.77	56.78
Syngas Density, kg/m ³	3.77	3.94	4.11
LHV of Syngas, Btu/lb	3360.2	3629.1	3892.1
HHV of Syngas, Btu/lb	3788.2	4058.2	4322.3
Cold-Gas Efficiency (HHV), %	67.5	73.7	79.9
Net Plant Power, MW	290	322	329
Plant Efficiency (HHV), %	40.7	45.0	46.1

Table 2.2.20. CFD Simulation Results (same operating conditions as in Table 2.2.19).

P, psia	400	400	400
Particle Size, μm	39.8	39.8	39.8
Slurry Temperature, K	298	298	298
Water Droplet Size, μm	25	25	25
Gasifier Diameter, m	1.00	1.00	1.00
Gasifier Length, m	1.175	1.742	3.000
Carbon Conversion, %	90.9	95.5	98.4
Exit Temperature, K	1766	1686	1657
Mole Fraction: CO	0.3863	0.3978	0.4068
H ₂	0.2413	0.2571	0.2650
H ₂ O	0.2368	0.2109	0.1980
CO ₂	0.1105	0.1063	0.1014
H ₂ S	0.0005	0.0033	0.0040
CH ₄	0.005680	0.005786	0.006057
COS	0.000321	0.000313	0.000323
HCl	-	-	-
N ₂	0.0178	0.0175	0.0173
Syngas Flow Rate, kg/s	54.95	55.89	56.43
Syngas Density, kg/m ³	-	-	-
LHV of Syngas, Btu/lb	3444.5	3683.1	3830.5
HHV of Syngas, Btu/lb	3877.8	4117.7	4265.7
Cold-Gas Efficiency (HHV), %	69.4	74.9	78.4
Net Plant Power, MW	302	325	342
Plant Efficiency (HHV), %	42.3	45.5	47.9

Comparing the values in Tables 2.2.19 and 2.2.20, it can be seen that there is good agreement between the process and reacting CFD models of the gasifier for the key indicators of gasifier performance. Hence, we can have confidence in using the process model of the gasifier to guide the selection of gasifier process conditions and identify improved overall plant performance, and then use the CFD models of the gasifier to investigate localized behavior within the gasifier (e.g., hot spots on walls, inadequate slagging behavior, etc.) or equipment directly connected to the gasifier.

2.2.4 Example Calculation: Soot and Tar Models for CFD Entrained Flow Gasifier

CFD simulations using REI's entrained flow gasifier model have been performed to examine the effects of the soot and tar model described in Appendix H versus the previously used soot correlation, also described in Appendix H. The soot and tar model solves transport equations for tar and soot whereas the previous soot correlation model calculates the soot concentration based on the local stoichiometry via algebraic correlations. Illustrated in Figure 2.2.26 is the comparison of the temperature and velocity field between using the previous soot correlations and the soot and tar model. The hot regions relatively close to the burner have expanded out toward the walls. The velocity down the center of the gasifier is lower as a result of lower overall

temperatures down the center. The hotter temperatures at greater radial locations within the gasifier may be explained by the presence of O_2 farther away from the centerline as shown in Figure 2.2.27. The high-temperature regions are associated with O_2 being transported into these same regions. This is a result of shrinking recirculation regions next to the radial wall.

Figure 2.2.26 Gas temperature and velocity distribution comparisons between the soot correlation model and the soot and tar model.

Figure 2.2.28 illustrates the difference in the concentration of CO and H_2 in the gasifier. When using the soot and tar model, the conversion to these key syngas constituents is delayed in the outer radial regions due to the presence of O_2 . However, the syngas composition at the exit of the gasifier is essentially the same. Therefore, the cold-gas efficiency is essentially the same regardless of which of the two soot models is used. The exit conditions are shown in Table 2.2.21.

Figure 2.2.27. Comparison of O_2 distribution between the soot correlation model and the soot and tar model.

Figure 2.2.28. Comparison of CO and H₂ distributions between the soot correlation model and the soot and tar model.

Figure 2.2.29. Comparison of soot volume fraction distribution between the soot correlation model and the soot and tar model. Tar mass fraction from soot and tar model.

Figure 2.2.29 shows comparisons of the soot volume fraction. The tar mass fraction is only shown for the soot and tar model because the soot correlation model does not predict the tar mass fraction. Whereas the soot and tar model shows very little soot away from the center of the gasifier, the soot correlation model shows a much higher concentration because the soot

correlation model does not involve the solution of transport equations. It is only dependent on the local equivalence ratio (see Appendix H). The soot and tar model provides a more correct physical picture of the soot formation in pressurized fuel-rich environments such as those found in gasifiers.

Table 2.2.21. Exit Temperature and Composition Comparison between Soot Correlation and the Soot and Tar Model.

	Soot Correlation	Soot and Tar Model
Temperature	1624 °K	1619 °K
CO, dry	51.7%	51.7%
H ₂ , dry	35.0%	35.2%
H ₂ S, dry	0.9%	0.9%
H ₂ O	17.2%	17.1%

Figure 2.2.30 shows the difference in the net radiative wall heat flux for both soot models. The soot and tar model results in negative wall heat flux at the top of the gasifier. This is a result of higher local wall convection related to the very high gas temperature adjacent the walls in addition to lower optical thicknesses for the radiation heat transfer. The net heat transfer is still positive (into the wall) when adding both radiation and convection.

Figure 2.2.30. Net wall radiative heat flux comparison between soot correlation and the soot and tar model.

To summarize, the predicted flowfield properties that results from using the more refined submodel for soot and tar production/destruction implemented into the CFD have been compared to the flowfields predicted using a correlation-based soot model. Although the exit conditions predicted by the original and improved gasifier model are similar, differences in localized values are noticeable. The model results have been shown for a single-stage, slurry-feed gasifier, but similar trends would be expected for a two-stage gasifier or a gasifier with a dry-feed system. Including the enhanced submodels had only a minor impact on the overall computation time and effort for the models; the additional partial differential equations that must be solved increased the required cpu time by only about 5-10%, depending on the type of gasifier modeled. The improved gasifier model will be a useful tool in studies targeting improvements to entrained flow gasifier performance, such as improving refractory life or fuel-injector life by eliminating localized hot spots and other heat transfer-related design issues.

2.2.5 Impact of Coal Gasification Kinetics on CFD Gasifier Model Results

In most of the CFD gasifier simulations performed within this project, we have used the global gasification kinetic parameters found in [Lupa and Kliesch, 1979] which was originally developed for modeling Illinois #6 coal. For the following we applied the PREKIN tool described in Appendix G to obtain global gasification kinetic parameters from intrinsic gasification data for Illinois #6 coal that has recently been published in the open literature [Liu et al., 2004]. A comparison of the global kinetic parameters is given in Table 2.2.22. The revised global kinetic parameters obtained from PREKIN were used in the CFD model of the one-stage gasifier. Figure 2.2.31 presents a comparison of predicted gas temperature and oxygen distributions in the one-stage, down-fired, slurry-feed gasifier. Only minor differences are noted. Applying the kinetics from PREKIN results in an increase in the carbon conversion from 96.0 to 97.2%. There is a slight increase in cold-gas efficiency (from 78.2 to 79.5%) and an associated increase in plant efficiencies by one percentage point. Overall, the differences in the predicted values for the two cases are not significantly different.

Table 2.2.22. Global Gasification Kinetic Parameters.

	PREKIN Kinetics	Lupa and Kliesch Kinetics
CO ₂ Gasification		
A, kg/(s m ² Pa ⁿ)	0.0113	0.0244
n	0.887	1
E, J/kmol	1.75E+08	1.75E+08
H ₂ O Gasification		
A, kg/(s m ² Pa ⁿ)	0.0609	0.0244
n	0.733	1
E, J/kmol	1.75E+08	1.75E+08
O ₂ Oxidation		
A, kg/(s m ² Pa ⁿ)	0.00107	0.0139
n	0.823	
E, J/kmol	1.00E+08	1.00E+08

Figure 2.2.31 Comparison of gas temperature and oxygen distribution for using kinetics from [Lupa and Kliesch, 1979] (A,C) versus kinetics determined with *PREKIN* (B,D).

2.2.6 IGCC-FCT Simulations for Vision 21 Reference Configuration and Parametrics

During the course of the project numerous simulations were performed for the Vision 21 reference configuration including variations (parametric) changes. The majority of these simulations were performed using the SCIRun-based IGCC-FCT framework. Hence, in this section we provide an overview of some of these simulations to provide a sense of the breadth and extensibility of this framework. Note that most of the models and capabilities of the IGCC-FCT were subsequently implemented into the VE-Suite based VEF.

Vision 21 Reference Configuration: One- and Two-Stage Gasifier Firing Illinois #6 and Petcoke Simulations were performed for the Vision 21 reference configuration shown in Figure 1.3.10-11. The simulations were performed for two gasifier types (two stage vs. one stage) and two fuels (Illinois #6 vs. Petcoke). Although Illinois #6 is the reference fuel for the plant configuration, we have also investigated the impact of using Petcoke. Petcoke is an attractive fuel for economic reasons, but is more difficult to use than coal because it burns hotter and produces much less ash for slagging than coal. Note that the IGCC plants at Polk Station and Wabash River have explored the use of Petcoke.

The network of modules used to perform the simulations in the SCIRun-based IGCC-FCT framework is shown in Figure 2.2.32. Note that the plant configuration used for the simulation uses a WGPU system rather than the hot gas clean up system shown in the Vision 21 reference configuration.

Process Conditions

The baseline gasifier conditions were determined from information provided by DOE (e.g., Table 1.3.1-1.3.2 and Figure 1.3.11). For the baseline we assume the gasifier is a two-stage, oxygen-blown gasifier, operating at 18 atm and firing (nominally) 3000 tpd Illinois #6 coal. The baseline slurry feed is assumed to be 66% solids by weight (dry basis). The slurry temperature is assumed to be 422K and the oxidant temperature is assumed to be 452.5K. The oxidant feed rate is assumed to be 2200 tpd (oxidant =95% O₂ , 5% N₂). REI did not have access to the models (or details on calculations) used by DOE to determine the values indicated in Table 1.3.2 and Figure 1.3.11. In the discussion below, we assume that the results for using a two-stage gasifier firing Illinois #6 (labeled 2 Stage, Illinois #6) are representative of the DOE baseline conditions.

Using the process (0D) entrained flow gasifier model, process conditions were created for the other simulations. For the one-stage gasifier firing Illinois #6, it was assumed that the coal flow rate and slurry loading should be the same as used in the two-stage gasifier simulations. However, operating a one-stage gasifier in this manner would result in too low of a bulk gas temperature and lead to slagging problems. Hence, the oxidant flow rate was increased slightly (to ~2400 tpd) to obtain a gas temperature in the gasifier of 2500°F, as determined with the process gasifier model. Due to the much higher heating value of Petcoke, the fuel feed rate must be reduced for both gasifiers. In addition, the solids loading in the slurry feed is typically less with Petcoke as compared to firing coal. Here we have assumed a solids loading of ~56% (dry basis) for the Petcoke simulations. The process gasifier model was used to define the process conditions for firing with Petcoke, subject to the constraint that the gasifier temperature should be the same as for firing with coal.

Figure 2.2.32. UI for IGCC-FCT representation of Vision 21 reference configuration.

Summarized in Tables 2.2.23 and 2.2.24, respectively, are the fuel properties and process conditions used for the plant simulations.

Table 2.2.23. Fuel Properties for IGCC-FCT Simulations.

	Illinois #6	Petcoke
Proximate Analysis	As-Received (wt%)	As-Received (wt%)
Moisture	11.12	7.00
Ash	9.70	0.48
Volatile Matter	34.99	12.40
Fixed Carbon	44.19	80.12
TOTAL	100.00	100.00
HHV (Btu/lb)	11666	14282
Ultimate Analysis	As-Received (wt%)	As-Received (wt%)
Moisture	11.12	7.00
Carbon	63.75	81.37
Hydrogen	4.50	2.55
Nitrogen	1.25	0.92
Sulfur	2.80	4.81
Ash	9.70	0.48
Oxygen (by difference)	6.88	2.87
TOTAL	100.00	100.00

Table 2.2.24. Entrained Flow Gasifier Conditions for IGCC-FCT Simulations.

Item	2 Stage Ill. #6	2 Stage Petcoke	1 Stage Ill. #6	1 Stage Petcoke
Fuel Flow Rate (tpd)	3000	2520	3000	2500
Slurry – wt % (dry basis)	66 %	56%	66 %	56%
Oxidant Flow Rate (tpd)	2200	1940	2420	2140
Slurry Temperature (K)	422	422	422	422
Oxidant Temperature (K)	452	452	452	452

For equipment other than the gasifier, inputs for the associated component model were taken directly from the reference configuration. In cases where data was not provided, data from similar units was used or the component was configured to obtain the proper results for the baseline simulation. The inputs for these components were not changed for subsequent simulations. As a result, some downstream equipment might not be configured to operate in an optimal manner for the non-baseline simulations.

Results – Baseline Simulations

Illustrated in Figures 2.2.33 and 2.2.34 are the simulation results obtained for the Vision 21 reference configuration using the IGCC-FCT framework. Shown in Figure 2.2.33 is the predicted overall plant efficiency, and illustrated in Figure 2.2.34 is the predicted net power for the principal power producing components.

Figure 2.2.33. Predicted plant efficiency for Vision 21 reference configuration.

Several items can be seen from the plots in Figures 2.2.33 and 2.2.34. Although the overall plant efficiency is slightly less for the simulations as compared to the DOE values, there is remarkably good agreement between the two despite having to make many assumptions about model inputs, equipment, etc. The DOE overall plant efficiency is 59.5%, which is only slightly less than the Vision21 target value of 60%. As expected, the plant efficiency is slightly higher for the two stage as opposed to the one-stage gasifier and the plant efficiency increases when firing Petcoke.

It should be noted that the gasifier cold-gas efficiency shown in Figure 2.2.33 and 2.2.34 is a computed value for the plant simulations, but an *assumed* value in the DOE information. The computed cold-gas efficiency for the models appears to have the expected trend: the two-stage gasifier has a higher cold-gas efficiency than the one-stage gasifier and the cold-gas efficiency increases with either gasifier when firing Petcoke.

Figure 2.2.34. Predicted net power generated by main components in Vision 21 reference configuration.

Comparing the net power results in Figure 2.2.34, again there is good agreement between DOE provided values and the values predicted with the framework. Comparing the DOE and computed net power for the fuel cell, there appears to be very good agreement. However, there does appear to be a noticeable difference between the DOE and computed net power values at the steam turbine. This is likely due to the relatively simple HSRG model used due to the lack of detail provided within the reference configuration

Additional Output Information

A key aspect of the framework is the ability to drill-down into the simulation results to obtain and organize more details on the predicted performance of individual devices or subsystems within the plant. Illustrated in Figures 2.2.35-2.2.36 are examples of additional summary information that can be extracted from the plant simulations to allow the engineer to better evaluate which components need improvement. The information shown here can be accessed by the user in addition to the very detailed information that can be obtained about an individual equipment piece.

Figures 2.2.35-2.2.36 highlight the ability to track and plot data within a plant simulation performed with the IGCC-FCT framework. As can be seen, exploiting such data gathering features provides a powerful tool for accessing a substantial amount of information. Shown are plant-wide bar charts for user-selected variables and how these variables vary across different pieces of equipment within the plant. Variables available for viewing are: gas and water variables (temperature, pressure, flow rate), gas specific variables (species concentration), water-specific variables (enthalpy, quality), and component power generation/consumption. The charts are accessible by each module in a network and can be archived by the user to Postscript format.

Figure 2.2.35. Example plot from IGCC-FCT framework of changes in user-selected variable (gas temperature) through the Vision 21 reference plant configuration.

Figure 2.2.36. Example plot from IGCC-FCT framework for changes in user-selected variable (top: component power generation; bottom: CO₂ concentration in syngas) through the Vision 21 reference plant configuration.

Parametric Cases – Process Conditions

During the course of the project, additional plant simulations were performed to explore the impact on plant performance for “one-off” variations on the Vision 21 conditions. Some of the parametric cases included:

- Oxidant Variation (*baseline*: oxidant composition, 95% O₂, 5% N₂)
 - Decreased Oxygen Concentration (75% O₂, 25% N₂)
- Slurry Temperature Variations (*baseline*: 422 K)
 - Room Temperature Slurry (293 K)
 - Preheated Slurry (450 K)
- Coal Type Variations (*baseline*: Illinois #6)
 - Petcoke
 - Pittsburgh #8
- Feed Variation (*baseline*: 74.65 wt % coal slurry)
 - Dry feed (N₂ transport)
 - Dry feed (CO₂ transport)

Selected results are summarized below.

Oxidant Concentration and Slurry Properties

The ASU module was altered to generate an oxidant stream with increased nitrogen concentration to demonstrate the effects of varying oxidant concentrations on plant performance. As would be expected, an oxygen-rich oxidant stream proved to best effect high efficiency and power output. Similarly, the effects of slurry temperature were investigated by altering the temperature of the slurry as it entered the gasifier. Results show that high slurry temperatures lead to better coal conversion as less thermal energy is required to vaporize the accompanying water. Similar trends were demonstrated in both one- and two-stage gasifiers. Figure 2.2.37 summarizes the results of these calculations for a two-stage gasifier.

Figure 2.2.37. Comparison of net power generation for the baseline network and three other configurations. Net plant power is summarized in the last column and overall plant efficiency is listed in the legend.

Coal and Gasifier Type

The impact of different fuel and gasifier types was explored. To create a standard for comparison, a network for each coal/gasifier combination was configured such that it would closely match the DOE assumed cold-gas efficiency of 84%. Figure 2.2.38 contains a comparison of the predicted plant efficiencies.

Figure 2.2.38. Comparison of net plant power generation for different fuels. Calculations were performed such that gasifier cold-gas efficiency was similar between cases. Properties of the generated syngas were also monitored for uniformity.

Dry Feed

In addition to using a slurry of pulverized coal mixed with water to feed coal into the gasifier, the coal can be transported and injected into the gasifier using pressurized CO₂ or N₂ gas. Calculations were performed to identify differences in plant performance between configurations using dry and slurry feed (see Figure 2.2.39). Both one- and two-stage gasifiers were used to evaluate plant performance. The slurry-feed calculations were performed using the baseline conditions. The dry-feed calculations were made using N₂ gas as the coal transport (carrier) gas, in the ratio of .07 lb of N₂ per 1 lb of coal. All other flow rates were maintained the same as per the baseline configuration.

Figure 2.2.39. Comparison of power generation for dry and slurry feeds for the one-stage downflow and two-stage upflow gasifier. The feed type, cold-gas efficiency and plant efficiency are shown at bottom of plot. Dry-feed calculations were made using N₂ gas as the coal transport in the ratio of .07 lb of N₂ per 1 lb of coal.

Parametric Cases – Equipment Variations

Parametric cases were performed to investigate the impact of altering some of the equipment upstream and downstream of the entrained flow gasifier. It should be noted that in the time period between performing the simulation described above and those reported in this section, improvements were implemented to selected models (in particular the HRSG) that resulted in much closer agreement with the Vision 21 reference configuration net power generation and overall plant efficiency. In the following, the differences should be compared only to each other and not necessarily to previous cases.

Parametric cases investigated included:

- Calculating Water Gas Shift of Syngas During Quench
- Dry Feed by Flashing Slurry and Using Flashed Steam as Quench
- Replacement of Equilibrium Reactor with Dump Combustor Downstream of Fuel Cells
 - 95 % conversion of low BTU gas
 - 99 % conversion of low BTU gas
- Replace Equilibrium Reactor with Catalytic Combustor Downstream of Fuel Cells
 - 95 % conversion of low BTU gas
 - 99 % conversion of low BTU gas
- Addition of Membrane Shift Reactor Upstream of Fuel Cells

Illustrated in Figure 2.2.40 shows the trends in overall plant efficiency with the cases identified above. Figure 2.2.41 shows the respective trends of the power generation of key equipment.

Figure 2.2.40. Predicted plant efficiency trends for parametric variations of the Vision 21 reference configuration.

Figure 2.2.41. Predicted plant power generation trends for parametric variations of the Vision 21 reference configuration.

By inserting a PFR kinetic reactor model downstream of the gasifier, the effect of the syngas undergoing a water gas shift during quench was calculated. This result is shown in Figures 2.2.40 and 2.2.41 labeled “quench (0.5s 1439 K/s),” which indicates the quench residence time and quench rate. The water gas shift occurring during this quench resulted in about a half % drop in plant efficiency.

Plant simulations were performed to evaluate the approach of heating a coal water slurry to the point of flashing to create a dry feed to the gasifier with N_2 or CO_2 carrier gas. The steam from the flashed water is fed to the syngas stream exiting the gasifier to provide a quench as well as additional reforming of the syngas to H_2 . This was modeled by applying some of the new modules (water heat exchanger and water-to-gas converter). The result is shown in Figures 2.2.40 and 2.2.41 labeled “Slurry Flash/Dry Feed.” This approach resulted in an efficiency increase of a few percentage point.

The dump combustor and catalytic combustor cases shown in Figures 2.2.40 and 2.2.41 are the result of replacing the equilibrium reactor in the network just downstream of the fuel cells with the indicated combustor. These reactors or combustors are intended to combust the remaining low BTU gas exiting the fuel cells (the fuel utilization of the fuel cells are about 85%). In these cases the design mode of the combustors was selected. The % conversion selected in these combustors is shown in the bar chart labels of the figures. Very little difference in plant efficiency was obtained by using the dump combustor model or catalytic combustor in place of

the equilibrium reactor model. The catalytic combustor at 95% conversion is not shown in Figures 2.2.40 and 2.2.41 because it is identical to the dump combustor results. The efficiency slightly decreased with the dump combustor since the combustion efficiency of the equilibrium reactor is always 100%. The size of the catalytic combustor needed to obtain a given conversion efficiency is many times smaller than that needed for the dump combustor since the former relies on catalyzed combustion.

The final case involved the addition of a membrane shift reactor, inserted just upstream of the fuel cells. The membrane of the shift reactor is permeable to only H_2 , and steam is added to shift the CO and steam to H_2 and CO_2 . Shift reactors are of interest in the application of CO_2 sequestration and for enriching the H_2 concentration of syngas streams. Here we wanted to demonstrate how easily it is to insert models into a given network. Again, the results are shown in Figures 2.2.40 and 2.2.41. There is a significant drop shown for the overall plant efficiency. A drop in power generation is also noted. It should be emphasized that in each of these cases no changes were made in the design or operation of downstream equipment. Optimization of the downstream equipment may improve the performance of this last case.

Parametric Cases – Framework Robustness

As part of developing the IGCC-FCT framework, several cases were run simply to test the robustness of the system; in general these simulations did not incorporate realistic data. Hence, some of the test cases may not be very practical because very different downstream equipment or different-sized equipment might be required (e.g., power generation within a system operating at 90 atm.). However, the cases tested the limits of network stability and included the following simulations:

- Increased Operating Pressure (*baseline*: 18 atm)
 - 30 atm Operating Gasifier Pressure
 - 60 atm Operating Gasifier Pressure
 - 90 atm Operating Gasifier Pressure
- Partial Networks (*baseline*: one gas turbine generator, two SOFC)
 - Removed Gas Turbine Generator
 - Removed single SOFC
 - Removed both SOFC's
- Increased Operating Temperatures (*baseline*: damper stream 290 K)
 - Damper Stream Increased to 1200 K
 - Damper Stream Increased to 1500 K

Though numerous tests have provided insight to the individual gasifier module's response to various conditions, it is important to understand how downstream modules react to changes in the plant network. Calculations, for example, do not illustrate the downstream results of operating the gasifier at pressures up to 90 bar (i.e., the plant system pressure required if the IGCC plant includes CO_2 sequestration). To test the robustness and integrity of downstream processes the network was configured to maintain the high pressures generated in the gasifier throughout the gas clean up and power generation cycles. Because the cases were designed simply to test framework and model stability under extreme conditions, downstream module configurations were not altered to account for the higher pressures. As a result, though each high-pressure case completely executed *successfully*, module calculations and configurations may not represent reasonable values.

In similar fashion, cases were designed to illustrate network stability under conditions of varying temperature, slurry % coal composition, flow rate, inlet stream properties, and some cases even removed selected modules from the network. No runtime errors were encountered, suggesting the need for “reasonability” checks and warnings embedded into module code to enhance framework usefulness. Such code enhancements would offset the dependency of successful framework utilization upon a knowledgeable user.

2.2.7 VEF Simulation of Vision 21 Reference Configuration

Extensive testing was performed in order to confirm that all component models had been successfully ported from the SCIRun-based IGCC-FCT framework to the VE-Suite-based framework, VEF. In addition to running tests to compare individual module calculations against previous models, the modules were also wired together in a full network with inputs identical to those of benchmarked configurations. The primary test case used was the DOE-provided Vision 21 reference configuration (see Figures 1.3.10-1.3.11 and Tables 1.3.1-1.3.2) which includes a two-stage, oxygen-blown gasifier, WGPU system, and a hybrid fuel cell/turbine power block. The UI for the VEF, when operating on a standard PC, is shown in Figure 2.2.42.

Close inspection of stream properties at key points within the network showed that calculations from the VEF matched closely with values from the IGCC-FCT framework. Slight differences can occur due to differences in compiler options, software libraries used and numerical round-off issues for Linux and Windows platforms. The IGCC-FCT framework was SCIRun-based and thus could only execute on a Linux platform, whereas the VEF makes use of both Linux and Windows systems. For the calculations presented in this section, the component models were executed on a Windows-based PC. Overall, comparing individual module results has demonstrated good agreement between the different frameworks, providing confidence that module codes were successfully ported into the VEF.

As an example, illustrated in Table 2.2.25 are summary tables showing comparisons of the stream properties exiting the syngas clean up and second (low pressure) SOFC for the SCIRun based IGCC-FCT and VE-Suite based VEF frameworks. Comparing the tabulated values, there is very close agreement.

Illustrated in Table 2.2.26 is a summary table for power consumed/generated for several pieces of equipment in the plant configuration. Again, there is close agreement between the SCIRun based IGCC-FCT and VE-Suite based VEF frameworks; discrepancies, where they occur, are on the order of fractions of a %.

Illustrated in Figure 2.2.43 are the results windows for the gasifier model, captured directly from the old and new frameworks (i.e., summary output windows). Due to differences in software used for the SCIRun based IGCC-FCT framework (TCL) and the VE-Suite based framework (wxWindows which is platform independent), the summary windows are not the same in appearance. In addition, the results window for modules in the VEF has been enhanced to include additional parameters, such as soot and tar content in the syngas, to facilitate a more detailed examination of the properties and trends when performing comparative studies. Nevertheless, close inspection of the numerical values listed in Figure 2.2.43 demonstrate there

is close agreement in the predicted values for the gasifier module – a key element within the plant configuration.

Illustrated in Figure 2.2.27 are comparisons of results for overall plant performance parameters. As can be seen from the tabulated results, there is close agreement between the SCIRun based IGCC-FCT framework and the VE-Suite based VEF.

Figure 2.2.42. UI for the VE-Suite-based VEF operating on a 2D screen. Shown is the Vision 21 reference configuration.

Table 2.2.25. Comparison of Predicted Values for SCIRun-based IGCC-FCT Framework and VE-Suite-Based VEF for Vision 21 Reference Configuration.

Stream Properties Exiting Gas Clean up			Stream Properties Exiting SOFC B		
Property	IGCC-FCT	VEF	Property	IGCC-FCT	VEF
Temperature (K)	639.904	639.904	Temperature (K)	1144.52	1143.86
Pressure (Pa)	1.517220E+06	1.517220E+06	Pressure (Pa)	337505	337513
Flowrate (kg/s)	64.568	64.568	Flowrate (kg/s)	391.872	391.875
Pressure Drop (Pa)	130481	130481			
AR	0.000775616	0.000775616	CO	0.00843502	0.00838443
CO	0.441273	0.441273	CO2	0.116333	0.115867
CO2	0.0783085	0.0783085	H2	0.00660089	0.00657404
H2	0.337171	0.337171	H2O	0.105016	0.1046
H2O	0.126657	0.126657	N2	0.663396	0.672065
N2	0.0148493	0.0148492			
ASH	0.753855	0.753855			
CHAR	0.246145	0.246145			

Table 2.2.26. Comparison of Predicted Power Values for SCIRun-based IGCC-FCT Framework and VE-Suite-Based VEF for Vision 21 Reference Configuration.

Module Results		IGCC-FCT	VEF
Component	Property		
Compressor 1	Power Req/Gen (MW)	-3.51 MW	-3.51 MW
Compressor 2	Power Req/Gen (MW)	-0.35 MW	-0.35 MW
Compressor 3	Power Req/Gen (MW)	9.11 MW	9.11 MW
Compressor 4	Power Req/Gen (MW)	137.75 MW	137.75 MW
Compressor 5	Power Req/Gen (MW)	132.70 MW	133.03 MW
Compressor 6	Power Req/Gen (MW)	-54.67 MW	-54.67 MW
Compressor 7	Power Req/Gen (MW)	-85.55 MW	-85.55 MW
Bulk Desulfurizer	COS Reduction Eff.	99.67	99.67
	H2S Reduction Eff.	99.99	99.99
	Temperature Out (K)	639.9	639.9
Fuel Cell A	Anode Temperature (K)	1129.92	1129.19
	Fuel Cell Power (MW)	141.48	140.45
Fuel Cell B	Anode Temperature (K)	1144.52	1143.86
	Fuel Cell Power (MW)	158.87	158.03
Steam Turbine 1	Power Generated (MW)	48.82	49.14
Steam Turbine 2	Power Generated (MW)	25.23	25.53

Figure 2.2.43. Summary information for the gasifier module in the SCIRun-based IGCCT (left) and VE-Suite-based VEF (right) for the Vision 21 reference configuration.

Table 2.2.27. Comparison of Overall Plant Performance for the SCIRun-Based IGCC-FCT Framework (left) and VE-Suite-Based VEF Framework (right) for the Vision 21 Reference Configuration.

Network Summary Comparison		
	IGCC-FCT	VEF
Gas T-G Net Power (MW)	135.48	135.81
Fuel Cell Power (MW)	300.35	298.48
Steam T-G Power (MW)	74.05	74.67
Net Power Gen. (MW)	509.88	508.96
Thermal Input (MW)	875.69	875.69
Plant Efficiency	58.23%	58.12%

2.2.8 Impact on Plant Efficiency of Cold Gas Clean Up for Hg Removal

The framework has been used to study the impact of using conventional CGCU technology on plant performance. In this study the WGPU equipment in the baseline plant configuration of Figure 2.2.43 is replaced by the CGCU equipment shown in Figure 2.2.44. The CGCU equipment includes a carbon bed unit for Hg removal and an AGR unit. These CGCU models are described in Section 1.3.2. CGCU has an adverse impact on the plant efficiency because the syngas must be cooled prior to the gas clean up process and then must be reheated prior to the next process at the plant. The impact of the location of the carbon bed was also investigated. Three locations of the Hg removal were studied.

The resulting plant efficiencies as calculated by the framework and the plant effluent Hg are given in Table 2.2.28 for the baseline WGPU configuration and the three CGCU configurations. The reduction in plant efficiency is the result of having to cool the syngas from 650 K to 313 K, cleaning the gas, and then reheating it back to 650 K. The additional heat required to raise this sensible enthalpy of the syngas drops the efficiency by 3 percentage points. This drop is not as large as might be expected because the majority of the sensible enthalpy in the syngas exiting the gasifier at about 1470 K is used to initially heat the water stream for generating power in the steam turbines. However, the plant efficiency for the CGCU cases assumes 100% efficiency in the reheater. Therefore, this calculated plant efficiency for CGCU is an upper bound by as much as another percentage point.

Figure 2.2.43. Baseline configuration with WGCU.

Figure 2.2.44. WGCU configuration with three possible locations of the carbon bed Hg removal unit.

Table 2.2.28 Predicted Plant Efficiencies.

	WGPU	CGCU Location 1	CGCU Location 2	CGCU Location 3
Plant Efficiency, %	58.0	55.0	55.0	55.0

The required size of the carbon bed unit for location 3 is significantly larger than for the other locations due to the larger gas volume flow that must be treated. Whereas the required bed size for locations 1 and 2 is about 5.5 m diameter and 3.9 m high as calculated by the model, and the size for location 3 is 27 m diameter and 11 m high. This same larger size is also required for the WGPU configuration of Figure 2.2.28. This larger size would result in significant capital cost increases. Note that the H₂S removal efficiency is identical in all the cases with four nines of removal assumed to occur in the AGR unit. Likewise, each carbon bed is assumed to reduce the Hg concentration to 1 ppm.

2.2.9 Demonstration of Coupling the VEF to the IECM Framework

A prototype Virtual Engineering-based framework that utilized a computational engine developed by REI, a visualization engine developed by ISU, component models from REI and CMU to predict performance (efficiency, power generated, emissions, etc.), and CMU financial models to predict plant economics (cost of electricity) was demonstrated at the Clearwater Conference 2004. At the conference a joint technical presentation was provided by team members from CMU, ISU and REI [Rubin et al., 2004]. In addition, one-on-one demonstrations of the coupled frameworks were provided at the REI exhibit booth for the conference; for these demonstrations, REI coordinated efforts with a NETL exhibit booth.

For the demonstration, the framework was used to simulate an IGCC plant with CO₂ capture. Hierarchical model support and plug-and-play capabilities were demonstrated by replacing the IECM gasifier with REI's detailed model. The demonstration highlighted the heterogeneous-computing capability of the framework. The demonstration was executed across multiple computational platforms and operating systems – the computational engine and CMU unit models were executed on a Linux workstation, the visualization engine on a Linux cluster, and the detached user interface on a Windows-based laptop and tablet PC. For the demonstration, we made use of a single-wall VR projection system provided by ISU and NETL.

The Virtual Engineering space took advantage of a tight coupling to the integrated IECM model by: dynamically altering its appearance to accurately reflect the configuration chosen by the user; adding 3D gauges to display important plant results/parameters; and adding color mapping of plant components based on data values obtained from model results.

The demonstration allowed full interaction within the framework. The user was able to configure, run, and view results for the plant design of their choice, limited only by the capabilities of the models themselves. The VE space was attached to the computational engine for displaying results and creating a virtual environment to reflect the current plant configuration. Figures 2.2.45-2.2.52 are intended to showcase the Virtual Engineering space and the interactive framework UIs.

The following is a script demonstrating key features of the framework used in the Clearwater Conference demonstration. The script and the corresponding figures illustrate how a user interacts with the framework, and the types of visual feedbacks provided to show model results.

- 1) Initiate the computational engine - the engine is now open via its interfaces and can receive network configurations and data.
- 2) Initiate a CMU Unit model - upon instantiation, the CMU model registers itself with the engine and waits (also via its interface) for data and instructions.
- 3) Initiate the user interface – the UI begins with a "blank slate" (Figure 2.2.45), completely isolated and autonomous from the computational engine and attached models.
- 4) Attach the UI to the computational engine (Figure 2.2.46) – the UI registers itself with the engine, creating a communication path to create and control a plant simulation.
- 5) Load desired pre-configured network (Figure 2.2.47) – available configurations correspond to those available under IECM and are reflected in the VR space (Figure 2.2.48).
- 6) Adjust component model values (Figure 2.2.49) and submit network to computational engine (Figure 2.2.46) – the network (models and connections) and model inputs are passed to the computational engine for storage. The computational engine will use this information for scheduling, resource allocation, and error checking.
- 7) Execute the network (Figure 2.2.46) – the UI signals the computation engine to commence network execution.
- 8) Examine results – the user can view plant results (Figure 2.2.50) and port results (Figure 2.2.51) in both the VR space and the detachable UI environment.
- 9) Demonstrate model plug-n-play capabilities by replacing IECM gasifier model with CFD gasifier model – the configuration change is reflected in the VE space (Figure 2.2.52).
- 10) Resubmit and execute the network – this injects CFD results into the simulation network.
- 11) Examine results - in addition to the visualization options described in #8, the user can now use the VE-Suite interface to examine detailed CFD results directly in the VR space.
- 12) Detach the UI from the computational engine (Figure 2.2.46) – the engine continues to exist independently from the UI. The UI can be reattached at any point to continue running simulations.

Figure 2.2.45. Framework UI.

Figure 2.2.46. Framework UI connection and execution pull down

Figure 2.2.47. Framework UI pre-configured networks.

Figure 2.2.48. Virtual Reality pre-configured networks representation.

Fuel Specification

Reset Coal:

Edit/New Coal:

Ultimate (wt.%)		Proximate (wt.%)		Ash Composition (wt.%)	
C	77.74	H2O	5.05	SiO2	54.14
H	5.14	VM	33.00	Al2O3	17.33
O	5.70	ASH	7.24	TiO2	0.71
N	1.50	FC	54.71	Fe2O3	4.55
S	2.24			CaO	10.83
Cl	0.06			MgO	2.43
Ash	7.62			Na2O	1.50
				K2O	1.12
				SO3	7.12
				P2O5	0.27
				BaO	0.00
				SrO	0.00

Heating Value
HHV (BTU/lb)

Fuel Cost
Minemouth Cost (\$/ton)
Delivered Cost (\$/ton)
Delivered Cost (\$/MBtu)

Figure 2.2.49. Sample framework UI GUI.

Figure 2.2.50. Framework plant results.

Figure 2.2.51. Framework port data results.

Figure 2.2.52. REI gasifier model.

2.2.10 Demonstration of Coupling the VEF to Aspen Plus

To maximize the capabilities of the VEF, the VE-Suite-based framework, special attention was given in the software design to ensure that coupling to other simulation packages was both feasible and practical. As a proof-of-concept test, REI software engineers created a simple coupling to the Aspen Plus process simulation software. Aspen Plus has a wide variety of

component models, and thus represented an ideal test case for framework-to-framework coupling. For this test AspenTech provided REI with an evaluation license of Aspen Plus.

The coupling component made use of the Aspen Plus ActiveX Automation Server for controlling Aspen with software commands from C++. The simple prototype was used to set stream attributes, execute the flow sheet, and to retrieve simulation results. While the coupling component was not generalized, it did illustrate the ability of the framework to make use of Aspen for future upgrades in capabilities.

Based on the success of the proof-of-concept test performed here, in future work it would be possible to implement a more general coupling between the VEF and Aspen Plus to leverage the many equipment component models and Aspen Plus flowsheets of plant configurations (or subsystems within the plant) that have been developed by NETL or NETL-funded researchers working on advanced power systems.

It should be noted that the software modifications to the VEF required to couple the VEF to Aspen Plus were implemented for demonstration purposes only and are not included in the software delivered to NETL.

2.2.11 Demonstration of Using VES-Open for Advanced Data Passing

The software infrastructure of the VEF imposes no limitations on the quantity or type of data that can be passed between component models. This concept was a guiding force in the development of VES-Open, the open source software used to interface models to the framework.

To demonstrate the power and importance of this attribute REI has implemented additional CFD models for a Pipe and Heat Exchanger. Both CFD models are placed immediately downstream of the CFD Gasifier model and utilize REI's *GLACIER* code (see Appendix D for details) as their core computational model. Figure 2.2.53 illustrates the test problem within the framework.

Figure 2.2.53. Three CFD models connected in series.

Dataflow that occurs between the CFD models contains not only the simple scalar data that is utilized by a majority of the models within the framework, but also contains detailed profile information that is extracted directly from model results. This profile information is interpolated onto the inlet plane for the downstream module and becomes a set parameter for the CFD simulation for the downstream device (see Figure 2.2.54).

Figure 2.2.54. Profile data being passed between the CFD models.

Results can be viewed and interacted with in the framework's virtual engineering space in the context of a complete energypex plant (Figure 2.2.55).

Figure 2.2.55. Interacting with coupled CFD models in virtual engineering space.

As is evident from Figures 2.2.54 and 2.2.55, passing only a single point value (e.g., only bulk values) would not suffice for this situation. Here, the profile data passed between subsequent models has a strong impact on the flowfield and the pattern for deposition of material in the downstream heat exchanger. For this example, the CAPE-Open interface would result in the loss of important data, resulting in an inaccurate (and mis-leading) simulation for the downstream

device. In contrast, VES-Open allows more flexible and extensive data passing between the two models and thus enables correctly computing the flowfield solution in the downstream equipment.

2.2.12 Time-Dependent CFD Simulation of Entrained Flow Gasifier

To investigate the ability to perform transient computations for an entrained flow gasifier, the *AIOLOS* reacting CFD tool was used to simulate a startup scenario for the generic, two-stage, slurry-feed gasifier model ($L/D = 6$, see Figure 2.2.56). The integration of the solution through time was performed in a time accurate mode. This simulation was performed by project team members at RECOM Services and the simulations were executed at the supercomputer center at the University of Stuttgart.

Figure 2.2.56. Two-stage industrial gasifier configuration (left) and geometry model (right).

Steady-state results have been generated for the following operating conditions using an Illinois coal #6 (see Table 2.2.29) with a uniform size of $39.8 \mu\text{m}$ as the base fuel:

Coal flow rate:	32.274 kg/s
O ₂ (95% vol.) and N ₂ (5% vol.) flow rate:	23.128 kg/s
H ₂ O (for wet slurry) flow rate:	11.188 kg/s
Gasifier pressure:	18 atm
Inlet coal temperature:	422 K
Inlet O ₂ temperature:	475 K

Table 2.2.29. Fuel Properties of Illinois coal #6.

Proximate Analysis	As-Received (wt-%)
Volatile Matter	34.99
Fixed Carbon	44.19
HHV (Btu/lb)	11666
Ultimate Analysis	As-Received (wt-%)
Carbon	63.75
Hydrogen	4.50
Nitrogen	1.25
Sulfur	2.90
Moisture	11.12
Ash	9.7
Oxygen	6.78

Steady-state results have been generated assuming a completely dried coal with 100 % vaporized slurry water. Furthermore, the injectors have been modeled assuming ideal mixing between the streams. Results showing average profiles of major species concentrations and average temperature over gasifier height are shown in Figures 2.2.57 and 2.2.58. The gasifier exit conditions predicted with *AIOLOS* are summarized in Table 2.2.30 and compared to the corresponding *GLACIER* simulations performed by REI.

Figure 2.2.57. Average profiles of major species concentrations over gasifier height.

Figure 2.2.58. Profiles of average and peak temperature over gasifier height.

Table 2.2.30: Two-Stage Gasifier Exit Conditions Predicted by *AIOLOS* and *GLACIER*.

	<i>AIOLOS</i>	<i>GLACIER</i>
CO-Concentration	45.5 Vol.-%	43.0 Vol.-%
H ₂ -Concentration	34.1 Vol.-%	32.3 Vol.-%
H ₂ O-Concentration	10.9 Vol.-%	14.0 Vol.-%
CO ₂ -Concentration	7.0 Vol.-%	8.2 Vol.-%
CH ₄ -Concentration	0.5 Vol.-%	0.18 Vol.-%
O ₂ -Concentration	0.0 Vol.-%	0.00 Vol.-%
Heating Value and Mass Flow	12260 kJ/kgGas (62.61 kgGas/s)	11499 kJ/kgGas (62.57 kgGas/s)
Cold-gas efficiency	87.5 %	82.2 %

A startup scenario going from 50% load to 100% load by increasing the load in 10% increments has been defined and modeled. The initial conditions used assumed a gas composition of air (23.3 wt% O₂ and 76.7 wt% N₂) at a pressure of 18 atm and a temperature of 1000°C. The 100% load settings of the steady-state analysis were used to determine the 50%-100%-load gasification conditions by simply reducing all the mass flows according to the load:

The time-marching arrangement summarized in Table 2.2.31 has been used to simulate the startup scenario:

Table 2.2.31: Time-Marching Arrangement for the Two-Stage Gasifier Startup Scenario.

Load	Time	Time Steps	Δt	Iterations	SX5-CPUh
50 %	0.0 - 0.5 s	50	0.01 s	250,000	18.50
50 %	0.5 - 1.5 s	50	0.02 s	300,000	22.20
50 %	1.5 - 4.0 s	50	0.05 s	600,000	44.40
50 %	4.0 - 4.5 s	5	0.10 s	110,000	08.14
50 %	4.5 - 5.5 s	5	0.20 s	110,000	08.14
50 %	5.5 - 10.5 s	10	0.50 s	400,000	29.60
50 %	10.5 - 20.5 s	10	1.00 s	450,000	33.30
60 %	20.5 - 21.5 s	10	0.10 s	200,000	14.80
60 %	21.5 - 26.5 s	10	0.50 s	400,000	29.60
60 %	26.5 - 31.5 s	5	1.00 s	225,000	16.65
70 %	31.5 - 32.5 s	10	0.10 s	200,000	14.80
70 %	32.5 - 37.5 s	10	0.50 s	400,000	29.60
70 %	37.5 - 42.5 s	5	1.00 s	225,000	16.65
80 %	42.5 - 43.5 s	10	0.10 s	200,000	14.80
80 %	43.5 - 48.5 s	10	0.50 s	400,000	29.60
80 %	48.5 - 53.5 s	5	1.00 s	225,000	16.65
90 %	53.5 - 54.5 s	10	0.10 s	200,000	14.80
90 %	54.5 - 59.5 s	10	0.50 s	400,000	29.60
90 %	59.5 - 64.5 s	5	1.00 s	225,000	16.65
100 %	64.5 - 65.5 s	10	0.10 s	200,000	14.80
100 %	65.5 - 67.5 s	5	0.50 s	200,000	14.80
100 %	67.5 - 68.5 s	1	1.00 s	45,000	03.33
Total	68.5 s	296		5,965,000	441.41

In the applied time-marching arrangement (see Table 2.2.31) time steps ranging from 0.01 s to 1 s have been used to describe the process. An iterative SIMPLE method requiring 5,000 ($\Delta t = 0.01$ s) to 45,000 iterations ($\Delta t = 1$ s) per time step was applied to converge each time level. A total number of 296 time steps covering 68.5 real-time seconds have been computed requiring a total number of 5,965,000 iterations. The calculations have been performed on a Vector Supercomputer (NEC SX5) consuming a total number of 441.41 SX5-CPUh. If the same simulation were to be performed on a more affordable machine, such as a sixteen CPU Linux cluster (P4 cpus), we estimate that the same simulation would require ~170 hrs of continuous compute time.

In the startup simulation, 20.5 real-time seconds were modeled for the initial 50%-load increase to reach acceptable steady-state conditions. In order to reduce the computational expenditure for the entire calculation, it has been decided to calculate a constant time period of 11 s on each load level before switching to the next load level (disregarding the fact that this might be too short to achieve steady-state conditions on every load level).

The transient results are exemplified in Figures 2.2.59-2.2.74, which show time-dependent temperature and CO values for the 50%-load startup. The results after 0.2 s (Figures 2.2.59 and 2.2.60) show a deep jet penetration into the center region of the geometry in the second stage. The jets in the first stage tend to build a concentric ring along the gasifier wall. In the following 0.2 s (Figures 2.2.61-2.2.62) the rotating flow from the first stage reaches the second stage and produces a CO rich center region and very high local temperatures in the geometry and at the furnace walls. In the following 0.6 s (Figures 2.2.65-2.2.72) the center CO bubble from the second stage moves downwards into the center part of first stage producing a homogenous well-mixed CO field in the bottom part of the gasifier. At the same time, the near wall flow from the first stage is moving upwards to the gasifier exit. During this process, local temperatures can reach very high values $> 2500^{\circ}\text{C}$. After 2 s the entire gasifier is filled with a homogenous CO-level with some peak areas in the bottom part of the gasifier (Figures 2.2.73 and 2.2.74). In the subsequent time, the CO level slowly increases to the steady-state value that is reached at time level 20.5 s (see movie-file 2Stage-T-50-100%Load.mpg).

More detailed results are available in the corresponding movie-files:

- 2Stage-T-50-100%Load.mpg
- 2Stage-CO-50-100%Load.mpg
- 2Stage-CO2-50-100%Load.mpg
- 2Stage-O2-50-100%Load.mpg
- 2Stage-H2-50-100%Load.mpg

A copy of these movie files was provided to the DOE during the course of this project.

The transient gasifier simulation described above was executed at a supercomputer center and thus was performed in a standalone manner. The simulation could have been performed within the SCIRun- or VE-Suite-based frameworks developed within this project using localized computational resources (e.g., Linux cluster). In this manner, the framework would be able to control, monitor, and adjust (“steer”) the simulation as it executes. From a pure technical viewpoint, the desired degree of control of the simulation can be achieved. However, to have the same level of control over a simulation executing at a supercomputer center requires resolving many administrative issues (e.g., firewalls and other security issues) that go beyond the scope of this project.

Figure 2.2.59. Computational results of inner, near wall, and mean CO concentrations ($t = 0.2$ s).

Figure 2.2.60. Computational results of inner, near wall, and mean temperature ($t = 0.2$ s).

Figure 2.2.61 Computational results of inner, near wall, and mean CO concentrations ($t = 0.3$ s).

Figure 2.2.62. Computational results of inner, near wall, and mean temperature ($t = 0.3$ s).

Figure 2.2.63. Computational results of inner, near wall, and mean CO concentrations ($t = 0.4$ s).

Figure 2.2.64. Computational results of inner, near wall, and mean temperature ($t = 0.4$ s).

Figure 2.2.65. Computational results of inner, near wall, and mean CO concentrations ($t = 0.5$ s).

Figure 2.2.66. Computational results of inner, near wall, and mean temperature ($t = 0.5$ s).

Figure 2.2.67. Computational results of inner, near wall, and mean CO-concentrations ($t = 0.6$ s).

Figure 2.2.68. Computational results of inner, near wall, and mean temperature ($t = 0.6$ s).

Figure 2.2.69. Computational results of inner, near wall, and mean CO concentrations ($t = 0.8$ s).

Figure 2.2.70. Computational results of inner, near wall, and mean temperature ($t = 0.8$ s).

Figure 2.2.71. Computational results of inner, near wall, and mean CO concentrations ($t = 1.0$ s).

Figure 2.2.72. Computational results of inner, near wall, and mean temperature ($t = 1.0$ s).

Figure 2.2.73. Computational results of inner, near wall, and mean CO-concentrations ($t = 2.0$ s).

Figure 2.2.74. Computational results of inner, near wall, and mean temperature ($t = 2.0$ s).

Chapter 3 - Conclusions

In this report, REI has described our work effort to develop and demonstrate a software framework to support advanced process simulations for evaluating the performance of Advanced Power Systems. Integrated into the framework are a broad range of models, analysis tools, and visualization methods that can be used for the plant evaluation. The framework provides a tightly integrated problem-solving environment, with plug-and-play functionality, and includes a hierarchy of models, ranging from fast running process models to detailed reacting CFD models. The framework places no inherent limitations on the type of physics that can be modeled, numerical techniques or programming languages used to implement the equipment models, or the type or amount of data that can be exchanged between models. Tools are provided to analyze simulation results at multiple levels of detail, ranging from simple tabular outputs to advanced visualization methods commonly used in CFD analysis. By design, the framework provides seamless communication between all models and tools. In addition, the framework can be coupled to other software frameworks that provide different modeling capabilities.

The focus and capabilities of the framework have evolved during the course of the project resulting in the development of three distinct frameworks.

- 1) The initial efforts focused on creating a framework for simulating the DOE Low Emissions Boiler System Proof of Concept (LEBS-POC) facility, an advanced pulverized-coal combustion-based power plant. Included in the framework were a CFD model for the LEBS boiler and process models for the downstream equipment, which included a heat exchanger, baghouse, and SCR unit.
- 2) Subsequent efforts focused on developing a framework to simulate an Integrated coal Gasification Combined Cycle - Fuel Cell Turbine (IGCC-FCT) plant configuration. For this framework, models were developed for entrained flow and transport reactor coal gasifiers as well as numerous pieces of downstream equipment to simulate the performance of the syngas clean up system, fuel cells (SOFCs), a HRSG, direct-fired (combustion) turbine and a hybrid power block that contained a SOFC, SOFC tail gas combustor, and simple turbine. In addition, models for balance of plant equipment were implemented. The coal gasifier models included CFD and process models with state-of-the-art capabilities for the commercially dominant systems. Submodels implemented included high-pressure coal gasification kinetics to better predict carbon conversion, a flowing slag wall model to estimate the slagging behavior of mineral matter deposited on the gasifier walls and its impact on heat transfer properties, and models for soot and tar evolution, which will also impact syngas heat transfer properties in the gasifier. Interfacing models to the framework was performed using VES-Open, and tests were performed to demonstrate how to interface CAPE-Open-compliant models to the framework.
- 3) The IGCC-FCT framework was subsequently extended to support Virtual Engineering concepts in which plant configurations can be constructed and interrogated in a three-dimensional (3D), user-centered, interactive, immersive environment. The Virtual Engineering Framework (VEF) was developed through close collaboration with NETL supported research teams from Iowa State University Virtual Reality Applications Center (ISU-VRAC) and Carnegie Mellon University (CMU). The VEF is *open source*, compatible across systems ranging from inexpensive desktop PCs to large-scale,

immersive facilities, and provides support for heterogeneous distributed computing of plant simulations. The ability to compute plant economics through an interface that coupled the CMU IECM tool to the VEF was demonstrated. Likewise, the ability to couple the VEF to Aspen Plus, a commercial flowsheet modeling tool, was demonstrated. Software support is included for interfacing models to the framework with VES-Open. CAPE-Open-compliant models can be interfaced to the framework by using VES-Open.

Throughout the course of the project, evaluations and comparisons to available data have been performed for individual equipment components and of overall plant performance to build confidence in the developed models and analysis capability. Simulations were performed to explore the impacts of a broad range of conditions, including alternative process conditions, fuel switching, coal kinetics, operating at elevated pressure, as well as altering the equipment used to allow Hg capture and improved heat integration.

The frameworks provide simulation capabilities not available in currently available commercial tools. The functionality and capabilities provided by the frameworks, as well as model validation results, have been highlighted through participation at NETL sponsored technical conferences focused on coal utilization and gasification, NETL program workshops and NETL program reviews, and project-specific meetings held between REI and NETL personnel. The software frameworks, including the component models, have been installed at NETL and training has been provided to NETL personnel. The knowledge base developed during this project has been used to provide guidance and suggestions to gasification industry personnel on improvements to equipment and process and also in discussions with personnel from the electric utility industry and fuel suppliers to the utility industry for IGCC issues. In addition to advanced power systems, REI has successfully reused software elements and lessons learned from the frameworks created in this project to develop frameworks for addressing problems in other industries and other applications. Discussions with a potential commercialization partner for the framework are in progress. Likewise, discussions are in progress with potential customers on applying the developed modeling capability to novel coal gasification systems.

NETL will benefit in several ways from the Virtual Engineering-based software framework and plant performance modeling capability provided in the VEF. In particular, the VEF can be used as an important next step toward the ultimate goal for simulation for the NETL Advanced Power Systems Research program - a fully integrated environment for performing dynamic plant simulation and engineering, which DOE has targeted to achieve by 2010. The VEF also provides DOE with a mechanism to enable and foster collaborations amongst a broad range of researchers from universities, industry, or DOE, whether US based or International, that are developing technologies for the gasification industry. In addition, other DOE programs focused on advanced power generation systems, such as Ultra Super Critical boiler development or the proposed FutureGen initiative, can benefit from the developed software frameworks.

References

Allam, R. J., Topham, A., "Integrated Air Separation Plant-Integrated Gasification Combined Cycle Power Generator," U.S. Pat. No. 5081845, Jan. 21, 1992.

B&W, *Steam – its generation and use*, 40th edition, Babcock & Wilcox, 1992.

Benyon, P., Inumaru, J., Otaka, M., Hara, S., Watanabe, H. and Kent J. "Engineering Modelling of High Pressure and Temperature Entrained-Flow Gasifiers," Japan-Australia Joint Technical Meeting on Coal, December 5-6, 2000, Fukuoka, Japan.

Bessette, N.F., "Modeling and Simulation for Solid Oxide Fuel Cell Power Systems," Ph.D. Thesis, 1994.

Black & Veatch, Shell synthetic fuels IGCC 500 MW reference plant EPRI project report, November 1994.

Bockelie, M.J., Swensen, D.A., and Denison, M.K., "Computational Workbench Environment for Virtual Power Plant Simulation", in Proceedings of the 26th International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, FL, USA, March 5-8, 2001(a).

Bockelie, M.J., Swensen, D.A., and Denison, M.K., and Sarofim, A., "A Computational Workbench for Simulating Power Plant Systems", Presented at the ASME International Joint Power Generation Conference 2001, New Orleans, Louisiana, June 4-7, 2001(b).

Bockelie, M.J., Swensen, D.A., Denison, M.K., Sarofim, A.F., "A Computational Workbench Environment For Virtual Power Plant Simulation," presented at the Vision 21 Program Review Conference, Morgantown, WV, Nov. 6-7, 2001(c).

Bockelie, M.J., Swensen, D.A., Denison, M.K., Chen, Z., Senior, C.L., Sarofim, A.F., "A Computational Workbench Environment for Virtual Power Plant Simulation", *Proceedings of the 27th International Technical Conference on Coal Utilization and Fuel Systems*, Clearwater, FL, USA, March 4-7, 2002(a).

Bockelie, M.J., Swensen, D.A., Denison, M.K., Chen, Z., Senior, C.L., Sarofim, A.F., "A Computational Workbench Environment for Virtual Simulation of a Vision 21 Energyplex", *Proceedings of the ASME International Joint Power Generation Conference 2002*, Phoenix, AZ, USA, June 24-27, 2002(b).

Bockelie, M.J., Denison, M.K., Chen, Z., Senior, C.L., Linjewile, T., Sarofim, A.F., "CFD modeling of Entrained Flow Gasifiers for Vision 21 Energyplex Systems," *Proceedings of the 19th Annual International Pittsburgh Coal Conference*, Pittsburgh, PA, USA, Sept. 24-26, 2002(c).

Bockelie, M.J., Denison, M.K., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., Holt, N., "CFD modeling for Entrained Flow Gasifiers," *Proceedings of the Gasification Technologies Conference, 2002*, San Francisco, CA, Oct.28-30, 2002(d).

Bockelie, M.J., Swensen, D.A., Denison, M.K., Chen, Z., Senior, C.L., Sarofim, A.F., "A Computational Workbench Environment for Virtual Power Plant Simulation", Presented at the NETL Simulation Workshop held at Iowa State University, Ames, IA, USA, Nov. 19-20, 2002(e).

Bockelie, M.J., Swensen, D.A., Denison, M.K., Maguire, M., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., "A Process Workbench for Virtual Simulation of Vision 21 Energyplex Systems," *Proceedings of the 28th International Technical Conference on Coal Utilization & Fuel Systems*, Clearwater, Florida, USA, March 10-13, 2003(a).

Bockelie, M.J., Swensen, D.A., Denison, M.K., Maguire, M., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., "Vision 21, The Next Generation Energy Plant, Description of its Goals and Progress in Developing Simulation Tools for It," Presented at the International Symposium of Utilization of Coal and Biomass: Energy and Environment, to be held in Newcastle, Australia, August, 28-29, 2003(b).

Bockelie, M.J., Sarofim, A.F., Denison, M.K., Swensen, D.A., Maguire, M., Weinstein, D., Davison de St. Germain, J., "Computational Workbench Environment for Virtual Power Plant Simulation," poster presented at the 28th International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, USA, March 10-13, 2003(c).

Bockelie, M.J., Denison, M.K., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., "Using Models To Evaluate Gasifier Performance," to be included in the *Proceedings of the 20th Annual International Pittsburgh Coal Conference*, Pittsburgh, PA, USA, Sept. 15-19, 2003(d).

Bockelie, M.J., Swensen, D.A., Maguire, M., Yang, C., Denison, M.K., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., "A Process Workbench for Virtual Simulation Of Advanced Power and Polygeneration Systems" *Proceedings of the 29th International Technical Conference on Coal Utilization & Fuel Systems*, Clearwater, Florida, USA, April 18-22, 2004.

Bockelie, M.J., Swensen, D.A., Yang, C., Denison, M.K., Senior, C.L., Sarofim, A.F., "A Software Framework For Modeling Advanced Power generation Systems" to be presented at the *30th International Technical Conference on Coal Utilization & Fuel Systems*, Clearwater, Florida, USA, April 16-21, 2005.

Bond, T. C., Noguchi, R.A., Chou, C-P., Mongia, R.K., Chen, J-Y and Dibble, R.W., "Catalytic combustion of natural gas over supported platinum: Flow reactor experiments and detailed numerical modeling." *American Society of Mechanical Engineers Technical Papers*. 96-GT-130, 1996.

Bool, L.E., Helble, J.J., Shah, N., Shah, A., Huffman, G.P., Huggins, F.E., Rao, K.R.P.M., Sarofim, A.F., Zeng, T., Raschke, R., Gallien, D., and Peterson, T.W., "Fundamental Study of Ash Formation and Deposition: Effect of Reducing Stoichiometry," Final Report for DOE Contract No. DE_AC22-93PC92190, 1995.

Boras, G., and Holt, N., "Pulverized Coal and IGCC Plant Cost and Performance Estimates," *Proceedings of the Gasification Technologies Conference 2004*, Washington, DC, CA, Oct.3-6, 2004.

Bracht, M., P.T. Alderliesten, R. Kloster, R. Pruschek, G. Haupt, E. Xue, J.R.H. Ross, M.K.Koukou, N. Papyannokos, "Water gas shift membrane reactor for CO₂ control in IGCC systems: techno-economic feasibility study," *Energy Convers. Mgmt Vol. 38, Suppl.*, pp. S159-S164, 1997.

Brown AL, and Fletcher TH., *Energy Fuels*, 1998, 12, 745-757.

Calgon Carbon Corporation, "Product Bulletin: HGR for Mercury Removal," PB-1047-12/99.

Campanari S., "Thermodynamic model and parametric analysis of a tubular SOFC module," *Journal of Power Sources*, Jan., 2001.

Chan, W.R.; Kelbon, M.; Krieger, B.B.: "Modelling and Experimental Verification of Physical and Chemical Processes During Pyrolysis of a Large Biomass Particle", *FUEL*, Vol. 64, pp. 1505-1513, 1985.

Chen, J-Y., "Development of Reduced Mechanisms for Numerical Modeling of Turbulent Combustion," Workshop on Numerical Aspects of Reduction in Chemical Kinetics, CERMICS-ENPC, Cite Descartes, Champs sur Marne, France, Sept. 2, 1997.

Chen, C. Miyoshi, T., Kamiya, H., Horio, M., and Kojima, T., "On the Scaling-up of a Two-Stage Air Blown Entrained Flow Coal Gasifier", *The Canadian Journal of Chemical Engineering*, **77**, 745-750 (1999).

Chen, C., Horio, M., and Kojima, T., "Numerical Simulation of Entrained Flow Coal Gasifiers", *Chemical Engineering Science*, **55**, 3861-3883 (2000).

Chou, C-P., Chen, J-Y., Evans, G.H. and Winters, W.S., "Numerical Studies of Methane Catalytic Combustion Inside a Monolith Honeycomb Reactor Using Multi-Step Surface Reactions," *Combustion Science and Technology*, Vol. 150 pp27-57, 2000.

Coulson, J. M., and Richardson, J. F., with Backhurst, J. R., and Harker, J. H., *Chemical Engineering Volume 2, Fourth Edition*, Pergamon Press, Oxford. 1991.

Damle, A.S., Gangwal S.K., Venkataraman V.K., "A Simple Model for a Water Gas Shift Membrane Reactor," *Gas Sep. Purif.* 8, p. 101. 1994.

Davis, K., Shim, H., Lignell, D., Denison, M., Felix, L., Giaer, T., Morrow, R., Risio, B., "Evaluation of Wood Firing Strategies Using CFD Simulations," The Electric Power Conference, Houston, TX, March 2003.

Davis B.M., Vimalchand P., Liu G., Smith P.V. and Longanbach J., Operation of the PSDF transport gasifier, 19th Annual Pittsburgh Coal Conference, September 23-27, 2002, Pittsburgh, Pennsylvania.

De Nevers, N., *Air Pollution Control Engineering*, 2d ed., McGraw-Hill, New York, Chapter 9, 2000.

Denison, M.K., Bockelie, M.J., Chen, Z., Senior, C.L., Linjewile, T., Sarofim, A.F., "CFD-Based Models of Entrained-Flow Coal Gasifiers with Emphasis on Slag Deposition and Flow," presented at the Colloquium on Black Liquor Combustion and Gasification, Park City Utah, USA, May 13-16, 2003.

Denison, M.K., Zhao, W., Bockelie, M.J., Sarofim, A.F., "Modeling Support for Incineration of Building", Final Report for EPA contract 4C-R010-NASX, to be published April, 2005.

Devarajan T.S, Peter N. Pintauro, "The water gash shift reaction assisted by a palladium membrane reactor," *Ind. Eng. Chem. Res.* 30, pp 585-589, 1991.

Dhir, V.K. and Lienhard, J.H., "Laminar Film Condensation on Plane and Axisymmetric Bodies in Non-uniform Gravity," *J. Heat Transfer*, Vol. 93, p. 97, 1971.

DOE, Vision 21 Program Plan: Clean Energy for the 21st Century, Federal Energy Technology Center, Office of Fossil Energy, U.S. Department of Energy, 1999.

DOE-NETL, Texaco Gasifier IGCC Base Cases, PED-IGCC-98-001, July 1998, Latest Revision, June 2000a.

DOE-NETL, DESTEC Gasifier IGCC Base Cases, PED-IGCC-98-003, September 1998, Latest Revision, June 2000b.

Dumesic, J.A., Topsoe, N.Y., Slabiak, T., Morsing, P., Clausen, B.S., Tornqvist, E., and Topsoe, H., 1993, "Microkinetic Analysis of the Selective Catalytic Reduction (SCR) of Nitric Oxide over Vanadia/Titania-Based Catalysts," in *Proceedings 10th International Catalysis Congress*, July 19-24, Elsevier, Vol. B, pp. 1325-1337.

Dumesic, J.A., Topsoe, N.Y., Topsoe, H., Chen, Y., and Slabiak, T., "Kinetics of Selective Catalytic Reduction of Nitric Oxide by Ammonia over Vanadia/Titania," *Journal of Catalysis*, Vol. 163, 1996, pp. 409-417.

Edlund, D.J., "A catalytic membrane reactor for facilitating the water-gas shift reaction at high temperature," DOE Contract No. DE-FG03-91ER81229, in Coal-Fired Power Systems 94 – Advances in IGCC and PFBC Review Meeting, Morgantown, WV, July 21-23, 1994.

Eurlings J.Th.G.M. and Ploeg J.E.G., Process performance of the SCGP at Buggenum IGCC, Gasification Technologies Conference, San Francisco, California, October 18-20, 1999.

Fletcher T.H., Kerstein A.R., Pugmire R.J. and Grant D.M., *Energy & Fuels*, 4, 54, 1990.

FutureGen, <http://www.fossil.energy.gov/programs/powersystems/futuregen>, 2004

Gemmen, R.S., "Oxidation of Low Calorific Value Gases—Applying Optimization Techniques to Combustor Design," U.S. DOE FETC, Presented at the 1998 IJPGC, Baltimore, MD, Aug 23-26, 1998.

Gemmen, R.S., Liese, E., Rivera, J.G., Faryar J. and Brouwer, J. "Development of dynamic modeling tools for solid oxide and molten carbonate hybrid fuel cell gas turbine systems". ASME, May 8-12, 2000.

Ghezel-Ayagh, H. and Maru, H. "Direct Fuel Cell/Turbine System for Ultra High efficiency Power Generation." *2002 Fuel Cell Seminar*, November 18-21, Palm Springs, California, pp.356-359. 2002

Gordon, S and McBride B.J., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications," NASA Reference Publication 1311, October 1994.

Guenther C., Shahnam M., Syamlal, M., Longanbach J., Cicero D. and P.V. Smith, "CFD modeling of a transport gasifier", 19th Annual Pittsburgh Coal Conference, September 23-27, 2002.

Hannes J.P., Svoboda K., van den Bleek and Renz U. "Mathematical modeling of CFBC: An overall modular programming frame using a 1.5-dimensional riser model", *proceedings of the 12th International Conference on Fluidized Bed Combustion*, (L.N. Rubow ed.), San Diego, CA, 455-463, 1993.

Harding, S.; Adams, B., Biomass as a reburning fuel: a specialized cofiring application. *Biomass & Bioenergy* **2000**, 19, 429-445.

Holt, N., "Coal Gasification Research, Development and Demonstration – Needs and Opportunities," presented at the Gasification Technologies 2001 Conference, San Francisco, CA, Oct. 8-10, 2001.

Holt, N., "Pulverized Coal and IGCC Plant Cost and Performance Estimates," Proceedings of the Gasification Technologies Conference 2004, Washington, DC, CA, Oct.3-6, 2004.

Howard, J.B., Williams, G.C., Fine, D.H.: "Kinetics of Carbon Monoxide Oxidation in Post-Flame Gases", 14th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, pp. 975-986, 1972.

Johnson C., "Interactive simulation and visualization," *COMPUTER* 32 (12), DEC, 1999

Jones, W.J.; Lindstedt, R.P.: "Global scheme for hydrocarbon combustion", *Combustion and Flame*, Vol. 73, p. 233, 1988.

Keating, M.H., et al. Mercury Study Report to Congress, Volume I: Executive Summary, EPA-452/R-97-003, December 1997.

Kobayashi, H., Howard, J.B. and Sarofim, A.F., Coal devolatilization at high temperatures, *6th Symposium (Int) on Combustion*, The Combustion Institute, 411-425, 1977.

Kohl, Arthur L., and Nielsen, Richard B., "Gas Purification." Fifth Edition, Gulf Publishing Company, Houston, Texas. 1997.

Kolaczowski, S.T., "Catalytic Stationary Gas Turbine Combustors: A Review of the Challenges Faced to Clear the Next Set of Hurdles." *Trans IchemE*, vol 73, Part A, 1995 pp168-190.

Korens, Nick, and Simbeck, Dale R., and Wilhelm, Donald J., "Process Screening Analysis of Alternative Gas Treating and Sulfur Removal for Gasification." Prepared for U.S.D.O.E./N.E.T.L. Task Order No. 739656-00100. December 2002.

Kunii, D., and Levenspiel, O., *Fluidization Engineering*, John Wiley and Sons Inc., 1969, pp 698-699.

Kunii D. and Levenspiel O., *Fluidization Engineering*, 2nd, John Wiley & Sons, New York, 1991.

Leonard R., Pinkston T., Rogers L. and Wheeldon J., The PSDF – Commercial readiness for coal power – revisited, 2002.

Liese, E., Gemmen, R. S., et al., "Development of Dynamic Modeling Tools for Solid Oxide and Molten Carbonate Hybrid Fuel Cell Gas Turbine Systems", Submitted for presentation at the International Gas Turbine Institute meeting of ASME, May 2000.

Liese, E., Gemmen, R. S., "Dynamic Modeling Results of a 1 MW Molten Carbonate Fuel Cell/Gas Turbine Power System," Proceedings of ASME TURBO EXPO 2002, Amsterdam, The Netherlands

Liu, G., Niksa, S., "Coal Conversion Submodels for Design Applications at Elevated Pressures. Part II. Char Gasification," *Progress in Energy and Combustion Science*, 30, 2004

Lupa, A.J. and Kliesch, H.C., "Simulation of a Texaco gasifier, Volume 1: A steady-state model," EPRI final report, September 1979.

Marigliano, G., G. Barbieri, E. Drioli, "Effect of energy transport on a palladium-based membrane reactor for methane steam reforming process," *Catalysis Today* 67, pp. 85-99, 2001.

McClintock, R.B. and Silvestri, G.J., "Some Improved Steam Property Calculation Procedures," *Journal of Engineering for Power*, April 1970.

McCabe, Warren L., and Smith, Julian C., and Harriott, Peter, "Unit Operations of Chemical Engineering," Mc-Graw-Hill Book Company, New York. 1985.

Monazam E.R. and Shadle L.J., Cold flow testing in a large circulating fluidized bed and verification of CFB loop model, 2001.

Montgomery, C., Swensen, D., Shino, D., Yang, C., Brunson, S., Parkinson, A., and Chen, J.-Y. "Selecting the Optimum Quasi-Steady State Species for Reduced Chemical Kinetic Mechanisms," 2003 SIAM Conference on Computational Science and Engineering, San Diego, CA, Feb. 10-13, 2003.

Niksa S. and Kerstein A.R., FLASHCHAIN theory for rapid coal devolatilization kinetics 1. Formulation, *Energy & Fuels*, 5, 673-683, 1991.

Norman, J.; Pourkashanian, M.; Williams, A.: "Modelling the formation and emissions of environmentally unfriendly coal species in some gasification processes", *Fuel*, Vol. 76, No. 13, 1997.

Parker, S.G., Miller, M., Hansen, C.D, Johnson, C.R., "An Integrated Problem Solving Environment: The SCIRun Computational Steering System," 31st Hawaii International Conference on System Sciences (HICSS-31), volume VII, pp. 147-156, Jan. 1998.

Patterson, J.H. Hurst, H.J. Quintanar, A. Boyd, B.K. and Tran, H, "Evaluation of the slag flow characterization of Australian coals in slagging gasifiers," *Research Report 19, Volume 1. Cooperative Research Centre for Black Coal Utilisation*, University of Newcastle, Australia, May, 2001.

Perry, R.H., Green, D.W., *Perry's Chemical Engineers' Handbook 7th ed.*, McGraw-Hill, New York, 1997.

Pontius, D.H., Robinson, M.S., and Vann Bush, P., "Fabric Filter Model – User's Manual", Southern Research Institute, SRI-ENV-92-161-4517, February, 17, 1992.

PSDF, Technical Progress Report, Gasification Test Run GCT3: December 1, 2000 – February 1, 2001, DOE Cooperative Agreement: DE-FC21-90MC25140, Southern Company Services Inc., May 2002.

Ruth, L., and Gemmen, R.S., private communication, July, 2002.

Ruth, L., and James, R., private communication, July, 2002.

Ratafia-Brown, J., Manfredo, L., Hoffman, J., Ramezan, M., "Major Environmental Aspects of Gasification-Based Power Generation Technologies," Prepared for: U.S.D.O.E/N.E.T.L. Gasification Technologies Program, December 2002.

Rubin, E., Bryden, K.M., Bockelie, M.J., Berkenpas, M., McCorkle, D., Swensen, D.A., "A Framework for Virtual Simulation of Advanced Power Systems", presented (no paper) at The 29th International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, USA, April 18-22, 2004.

Sarofim, A.F., Bockelie, M.J., Denison, M.K., Chen, Z., Ma, J., "A Process Workbench for Virtual Simulation Of Advanced Power and Polygeneration Systems" *Proceedings of the 14th IFRF Members Conference, "A Sustainable Energy Supply for Industry: A Challenge for the IFRF"*, Noordwijkerhout, The Netherlands, May 11-14, 2004.

Schneyer, G.P., Cook, J.L., Brownell, D.H., Jr. and Blake, T.R., "Dynamic simulation of a single-stage entrained flow coal gasifier," EPRI final report, December, 1982.

Seader, J. D., Henley, E. J., *Separation Process Principles*, John Wiley & Sons, Inc., New York, 1998, p 776.

Seggiani, M., Modelling and simulation of the time varying slag flow in a Prenflo entrained-flow gasifier. *Fuel*, **77**, 1611, 1998.

Shelton, W., and Lyons, J., Texaco Gasifier IGCC Base Cases, US DOE / NETL report number PED-IGCC-98-001, July 1998, Latest Revision June 2000.

Shim, H., Sarofim, A., Davis, K., Bockelie, M. "Modeling the Impacts of Soot From Low-NOx Combustion Systems", *Proceedings of The 28th International Technical Conference on Coal Utilization & Fuel Systems*, Clearwater, FL, March 2003.

Solomon P.R., Hamblen D.G., Carangelo R.M., Serio M.A. and Deshpande G.V., General model of coal devolatilization, *Energy & Fuels*, **2**, 405, 1988.

Solomon P.R., Serio M.A. and Suuberg E.M., Coal pyrolysis: experiments, kinetic rates and mechanisms, *Prog. Energy Combustion Sci.*, **18**, 133-220, 1992.

Sun, J. and Hurt, R.H., "Mechansisms of Extinction and Near-Extinction in Pulverized Solid Fuel Combustion," *Proceedings of the Combustion Institute*, **28**, 2205-2213, 2000.

Swensen, D.A., Maguire, M., Spencer, R., Shino, D., Li, X., Bockelie, M.J., "Visualization Techniques for CFD Simulations of Industrial Systems, presented at the 27th International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, FL, USA, March 4-7, 2002.

Swensen, D.A., Denison, M.K., Maguire, M., Bockelie, M.J., Montgomery, C.J., Davison de St. Germain, J., "Computational Simulation Environments," poster presented at the Society of Industrial and Applied Mathematicians (SIAM) Computational Sciences and Engineering Conference 2003, San Diego, California, USA, February 10-14, 2003(a).

Swensen, D.A., Yang, C., Maguire, M., Shino, D., Parker, S., Weinstein, D., Davison de St. Germain, J., "Model Interchangeability via Component Architectures for Vision 21 Simulation Environments," poster presented at the 28th International Technical Conference on Coal Utilization & Fuel Systems, to be held in Clearwater, Florida, USA, March 10-13, 2003(b).

Swensen, D.A., Yang, C., Maguire, M., Denison, M.K., Bockelie, M.J., "A Virtual Engineering Framework for Advanced Power Plant Simulation," an exhibit booth demonstration presented at the Super Computing 2004 Conference, Pittsburgh, PA, USA, Nov. 6-12, 2004.

Swensen, D.A., Maguire, M., Yang, C., and Bockelie, M.J., "Computational Frameworks for Practical, Engineering Applications," submitted for presentation at the *SIAM Computational Sciences and Engineering Conference 2005*, Orlando, Florida, USA, February 12-15, 2005.

Steigel, G.J., Clayton, S.J., and Wimer, J.G., DOE's Gasification Industry Interviews: Survey of Market Trends, Issues, and R&D Needs, *Proceedings of the Gasification Technologies 2001 Conference*, San Francisco, CA, Oct. 8-10, 2001.

Tucci, E.R. "Use Catalytic Combustion for LHV Gases." *Hydrocarbon Processing*, pp159-166, 1982.

USDOE, U.S. Department of Energy and Tampa Electric Company, Tampa Electric integrated gasification combined-cycle project, an update, July 2000.

USDOE, U.S. Department of Energy, NETL, Wabash River coal gasification repowering project: A DOE assessment, January 2002.

Wen, C.Y., and Galli, A.F., "Dilute Phase Systems," in *Fluidization*, Davidson, J.F., and Harrison, D., eds., Academic Press Inc., London, 1971, pp 698-699.

Woodward, D. W., Agrawal, R. "Air Separation Process for the Production of Oxygen-rich and Nitrogen-rich Products," U.S. Pat. No. 4936099, June 26, 1990.

Zimont, V.L., Trushin, Y.M.: 'Total Combustion Kinetics of Hydrocarbon Fuels', Comb. Explosion and Shock Waves, Vol. 5, No. 4, pp. 391-394, 1969.

Appendix A

Component Software Issues for Advanced Power Plant Simulation and Engineering – Findings and Recommendations

Contained in this section is a whitepaper authored by REI and distributed to selected personnel at the Clearwater Conference 2003, held in Clearwater, Florida, March 10-14, 2003.

Abstract

During the last two years there has been substantial effort invested by DOE and DOE contractors to better define the needs of Vision 21 simulations. The goal of these efforts has been to identify the appropriate software techniques and capabilities to embody within Vision 21 plant simulator systems to ensure these simulators can support the hierarchy of models and simulation techniques that will be used in near term and future Vision 21 plant simulations.

In this manuscript we summarize our findings and recommendations on the issues of component architectures and component interfaces that are relevant to Vision 21 plant engineering and simulation. These concepts relate to advanced software engineering techniques, originally developed for business applications that have recently been adopted by the scientific computing community. The advent of the Vision 21 program has probably been the first instance of these software techniques being used in simulations for power generation applications. To keep our descriptions brief, we provide summaries, written in “layman terms”, on component architectures (e.g., COM, CORBA, CCA), component interfaces (e.g., Cape-Open) and software frameworks (e.g., ASPEN, SCIRun). We highlight only the key concepts that are relevant to Vision 21 simulation. As described below, direct comparisons between items at different levels of the software engineering hierarchy (e.g., CCA .vs. Cape-Open) are not appropriate.

Our findings are based on research performed within our Vision 21 project, in conjunction with discussions with personnel involved with Vision 21 and with leading researchers in the fields of HPC and scientific computing.

Our findings lead to the following recommendations:

- 1) Near term: Vision 21 simulator frameworks should support both COM and CORBA component architecture versions of the Cape-Open interface standard. We anticipate continued, extensive use of process flow sheet models within Vision 21 plant simulations and engineering. This component interface will allow use of process models developed for process flow sheet simulations from commercial and research sources.
- 2) Long term: an improved component model interface should be developed and deployed to support specific needs of the Vision 21 simulator. In particular, the inherent limitations on data transfer between components imposed by the Cape-Open interface should be eliminated to allow utilization of more comprehensive modeling techniques. The enhanced component interface could be developed through judicious extensions to the Cape-Open standard or by creating a new specification targeted for Vision 21.
- 3) Frameworks: We recommend continued development of Vision 21 simulator framework(s) that can support the hierarchy of models anticipated for future Vision 21 plant simulations. In the near term, commercially available frameworks (e.g., ASPEN) will continue to play an important role in Vision 21 simulation. However, it is unclear that there is sufficient motivation for commercially available frameworks to invest the funds needed to extend their simulation tools to have the flexibility and extensibility desired for advanced plant simulation.

Introduction

Over the course of the last decade, component architectures have revolutionized business software design and implementation. Based on the successes attained in the business software world, developers of scientific computing applications have, over the last several years, taken significant interest in this paradigm. The key features of component methods that make them so attractive for scientific computing are:

- interoperability of software (reuse);
- programming language independence; and
- location transparency.

It is the goal of this document to educate the reader regarding component architecture technology being used to target scientific applications and provide recommendations on how this technology applies to Vision 21 plant simulations.

Background

As software engineering techniques evolved during the early 1990's, it was recognized that the current model for code reuse and application engineering was constrained at best. This original model relied on the use of static and dynamic libraries that contained code (both modular and/or object-oriented) could be directly linked to an application core.

One of the problems with this paradigm is that developers were highly constrained by the language used to generate the libraries. If an application developer was using a language different from that of the libraries, a significant amount of specialty, platform-specific code needed to be generated to utilize the libraries. Also, this paradigm provided no inherent capabilities for platform independence or location transparency. Finally, code reuse was very limited due to the aforementioned language problems and also as a result of non-standard software interfaces (data structures, function parameters etc) used by functions and objects in the libraries.

How did these problems affect scientific and engineering applications? Most notably by limiting code reuse (interoperability), by causing programming language incompatibilities and by requiring extra development effort for any distributed parallelism (executing on remote computational resources).

Component Architecture Concepts

To address these shortcomings, component architectures and component programming models were developed. Component methods specifically target the problems of language independence, location transparency, and interoperability of software. The component programming model is the end of a natural progression, starting from the monolithic application (the old paradigm), and moving toward applications built from increasingly more modularized pieces.

Historically, work on component architectures has been motivated by business-oriented computing. Application of component architectures to scientific and engineering applications is a relatively new endeavor (within last ~5 years).

Component architectures are a step beyond object-oriented programming, where software exists as components of functionality, which interact through well-defined interfaces. This is a bit of a fuzzy concept, which requires some elaboration.

Example: Let's begin with an example of a relatively simple component, which would have broad applications to scientific computing. Assume we want to create a component that will be capable of solving a linear system of the form $Ax=b$.

To begin with, we would write a component interface in a special language called IDL (Interface Definition Language). This language, which is a function of the component architecture chosen, is specifically designed to create *interfaces* – not the equation solver software itself. The IDL written for this example would define language-independent data structures for the matrices, methods (functions) for changing the solution techniques and for setting problem parameters. This is the first step in creating a component.

After the IDL has been written, we use an IDL compiler to compile the IDL code. When we compile the IDL code, we must tell the compiler which programming language to use (C++, FORTRAN, Java, etc). The IDL compiler then creates a programming language specific implementation of our language-independent IDL. We can then take the code generated by the IDL compiler and write the actual implementation of the solver in the appropriate methods of the component.

A developer wishing to use our component would obtain a copy of the IDL code from us and would then compile the code using their language of choice. The developer will now have access to language specific prototype information for the component, which they would then use to access the desired functionality.

One should note that the component developed in this example could be executed on any platform that has an implementation of the target component architecture. Also, the developer need not execute the component on the same computer as their application, which makes use of this component. The details of this location transparency are encapsulated in the specific component architecture being used.

To summarize, the following steps are required to construct and utilize a component in an application (see Figure A.1):

- choose the component architecture of interest (depends on platform, performance requirements, required data structures);
- write the *software interface* to the component using the IDL belonging to the component architecture chosen in previous step;
- compile the IDL code using the IDL compiler; and
- flush out the code generated by the IDL compiler with the details of component's implementation (i.e., code to solve $Ax=b$).

An application requiring the component's functionality can now include client-side code generated by the IDL compiler and make calls to the component via the *software interface*.

Figure A.1. Component creation steps.

Standard Interfaces

While components have allowed us to solve most of the problems associated with language interoperability and location transparency, we haven't discussed the issue of *standard interfaces*. This is a very important topic, especially when we are interested in code reuse and interoperability. *There is tremendous motivation to make use of software components, created by other developers, in new software we are creating.* One can imagine the power of being able to construct scientific applications as compositions of pre-existing functional components.

To make this a reality, we must define standard, domain-specific *interfaces*, which clearly define how components with different types of functionality interact with the outside world. Such standard interfaces make possible a paradigm where a host software application (the *framework*)

can be used to instantiate and interconnect various components with well-defined interfaces to construct an application.

To date, the most significant set of standard interfaces for a domain-specific scientific application is CAPE-Open. CAPE (Component Architectures for Process Engineering) was created to address the needs of the chemical process modeling industry. The goal was to create interoperability and reuse of models developed for use in the large process simulation frameworks (Aspen Plus, Hysys, etc). CAPE is an excellent step in the direction of increased reuse and interoperability for the process simulation community. CAPE interfaces have been created for both COM and CORBA IDLs (see section entitled Flavors of Component Architectures, which is provided below).

Although the CAPE interface specifications are very capable for process engineering problems, one must keep in mind that they were designed specifically for process engineering applications where simple single point scalar data (bulk temperature, pressure, species concentrations, flow rate, etc) is passed to and from components. This in no way detracts from the capabilities of CAPE for process engineering, but must be considered when higher order models and other functional entities must be included in a simulation framework composition.

In the HPC community, numerous efforts are underway to generate standard interfaces for various problem domains such as solvers, mesh manipulation, visualization components, etc. Continued work in this area will lead to a new era in modular HPC applications.

Flavors of Component Architectures

What exactly is a component architecture? A given component architecture is the low-level software that provides all the capabilities that we have discussed in the previous sections. These include the IDL language and IDL compiler, the necessary libraries to perform network communications (where applicable), the “controller” software, which receives and processes requests to instantiate components and numerous other low-level capabilities. There are three main component architectures that are of interest to scientific application developers.

COM/DCOM

COM/DCOM (Component Object Model/DistributedCOM) is the component architecture developed by Microsoft Corporation. It is by far the most widely used general purpose CA. Anyone who uses Microsoft Windows in any of its recent incarnations makes extensive use of COM without even knowing it. Windows uses COM for virtually everything, including their user interface and many core operating system elements. There exists a somewhat small but growing interest in applying COM to scientific applications.

CORBA

CORBA (Common Object Request Broker Architecture) is a widely used, business-oriented component architecture standard developed by the Object Management Group (OMG). The OMG is an open-membership, not-for-profit consortium that produces and maintains computer industry specifications for interoperable enterprise applications. Membership includes virtually every large company in the computer industry and hundreds of smaller ones. While lacking in

the high-performance features of the CCA, the wide user base of CORBA and its mature implementations makes it a logical choice for small- to medium-sized computational models.

CCA

CCA (Common Component Architecture) is the newest component architecture and the only one that is targeted specifically to HPC applications. The CCA effort is funded through the Center for Component Technology for Terascale Simulation Software (CCTSS), which is dedicated to the development of a component-based software development model suitable for the needs of high-performance scientific simulation (CCA).

The Center is funded by the U. S. Dept. of Energy (DOE) as an Integrated Software Infrastructure Center (ISIC) under the Scientific Discovery through Advanced Computing (SciDAC) program and includes members from Argonne, Livermore, Los Alamos, Oak Ridge, Pacific Northwest, Sandia National Laboratories, Indiana University, and the University of Utah.

The CCA specification is still under development although numerous applications have been developed using the current specification. CCA was created to overcome the limitations of the business-oriented CAs (COM/CORBA) with regard to data passing, parallelism, memory management etc. CCA is seeing tremendous growth in the HPC community.

In addition to enhanced performance, CCA boasts some unique capabilities, which further differentiate it from the traditional CAs. Of particular note is its rich IDL (SIDL – Scientific Interface Definition Language), which contains a wide array of datatypes and data structures needed in scientific computing. CCA's SIDL compiler is also the only IDL compiler that can generate FORTRAN 77 and FORTRAN 90 bindings making it particularly useful for legacy scientific application porting.

Although CCA is the clear winner in terms of targeting HPC applications, it is still quite early in development. The available frameworks and associated tools are currently limited to Unix/Linux platforms and require significant expertise to configure and use. With the current significant interest in CCA and continued funding for its development, CCA is and will continue to be the CA of choice for HPC scientific applications.

It should be emphasized that CCA is targeted at HPC software. Specifically, CCA is intended to be used to componentize submodels of detailed computational models. When used in this manner, CCA is far superior to both COM and CORBA. This intra-model componentization is a more demanding application than that of providing a plug-and-play environment for connecting elements of a Vision21 plant together. Although CCA could certainly be used for the plant coupling, the additional complexity of CCA is really overkill for the application.

Overall Structure of Component-based Software with Standard Interfaces

Now that we have discussed the various entities that constitute a component-based application, let's see how the pieces fit together. Figure A.2 provides an overview of the software structure. As a result of using standard interfaces, we are able to utilize a host application framework (center) that “speaks the language” of the standardized component interfaces. This allows us to plug-and-play compliant components within the framework with no coding required.

The standard interfaces shown in Figure A.2 are represented by circles that lie between the framework and the underlying components. Interfaces shown in the figure include CAPE-Open and V21, with COM, CORBA and CCA underlying CAs. Note that the V21 software interface does not currently exist (see section entitled Recommendations for Application of CAs to Vision21 Simulation Environments, which is provided below).

Figure A.2. Use of standard component interfaces.

Recommendations for Application of CAs to Vision21 Simulation Environments

Clearly, the advantages of CAs and standard interfaces would be very beneficial to Vision21 simulators. By supporting CAs, the Vision21 simulation projects will benefit by gaining access to software components being developed by numerous groups, unrelated to the Vision21 program, as well as software being developed internal to the Vision21 project. Also, software developed for the Vision21 program using these principals will be significantly more extensible and usable as the program continues to evolve and possibly mutate into other efforts.

Roadmap

To achieve these capabilities for Vision21 simulators, we suggest a phased approach to transitioning to CA and standard interfaces. First, we must define which CAs will be targeted and then select or create appropriate standard interfaces. Second, we must choose frameworks that are capable of utilizing these types of components.

CA and Standard Interfaces

As a first step, we suggest supporting both the COM and CORBA versions of the CAPE-Open interface. As noted earlier, CAPE is a very viable choice for process engineering models with limited data transfer needs. As a second step, to address the needs of more comprehensive models in the simulation, we suggest creating an interface specification, specific to the Vision21 program (V21 in Figure A.2). The target CAs for this specification would be COM, CORBA and CCA. Note that the initial V21 interface specification would be limited to defining how Vision21 plant component models communicate and interact with one another. Future enhancements to V21 would likely include interface capabilities for lower level detailed modeling, which would mandate implementing this portion of the interface using CCA SIDL.

By using the appropriate framework, both the CAPE and V21 interface specifications could be used. Using this approach, we achieve the “best of both worlds” by leveraging all the work done by the CAPE/processing engineering community, while using the V21 interface specification for more complex development tasks.

COM and CORBA CAs, with appropriate interface specifications, will meet the short term needs of the Vision21. However, long term, we believe CCA will be an important element of future Vision21 simulations. There is a significant amount of sophisticated modeling software currently being developed as CCA components. It would be beneficial to the Vision21 program to leverage this future source of HPC components. As a result of this consideration, we recommend that the framework chosen for use with Vision 21 simulators should be capable of working with CCA components.

Frameworks

For doing more simplistic modeling, Aspen Plus is a viable framework because it supports CAPE-Open components and is currently capable of using Fluent (via CAPE) to perform detailed simulations which return point (bulk) data. The problem with using Aspen Plus as a

framework for the future of Vision21 stems from the limitation that only single-point information is passed between models. This limitation exists not only with the CAPE-Open interface, but also with Aspen itself. Being a commercial product, it is highly unlikely that Aspen would be modified to support other CA standards (V21) that would have very limited commercial application.

To support the hierarchy of models required for Vision21 (ranging from very simple response surface models to fully detailed CFD models), we need a framework that can support not only the simple models implemented with CAPE, but also the models developed using the more sophisticated interface developed for Vision21. This framework could be created by modifying an existing framework (such as SCIRun) or by creating a new framework specifically targeting Vision21 simulations. These decisions will depend in large part on who the end users of the simulation environments will be (and their level of expertise) and also the computer platforms they will be using for the simulations (Windows, Linux, Unix, etc).

Appendix B

VES-Open – IDL used in Virtual Engineering Framework

Listed below is the CORBA interface definition language (IDL) code used by VES-Open. The IDL defines the communication and data exchange between the various software components of the Virtual Engineering Framework. The interface “unit” is of particular importance as it defines how computational models are integrated and accessed with the framework.

VES-Open is an open-source tool that is maintained at ISU. For further information, please see <http://www.vrac.iastate.edu/~kmbryden/vesuite/vesopen.htm>.

```

/***** <auto-copyright.pl BEGIN do not edit this line> *****/
*
* VE-Suite is (C) Copyright 1998-2004 by Iowa State University
*
* Original Development Team:
* - ISU's Thermal Systems Virtual Engineering Group,
*   Headed by Kenneth Mark Bryden, Ph.D., www.vrac.iastate.edu/~kmbryden
* - Reaction Engineering International, www.reaction-eng.com
*
* This library is free software; you can redistribute it and/or
* modify it under the terms of the GNU Library General Public
* License as published by the Free Software Foundation; either
* version 2 of the License, or (at your option) any later version.
*
* This library is distributed in the hope that it will be useful,
* but WITHOUT ANY WARRANTY; without even the implied warranty of
* MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU
* Library General Public License for more details.
*
* You should have received a copy of the GNU Library General Public
* License along with this library; if not, write to the
* Free Software Foundation, Inc., 59 Temple Place - Suite 330,
* Boston, MA 02111-1307, USA.
*
* -----
* File:      $RCSfile: module.idl,v $
* Date modified: $Date: date $
* Version:    $Rev: 999999 $
* -----
*
*****/

```

```

module Types{
  // Array type def

  typedef sequence<long>    ArrayLong;
  typedef sequence<double>  ArrayDouble;
  typedef sequence<string>  ArrayString;

```

```
typedef sequence<boolean>  ArrayBoolean;
typedef sequence<any>      ArrayAny;
```

```
typedef sequence<ArrayLong>   ArrayLong2D;
typedef sequence<ArrayDouble> ArrayDouble2D;
typedef sequence<ArrayString> ArrayString2D;
typedef sequence<ArrayBoolean> ArrayBoolean2D;
typedef sequence<ArrayAny>    ArrayAny2D;
```

```
typedef sequence<ArrayLong2D>   ArrayLong3D;
typedef sequence<ArrayDouble2D> ArrayDouble3D;
typedef sequence<ArrayString2D> ArrayString3D;
typedef sequence<ArrayBoolean2D> ArrayBoolean3D;
typedef sequence<ArrayAny2D>    ArrayAny3D;
```

```
typedef sequence<ArrayDouble3D> ArrayDouble4D;
```

```
struct Profile {
    ArrayString  profile_vars;
    ArrayDouble2D profile_vals;
};
};
```

```
module Error{
    exception EUnknown{
        long code;
        string description;
        string interfacename;
        string operatio;
    };
};
```

```
module Body{
    interface Unit{          // this is the calculation module
```

```
    //This start the calculation
    void StartCalc() raises(Error::EUnknown);
```

```
    //This stop the calculation
    void StopCalc() raises(Error::EUnknown);
```

```
    //This is to pause the calculation
    void PauseCalc() raises(Error::EUnknown);
```

```
//This is to Resume the calculation
void Resume() raises(Error::EUnknown);
```

```
//This is for querying the status of the module
string GetStatusMessage() raises(Error::EUnknown);
```

```
//This is to get the 3D data
string GetUserData() raises(Error::EUnknown);
```

```
//This is to Set the Module up
void SetParams(in string param) raises(Error::EUnknown);
```

```
//This is to Set the ID
void SetID(in long id) raises(Error::EUnknown);
```

```
//This is to Get the ID
long GetID() raises(Error::EUnknown);
```

```
//This is to Set the name
void SetName(in string name) raises(Error::EUnknown);
```

```
//This is to Get the name
string GetName() raises(Error::EUnknown);
```

```
};
```

```
interface UI { //This is the UI;
```

```
//This is to update the network, called by the Executive
void UpdateNetwork(in string network) raises(Error::EUnknown);
```

```
//This is to update the module UI, called by the Executive
void UpdateModuleUI(in long module_id, in string msg) raises(Error::EUnknown);
```

```
//This is to update the Result UI, called by the Executive
void UpdateModuleResult(in long module_id, in string msg) raises(Error::EUnknown);
```

```
//This is to update the Link content UI, called by the Executive
void UpdateLinkContent(in long id, in string msg) raises(Error::EUnknown);
```

```
//This is to Raise the Notification or warning or error message
void Raise(in string notification) raises(Error::EUnknown);
```

```
};
```

```
interface Executive { // This is the Executive Engine;
```

//This is to Get the Flow in Data for Module module_id, port port_id, Called by the Unit and/or UI to display the port data

```
string GetImportData(in long module_id, in long port_id) raises(Error::EUnknown);
```

//This is to Set the Flow out Data for Modle moduel_id, port port_i, Called by the Unit

```
void SetExportData(in long module_id, in long port_id, in string data)
raises(Error::EUnknown);
```

//This is to Get the Flow out Data for Modle moduel_id, port port_i, Called by the UI to display the port data

```
string GetExportData(in long module_id, in long port_id) raises(Error::EUnknown);
```

//This is to set the Multi Dimention Profile Data, call by the upstream Unit Module

```
void SetProfileData(in long module_id, in long port_id, in Types::Profile data)
raises(Error::EUnknown);
```

//This is to get the Multi Dimention Profile Data, call by the upstream Unit Module, put the result in the out parameter to save data copying

```
void GetProfileData(in long module_id, in long port_id, out Types::Profile data)
raises(Error::EUnknown);
```

//This is the Set the Module Message, called by Unit

```
void SetModuleMessage(in long module_id, in string msg) raises(Error::EUnknown);
```

//This is the Set the Module Result, called by Unit

```
void SetModuleResult(in long module_id, in string result) raises(Error::EUnknown);
```

//This is the Get the Module Result, called by UI

```
string GetModuleResult(in long module_id) raises(Error::EUnknown);
```

//This is the set the network, called by the UI

```
void SetNetwork(in string network) raises(Error::EUnknown);
```

//This is the set the network, called by the current Editing UI

```
void SetModuleUI(in long module_id, in string ui) raises(Error::EUnknown);
```

//This is to get the network, called by the UI

```
string GetNetwork() raises(Error::EUnknown);
```

//This is to set up the executive watch list, Called by the UI (the editable one)

```
void SetWatchList(in Types::ArrayLong id) raises(Error::EUnknown);
```

//This is to get the watch list, Called by the UI

```
Types::ArrayLong GetWatchList() raises(Error::EUnknown);
```

//This is to get the status message of Executive, called by the UI


```

string GetStatus() raises(Error::EUnknown);

//This start the network calculation, Called by the UI
void StartCalc() raises(Error::EUnknown);

//This stop the network calculation, Called by the UI
void StopCalc() raises(Error::EUnknown);

//This is to pause the calculation, Called by the UI
void PauseCalc() raises(Error::EUnknown);

//This is to Resume the calculation, Called by the UI
void Resume() raises(Error::EUnknown);

//This is to Register a UI to the Executive, make it aware that this UI is connected in
void RegisterUI(in string UIName, in Body::UI ui) raises(Error::EUnknown);

//This is to disconnect the UI to the Executive,
void UnRegisterUI(in string UIName) raises(Error::EUnknown);

//This is to disconnect the Unit to the Executive
void UnRegisterUnit(in string UnitName) raises(Error::EUnknown);

//This is to Register a Unit to the Executive, flag=0 is normal module, flag=1 will be the
global module
void RegisterUnit(in string UnitName, in Body::Unit unit, in long flag)
raises(Error::EUnknown);

//This is to Get the global modules's ID, so the output of the global module can be used by all
modules (for example, coal module), return value is the number of the global modules, the output
parameter is the ids fo the global modules. So the Unit can call the GetExportData(id) to the get
the global data
long GetGlobalMod(out Types::ArrayLong ids) raises(Error::EUnknown);

};

};

```

Appendix C

Virtual Engineering Framework User Guide

Note - All figures, tables and literature citations refer to information in this Appendix.

AGR Module (Acid Gas Removal)

A process engineering (0D) model is used to simulate the performance of the Acid Gas Removal (AGR) unit. For advanced power generation configurations that involve a SOFC, the primary purpose of the AGR is to remove the H₂S in the syngas down to less than 1ppm to avoid damaging the SOFC materials.

The solvents used in an AGR fall into two broad categories: physical and chemical solvents. The choice of solvent is usually dictated by the H₂S/CO₂ ratio in the syngas, the solvent's selectivity for H₂S over CO₂, carbonyl sulfide removal, and whether total removal of CO₂ is desired. Physical solvents rely upon variations in the physical solubility of gases to effect separation. Examples are Selexol and Rectisol. Chemical solvents are usually amine-based and remove H₂S and CO₂ through an acid-base reaction path. One of four amine-based solvents is usually employed (MEA, DGA, TEA and MDEA). In IGCC, selectivity of H₂S over CO₂ is important. Thus the best chemical solvent for this task is MDEA (Methyldiethanolamine). MDEA actually reacts with H₂S but only as a catalyst for hydrolysis of CO₂ [Kohl and Nielsen, 1997]. MDEA has the lowest capital cost in comparison with Selexol and Rectisol, which may also be selected for IGCC service. Rectisol is the costliest solvent but may be the best choice if complete removal of CO₂ is preferred.

Modeling the AGR unit provides information on the amine circulation rate required to meet the H₂S removal levels, and the size of the absorption tower and the number of stages required to effect the removal of H₂S. The key design equations used in the model are:

1) The amine circulation rate:

$$\text{GPM} = \frac{0.206 \cdot \text{MM} \cdot (\text{H}_2\text{S} + \text{CO}_2) \cdot \text{MolWT}}{\text{ML} \cdot \text{WT}}$$

where

GPM = amine circulation rate

MM = actual gas flow rate, million cubic ft/day

H₂S = Mol% of H₂S in gas mixture to be removed

CO₂ = Mol% of CO₂ in gas mixture to be removed

ML = Mol loading or (moles of acid gas) / (mol of syngas)

WT = Amine solution wt% circulated

2) Absorber bubbling gas velocity:

$$U_{al} = K \left(\frac{\rho_L - \rho_G}{\rho_G^{0.5}} \right)^{0.5}$$

where

$K = 0.25$ for valve trays, 0.20 for bubble cap trays

U_{al} = Allowable velocity of gas through bubbling area, ft/s

ρ_L = Density of amine solution, lb/ft³

ρ_G = Density of syngas at tray conditions, lb/ft³

3) Theoretical number of stages (see [[Perry, Seventh Edition Chapter 14](#)]):

$$N = \frac{\ln[(1 - A^{-1})(y_1 - y_2^0)/(y_2 - y_2^0) + A^{-1}]}{\ln(A)}$$

where

N = Number of Stages, N

$A = L_m/mG_m$ is the Absorption factor

L_m = liquid molar flow rate/unit area (i.e. solvent entering at the top of tower)

G_m = Gas molar flow rate/unit area (i.e. syngas entering at bottom of tower)

m = slope of equilibrium curve

note: this analysis is valid only if the equilibrium curve is represented by $y_e =$

mx

4) Absorption Factor

$$A = \frac{L_m}{mG_m}$$

where

A , L_m , G_m and m are defined as above.

Connections

- **Inlet Port 0** : Inlet gas stream.
- **Outlet Port 0** : Outlet gas stream.

Graphical User Interface (UI)

The inputs for the AGR model are the solvent properties (molecular weight and density). The UI for entering model inputs for an example case is shown in the left figure. The model outputs include the amine circulation rate, size of the absorption tower, number of stages required to effect the removal of H₂S, clear liquor

residence time and the exit gas composition.

Summary Data (SUM)

After the module has executed, the *Summary Data* button provides summary information. The module outputs calculated absorber height (ft), amine circulation rate (gpm), area of downcomer (ft²), mole fraction of CO₂, number of trays and their diameter (ft).

References

1. Kohl, Arthur L., and Nielsen, Richard B., "Gas Purification." Fifth Edition, Gulf Publishing Company, Houston, Texas. 1997.
2. Keating, M.H., et al. *Mercury Study Report to Congress, Volume I: Executive Summary*, EPA-452/R-97-003, December 1997.

3. Korens, Nick, and Simbeck, Dale R., and Wilhelm, Donald J., "Process Screening Analysis of Alternative Gas Treating and Sulfur Removal for Gasification." Prepared for U.S.D.O.E./N.E.T.L. Task Order No. 739656-00100. December 2002.
 4. Ratafia-Brown, Jay, and Manfredo, Lynn, and Hoffman, Jeffrey, and Ramezan, Massood, "Major Environmental Aspects of Gasification-Based Power Generation Technologies." Prepared for : U.S.D.O.E./N.E.T.L. Gasification Technologies Program. December 2002.
-

ASU Module (Air Separation Unit)

The ASU module is designed to emulate an air separation unit which separates an incoming air stream into a high purity oxygen stream and a nitrogen-rich side stream. The ASU module is intended to provide oxygen to a gasifier, so the products (O_2 and N_2) exit the module as gases, not as liquids.

SIMPLIFIED ASU SCHEMATIC

An ASU is based on a cryogenic distillation process--the only economical option at large capacities. Cryogenic distillation separates a vapor/liquid mixture based on differences in the vapor pressures of various components. The distillation column operates at pressures from 8-20 bar, and at temperatures on the order of 100 K [Seader 1998]. Air is first compressed, then passed through a molecular sieve bed to filter out any water, CO_2 , or hydrocarbons that would freeze at the low operating temperatures. Cold product streams are used to cool the incoming air stream in the heat exchanger before the inlet air enters the distillation column. Upon exiting, the products are at near-ambient temperatures of high pressure. Product purities are typically 95% oxygen, and >99% nitrogen. If desired, the high pressure gases can be expanded through turbines to produce power. The primary energy requirements for the ASU are a result of gas compression.

The ASU model assumes that air is compressed outside the unit in a separate compressor module. All of the oxygen entering the unit is assumed to exit in the oxygen product stream [Allam 1992]. The inlet argon is assumed to partition 75% to the oxygen stream and 25% to the nitrogen stream based on the relative vapor pressure of argon with respect to oxygen and nitrogen [Woodward 1990]. All separation and heat exchange are accounted for internally within the model. All components except oxygen, nitrogen, and argon are removed from the unit and are therefore only accounted for in the energy

balance. The model checks the user specified temperature, pressure, and composition to ensure vapor-phase effluents.

Connections

- **Inlet Port 0** : Inlet gas stream.
- **Outlet Port 0** (up) : High purity oxygen outlet gas stream.
- **Outlet Port 1** (down) : Nitrogen outlet gas stream.

Graphical User Interface (UI)

The UI window prompts the user for the desired properties of the two outlet gases: O₂ and N₂. These properties act as the target values by which the ASU module operates. Module calculations are governed by the temperature, pressure, and purity of the exiting oxygen gas, as well as by the temperature and pressure of the exiting nitrogen gas.

High pressure products at ambient temperatures represent typical outlet gas properties.

Summary Data (SUM)

Description	Value
+++++	
Q (MW)	-0.00

The summary table indicates the energy required by the module.

References

1. Allam, R. J., Topham, A., "Integrated Air Separation Plant-Integrated Gasification Combined Cycle Power Generator," U.S. Pat. No. 5081845, Jan. 21, 1992.
 2. Seader, J. D. and Henley, E. J., Separation Process Principles, John Wiley & Sons, Inc., New York, 1998, p 776.
 3. Woodward, D. W., Agrawal, R. "Air Separation Process for the Production of Oxygen-rich and Nitrogen-rich Products," U.S. Pat. No. 4936099, June 26, 1990.
-

Bulk Desulfurizer Module

The Bulk Desulfurizer module is a part of the warm (hot) gas cleanup unit designed for bulk removal of sulfur species from the gas stream. The primary sulfur species of concern are H_2S and COS , and the unit is designed to achieve exit concentrations of about 10 ppm H_2S and 1 ppm COS . Sulfur species must be removed because of emissions requirements and adverse interactions in downstream equipment such as poisoning of fuel cells and other catalytic units.

The Bulk Desulfurizer is based on a transport reactor that has been demonstrated for high temperature operation. The reactor consists of a recirculating system in which the syngas flows co-currently with sorbent in a riser section. A cyclone separates the cleaned syngas from the sorbent and the sorbent falls through a return leg, at the bottom of which it contacts incoming dirty syngas. A portion of the sorbent is removed in a return leg and sent to a regeneration riser. Off-gas from regeneration is processed to produce elemental sulfur or sulfuric acid using conventional technology. Regenerated sorbent is injected back into the riser section of the desulfurization reactor. The Bulk Desulfurizer is intended to be placed downstream of the [Chlorine Guard Bed](#), and upstream of the [Sulfur Polisher](#). A heat exchanger may be required upstream of the unit to achieve the desired operating temperature (~ 672 K for warm gas operation). The module is assumed to be of use in both hot and warm gas cleanup systems, provided a suitable sorbent is used.

The Bulk Desulfurizer module acts as a component separator. The user provides either a removal efficiency or an exit concentration for COS and H_2S . A temperature change can

be specified to account for heat effects. Pressure drop across the unit can be specified or computed using specific module configuration details as shown in the User Interface (see below). The pressure drop is based on the Ergun equation and includes terms to account for the static head pressure drop (pressure lost in suspending the solid particles,) and the wall friction. The computed pressure drop option requires the bed diameter, depth, void fraction, nominal particle size, particle sphericity, particle density, and solids mass flow. The unit outputs are the exit gas state: temperature, pressure, and composition.

Connections

- **Inlet Port 0:** Inlet gas stream
 - **Outlet Port 0:** Desulfurized outlet gas stream
-

Graphical User Interface (UI)

The screenshot shows a window titled "BulkDesulfurizer" with a close button (X). The interface is organized into several sections:

- Temperature change (F):** A text input field containing the value "0".
- H2S section:**
 - ☐ H2S efficiency (%): A text input field containing "0".
 - ☒ H2S ppm: A text input field containing "1".
- COS section:**
 - ☐ COS efficiency (%): A text input field containing "0".
 - ☒ COS ppm: A text input field containing "1".
- Pressure Drop section:**
 - ☒ Specify Pressure Drop (psi): A text input field containing "24".
 - ☐ Calculate Pressure Drop:
 - Below the radio buttons are several text input fields for parameters used in the calculation:
 - Bed diameter (m): "0"
 - Bed depth (m): "0"
 - Bed void fraction: "0"
 - Particle size (m): "0"
 - Particle sphericity: "0.65"
 - Particle density (kg/m3): "2000"
 - Solids Mass Flow (kg/s): "-1"

At the bottom of the window are two buttons: "OK" and "Cancel".

This user interface first allows the user to specify the change in temperature of the gas through the module--thereby accounting for heat effects. Positive values represent an increase of temperature in the gas between inlet and outlet ports. (Note that the temperature change is measured in degrees **Fahrenheit**)

H2S and COS removal calculations can be made either by specifying the desired removal efficiencies or by specifying the desired exit concentrations.

Pressure drop across the module can either be *specified* (in **psi**) or *computed* within the module. If the exit concentration is *specified*, the value should be below that of the inlet. The *calculated* pressure drop is based on the Ergun equation, with terms to account for the static head pressure drop (pressure lost in suspending the solid particles,) and the wall friction. *Void fraction* is defined as 1 - sorbent volume / bed volume. The *particle size* can be computed as the diameter of a sphere of the same volume as the particle. The *sphericity* is the surface area of the sphere described above divided by the actual particle surface area.

Default values are provided for temperature drop, exit acid gas concentrations, specified pressure drop, and particle density and sphericity (for the computed pressure drop option).

Summary Data (SUM)

The image shows a software window titled 'Result Dialog' with a sub-header 'Summary Data'. Inside the window is a table with two columns: 'Description' and 'Value'. The table contains four rows of data. Below the table is an 'OK' button.

Description	Value

COS Reduction Eff	99.67
H2S Reduction Eff	99.99
Pressure Drop (ps	24.00
Temperature Out (	639.90

After the module has executed, the *Summary Data* button provides summary information. The module outputs the reduction/removal efficiencies for both COS and H₂S, the pressure drop across the module (in **psi**), and the temperature of the exiting gas stream (in **Kelvin**).

CarbonBed Module (Carbon Bed)

A process engineering (0D) model is used to simulate mercury removal from the syngas within the cold gas clean up stream. The use of carbon beds to remove mercury from syngas has been demonstrated at the Eastman Chemical plant in Kingsport, TN [Eastman Chemical Co, 2003].

Activated carbon, which can have internal surface area of the order of $10^6 \text{ m}^2/\text{kg}$ (Coulson et al, 1991), is effective in removing mercury from syngas streams. Calgon Carbon Corporation of Pittsburgh supplies two versions of sulfur-impregnated activated carbons in granular form in 4x10 US Mesh (HGR) and 4mm pellet as HGR-P. These carbons are made from bituminous coals. The sulfur in the carbon reacts with elemental mercury to form a stable mercuric sulfide compound (HgS). Calgon Product Bulletin (1994) states that adsorption systems using the HGR-type activated carbon can be designed to reduce mercury concentrations to below $0.001 \text{ ug}/\text{Nm}^3$ in the treated gas. The adsorptive capacity of these carbons can be as high as 20 weight percent. NORIT Americas Inc., of Texas, supplies sulfur-impregnated activated carbon in the form of powder (DARCO FGD) and 3 or 4mm pellets (RBHG) made from lignite coal. Both suppliers report that in a properly designed carbon system, the mercury removal process is not affected by inlet mercury concentration or changing the operating pressure. However, increasing the gas temperature or moisture content of the gas stream would drastically affect mercury removal.

Design calculations of a fixed bed adsorber can be readily made from feed and product gas specifications, equilibrium data, and knowledge of the bed saturation at the break point under the desired operating conditions. A theoretical basis for design of fixed bed adsorbers is given by Brown et al., (1955), McCabe et al., (1985) and Coulson et al., (1991). However, for adsorption with chemical reaction, the interrelation of these variables is so complex that methods of design usually rely heavily on experimental and operating data of existing plants. The purpose of an adsorber design is to determine the dimensions of the vessel and the quantity of activated carbon required to achieve a specified mercury removal rate. In the simplest of the design approach, the following steps are followed:

- Determination of allowable pressure drop
- Determination of the minimum fluidization velocity
- Determination of allowable superficial velocity through the bed
- Specification of residence time

- Determination of adsorber dimensions
- Calculation of quantity of carbon needed
- Specification of mercury content of coal
- Specify adsorbent lifetime
- Calculate mercury loading of the carbon bed

Connections

- **Inlet Port 0** : Inlet gas stream.
- **Outlet Port 0** : Outlet gas stream.

The screenshot shows a window titled "CarbonBed" with a close button (X) in the top right corner. The window contains a form with the following fields and values:

Parameter	Value
Allowable Pressure Drop (psi/ft)	0.26
Parameters	
Carbon Particle Diameter (mm)	3.38
Bulk Density (kg/m ³)	592.7
Operating Temperature (K)	313
Operating Pressure (psi)	255
Carbon Replacement Time (years)	2
Carbon Bed Porosity	0.7
Absorber Residence Time (sec)	20

At the bottom of the window are two buttons: "OK" and "Cancel".

Graphical User Interface (UI)

The UI window prompts the user for the desired properties of the Carbon and operation parameters. Module calculations are governed by these parameters, as well as by the properties of the input gas stream.

Summary Data (SUM)

The screenshot shows a 'Result Dialog' window with a 'Summary Data' tab. It contains a table with two columns: 'Description' and 'Value'. The table lists various parameters and their calculated values. An 'OK' button is located at the bottom right of the dialog.

Description	Value
Adsorber Diameter (m)	5.60
Bed Height (m)	29.20
Hg Leaving Adsorber (lb/hr)	3.42e+002
Min. Fluidization Vel. (m/sec)	27.30
Number of Adsorbers (#)	1.00
Pressure Drop (Pa/m)	5066.25
Superficial Velocity (m/sec)	30.30
Total Bed Pressure Drop (psi)	506625.00

After the module has executed, the *Summary Data* button provides summary information. The module outputs calculated absorber diameter (m), bed height (m), mercury leaving the adsorber (lbm/hr), minimum fluid velocity (m/sec), number of adsorbers, pressure drop per meter (Pa/m), superficial velocity (m/sec), and pressure drop across the bed (psi).

References

1. Kohl, Arthur L., and Nielsen, Richard B., "Gas Purification." Fifth Edition, Gulf Publishing Company, Houston, Texas. 1997.
2. Keating, M.H., et al. *Mercury Study Report to Congress, Volume I: Executive Summary*, EPA-452/R-97-003, December 1997.
3. Korens, Nick, and Simbeck, Dale R., and Wilhelm, Donald J., "Process Screening Analysis of Alternative Gas Treating and Sulfur Removal for Gasification." Prepared for U.S.D.O.E./N.E.T.L. Task Order No. 739656-00100. December 2002.
4. Ratafia-Brown, Jay, and Manfredo, Lynn, and Hoffman, Jeffrey, and Ramezan, Massood, "Major Environmental Aspects of Gasification-Based Power Generation Technologies." Prepared for : U.S.D.O.E./N.E.T.L. Gasification Technologies Program. December 2002.

Catalytic Combustor Module

In fuel cell applications, catalytic combustion offers an efficient means of recovering heat from the low heating value fuel cell effluent streams that may otherwise be difficult to burn directly. This is particularly manifest in molten carbonate fuel cell (MCFC) systems where the cell discharges unreacted fuel at about 600°C. In these systems, the anode exhaust containing the unreacted fuel is mixed with air and then oxidized completely in a catalytic combustor (Ghezel-Ayagh and Maru, 2002). At present, solid oxide fuel cell (SOFC) systems operate at temperatures in the window of 800 – 1000°C, because the oxygen ion conduction in yttria stabilized zirconia (YSZ) is best in this temperature window. However, with the current push for low temperature solid electrolytes for SOFC systems, the operating temperature window is likely to fall in the range 700 – 800°C where catalytic oxidation of the lean fuel/air mixtures is an attractive option. In addition to the ability to burn lean fuel/air mixtures completely (Tucci, 1982), catalytic combustors operate at low enough temperatures such that NO_x emissions are minimized (Kolaczowski, 1995).

Connections

- **Inlet Port 0:** Inlet gas stream.
- **Outlet Port 0:** Outlet gas stream.

Graphical User Interface (UI)

The screenshot shows a window titled "CatalyticCombustor" with two radio buttons: "Evaluation Mode" (selected) and "Design Mode". Below the radio buttons are several input fields with the following values:

Parameter	Value
Effectiveness Factor	1
Site Density	2.7e-005
Hydraulic Diameter (m)	0.0012
Length (m)	0.078
Conversion (%)	0.99
Inlet Velocity (m/sec)	16.7

At the bottom of the window are "OK" and "Cancel" buttons.

This User Interface requires the user to first specify the method of module calculation. *Evaluation Mode* (shown) allows the user to input the existing *Length* of a combustor and the module will thereby calculate the maximum possible conversion. When *Design Mode* is specified, the user inputs a *Desired Conversion*, and the module calculates the necessary combustor geometry to achieve that specified conversion.

Additional required user inputs include the *Inlet Velocity* through the unit.

Summary Data (SUM)

The screenshot shows a window titled "Result Dialog" with a tab labeled "Summary Data". Inside the window is a table with two columns: "Description" and "Value".

Description	Value
+++++	
Pressure Drop (Pa)	506625.00
Res. Time (sec)	1.00000e+000

At the bottom of the window is an "OK" button.

The Summary screen shows the computed values for the *Pressure Drop*, as well as the *Residence Time* from the computations. When *Evaluation Mode* is specified in the UI, the *Conversion Rate* will also be displayed. When *Design Mode* is specified in the UI, then the *Calculated Length* will be displayed.

Chlorine Bed Module

The Chlorine Guard Bed (CGB) module is part of the warm (hot) gas cleanup system designed to remove chlorine from the gas stream. Chlorine removal is required prior to desulfurization because chlorine tends to react with sulfur sorbents. A commercially available nahcolite sorbent operating at 1000° F has been proposed to remove chloride (and other halogens). The CGB module is intended to be placed after the syngas has been cooled to the appropriate temperature (about 1000° F), and before the desulfurization steps. It is assumed that a chlorine guard bed would be used for both warm and hot gas cleanup, provided the appropriate sorbent is used.

The CGB model acts as a component separator. The user provides either an HCl removal efficiency or an exit HCl concentration (required to be below the inlet concentration). In addition, a temperature drop can be specified to account for heat losses. Pressure drop across the unit can either be specified or computed using required unit configurations specified by the user in the User Interface (UI). The pressure drop is based on the Ergun equation [Kunii and Levenspiel, 1969] and requires the bed diameter, depth, void fraction, nominal particle size, and particle sphericity. The unit outputs are the exit gas state: temperature, pressure and composition.

CHLORINE BED UNIT

Connections

- **Inlet Port 0:** Inlet gas stream
- **Outlet Port 0:** Low-chlorine outlet gas stream

Graphical User Interface (UI)

This user interface first allows the user to specify the change in temperature of the gas through the module. Positive values represent an increase of temperature in the gas between inlet and outlet ports. (Note that the temperature change is measured in degrees **Fahrenheit**)

HCl removal calculations can be made either by specifying the desired HCl removal efficiency or by specifying the desired exit HCl concentration.

Pressure drop across the module can either be specified (in **psi**) or computed within the module. The calculated pressure drop is based on the Ergun equation and requires several module parameters. *Void fraction* is defined as $1 - \text{sorbent volume} / \text{bed volume}$. The *particle size* can be computed as the diameter of a sphere of the same volume as the particle. The *sphericity* is the surface area of the sphere described above divided by the actual particle surface area.

Default values are provided for

temperature drop, exit HCl concentration, specified pressure drop, and particle sphericity (for the computed pressure drop option).

Summary Data (SUM)

After the module has executed, the *Summary Data* button provides summary information. The module outputs the *HCL reduction efficiency*, *pressure drop* (in **psi**) and the *temperature out* (in **Kelvin**).

References

1. Kunii, D., and Levenspiel, O., Fluidization Engineering, John Wiley and Sons Inc., 1969, pp 698-699.
-

Compress/Expand Module

This module emulates either a compressor or expander. The thermodynamic calculations involve the assumption of an isentropic compression/expansion process coupled with an isentropic efficiency. The user specifies the isentropic efficiency and pressure change through the module.

Connections

- **Inlet Port 0:** Inlet gas prior to compression/expansion.
- **Outlet Port 0:** Outlet gas following compression/expansion.

Graphical User Interface (UI)

The User Interface first allows the user to input an *Isentropic Efficiency* for the Compressor/Expander (as fraction).

The user must also specify a desired *Pressure Change*. Negative values decrease pressure through the module--modeling an Expander. Positive values increase pressure--modeling a Compressor.

Summary Data (SUM)

The summary table indicates the energy required by the module. When used to model compressors, the resultant number will be negative and will represent the power required to compress the inlet gas. When the module is used to model expanders, the number will be positive and represents the power generated as a result of the pressure drop.

References

1. Schematic modified from www.smud.org/cpp/construc/schemati.pdf
-

Condenser Module

The condenser model is a heat exchanger model that involves heat transfer between two water streams. The first is superheated water vapor (flows top to bottom on icon) that is to be condensed to liquid, and the second (flows left to right on icon) is a liquid stream used for the cooling. The heat transfer correlations used are for condensation heat transfer on tube banks.

Connections

- **Inlet Port 0** (top): Inlet water stream to be cooled.
 - **Inlet Port 1** (left): Inlet water stream to serve as heat sink.
 - **Outlet Port 0** (bottom): Cooled outlet water stream.
 - **Outlet Port 1** (right): Sink outlet.
-

Graphical User Interface (UI)

A screenshot of the 'Condenser' graphical user interface. It features a title bar with the text 'Condenser' and a close button. Below the title bar, there are seven input fields arranged in two columns. The first column contains labels for 'Number of Tubes (Horiz)', 'Number of Tubes (Vert)', 'Tube Inner Diameter (m)', 'Tube Outer Diameter (m)', 'Tube Length (m)', 'Internal Pressure Drop (Pa)', and 'External Pressure Drop (Pa)'. The second column contains corresponding numerical input boxes with values: 142, 33, 0.0381, 0.0508, 11.948, 0, and 0. At the bottom of the window, there are two buttons: 'OK' and 'Cancel'.

This user interface prompts the user for properties of the condensing unit. These data fields are necessary in order to compute the transfer heat rate effectiveness of the unit.

The *Internal Pressure Drop* field allows the user to specify a desired pressure drop for the water stream as it flows through the module, whereas the *External Pressure Drop* specifies the change in pressure of the vapor stream through the module.

Cyclone Module

A Cyclone unit eliminates particulate matter from syngas and is usually placed upstream of the gas cleanup system. The Cyclone Module is a 0D model that makes use of engineering correlations to calculate the pressure drop and the particulate removal efficiency as a function of particle diameter. Collected solids from Cyclone units is typically refed to the Gasifier through the particle inlet port (see [Gasifier](#) module.)

Connections

- **Inlet Port 0:** Inlet gas stream prior to particulate removal
- **Outlet Port 0** (top right): Outlet gas stream following particulate removal
- **Outlet Port 1** (bottom): Outlet of accumulated solid particles

Graphical User Interface (UI)

Module specifications including *Cyclone Diameter*, *Particle Turn Count* and *Velocity Heads*.

Summary Data (SUM)

The summary table entries include properties such as *Cyclone Cut Diameter* (in microns), the stream's *Inlet Gas Velocity* (m/s) upon entering the cyclone chamber, the *Mass Mean Diameter* (microns) of the particles, total *Particle Flowrate* (kg/s), the percent of the *Particle Flow Collected*, the percent of the *Particle Flow Passed*, the *Pressure Drop* across the module (kPa), and the *Standard Deviation* (microns) for the Mean Diameter calculation.

References

1. De Nevers, N., *Air Pollution Control Engineering* , 2d ed., McGraw-Hill, New York, Chapter 9, 2000. p 29 (image)
-

Dump Combustor Module

The Dump Combustor Module is typically placed downstream of solid oxide fuel cells in order to burn out any remaining unreacted fuel. Though the SOFC exhaust stream is dilute and the energy density is low, use of a dump combustor harnesses a significant amount of energy from the lean gas exhaust of fuel cells, and improves overall plant efficiency.

Combustion stability and reaction rate are typically of concern in combustion. Kinetic simulations have shown that combustion occurs over a wide range of temperatures and pressures, with no observed blowout condition for combustion of typical SOFC exhaust. Increasing pressure affects the reaction by decreasing the required residence time and increasing combustion rates. High temperatures also increase the required residence time. Though combustion is possible over a wide range of temperatures, the residence time is so high at low temperatures that a prohibitively large combustion chamber would be required. For these conditions, an alternate combustion process would be required. Options for combustion include preheating the inlet gas, or using a catalytic combustion in place of a dump combustor.

The Vision 21 dump combustor model is based on a plug flow reactor. These types of reactors describe the time evolution of a well-mixed reacting fluid, such as the flow in a pipe with perfect radial mixing and zero axial mixing. The model makes use of the GRI mech 3.0 kinetic mechanism (Smith et al), and is designed to provide the combustor volume required for a given fuel conversion, or the fuel conversion for a given volume. The model can be run in one of two modes: (1) Evaluation mode, in which the combustion volume is specified, and the fuel conversion and exit properties are computed, and (2) Design mode, in which the program computes the required volume for a user-specified degree of fuel conversion. A heat loss and pressure drop over the unit can be specified. Outputs include heat loss and pressure drop, if any, combustor volume (for design mode), fuel conversion (for evaluation mode), and residence time. Full error handling is provided to alert the user of error or warning conditions, and to enforce proper input specifications. For example, an error occurs if the equilibrium fuel conversion is below the specified fuel conversion.

Connections

- **Inlet Port 0:** Inlet gas stream
- **Outlet Port 0:** Outlet gas stream

Graphical User Interface (UI)

A screenshot of the 'DumpCombustor' graphical user interface. It features a title bar with a close button. Below the title bar, there are two radio buttons: 'Evaluation Mode' (selected) and 'Design Mode'. Below these are four input fields: 'Combustor Volume' (0.99), 'Desired Conversion' (10), 'Fraction Heatloss' (0), and 'Pressure Drop (psi)' (0). At the bottom, there are 'OK' and 'Cancel' buttons.

This User Interface requires the user to first specify the method of module calculation. *Evaluation Mode* (shown) allows the user to input the existing *Volume* of a combustor and the module will thereby calculate the maximum possible conversion. When *Design Mode* is specified, the user inputs a *Desired Conversion*, and the module calculates the necessary combustor geometry to achieve that specified conversion.

Additional required user inputs include the *Fraction Heatloss* and *Pressure Drop* through the unit.

Summary Data (SUM)

A screenshot of the 'Result Dialog' graphical user interface. It has a title bar with a close button. Below the title bar, there is a section titled 'Summary Data'. Inside this section is a table with two columns: 'Description' and 'Value'. The table contains three rows of data: 'HeatLoss (MW)' with value '2.30', 'Pressure Drop (psi)' with value '50662.50', and 'Tau Average (sec)' with value '1.30'. Below the table is an 'OK' button.

The Summary shows the computed values for the *Heatloss* and *Pressure Drop*, as well as the *Tau Average* from the computations. When Evaluation Mode is specified in the UI, the *Conversion Rate* will also be displayed. When Design Mode is specified in the UI, then the *Calculated Volume* (as shown) will be displayed.

References

1. Gremmen, R.S., "Oxidation of Low Calorific Value Gases--Applying Optimization Techniques to Combustor Design," U.S. DOE FETC, Presented at the 1998 IJPGC, Baltimore, MD, Aug 23-26.
 2. Smith, Gregory P., David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, Jr., Vitali V. Lissianski, and Zhiwei Qin
http://www.me.berkeley.edu/gri_mech/
-

Equilibrium Reactor Module

The equilibrium reactor module is a process engineering (0D) model that calculates full chemical equilibrium for the provided conditions. This model can be used to estimate the performance of the combustor in a direct-fired gas turbine. The model is implemented in a general manner and thus can be used for calculating equilibrium gas compositions in other devices as well. The equilibrium calculation is implemented as a member function within the thermodynamics class contained within the framework.

Connections

- **Inlet Port 0:** Inlet gas stream
 - **Outlet Port 0:** Outlet gas stream
-

Evaporator Cooler Module

The evaporation cooler model is used to simulate a cooling tower for cooling the heated liquid water from the condenser via a direct contact heat exchange evaporation process. The ambient relative humidity and desired outlet water temperature are included as inputs. Model calculations range from the required air flow to evaporated water loss from the process.

Connections

- **Inlet Port 0:** Inlet water stream.
- **Outlet Port 0 :** Cooled outlet water stream.

Graphical User Interface (UI)

A screenshot of a graphical user interface (GUI) window titled "EvaporationCooler". The window has a blue title bar with a close button (X) on the right. Inside the window, there are four input fields with labels: "Desired Temperature (K):" with a value of 305, "Air Temperature (K)" with a value of 298, "Air Relative Humidity (%)" with a value of 20, and "Ambient Pressure (Pa)" with a value of 101325. At the bottom of the window, there are two buttons: "OK" and "Cancel".

User inputs *Desired Temperature* of water stream (K) and ambient air properties such as *Temperature*, *Relative Humidity*, and *Pressure*.

Summary Data (SUM)

Following a successful model run the summary table provides: *Air Flow Required* (kg/s) in order to obtain desired temperature and the resultant *Evaporation Rate* (kg/s) associated with the tower.

Gas Feedback Module

The Gas Feedback Module facilitates feedback loops like the one shown on the right where inlets to a given module are dependent on the same module's outlets.

The Gas Feedback Module executes a series of iterations until properties of the cycling gas between sequential iterations fall within certain user-specified parameters.

EXAMPLE GAS FEEDBACK LOOP

The Gas Feedback module is always coupled with a [GasSource](#) Module that serves as a "first guess" of the properties of the gas at the feedback inlet (site "A" above). A simplified model of the above schematic would look like the network shown on the left.

Connections

- **Inlet Port 0** (top): Inlet gas stream to serve as an initial guess
- **Inlet Port 1** (left): Inlet gas stream as feedback
- **Outlet Port 0**: Outlet gas stream as feedback

Graphical User Interface (UI)

This User Interface allows the user to specify the desired accuracy and computational method of a gas feedback loop. The *Max. Iterations* box gives the total number of iterations allowed in the case that the specifications listed below are not met. The lower list allows the user to define a set of conditions that, if met, end iterations and signify an achieved suitable outcome.

Example: The loop defined by the specifications shown at left will cycle until the change in CO level between iterations is less than 1%, the change in NO levels is less than 1%, and the change in temperature is less than 1%, or until the number of iterations reaches 12. Once one of those two condition sets is reached, the module network ends the loop and will continue using the gas properties from the most recent iteration.

Gas Heat Exchanger Module

The Gas Heat Exchanger module allows the user to heat or cool a gas stream to a desired temperature. The module calculates both the heat transfer necessary to bring the gas stream to the specified temperature, and also outputs the resultant *Temperature Change* between inlet and outlet streams.

Connections

- **Inlet Port 0**: Inlet gas stream.
- **Outlet Port 0**: Outlet gas stream of desired temperature.

Graphical User Interface (UI)

The desired outlet gas temperature is input here.

Summary Data (SUM)

Description	Value
Q (MW)	-0.83
Temperature Chang	-194.57

Upon completion, the total heat energy transferred, Q (expressed in MW), as well as the resultant *Temperature Change* expressed in **Kelvin**. Negative values indicate that heat was **removed** from the gas stream.

Gasifier CFD Module

The computer model used for the Gasifier Module is a CFD-based reacting flow code, GLACIER, developed by Reaction Engineering International (REI). The code couples the effects of turbulent fluid mechanics, gas-phase combustion chemistry, turbulent particle dispersion, heterogeneous particle reactions, and convective and radiative heat transfer. The REI combustion code assumes that the flow field is a continuum field that can be described locally by general conservation equations. The flow is assumed to be steady state and gas properties are determined through local mixing calculations. The fluid is assumed to be Newtonian and dilatation is neglected. The comprehensive model uses an Eulerian framework and handles either Reynolds- or Favre-averaging. The code couples the turbulent fluid mechanics and the chemical reaction process, using progress variables to track the turbulent mixing process and equilibrium chemistry to describe the chemical reaction process.

Within the model, the rate at which the primary combustion reactions occur is assumed to be limited by the rate of mixing between the fuel and the oxidizer, which is a reasonable assumption for the chemical reactions governing heat release. The thermodynamic state

at each spatial location is a function of the enthalpy and the degree of mixing of mixture fractions, one of which corresponds to the coal off-gas. The effect of turbulence and mixing on

mean chemical composition is incorporated by assuming that the mixture fractions are defined by a "clipped Gaussian" probability density function (pdf) having a spatially varying mean and variance. The mean and variance are computed numerically at each grid point and mean chemical species concentrations are obtained by convolution over the pdf. Specie concentrations are calculated as properties based on the local stream mixture and enthalpy. This is much more computationally efficient than tracking individual species.

Particle mechanics are solved by following the mean path or trajectory for a discretized group or ensemble of particles in a Lagrangian reference frame. Particle mass and momentum sources are converted from a Lagrangian to an Eulerian reference frame where they are coupled with gas phase fluid mechanics. The radiative intensity field is solved based on properties of the surfaces and participating medium and the resulting local flux divergence appears as a source term in the gas-phase energy equation.

Connections

- **Inlet Port 0:** Inlet gas stream
 - **Outlet Port 0:** Outlet gas stream
-

Graphical User Interface (UI)

The Gasifier module can be used to model either one stage or two stage gasifiers. One stage gasifiers are typified by a single set of injectors positioned in either a down flow (shown below) or upflow design. Two stage gasifiers usually have two larger compartments separated by a thin necked center section. Two stage gasifiers use two sets of injectors fired directly into each of the larger compartments (shown at right).

ONE STAGE DOWN-FIRED GASIFIER

T-FIRED TWO STAGE GASIFIER

The first folder, *Flows*, allows the user to specify the injector properties. The user interface is organized such that each of the three available injectors is configured **separately**, toggled by the radio button at the top of the screen. When the *One-stage* Gasifier button is toggled, only the first injector level is activated. When the *Two-stage* Gasifier button is toggled, then all three injector levels are activated (see schematic above). Required fields include steam *Flowrate* as well as slurry properties including *Temperature*, *Flowrate*, and percent *Coal*. The *Re-Cycled Char* is an externally computed value specified by the user to represent the percent char returning to the gasifier (typically from a feedback loop running through a [Cyclone](#) unit).

The *Misc* folder prompts for the *Pressure Drop* across the module, as well as for information regarding the chemical properties of the coal in the slurry. The workbench provides several preprogrammed coal types:

- E-Gas AppLS
- E-Gas AppMS
- E-Gas_Illinois_#6
- E-Gas_Utah
- E-Gas_Wyodak
- E-Gas_Wyoming
- Illinois_#5
- Illinois_#6
- Petcoke
- Pike_County
- Pittsburg_#8
- Pocahantas_#3

Summary Data (SUM)

The screenshot shows a 'Result Dialog' window with a 'Summary Data' tab. The window contains a table with two columns: 'Description' and 'Value'. The table lists four items: 'Soot Mass Fraction' (2.0E-002), 'Soot Part #/Mass Fraction' (5.0E-003), 'Tar Mass Fraction' (3.0E-002), and 'Thermal Input (MW)' (2.03e+001). The window has an 'OK' button at the bottom.

Description	Value
Soot Mass Fraction	2.0E-002
Soot Part #/Mass Fraction	5.0E-003
Tar Mass Fraction	3.0E-002
Thermal Input (MW)	2.03e+001

After the module has executed, the *Summary Data* button provides summary information. The module outputs calculated soot mass fraction, soot particle #/mass fraction, tar mass fraction and thermal input (MW).

References

1. Bockelie, M.J., Denison, M.K., Chen, Z., Senior, C.L., Linjewile, T., Sarofim, A.F., "CFD modeling of Entrained Flow Gasifiers for Vision 21 Energyplex Systems," Proceedings of the 19th Annual International Pittsburgh Coal Conference, Pittsburgh, PA, USA, Sept. 24-26, 2002(c).
 2. Bockelie, M.J., Denison, M.K., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F. and Holt, N., "CFD modeling for Entrained Flow Gasifiers," Proceedings of the Gasification Technologies Conference 2002, San Francisco, CA, Oct.28-30, 2002(e).
 3. Bockelie, M.J., Swensen, D.A., Denison, M.K., Chen, Z., Senior, C.L., Sarofim, A.F., "A Computational Workbench Environment for Virtual Power Plant Simulation" , Proceedings of the 27th International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, FL, USA, March 4-7, 2002(a).
 4. Bockelie, M.J., Swensen, D.A., Denison, M.K., Maguire, M., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., "A Process Workbench for Virtual Simulation of Vision 21 Energyplex Systems," to be presented at the 28th International Technical Conference on Coal Utilization & Fuel Systems, to be held in Clearwater, Florida, USA, March 10-13, 2003
-

Gasifier_0D Module

The 0-D gasifier model consists of two submodels: a zonal equilibrium submodel with heat transfer and an optional coal burnout submodel. The zonal submodel calculates the equilibrium exit gas concentration and

temperature given the calculated heat transfer through the walls. An ash viscosity submodel from the CFD gasifier slag model is used to calculate a representative ash viscosity and critical viscosity temperature. The fuel burnout is required by the zonal submodel that may be obtained from either the burnout submodel or simply specified as a user input. If the geometry is

input, the burnout is calculated by the burnout submodel. If the desired burnout is specified by the user, the burnout submodel is optional to determine the residence time and the geometry needed to produce the input burnout. The gas and radiation temperatures needed by the burnout submodel are obtained from the zonal submodel.

Schematic diagrams for the 0D model in a one and two stage gasifier are illustrated in the figures above and at right, respectively.

Connections

- **Inlet Gas Port 0** (top): Inlet gas stream for first stage
- **Inlet Gas Port 1** (middle): Inlet gas stream for second stage
- **Inlet Recycled Particle Port 2** (bottom): Inlet particle stream (usually feedback from Cyclone)
- **Outlet Port 0**: Outlet gas stream

Graphical User Interface (UI)

The Gasifier Module's graphical **User Interface** is divided into two folders.

The first folder, *Flows*, allows the user to specify the injector properties. The folder is organized such that each level of the three available injectors is configured **separately**. Required fields include steam *Temperature* and *Flowrate* as well as slurry properties including *Temperature*, *Flowrate*, and *Percent Coal*.

The Gasifier module can be used to model either one stage or two stage gasifiers. One stage gasifiers are typified by a single set of injectors positioned in either a down flow (shown below) or upflow design. Two stage gasifiers usually have two larger compartments separated by a necked center section. Two stage gasifiers use two sets of injectors fired directly into each of the larger compartments (shown at right).

When the one stage type is specified, only the first injector of the **User Interface** is active. When a two stage gasifier is selected, the user must input values for each of the three injectors (see diagram at right).

ONE STAGE DOWN-FIRED GASIFIER

The screenshot shows the 'Gasifier0D' window with the 'Misc' tab selected. The interface is divided into several sections:

- Geometry Specified:** Contains a 'Specify Geometry' checkbox (checked), a 'Dimensions' section with 'Diameter (m)' (2.2) and 'Length (m)' (5.5), and 'Rwall (m2-K/W)' for '1st Stage' (1) and '2nd Stage' (1).
- Burnout Specified:** Contains 'Burnout (%)' (98), 'Heatloss (%)' for '1st Stage' (0) and '2nd Stage' (0), a 'Design Mode' checkbox (unchecked), and 'L/D' (3).
- Emis:** Contains '1st Stage' (0.75) and '2nd Stage' (0.75).
- Misc:** Contains 'Backside Temp (K)' (300), 'Slag Efficiency (%)' (50), and 'Pressure Drop (Pa)' (502042).
- Coal Info:** Contains a 'Coal Type' dropdown (Illinois_#6), 'Size percent thru 50' (99.9), and 'Size percent thru 200' (90).

At the bottom are 'OK' and 'Cancel' buttons.

The *Miscellaneous* folder controls the calculation mode of the model. If the *Specify Geometry* button is selected, dimensions of the gasifier and the wall thermal resistance, R_{wall} , are input. Otherwise, the percent *Burnout* is input. With the *Specify Geometry* button unselected, the *Design Mode* button is available where, if selected, the user specifies the length over diameter ratio (L/D) and the model calculates the dimensions required to produce the specified *Burnout*. These results would be reported along with other module results.

Stage *Emis* are also specified in this folder, as well as *Backside Temp*, *Slag Efficiency*, and *Pressure Drop*. The *Coal Type* input allows the user to select coal characteristics from a number of pre-programmed coal types. Coal choices include:

- E-Gas AppLS
- E-Gas AppMS
- E-Gas_Illinois_#6
- E-Gas_Utah
- E-Gas_Wyodak
- E-Gas_Wyoming
- Illinois_#5
- Illinois_#6
- Petcoke
- Pike_County
- Pittsburg_#8
- Pocahantas_#3

Summary Data (SUM)

The screenshot shows a software window titled 'Result Dialog <3>' with a sub-header 'Summary Data'. It contains a table with two columns: 'Description' and 'Value'. The table lists various gasifier parameters and their calculated values. An 'OK' button is located at the bottom of the window.

Description	Value

1st Stage Wall He	0.00
2nd Stage Wall He	0.00
Burnout (%)	98.00
Cold gas efficien	87.29
Cold gas efficien	82.97
HHV (BTU/lb)	5018.07
LHV (BTU/lb)	4566.27
Output Temperatur	1389.06
Slag Critical Vis	1627.59
Slag Flow (kg/sec	1.57
Slag Surface Temp	1993.82
Slag Viscosity (P	2.42
Thermal Input (MW	875.69
Thermal Output (M	764.38

The Summary box shows the results of gasifier module calculations. The first values indicate the *Stage Wall Heat Transfer* (W), followed by the percent *Burnout*. The *Cold Gas Efficiencies* are expressed both as a percent of the higher heating value (*Thermal Output/Thermal Input*) as well as a percent of the lower heating value. The exiting gas stream's *Output Temperature* as well as the *Slag Critical Viscosity Temperature* (minimum temperature required for slag to flow) are both displayed in Kelvin. Further slag information is included such as *Slag Flow* (kg/s), *Slag Surface Temperature* (K), and *Slag Viscosity* (Pa-s). The calculated *Thermal Input and Output* (MW) are also included as computed using the higher heating value.

References

1. Bockelie, M.J., Denison, M.K., Chen, Z., Senior, C.L., Linjewile, T., Sarofim, A.F., "CFD modeling of Entrained Flow Gasifiers for Vision 21 Energyplex Systems," Proceedings of the 19th Annual International Pittsburgh Coal Conference, Pittsburgh, PA, USA, Sept. 24-26, 2002(c).
 2. Bockelie, M.J., Denison, M.K., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F. and Holt, N., "CFD modeling for Entrained Flow Gasifiers," Proceedings of the Gasification Technologies Conference 2002, San Francisco, CA, Oct.28-30, 2002(e).
 3. Bockelie, M.J., Swensen, D.A., Denison, M.K., Chen, Z., Senior, C.L., Sarofim, A.F., "A Computational Workbench Environment for Virtual Power Plant Simulation", Proceedings of the 27th International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, FL, USA, March 4-7, 2002(a).
 4. Bockelie, M.J., Swensen, D.A., Denison, M.K., Maguire, M., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., "A Process Workbench for Virtual Simulation of Vision 21 Energyplex Systems," to be presented at the 28th International Technical Conference on Coal Utilization & Fuel Systems, to be held in Clearwater, Florida, USA, March 10-13, 2003
-

Gas Mixer Module

The Gas Mixer is a utility module for mixing gas streams. The module calculates the outlet composition and temperature based on the relative flow rates of the individual inlet streams. The mixture temperature is determined to match the sum of the total enthalpy of the individual inlet streams. The higher pressure input stream is assumed throttled to the lower pressure input stream and therefore the pressure of the outlet mixture is calculated to be the lesser of the inlet pressures.

Connections

- **Inlet Ports 0,1,2,3** (where 0 = top): Inlet gas streams to be mixed
 - **Outlet Port 0**: Resultant outlet gas stream
-

Gas Separator Module

The Gas Separator module is used to separate a single specie out of a mixed gas stream.

Connections

- **Inlet Port 0:** Inlet gas stream.
- **Outlet Port 0 (top):** Outlet gas stream.
- **Outlet Port 1 (bottom):** Outlet concentrated gas stream containing targeted specie.

Graphical User Interface (UI)

A screenshot of the 'GasSeparator' dialog box. It has a title bar with 'GasSeparator' and a close button. Inside, there are three input fields: 'Specie' with a dropdown menu showing 'AR', 'Purity (%)' with a text box containing '95', and 'Remaining (%)' with a text box containing '1'. At the bottom, there are 'OK' and 'Cancel' buttons.

The user inputs which specie is to be separated from the gas stream as well as the desired purity. The *Remaining* input is the percentage of the specie that will remain in the non-pure stream. For example, from the inputs shown at left, the separated stream will be 95% argon, whereas the main gas stream will have only 1% argon concentration.

Gas Source Module

The Gas Source Module serves to initiate a module network by allowing the user to specify the initial properties of a gas stream. The module carries only a single output and is therefore used only when beginning a network or feedback loop within a network. When coupled with a gas feedback loop (see also [GasFeedback](#) module) the Gas Source Module is used as an "initial guess" of gas properties at a given point on the feedback loop.

Connections

- **Outlet Port 0:** Outlet gas stream with user-specified properties

Graphical User Interface (UI)

GasSource

Gas | Particle

Gas Average

Temperature (K): 290.8

Pressure (Pa): 101325

Flowrate (kg/s): 94.85

Specie	Composition	Mole Fraction
AR	AR	0.001
C(GR)	N2	0.789
C2H2	O2	0.21
C2H6		
CH		
CH4		
CO		
CO2		
COS		
H		
H2		
H2O		
H2O(L)		
H2S		
HCL		
HCN		
N		
N2		
N2O		
NH3		
NO		
NO2		
O		
O2		
OH		
OIL		
SO2		

Add Del

OK Cancel

User Interface-Gas

This first tab of the User Interface allows the user to specify the necessary temperature, pressure, and flowrate of the gas source. To specify gas composition first select a gas from the lower section and select *add*. Once the gas appears on the right side its molar fraction within the gas mixture can be specified (as a decimal) by clicking on the specie under the *Composition* column. The data is then stored when the user presses the *OK* button.

GasSource [X]

Gas | **Particle**

Particle Average

Particle Temperature (K):

Particle Flowrate (kg/s):

Mean Particle Size (M):

Size Variance (M^2):

Coal Calcium (wt%):

Ash Calcium (wt%):

Ash pH:

Constituent	Composition	Mass Fraction
ASH	ASH	0.0
CHAR	CHAR	0
COAL	COAL	0
WATER	WATER	0

User Interface- Particle

This second page of the User Interface prompts the user for information regarding particles within the gas stream. As with gases, particle properties such as temperature, flowrate, and particle size are assigned above while composition is specified below.

Gas Splitter Module

The Gas Splitter Module is used to split a single inlet gas stream into multiple outlet gas streams. The module simply redirects gas, and therefore only the flowrates of the outlet gases will differ from the inlet gas. Compositions and gas properties remain the same through the module.

The user specifies the number of desired outlet streams as well as the percentage of the inlet stream to be diverted into each outlet stream.

Connections

- **Inlet Port 0:** Inlet gas stream
- **Outlet Ports 0,1,2,3** (where 0 = top): Separated outlet gas streams

Percentage Flow	
Gas Port 0	49.92
Gas Port 1	46.08
Gas Port 2	0
Gas Port 3	4

This User Interface allows the user to determine how much of the inlet gas stream to divert to each outlet gas stream. Values represent percentages and should sum to 100.

Example (shown): 49.92 means that 49.92% of the inlet gas will flow out through outlet port 0. Therefore, if the inlet gas stream had a flowrate of 100 kg/s, the exiting gas stream flowing through outlet port 0 would have a new flowrate of 49.92 kg/s.

Heat Exchanger Module

The Heat Exchanger Module utilizes the effectiveness-NTU method to calculate the heat transferred between a gas and liquid stream. In order to compute outlet fluid properties the NTU method requires only inlet gas and water stream properties in addition to unit effectiveness. The heat transfer rate

effectiveness is internally computed from an array of user-specified unit properties.

Module calculations incorporate the use of a digitized family of curves from "*Steam*"¹ and the module runs an interpolation routine to calculate outlet gas and water properties.

Connections

- **Inlet Port 0** (top left): Inlet gas stream
 - **Inlet Port 1** (bottom left): Inlet water stream
 - **Outlet Port 0** (top right): Outlet gas stream
 - **Outlet Port 1** (bottom right): Outlet water stream
-

Graphical User Interface (UI)

The screenshot shows a window titled "HeatExchanger" with a close button (X) in the top right corner. The window contains the following fields and controls:

Field Name	Value
Arrangement	Cross Flow
Tube Configuration	Inline
Number of Tubes (Long)	20
Number of Tubes (Cross)	36
Tube Long Pitch-SI (m)	0.127
Tube Cross Pitch-St (m)	0.0826
Tube Inner Diameter (m)	0.0381
Tube Outer Diameter (m)	0.0445
Tube Length (m)	5
Internal Pressure Drop (Pa)	0
External Pressure Drop (Pa)	109096
☒ Finned Tubes	Fin Effectiveness: 2

At the bottom of the window are two buttons: "OK" and "Cancel".

This user interface prompts the user for properties of the heat exchanger unit. These data fields are necessary in order to compute the transfer heat rate effectiveness of the unit.

The *Internal Pressure Drop* field allows the user to specify a desired pressure drop for the water stream as it flows through the module, whereas the *External Pressure Drop* specifies the change in pressure of the gas stream through the module.

The user can also toggle whether the unit uses *Finned Tubes* and (when toggled) the *Fin Effectiveness* of those tubes.

References

1. Kitto, John B and Stultz, Steven C. *Steam: its generation and use*, 40th ed., The Babcock & Wilcox Company, Barberton, Ohio, USA, ©1992. p 4-11.
-

Heat Exchanger CFD Module

The Heat Exchanger CFD Module utilizes the Glacier CFD code. It is an experiment module. It is use to demonstrate the CFD to CFD coupling capability of the framework. Do not use this module to replace Heat Exchanger Module in ordinary simulation.

Connections

- **Inlet Port 0** : Inlet gas stream
- **Outlet Port 0** : Outlet gas stream

Summary Data (SUM)

After the module has executed, the *Summary Data* button provides summary information. The module outputs calculated soot mass fraction, soot particle #/mass fraction and tar mass fraction.

Kinetic Reactor Module

This model provides a general purpose homogeneous gas phase kinetics integration capability. This allows for the effect of finite rate quench on the water-gas shift reaction occurring in the gasifier syngas to be calculated. Currently, only GRI Mech 3.0 is available as the detailed kinetic mechanism. The model has three modes of operation, two PFR modes and the PSR mode. The first PFR mode is the constant pressure variable temperature option. In this mode the temperature is integrated adiabatically or a heat loss may be specified. In the second mode the user inputs a linear temperature profile to simulate the effect of quench. These first two modes work as a PFR calculation. The third mode is a PSR calculation.

Connections

- **Inlet Port 0:** Inlet gas stream.
 - **Outlet Port 0:** Outlet gas stream.
-

Graphical User Interface (UI)

In the PFR mode, the residence time is a required input. In the PFR TTIM mode the quench rate is an additional input. In the PSR mode, the residence time and volumetric heat loss are required inputs.

Membrane Reactor Module

The importance of this reaction lies in the ability to convert CO to H₂, which is valuable both as a fuel and as a chemical feedstock.

The membrane reactor for WGS uses a two-zone catalytic, fixed-bed, reactor with an integrated hydrogen selective membrane to convert the CO in cleaned syngas to hydrogen. Compared to other possible configurations, the annular feed configuration (see Figure at right) gave higher conversions for the same reactor size, and this configuration is assumed in the model (Marigliano et. al., 2001). Syngas enters and reacts on the feed-side of the membrane, and hydrogen permeates to and is carried away by a sweep gas (typically nitrogen or steam) on the permeate side of the membrane. A membrane reactor module would be positioned after gas cleanup units and before fuel cells, combustors, or other equipment which would process the hydrogen product gas.

The MR is a one dimensional model that integrates the hydrogen flux across the catalyst over the length of the unit. The integration is performed numerically using a second order explicit predictor corrector method, and the adiabatic equilibrium is computed locally from the feed gas enthalpy and composition. The model assumes plug flow, with no axial dispersion.

The hydrogen permeation rate is assumed to be the limiting process; chemical reactions

are assumed fast compared to hydrogen permeation. Thus, the feed gas is assumed to be in chemical equilibrium, and all catalytic reaction dependencies are ignored. This assumption has been used and validated in models in the literature (Damle et. al. 1994), (Devarajan et. al. 1991). Only chemical equilibrium for the water gas shift reaction is assumed, all other species are assumed inert. This option simplifies the solution procedure and, more importantly, allows reasonable computation times.

It is important to note that the membrane reactor only works so long as there is a hydrogen partial pressure driving force. Once the feed side hydrogen pressure matches that of the sweep gas, the WGS reaction is limited by the equilibrium composition. The primary purpose of the sweep gas is to dilute the hydrogen enough to provide a sufficient driving force over the membrane, hence allowing high CO conversion. A feed-to-permeate pressure ratio of 15 atmospheres is typical (Bracht et. al., 1997).

Connections

- **Inlet Port 0** (top left): Inlet gas stream
 - **Inlet Port 1** (bottom left): Inlet sweep gas stream
 - **Outlet Port 0** (top right): Outlet gas stream
 - **Outlet Port 1** (bottom right): Outlet sweep gas stream
-

Graphical User Interface (UI)

The screenshot shows a software window titled "MembraneReactor" with a close button (X). It contains two radio buttons: "Evaluation Mode" (selected) and "Design Mode". Below these are several input fields with numerical values: Membrane Diameter (m) is 0.1, Membrane Thickness (m) is 1e-005, Reactor Length (m) is 1.5, Desired CO conversion is 0.9, Number of Modules is 1200, and Shell Diameter (m) is 0.15. There are two checked checkboxes: "Allow Preshift Reactor" and "Specify H2O : CO". Below these, the "M.R. inlet temp (K)" is set to 565, and the "H2O : CO (ratio)" is set to 1. At the bottom are "OK" and "Cancel" buttons.

The User Interface first asks the user to specify the method of module calculation. *Evaluation Mode* (shown) allows the user to input existing membrane geometries (*Diameter, Thickness, and Length*), and the module will use these values to calculate the resultant CO conversion. To work backwards,

the *Design Mode* allows the user to specify a *Desired CO Conversion*, and uses a user-specified *Diameter* and *Thickness* to determine the *Reactor Length* necessary to achieve the desired conversion.

To allow further flexibility, the model is configured with an option to simulate the requirements of a staged operation in which the feed gas is first introduced to a *Preshift* catalytic non-membrane *Reactor*, cooled and then fed to the membrane reactor. A schematic of this option is presented at right, taken from Bracht et. al. (1997). As equilibrium is assumed with the aid of a catalyst, the pre-shift reactor is simply modeled as an adiabatic equilibrium on the feed gas. The temperature of the gas is then dropped to the user-specified *M.R. inlet temp*, with the required heat duty computed and displayed in the summary window below.

In addition, the user can specify the H_2O to CO ratio when the *Specify H2O:CO* option is toggled.

Summary Data (SUM)

The screenshot shows a 'Result Dialog' window with a 'Summary Data' section. It contains a table with two columns: 'Description' and 'Value'. The table lists various process parameters and their computed values. An 'OK' button is located at the bottom of the dialog.

Description	Value

CO Conversion (fr	0.79
Catalyst Space Ve	2651.73
Exit Gas Temp (K)	621.17
Footprint (m2)	27.00
H2 Recovery (frac	0.32
Pre- MR CO Conver	0.64
Pre-Shift Heat Du	11.43
Steam Required (k	9.8819
Sweep H2 Concentr	0.41

The Summary screen displays computed values of the module given specifications in the UI. The categories shown at left represent those displayed when both the Preshift and H₂O:CO ratio options are toggled. The *CO Conversion* is displayed as a fraction, as is the *H₂ Recovery*, *Pre- MR CO Conversion*, and the *Sweep H₂ Concentration*. Also displayed are the *Catalyst Space Velocity*, *Exit Gas Temperature*, unit *Footprint*, *Pre-Shift Heat Duty* (in MW), and finally the *Steam Required* (in kg/s).

References

1. M. Bracht, P.T. Alderliesten, R. Kloster, R. Pruschek, G. Haupt, E. Xue, J.R.H. Ross, M.K.Koukou, N. Papyannokos, "Water gas shift membrane reactor for CO₂ control in IGCC systems: techno-economic feasibility study," *Energy Convers. Mgmt Vol. 38, Suppl.*, pp. S159-S164, 1997.
-

PipeCFD Module (Pipe CFD)

This is an experiment module to demonstrate CFD to CFD coupling simulation. Do not use this module for ordinary simulation.

Connections

- **Inlet Port 0** : Inlet gas stream.
 - **Outlet Port 0** : Outlet gas stream.
-

PREKIN Module (Kinetics Pre-processor)

The *PREKIN* tool is designed for easy use by engineers and scientists with an advanced level of understanding of the physics, chemistry and modeling methods used for high pressure gasification kinetics. It is not intended for the casual user.

PREKIN requires numerous, detailed inputs for coal parameters (typically obtained from laboratory tests), reaction conditions within the gasifier and model parameters. The inputs are organized into five panels

- general coal information
- devolittization kinetics
- oxidation kinetics
- char gasification kinetics
- reaction conditions in the gasifier

No Connections

- This module runs by itself to generate a profile used by GasifierCFD.
-

Graphical User Interface (UI)

Prekin

Coal | Devolatilization | Oxidation | Gasification | Reaction Conditions

Coal Name

Pittsburg_#8

Mode of Burning

0.2

Linear Swelling Factor

-1

Initial Fuel Carbon Density, g/cm3

-1

Ash Film Porosity

0.17

Ash Grain Size, um

5

Ash Thermal Conductivity, cal/cm-s-deg

0.005

Particle Size Distribution

% through 50 Mesh

97.4

% through 200 Mesh

73.4

Pore Structure Model

☐ Parallel Model

T/1

6

☒ Random Pore Model

Average Radii For Macropore, um

75

Average Radii For Micropore, um

0.1

Macroporosity

0.1

Porosity

0.58

OK

Gen Profile

Cancel

Prekin

Coal | Devolatilization | Oxidation | Gasification | Reaction Conditions

Model Selector

Model

☒ Manual Input of Volatile Yield

☐ 120% of ASTM

☐ CPD

☐ Two-Step

HTVL (%) (0~100)

-1

CPD parameters

AB

2.602e+01

EB

55400

EBSIG

1800

AC

0.9

EC

0

EGSIG

8100

AG

3e+015

EG

69000

ECR

65000

ACR

3e+015

ECR

65000

☐ Structure parameters: Manual Input

P0

0.61

C0

0

SIGP1

4.6

MW

267

MDL

29

Two-Step parameters

A1,1/s

962000

E1,cal/mol

17579

Y1

0.65

A2,1/s

1.5e+013

E2,cal/mol

59950

Y2

1

Devolatilization Conditions

Heating Rates, deg/s

100000

Maximum Temp, K

2000

Total Residence Time, sec

0.1

of Grid Points: Heating

30

of Grid Points: Isothermal

20

OK

Gen Profile

Cancel

Prekin

Coal | Devolatilization | **Oxidation** | Gasification | Reaction Conditions

☒ **Gasification Page**

☐ Fractional Order Power Law

FOPL Parameters

☐ Mass-specific Intrinsic Reactivity

$K_o S_o, \text{gC/gC-s-(mol/m}^3)^n$

$K_o, \text{gC/m}^2\text{-s-(mol/m}^3)^n$

$S_o, \text{m}^2\text{C/gC}$

Intrinsic Activation Energy, cal/mol

Intrinsic Reaction Order

☐ Semi-global

Semi-global Parameters

$K_{3o}, 1/\text{s}$ $E_1, \text{cal/mol}$

K_{2o}/K_{3o} $E_2, \text{cal/mol}$

K_{3o}/K_{1o} $E_3, \text{cal/mol}$

Intrinsic Reaction Order for Step 2

CO/CO₂ Ratio

A_{co} $E_{co}, \text{cal/mol}$

OK Gen Profile Cancel

Prekin

Coal | Devolatilization | **Oxidation** | Gasification | Reaction Conditions

☐ **Oxidation Page**

☒ Fractional Order Power Law

☒ CO₂ ☐ H₂O

$K_o, \text{gC/m}^2\text{-s-(mol/m}^3)^n$

$S_o, \text{m}^2/\text{gC}$

Intrinsic Activation Energy, cal/mol

Intrinsic Reaction Order

☐ Langmuire-Hinshelwood Kinetics

☒ CO₂ ☐ H₂O

$K_{1o}, 1/\text{atm-s}$ $E_1, \text{cal/mol}$

$K_{2o}, 1/\text{atm}$ $E_2, \text{cal/mol}$

$K_{3o}, 1/\text{atm}$ E_3

Product/Reactant Ratio

from to # of steps

OK Gen Profile Cancel

Prekin

Coal | Devolatilization | **Oxidation** | Gasification | Reaction Conditions

Simulation Conditions

Mean Rxn Temp, K +/- % # of Temp Steps

Reactant Fractions to # of Pressure Steps

Total Pressure, atm

Time Interval, sec # of Time Steps

Conversion Level, %

Optimization

Starting Values :

$k_G, \text{kgC/m}^2\text{-s-(Pa)}^m$

$E_G, \text{kcal/mol}$

m

Tolerance

Schema:

☒ Varying k_G only ☐ Varying k_G and m ☐ Varying All

Recommended Time Interval, sec

for oxidation : 0.01 sec

for gasification : >=10 sec

OK Gen Profile Cancel

Coal

This panel is used to enter general properties of the coal. Required items include the coal type (can select coal types contained in a database), coal swelling factor, ash characteristics, coal grind (mass of particles through 50 and 200 mesh), and pore structure information. More generic coal data such as ultimate and proximate analysis is accessed via the coal database capability within the framework.

Devolatilization

In this panel the user selects the devolatilization model to use. Options include manual input of volatile, 120% of ASTM volatile yield value determined in the ultimate/proximate analysis, CPD [Brown et al, xxxx], or a two step model [Kobayashi, 1978]. These models and their corresponding parameters are described in more detail in the section entitled Devolatilization located above.

Oxidation

In this panel the user selects the oxidation model to use and enters corresponding numerical parameters. The available options include re-use of values from the char gasification model inputs, fractional order power law, semi-global kinetic rates or specifying the CO:O₂ ratio. For additional detail on the different models and model parameters see the section entitled Oxidation located above.

Gasification

In this panel the user can select from different options on how to model the char gasification. Available models include using information from the oxidation model inputs (?), fractional order power law for CO₂ and/or H₂O, Langmuir-Hinshelwood kinetics or specifying the product/reactant ratio. Additional details on these models and their corresponding numerical parameters are provided above in the section entitled Gasification.

Reaction Conditions

This input panel is used to enter general conditions that are expected to occur within the gasifier as well as required numerical parameters.

The outputs from the model are gasification rates (numerical values) that can be used in most modeling tools intended for modeling coal combustion or gasification. Within the framework, the gasification rates computed by *PREKIN* are passed directly to the entrained flow model

References

1. Anthony D.B. and Howard J.B., Coal devolatilisation and hydrogasification, AIChE J., 22, 625-656, 1976.

2. Arendt P. and van Heek K.H., Comparative investigations of coal pyrolysis under inert gas and H₂ at low and high heating rates and pressures up to 10 MPa, *Fuel*, 60, 779-787, 1981.
3. Banin et al., *Combustion and Flame*, 108, 1-8 (1997)
4. Beath A.C., Mathematical modeling of entrained flow gasification, PhD thesis, University of Newcastle, Australia, 1996.
5. Benfell, K. E., Liu, G.-S., Roberts, D. G., Harris, D. J., Lucas, J. A., Bailey, J. D., and Wall, T. F., *Proceedings of the Combustion Institute*, 28, 2233-2241 (2000)
6. Benyon P.J., Computational modeling of entrained flow slagging gasifiers, PhD thesis, University of Sydney, Australia, 2002.
7. Biederman DL "A study of the oxidation of graphite by carbon dioxide", PhD Thesis, Penn. State Univ., 1965.
8. Chapman S, Cowling TG "Mathematical Theory of Non-Uniform Gases", Second Edition, Cambridge University Press (1951), Chapters 10 and 14.
9. Dobner S, Modeling of Entrained Bed Gasification: The Issues; LUPA AND KLIESCH (1979) Internal Report, 1/15/76.
10. Ergun S *J. Phys. Chem.* 1956, 60, 480.
11. Fletcher T.H., Kerstein A.R., Pugmire R.J. and Grant D.M., *Energy & Fuels*, 4, 54, 1990.
12. Frank-Kamenetskii DA, *Diffusion and Heat Transfer in Chemical Kinetics*, Plenum Press, New York (1969).
13. Gadsby J, Long FJ, Sleightholm P, Sykes KW *Proc. Roy. Soc. (London)* 1948, A193, 357
14. Gibbins J.R. and Kandiyoti R., The effect of variations in time-temperature history on product distribution from coal pyrolysis, *Fuel*, 68, 895-903, 1989.
15. Grant, D. M., R. J. Pugmire, T. H. Fletcher, and A. R. Kerstein, "A Chemical Model of Coal Devolatilization Using Percolation Lattice Statistics," *Energy and Fuels*, 3, 175 (1989).
16. Griffin T.P., Howard J.B. and Peters W.A., Pressure and temperature effects in bituminous coal pyrolysis: experimental observations and a transient lumped-parameter model, *Fuel*, 73, 591-601, 1994.

17. Harris D.J., Kelly M.D., Roberts D.G., Mill C.J., Stubington J.F. and Wall T.F., Determining coal reactivity parameters at elevated pressures using bench-scale techniques, 2002.
18. Harris, D. J., and Smith, I. W., Proceedings of the Combustion Institute, 23, 1185-1190 (1990)
19. Hurt RH, Calo JM Semi-Global Intrinsic Kinetics for Char Combustion Modeling Comb.Flame 125, 1138-1149 (2001).
20. Hurt RH, Sun JK, Lunden M, "A Kinetics Model of Carbon Burnout in Pulverized Coal Combustion," Combustion and Flame 113, 181 (1998).
21. Kobayashi H, Howard JB, Sarofim AF 16th Symp. (Int.) Comb., Combustion Inst., Pittsburgh, 411 (1977).
22. Joutsenoja et al., Energy and Fuels, 13, 130-145 (1999)
23. Lewis WK, Gilliland ER, McBride GT Jr., Ind.Eng.Chem. 31, 1213-26 (1949)
24. Liu, G., Benyon, P., Benfell, K.E., Bryant, G.W., Tate, A.G., Boyd, R. K., Harris, D.J., and Wall, T.F., Fuel, 79, 617-626 (2000)
25. Lupa and Kliesch, "Simulation of a Texcao Gasifier, Vol.1 A Steady State Model", LUPA AND KLIESCH (1979) Report AF-1179, Vol. 1 Research Project 1037-1. Final Report, 1979
26. Meijer R, Sibeijn M, van Dillen MRB, Kapteijn F, Moulijn JA I&EC Research., 30(8), 1760-1770 (1991).
27. Mentser M, Ergun S, "A study of the carbon dioxide carbon reaction by oxygen exchange", Bull.US Bur.Mines No. 664, 1973.
28. Mitchell RE A Theoretical Model of Chemically reacting Recirculating Flows, Sandia Technical Report, SAND79-8236, Sandia National Laboratory, Livermore, CA (1980)
29. Mitchell RE, Hurt RH, Baxter LL, Hardesty DR Compilation of Sandia Coal Char Combustion Data and Kinetic Analyses: Milestone Report Sandia Technical Report, SAND92-8208, 1992.
30. Monson et al., Combustion and Flame, 100, 669-683 (1995)
31. Mühlen H-J, van Heek KH, Jüntgen H "Kinetic studies of steam gasification of char in the presence of H₂, CO₂ and CO" Fuel, Vol 64, July, 944-949 (1985).

32. Niksa S. and Kerstein A.R., FLASHCHAIN theory for rapid coal devolatilization kinetics 1. Formulation, Energy & Fuels, 5, 673-683, 1991.
33. Okumura Y., Sugiyama Y. and Okazaki K., Evolution behavior of coal-nitrogen in high pressure pyrolysis processes, Fuel Chemistry Division Preprints, 46, 141-143, 2001.
34. Otaka et al., 26th International Conference on Coal Utilization and Fuel Systems, Clearwater, Fl., 2001
35. Roberts, D. G., and Harris, D. J., Energy & Fuels, 14, 483-489 (2000)
36. Roberts, D.G., Harris, D. J., and Wall, T. F. , "High-Pressure Intrinsic Char Gasification Kinetics: an Application of a modified nth-order rate equation", 18th Pittsburgh Coal Conference, Newcastle, Australia, 3-7 Dec, 2001.
37. Roberts GW, Satterfield CN, "Effectiveness Factor for Porous Catalysts", Ind. Eng. Chem. Fundamentals, Vol. 4, No. 3, 288 (1965)
38. Request forms, a booklet describing the entire Penn State Coal Sample Bank and Database, and assistance in acquiring samples and data can be obtained from:
 39. Coal and Organic Petrology Laboratories
 40. The Pennsylvania State University
 41. 105 Academic Projects Building
 42. University Park, PA 16802-2300
43. Senneca, O., Salatino, P., Masi, S., Fuel, 77, 1483 (1998).
44. Smith I.W., The combustion rates of coal chars: a review, Proceedings of the Combustion Institute, 1045-1065 (1982)
45. Solomon P.R., Hamblen D.G., Carangelo R.M., Serio M.A. and Deshpande G.V., General model of coal devolatilization, Energy & Fuels, 2, 405, 1988.
46. Solomon P.R., Serio M.A. and Suuberg E.M., Coal pyrolysis: experiments, kinetic rates and mechanisms, Prog. Energy Combustion Sci., 18,m 133-220, 1992.
47. Strange JF, Walker PL Jr. Carbon 1976, 14, 345.
48. Suuberg EM, Fundamental Issues in Control of Carbon Gasification Reactivity, Kluwer Academic Publishers, Dordrecht (1991).
49. Hampartsoumian JE, Pourkashanian M, Williams A Journal of the Institute of Energy, March, p. 48 (1989)

50. Suuberg E.M., Peters W.A. and Howard J.B., Product compositions and formation kinetics in rapid pyrolysis of pulverised coal - implications for combustion, Proceedings of the Combustion Institute, 17, 117-128, 1978.
 51. Tampa Electric Integrated Gasification Combined-Cycle Project, Clean Coal Technology Topical Report Number 19, July 2000.
 52. Ubhayakar SK, Stickler DB, von Rosenberg CW, Gannon RE 16th Symp.(Int.) Comb., Combustion Inst., Pittsburgh, 427 (1977).
 53. von Fredersdorff CG, Pyrcioch EJ, Pettyjohn ES Inst.Gas Technol., Research Bull., NO. 7, 71 (1957)
 54. Wakao N, Smith JM, Diffusion in Catalyst Pellets, Chem. Eng. Sci., 17, 825 (1962).
 55. Wall T.F., Liu G.-S., Wu H.-W., Roberts D.G., Benfell K.E., Lucas J.A. and Harris D.J., The effect of pressure on coal reactions during pulverized coal combustion and gasification, to be published, 2002.
 56. Wen C.Y. and Chaung T.Z., Entrained coal gasification modeling, Ind. Eng. Chem. Process Des. Dev., 18, 684-695, 1979.
 57. Wheeler A, Advances in Catalysis, Academic Press, New York (1951).
 58. Wu, H., Bryant, G. W., and Wall, T. F., Energy and Fuels, 14, 745-750 (2000).
 59. Wu PC "The kinetics of the reaction of carbon with carbon dioxide", ScD thesis Chem.Eng., Massachusetts Institute of Technology, 1949
 60. Wu P-C, Lower WE, Hottel HC "Reaction kinetics of carbon dioxide with electrode carbon particles", Fuel, Vol 67, February, 205 (1988).
-

Recuperator Module

The
Recuperator
Module utilizes
the
effectiveness-
NTU method to
calculate the
heat transferred
between two
gas streams. In
order to
compute outlet
stream

properties the

NTU method requires only inlet stream properties in addition to unit effectiveness. The heat transfer rate effectiveness is internally computed from an array of user-specified unit properties.

Module calculations incorporate the use of a digitized family of curves from "*Steam*"¹ and the module runs an interpolation routine to calculate outlet gas properties.

Connections

- **Inlet Port 0** (left): Inlet gas stream
 - **Inlet Port 1** (top): Inlet gas stream
 - **Outlet Port 0** (right): Outlet gas stream corresponding to Inlet Port 0
 - **Outlet Port 1** (bottom): Outlet gas stream corresponding to Inlet Port 1
-

Graphical User Interface (UI)

The image shows a Windows-style dialog box titled "Recuperator". It contains several input fields and checkboxes. The "Arrangement" dropdown is set to "Counter Flow" and "Tube Configuration" is set to "Inline". The "Number of Tubes (Long)" is 64 and "Number of Tubes (Cross)" is 28. The "Tube Long Pitch-SI (m)" is 0.127, "Tube Cross Pitch-St (m)" is 0.0826, "Tube Inner Diameter (m)" is 0.03, and "Tube Outer Diameter (m)" is 0.045. The "Tube Length (m)" is 10. The "Internal Pressure Drop (Pa)" and "External Pressure Drop (Pa)" are both set to 0. The "Finned Tubes" checkbox is checked, and the "Fin Effectiveness" is 0.7. At the bottom are "OK" and "Cancel" buttons.

Parameter	Value
Arrangement	Counter Flow
Tube Configuration	Inline
Number of Tubes (Long)	64
Number of Tubes (Cross)	28
Tube Long Pitch-SI (m)	0.127
Tube Cross Pitch-St (m)	0.0826
Tube Inner Diameter (m)	0.03
Tube Outer Diameter (m)	0.045
Tube Length (m)	10
Internal Pressure Drop (Pa)	0
External Pressure Drop (Pa)	0
Finned Tubes	☒
Fin Effectiveness	0.7

This user interface prompts the user for geometrical properties of the recuperator unit. These data fields are necessary in order to compute the transfer heat rate effectiveness of the unit.

The *Internal Pressure Drop* and *External Pressure Drop* fields allow the user to specify desired pressure drops for the two gas streams. The *Internal* field corresponds to the change in pressure for the gas stream that is heated by the recuperator whereas the *External* field corresponds with the change in pressure of the hot gas stream as it flows through the recuperator.

The user can also toggle whether the unit uses *Finned Tubes* and (when toggled) the *Fin Effectiveness* of those tubes.

References

1. Kitto, John B and Stultz, Steven C. *Steam: its generation and use*, 40th ed., The Babcock & Wilcox Company, Barberton, Ohio, USA, ©1992. p 4-11.
-

SOFC Module (Solid Oxide Fuel Cell)

This module makes use of the Nernst equation and equations for activation, concentration, and ohmic losses to calculate fuel cell electrical output. Thermodynamic calculations are performed using a combination of equilibrium and heat exchanger calculations. The anode temperature is iterated until the thermodynamic output from the fuel cell matches the electrical output. The model obtained from DOE-NETL was developed for use in Aspen-Plus and employed a combination of Aspen-Plus functions and imbedded FORTRAN. The DOE model was subsequently re-implemented using C++ for use in the workbench. Enhancements from the NETL fuel cell model include the ability to use coal derived syngas as the fuel gas, operate at elevated pressure, remove the fuel gas reformer (not needed for IGCC), and use more robust equation solvers.

This module is coded only to handle CO and H₂ coming into the anode as fuels. This is 'hardwired' in both the thermal and electrical calculations. The cathode 'air' stream, however, is **not** limited to just O₂ and N₂. The cathode composition is arbitrary - the code just pulls off enough O₂ to react with the CO and H₂ entering in the anode stream at the specified fuel utilization level.

Connections

- **Inlet Port 0** (left): Inlet anode gas stream (rich in CO and H₂)
- **Inlet Port 1** (top): Inlet cathode gas stream
- **Outlet Port 0**: Outlet gas stream

Graphical User Interface (UI)

The screenshot shows the SOFC GUI with the following fields and values:

Section	Parameter	Value
Construction	Anode Thickness (cm)	0.15
	Cathode Thickness (cm)	0.01
	Electrolyte Thickness (cm)	0.001
	Fuel Cell Pressure Drop (Pa)	27576
Cell Resistance: $R = A_e \cdot (E/t)$	Anode, A	0.00298
	Anode, E	-1392
	Cathode, A	0.008144
	Cathode, E	600
	Electrolyte, A	0.00294
	Electrolyte, E	10350
Cells	Area per unit cell (cm ²)	305
	Number of cells	70000
Fuel Utilization (%)		85

Buttons: OK, Cancel

This user interface allows the user to manipulate fuel cell characteristics and performance. The user can input not only fuel cell size and quantity, but also the cell resistance and general construction of the unit.

Summary Data (SUM)

This screen shows results after the module is executed. The first line shows the exiting *Anode Temperature* (outlet gas) while the second shows the *Fuel Cell Power* in MW.

References

1. Bessette, N.F., "Modeling and simulation for solid oxide fuel cell power systems," Ph.D. Thesis (1994), Georgia Institute of Technology.
 2. Gemmen, R.S., Liese, E., Rivera, J.G., Faryar J. and Brouwer, J. "Development of dynamic modeling tools for solid oxide and molten carbonate hybrid fuel cell gas turbine systems". ASME, May 8-12, 2000.
 3. Liese, E. and Gemmen, R.S., "Dynamic modeling results of a 1 MW molten carbonate fuel cell/gas turbine power system." Proceedings of ASME Turbo Expo 2002, June 3-6, Amsterdam, The Netherlands. GT 2002 30110.
-

SOFC 1D Module

The SOFC_1D model is of higher fidelity compared to the 0-D SOFC model also in the workbench. The model allows for steady-state spatial variation in one dimension along the fuel cell.

Connections

- **Inlet Port 0** (left): Inlet anode gas stream (rich in CO and H₂).
- **Inlet Port 1** (top): Inlet cathode gas stream.
- **Outlet Port 0** (up): Outlet anode gas stream.
- **Outlet Port 1** (bottom): Outlet cathode gas stream.

SOFC1D

Working Directory

Anode

Channel Height (m)
Channel Width (m)
Channel Spacing (m)
Exg.Cur.Den. (Amp/m2)
Trans. Coeff
Electrode Thickness (m)
Pressure Drop (Pa)

0.001

0.001

0.001

5

1e+006

5e-005

3250

Cathode

Channel Height (m)
Channel Width (m)
Channel Spacing (m)
Exg.Cur.Den. 'b' Coeff
Exg.Cur.Den. 'm' Coeff
Trans. 'B' Coeff
Trans. 'M' Coeff
Electrode Thickness (m)
Pressure Drop (Pa)

0.003

0.001

0.001

-13595

15

0.5

0

5e-005

431

Separator

Thickness (m)
Heat Capacity (J/kg-K)
Density (kg/m3)

0.002

400

8000

Electrolyte

Thickness (m)
Res. PreExpon. (ohm-cm)
Res. Expon. (K)

0.00018

0.002838

10300

Electrodes

Fuel Res. PreExpon. (ohm-cm)
Fuel Res. Expon. (K)
Air Res. PreExpon. (ohm-cm)
Air Res. Expon. (K)

0.0014

0

0.0186

0

Interconnect

Res. PreExpon. (ohm-cm)
Res. Expon. (K)

0.5

0

Cells

Number of Cells
Heat Capacity (J/kg-K)
Density (kg/m3)
Axial Length (m)
Axial Width (m)

1000

800

1500

1

1

Operational

Stop Time (sec)
Number of Axial Nodes
Load Resistance (ohm)

1000

5

0.006

OK

Cancel

Graphical User Interface (UI)

This user interface allows the user to manipulate fuel cell characteristics and performance. The user can input not only fuel cell size and quantity, but also the cell resistance and general construction of the unit.

Summary Data (SUM)

This shows results after the module is executed. The first line shows overall produced power and heat transfer of the unit.

Steam Turbine Module

The Steam Turbine module is based on thermodynamic calculations using adiabatic efficiency. The efficiency is applied to an isentropic expansion process using the ASME 67 steam properties.

Connections

- **Inlet Port 0:** Water supply, as superheated steam, to turbine
- **Outlet Port 0:** Turbine exhaust as condensed outlet water stream

Graphical User Interface (UI)

This User Interface allows the user to specify the desired *Isentropic Efficiency* (as a decimal fraction) and the *Pressure Drop* across the module.

Summary Data (SUM)

The summary table outputs *Power* generated by the turbine shaft unit.

References

1. Schematic modified from www.smud.org/cpp/construc/schemati.pdf
-

Sulfur Polisher Module

The Sulfur Polisher module is part of the warm (hot) gas cleanup unit, designed to follow the Bulk Desulfurizer and achieve very high removal of sulfur species from the gas stream. The primary sulfur species of concern are H_2S and COS , and the unit is designed to achieve exit concentrations of about 0.1 ppm H_2S and 0.01 ppm COS . While the Bulk Desulfurizer can reduce sulfur emissions to levels acceptable for gas turbine operation, very high removal is required for downstream equipment such as fuel cells and other catalytic units, and a sulfur polisher is needed. The Sulfur Polisher module is based on a non-regenerable, fixed sorbent bed (typically ZnO), operating at a nominal temperature of 672 K. The unit is intended to be placed downstream of the Bulk Desulfurizer and is assumed to be of use in both hot and warm gas cleanup systems, provided a suitable sorbent is used.

The Sulfur Polisher module acts as a component separator. The user provides either a removal efficiency or an exit concentration for COS and H_2S . A temperature change can be specified to account for heat effects. Pressure drop across the unit can be specified or computed using specific module configuration details as shown in the User Interface (UI). The calculated pressure drop is based on the Ergun equation [Kunii and Levenspiel, 1969]

and requires the bed diameter, depth, void fraction, nominal particle size, and particle sphericity. The unit outputs are the exit gas state: temperature, pressure, and composition.

Connections

- **Inlet Port 0:** Inlet gas stream
- **Outlet Port 0:** Outlet gas stream with low sulfur concentration

Graphical User Interface (UI)

This user interface first allows the user to specify the change in temperature of the gas through the module--thereby accounting for heat losses. Negative values represent a decrease of temperature in the gas between inlet and outlet ports (heat lost by the gas). (Note that the temperature change is measured in degrees **Fahrenheit**)

H₂S and COS removal calculations can be made either by specifying the desired removal efficiencies or by specifying the desired exit concentrations. Appropriate exit concentrations are on the order of .1 ppm for H₂S and .01 for COS.

Pressure drop across the module can either be *specified* (in **psi**) or *computed* within the module. If the exit concentration is *specified*, the value should be below that of the inlet. The *calculated* pressure drop is based on the Ergun equation, with terms to account for the static head pressure drop (pressure lost in suspending the solid particles,) and the wall friction. *Void fraction* is defined as 1 - sorbent volume / bed volume. The *particle size* can be computed as the diameter of a

sphere of the same volume as the particle. The *sphericity* is the surface area of the sphere described above divided by the actual particle surface area.

Default values are provided for temperature drop, exit acid gas concentrations, specified pressure drop, and sphericity (for the computed pressure drop option).

Summary Data (SUM)

After the module has executed, the *Summary Data* button provides summary information. The module outputs module *Reduction Efficiencies* for both COS and H2S, as well as the *Pressure Drop* (in **psi**) across the module and the *Temperature Out* (K) of the resultant outlet stream.

References

1. Kunii, D., and Levenspiel, O., Fluidization Engineering, John Wiley and Sons Inc., 1969, pp 698-699.
-

Water Pump Module

A water pump model has been added which calculates required power needed to achieve the input pressure rise based on an input isentropic efficiency of the pump.

Connections

- **Inlet Port 0:** Inlet water stream.
- **Outlet Port 0:** Pressurized outlet water stream.

Graphical User Interface (UI)

The User Interface first allows the user to input an *Isentropic Efficiency* for the Water Pump (as fraction).

When in evaluation mode the user must also specify a desired *Pressure Change* (outlet pressure - inlet pressure). In design mode, the user specifies the *desired outlet pressure* and the module accordingly calculates the required pressure change.

Summary Data (SUM)

The Summary screen displays the computed *Power* to coincide with specifications entered in the UI. Negative values represent the power required.

The Water Source Module serves to initiate a module network by allowing the user to specify the initial properties of a water stream. The module carries only a single output and is therefore only used as a specified water source. [Heat Exchangers](#), [Steam Turbines](#), HRSG's and syngas coolers all require water and would likely be coupled with the WaterSource module.

Connections

- **Outlet Port 0:** Outlet water stream with user-specified properties

Graphical User Interface (UI)

A screenshot of a graphical user interface window titled "WaterSource". It features two radio buttons at the top: "Temperature/Pressure" (selected) and "Pressure/Enthalpy". Below these are four input fields: "Temperature (K):" with the value "310", "Pressure (Pa):" with the value "3.73e+006", "Enthalpy (J/kg):" with the value "0", and "Flowrate (kg/s):" with the value "75". At the bottom are "OK" and "Cancel" buttons.

This User Interface allows the user to specify either the desired temperature and pressure or pressure and enthalpy of the water source. The water flowrate is also a required input. Selecting *OK* saves the data for future network execution.

Appendix D

REI Reacting CFD Model Capabilities

Note - All figures, tables and literature citations refer to information in this Appendix.

The CFD-based models used for the LEBS-POC and entrained flow gasifier models were created using REI's proprietary, comprehensive reacting CFD code *GLACIER*. An overview of the modeling capabilities provided in *GLACIER* is summarized below.

GLACIER is a comprehensive reacting CFD code that has been used to model approximately 150 different industrial furnaces. The algorithms used in the *GLACIER* code are robust, accurate, iterative solvers that extract the nonlinear coupling between turbulent fluid mechanics, gas-phase reaction chemistry, heat transfer (particularly radiation), particle-phase reaction, turbulent particle dispersion, and particle-wall or heat transfer surface interactions. Particle/fluid interphase coupling is included through a moving-Eulerian particle cloud tracking and source distribution technique. Computations of turbulent fluctuations include statistical distributions for all reaction and radiation properties. Reaction and radiation calculations can include any number of chemical species. *GLACIER* has the following model capabilities:

- complex 3D geometries;
- polydispersed phases of gases and particles, droplets or slurries with full mass, and momentum and energy coupling between phases;
- multiple reaction rate processes for liquid vaporization, coal devolatilization, and heterogeneous particle reactions;
- steady-state, laminar or turbulent flows;
- mixing and reaction of multiple fuels;
- full coupling between turbulent fluid mechanics, radiative and convective heat transfer, and chemical reactions;
- homogeneous combustion and gasification performed with equilibrium chemistry and turbulence-chemistry interaction accounted for with an assumed shape Probability Density Function (PDF);
- radiative heat transfer for scattering-absorbing-emitting, turbulent, sooting media;
- variable thermal boundary conditions including adiabatic, thermal resistance, heat exchanger;
- prediction of particle trajectories, concentrations and dispersion, particle deposition;
- slagging of material deposited on walls; and
- soot and tar production/destruction.

To compute pollutant emissions, vaporized metals and other trace species, finite-rate chemistry effects can be included in a post-processor mode.

Further details on the *GLACIER* CFD code and its application are available at <http://www.reaction-eng.com>.

Appendix E

RECOM Reacting CFD Model Capabilities

Note - All figures, tables and literature citations refer to information in this Appendix

Reaction and Combustion Modeling Services (RECOM), located in Stuttgart, Germany provides furnace modeling services to their customers using *AIOLOS*, a comprehensive, reacting CFD modeling code. *AIOLOS* was originally developed at the Institute of Process Engineering and Power Plant Technology (IVD) at the University of Stuttgart. Through a technology agreement with IVD, RECOM markets *AIOLOS* to industrial customer and uses *AIOLOS* to solve industrial furnace problems.

AIOLOS can be used to model a broad range of turbulent reacting flows. It can be used to model two-phase fuel applications, using either Eulerian-Eulerian or Eulerian-Lagrangian methods. *AIOLOS* employs an EDC technique for turbulence-chemistry coupling. It can employ multi-domain grids and perform time-dependent coal combustion simulations using either implicit or explicit time stepping. It can be used on virtually any level of hardware or operating system. *AIOLOS* is parallel-capable on both SMP and distributed architectures. It can be executed on single or dual cpu PCs/workstations, PC clusters and has been tuned for use on supercomputers. The general capabilities of the code include:

- General features
 - 3D Finite-Volume code for turbulent reactive flows
 - Cartesian, or cylindrical coordinates, body-fitted coordinates
 - Non-staggered, structured grid
 - SIMPLEC or PISO pressure correction scheme
 - Higher-order schemes for spatial discretization to minimize numerical diffusion
 - Temporal discretization by Euler Implicit
 - Hybrid parallelization strategy: Combined multiblock and microtasking methodology for distributed and shared memory computer architectures
 - Solution algorithms: SOR, Stone, CG methods, Multigrid (under development), optimized for vector- and parallel-processor computer systems
 - Domain decomposition techniques: Individual choice of coordinate system and grid resolution, and of physical models and numerical methods in different sub-domains
 - Installations in industry on various hardware platforms
- Turbulent two-phase flow
 - k-epsilon model and Differential Reynolds Stress model
 - Eulerian approach (particle phase treated as a continuous phase)
 - Eulerian/Lagrangian two-phase flow description (fully coupled)
- Heat transfer
 - Discrete Ordinates Method
 - Semistochastic Monte Carlo radiation model
 - Moment Method
 - Finite-Volume Method
 - Flux Method
 - Discrete Transfer Model
- Reaction model
 - Kinetic model using GRI Mech 3.0, advanced Eddy Dissipation Concept (EDC)
 - For pulverized-coal combustion (pyrolysis, tar formation and tar decomposition, char and volatile combustion). Consideration of particle-size distribution

- Model for pollutant formation (fuel NO, thermal NO) for unstaged, air-staged, and fuel-staged (reburn) combustion systems.

Further details on the *AIOLOS* CFD code and its use to solve practical problems are available at http://www.ivd.uni-stuttgart.de/english/frame_ru/aiolos_e_ru.html and at <http://www.recom-services.com>.

Appendix F

Entrained Flow Gasifier – Slagging Wall Model

Note - All figures, tables and literature citations refer to information in this Appendix.

Introduction

Slagging of hot mineral matter on the walls of an entrained flow coal gasifier is important for good gasifier operation and thus is included within our comprehensive gasifier model. The slagging wall model we have implemented is an extension of work carried out by Physical Sciences Inc. and United Technologies Research Center under the US Department of Energy's Combustion 2000 program [Senior and Sangiovanni, 2001]; the Collaborative Research Center for Coal and Sustainable Development (CCSD) in Australia [CCSD], most notably Professor Terry Wall, Dr. David Harris and Mr. Peter Benyon; and researchers developing models for the Prenflo gasifier being used at the IGCC plant in Puertollano, Spain [Seggiani, 1998]. Details of the model, predicted values and implementation into the CFD model are provided in [Bockelie et al., 2002], [Bockelie et al., 2003].

The model uses information from the gas flowfield in the gasifier (e.g., gas composition, gas temperature, incident heat transfer, and particle deposition rate) to predict the slag properties (e.g., slag flow, slag thickness, frozen slag thickness) and heat transfer through the walls of the gasifier (for an assumed refractory resistance and external ambient temperature). The model is sufficiently general to include the effects of using a cooling jacket/system on the outside of the gasifier. The equations used to describe the ash layer are the conservation equations for momentum, energy, and mass. The model is two-dimensional. The slag thickness is calculated as a function of vertical distance down the walls. At each vertical location, the temperature profile is calculated through the layer thickness. The model is fully integrated into our CFD model of the gasifier. The slagging model can be applied to three-dimensional geometries by applying it for every vertical column of wall computational cells. At each wall cell where there is liquid slag flow from above or a non-zero ash deposition rate, an adiabatic wall calculation is first performed to determine whether there is enough heat flux to drive a liquid layer. If so, the solid layer thickness is calculated such that the interface temperature between the solid and liquid layers is at the critical viscosity temperature (the temperature of the onset of slag flow). The critical viscosity is computed using a correlation from the literature, that utilizes the ash composition (wt % of SiO_2 , Al_2O_3 , Fe_2O_3 , CaO , MgO) and numerical parameters based on experimental data.

In the following are presented, in order,

- a description of the model;
- how the model is implemented into a CFD code; and
- example calculations with the model.

Model Description

The flowing slag model treats the flow of slag on a vertical surface as shown in Figure F.1. The equations used to describe the slag layer are the conservation equations for momentum, energy, and mass as first formulated by [Rogers, 1979].

Figure F.1. Gravity induced flow of a viscous slag layer down a solid surface.

Because inertial forces and the pressure gradient are negligible for a falling film at low Reynolds number with a free surface, the equation of motion (x-direction) for the slag layer is simply

$$\frac{\partial \tau}{\partial y} = \rho g \quad (F.1)$$

where τ and ρ are the viscous shear stress and mass density of the slag layer, respectively, and g is the gravitational constant. By further assuming that the slag can be represented as a Newtonian fluid, the viscous shear stress for the slag is related to the viscosity, μ , by the expression

$$\tau = \mu \frac{\partial u}{\partial y} \quad (F.2)$$

where $u = u(x, y)$ is the velocity of the slag layer in the y-direction. The equation of motion can be rewritten as

$$\frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) = \rho g. \quad (\text{F.3})$$

Because energy exchange due to convection and viscous dissipation is negligible for low Reynolds number flow and heat conduction across the slag layer is the dominant energy transport mechanism, the energy conservation equation for the slag layer is simply

$$q = k \frac{\partial T}{\partial y} \quad (\text{F.4})$$

where $q = q(x, y)$ is the heat flux normal to the slag layer, k is the thermal conductivity of the slag, and $T = T(x, y)$ is the temperature of the slag.

The conservation of mass can be expressed as the integral of the velocity profile,

$$\dot{M}_s = \int_0^s \rho u(x, y) dy \quad (\text{F.5})$$

where $\dot{M}_s$ is the mass flow per unit width of slag layer and the free surface of the slag layer is located at $y = s$. The mass flux is also equal to the integral of the ash deposition flux from the gas:

$$\dot{M}_s = \int_0^x \dot{m}_s(x) dx \quad (\text{F.6})$$

where $\dot{m}_s(x)$ is the local ash deposition flux. If the viscosity of a portion of the slag layer is less than the critical viscosity, as indicated by the temperature of the layer, that portion of the layer is assumed to have frozen and the integral of Equation (F.6) is only evaluated across the flowing portion of the slag. The boundary conditions can be stated as:

$$u(x, 0) = 0 \quad (\text{F.7})$$

$$T(x, 0) = T_w(x) \quad (\text{F.8})$$

$$\tau(x, s) = \tau_s(x, T_s) \quad (\text{F.9})$$

$$q(x, s) = q_s(x, T_s) \quad (\text{F.10})$$

where T_s is the temperature at the slag surface. Equation (F.8) assumes that the wall temperature varies axially. Equations (F.9) and (F.10) require that we assume a surface shear force, τ_s , and a surface heat flux, q_s , respectively.

A numerical solution was developed for the above set of equations which describe the development, flow, and heat transfer across a falling vertical slag layer. This numerical solution is based on transforming the governing equations with respect to the independent variables of the (x, y) coordinate system as follows:

$$\frac{\partial y}{\partial T} = \frac{k}{q(x, T)} \quad (\text{F.11})$$

$$\frac{\partial u}{\partial T} = \frac{k \tau}{\mu q(x, T)} \quad (\text{F.11})$$

$$\frac{\partial q}{\partial T} = 0 \quad (\text{F.12})$$

Examination of Equation (F.11) and the relevant boundary conditions leads to the following result

$$q(x, T) = q_s(x, T) \quad (\text{F.13})$$

that is, the heat flux through the slag layer is equal to the heat flux at the surface of the layer. Integration of Equation (F.11) gives the slag layer thickness, s , as

$$s(x) = \frac{k(T_s - T_w)}{q_s(x, T_s)} \quad (\text{F.14})$$

To complete the slag layer model, the density, ρ , and thermal conductivity, k , of the slag are assumed to be constant and the free surface shear force is assumed to be zero, while the viscosity of the liquid slag is assumed to vary with temperature according to the Weymann relation which is expressed as:

$$\mu = A T e^{B/T} \quad \text{for } T > T_{cv} \quad (\text{F.15})$$

where A and B are coefficients for the particular ash. This approach was originally proposed by [Urbain et al., 1981] for the prediction of viscosities of ceramics, glasses and steel slags.

By transformation of the equation of motion, Equation (F.3), using Equation (F.11), and integrating with respect to temperature, one obtains the viscous shear stress in the slag layer given by

$$\tau(x, T) = \frac{\rho g k(T_s - T)}{q_s(x, T_s)} + \tau_s \quad (\text{F.16})$$

where $\tau_s = 0$.

Then by substituting Equation (F.17) into Equation (F.12) and integrating again with respect to temperature, the velocity profile for the liquid slag layer is given by

$$u(x, T) = \rho g \left[\frac{k}{q_s(x, T_s)} \right]^2 \int_{T_w}^T \frac{(T_s - \theta)}{A \theta^n e^{B/\theta}} d\theta \quad (\text{F.17})$$

Once the velocity is known, the mass flux can be calculated from Equation (F.5) by the expression:

$$\dot{M}_s(x) = \frac{\rho k}{q_s(x, T_s)} \int_{T_i}^{T_s} u(x, \theta) d\theta \quad (\text{F.18})$$

where $T_i = T_w$ if there is no frozen slag layer. Otherwise T_i is assumed to be equal to the temperature of critical viscosity.

To complete the description of slag flow behavior in a gasifier, a model describing the interactions between a gravity-induced flow of slag on a hot, vertical wall and heat transfer through the slag layer must take into consideration the viscous behavior of the slag.

Entrained flow gasification units operate at high temperatures with the hot gases leaving the gasifier in the temperature range 1600 to 1800 K for a single stage gasifier. Because of the high temperatures, mineral matter present in the coal forms slag. The ash slag flows down the refractory walls of the gasifier under the influence of gravity and is removed at the bottom of the gasifier after dropping into a water quench vessel. For these gasifiers to operate well, the slag must be removed continuously. The critical condition for continuous removal of the slag is the maintenance of the slag in a liquid phase so that it can flow unrestrictedly into the slag quench vessel. For this reason, slag viscosity is an important property for determination of the performance of a given coal in a gasifier. As such, it is generally accepted that the optimum slag tapping viscosity is in the range 15 – 25 Pa·s at temperatures ranging from 1673 – 1773 K. It becomes apparent therefore, that the molten slag must have a low viscosity for good slag flow at the tapping temperature. The tapping temperature, however, must be high enough so as to avoid crystallization of the slag in the tapping hole but not high enough to have a negative impact on the cold gas efficiency of the gasifier. Therefore the removal of slag from a gasifier depends on the viscosity of the slag and the temperature at which the slag begins to crystallize.

A number of empirical correlations relating the viscosity of a slag to its composition and temperature have been reported in the literature. These include the correlations published by Reid and Cohen (1944), Hoy et al. (1965), Watt, (1969), Urbain et al. (1981) and Schobert et al. (1985) for a variety of operating conditions.

Spurred by the need for prediction of viscosity of slags in entrained flow gasifiers, Patterson et al., (2001) published an extensive report on the relationship between slag viscosity, ash composition and temperature for Australian coal ashes. The treatise is based on the modified Urbain model which yields viscosity-temperature relationships for gasifier slags with wt % FeO contents in the ranges 0-2.5, 2.5 – 5, 5 – 7.5, 7.5 – 10, 10 – 12.5 and 12.5 – 15. In the present work these viscosity models have been incorporated in a CFD code for prediction of gasifier performance. Figures F.2 and F.3 show a comparison between predicted and experimental slag viscosities. The model considers the composition of the ash to be limited to the weight percent of the major species, namely, SiO_2 , Al_2O_3 , CaO and Fe_2O_3 . In the model calculations, Fe_2O_3 is converted to FeO in order to account for the reducing environment in the gasifier.

Figure F.2. Predicted and experimental viscosities for a coal ash slag containing 52.2% SiO_2 , 24.9% Al_2O_3 , 4.83% CaO , 8.48% Fe_2O_3

Figure F.3. Predicted and experimental slag viscosities at 1723 and 1773 K. Coal ash contains 46.8% SiO_2 , 23.16% Al_2O_3 , 9.60% CaO and 11.56% Fe_2O_3 .

The flow behavior of coal slags has been described in detail by Watt (1969). Briefly, coal slags exhibit Newtonian flow at high temperatures where slag viscosity decreases with increase in

temperature. However, if a Newtonian slag is cooled, its viscosity will increase until the fluid transforms to a Bingham plastic. Further slow cooling of the slag below a threshold temperature value will result in a sharp increase in viscosity, caused by the formation of crystals in the liquid. This viscosity is called the critical viscosity. The temperature at which this occurs is the highest temperature at which solid and liquid slag can co-exist in equilibrium and is called the temperature of critical viscosity, denoted by T_{cv} . If the slag is cooled even further beyond T_{cv} , more crystals will separate out and eventually the slag will become a solid.

The temperature of critical viscosity is a function of the ash composition. Estimation of the temperature of critical viscosity is a difficult proposition because a large number of data points covering a wide range of compositions is needed to provide a meaningful correlation. We have developed a correlation for T_{cv} following the procedure laid out by Hoy et al. (1965) and the slag data of Patterson et al. (2001) given as

$$T_{cv} [K] = 3452 - 519.5\alpha + 74.5\alpha^2 - 67.8\beta + 0.86\beta^2 \quad (F.20)$$

where

$\alpha = \text{SiO}_2/\text{Al}_2\text{O}_3$ and

$\beta = \text{Fe}_2\text{O}_3 + \text{CaO} + \text{MgO} + \text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 + \text{CaO} + \text{MgO} = 100$ [weight%]

Figure F.4 shows the relationship between the T_{cv} correlation and the experimental data of Patterson et al. (2001).

Figure F.4. Correlation of predicted and measured temperature of critical viscosity for coal ash slags using experimental data of Patterson et al. (2001).

Numerical Solution

The numerical procedure developed to simultaneously solve for the net radiant heat transfer to the wall, the liquid slag layer thickness and its related characteristics, at each axial position of the gasifier is as follows:

- 1) Assume the thickness of the liquid slag layer. At the top of the gasifier, at $y = 0$, the slag layer thickness is defined to be zero. For $y > 0$, the slag layer thickness at the previous axial position is a good initial assumption for subsequent axial positions.
- 2) Using an iterative procedure based on the radiation and conduction equations, compute the surface temperature of the slag layer and the net heat flux to the wall slag surface.
- 3) Compute the velocity profile in the slag layer using Equation (F.18).
- 4) Compute the mass flux of liquid slag using Equation (F.19).
- 5) Compute the amount of slag which has frozen, as defined by the portion which is at a viscosity greater than the critical value. The temperature corresponding to the critical viscosity, T_{cv} , is used for this determination of the frozen slag fraction.
- 6) Compare the mass flux of liquid slag, computed in Equation (F.3), with the sum of the deposition of ash from the gas phase which is in the slag layer, computed in Equation (F.4). If these computed values for the slag mass flux agree within a reasonable tolerance (0.1% should be acceptable), the assumed slag layer thickness is correct.
- 7) Repeat the above procedure until accurate and consistent values have been found for the slag layer thickness and surface temperature.

CFD Implementation

The above flowing slag wall model has been integrated into the *GLACIER* gasifier model where the inputs (incident heat flux and particle deposition flux) needed for the slagging calculation are taken from the CFD heat transfer and particle calculations. The wall boundary of the gasifier model is divided into vertical strips, a slag calculation is performed as outlined above for each strip. The slag surface temperature solutions are then transferred back to the CFD heat transfer calculations as temperature boundary conditions. Iterations between the CFD and slagging model proceed until convergence.

Model Results

In this section, results for the two-stage gasifier are presented. Figure F.5 shows cross-sectional area averages of liquid and solid slag thickness as functions of the gasifier height. Slag formed only in the combustor section. Liquid slag thickness is in an order of a few millimeters, which is similar to that reported in Benyon et al. (2000), who simulated slag behavior in an air-blown gasifier with a similar geometry as used in this work. Solid slag also formed in the lower section of the gasifier, where the wall temperature changed dramatically, as shown in Figure F.6. T_s and T_i in the figure denote liquid slag surface temperature and liquid-solid slag interface temperature, respectively. Figure F.7 shows local slag thickness; the horizontal axis represents radial location of the gasifier, starting from the center of one of the injectors in the combustor section and moving counterclockwise. A few vertical strips of liquid slag can be observed; these strips are located above the middle-level injectors. Solid slag mainly formed in the section between the lowest-level injectors and the middle-level injectors and in a region above the highest-level injectors.

Figure F.5. Average slag thickness as a function of gasifier height.

Figure F.6. Average liquid slag surface temperature, liquid-solid slag interface temperature and wall temperature as functions of gasifier height.

Figure F.7. Local liquid and solid slag thickness.

References

- Benyon P.J., Computational modeling of entrained flow slagging gasifiers, PhD thesis, University of Sydney, Australia, 2002.
- Bockelie, M.J., Denison, M.K., Chen, Z., Senior, C.L., Linjewile, T., Sarofim, A.F., "CFD Modeling of Entrained Flow Gasifiers for Vision 21 Energyplex Systems," Proceedings of the 19th Annual International Pittsburgh Coal Conference, Pittsburgh, PA, USA, Sept. 24-26, 2002.
- Bockelie, M.J., Swensen, D.A., Denison, M.K., Maguire, M., Chen, Z., Linjewile, T., Senior, C.L., Sarofim, A.F., "A Process Workbench for Virtual Simulation of Vision 21 Energyplex Systems - Using Models To Select Operating Conditions for Gasifiers," presented at the International Symposium of Utilization of Coal and Biomass: Energy and Environment, to be held in Newcastle, Australia, August, 28-29, 2003. Conference proceedings to be published in Fuel.
- CCSD. URL = <http://www.newcastle.edu.au/research/centres/blackcoal.html>.
- Patterson, J.H. Hurst, H.J. Quintanar, A. Boyd, B.K. and Tran, H. Evaluation of the slag flow characterization of Australian coals in slagging gasifiers. *Research Report 19, Volume 1. Cooperative Research Centre for Black Coal Utilisation*, University of Newcastle, Australia, May, 2001.
- Hoy, H.R., Roberts, A.G. and Wilkins, D.M., Behavior of mineral matter in slagging gasification processes. *J. Inst. Gas Engrs*, **5**, 444, 1965.
- Reid, W.T. and Cohen, P., "The flow characteristics of coal-ash slags in the solidification range." *Trans. Amer. Soc. Mech. Engrs.*, **66**, 83(1944).
- Rodgers, M.W., Slag layers in coal-fired MHD generators. *PhD thesis*, Stanford University, Palo Alto, CA, 1979.
- Schobert, H.H, Streeter, R.C. and Diehl, E.K., "Flow Properties of low-rank coal ash slags: Implications for slagging gasification." *Fuel*, **64**, 1611(1985).
- Seggiani, M., Modelling and simulation of the time varying slag flow in a Prenflo entrained-flow gasifier. *Fuel*, **77**, 1611, 1998.
- Senior, C.L. and Sangiovanni, J.J., Numerical model of slag flow in a novel coal-fired furnace, *International Journal of Heat and Mass Transfer*, 2001.
- Urbain, G., Cambier, F., Deletter, M., and Anseau, M.R., Viscosity of Silicate Melts. *Trans. J. Br. Ceram. Soc.*, **80**, 139, 1981.
- Watt, J.D., The flow properties of slags formed from the ashes of British coals: Part 2. The crystallizing behavior of the slags. *J. Inst. Fuel*, **42**, 131, 1969.

Appendix G

Entrained Flow Gasifier – *PREKIN* – A Preprocessor for Modeling Coal Gasification Kinetics

Note - All figures, tables and literature citations refer to information in this Appendix.

Introduction

The heterogeneous reaction kinetics that describe coal gasification processes are important due to their direct impact on calculations performed to estimate gasifier size, expected carbon conversion and possible char recycle requirements. The wide range of conditions that exist in a commercial-scale gasifier makes it difficult to apply a simple correlation, such as global kinetic parameters, to describe the competing effects on reactions from oxygen firing, elevated operating pressure and small particle size. The impact of elevated system pressure (20-80 bar) shifts the coal reactions toward the diffusion-limited regime. In contrast, oxygen firing and small particle size shifts the reaction back toward the kinetically controlled regime. In addition, peak temperatures in an oxygen-fired gasifier can be very high, leading to low reactivity chars in the late stages of burning, which can shift the reaction mode to the chemical kinetics-controlled regime. To accurately describe the mixed reaction mode that occurs in the gasifier, a more fundamental and mechanistic approach is needed. The approach we have pursued uses detailed intrinsic kinetics coupled with a pore diffusion model. The intrinsic kinetics are based on the active surface area and can be combined with a diffusion model to generate overall reaction rates for combustion and gasification. In addition, the intrinsic kinetics model can be extended for broader conditions by including pressure/temperature effects on pore development/diffusion. This capability is important for evaluating gasifier performance or exploring potential changes in gasifier operation or design.

The increase in computational resources required to use such a reaction model is acceptable for a process model of a gasifier. However, the required computational time for such a model would be intractable for a 3D CFD model executing on a workstation in a typical engineering office. Hence, our approach has been to develop a kinetic preprocessor that accounts for the details of the heterogeneous reaction under gasifier specific conditions and generates kinetic parameters that can be directly used in a typical two-phase, reacting CFD code.

Within this project, a literature survey on oxidation/gasification kinetics including devolatilization has been performed and relevant features in determining the rates examined. Based on the survey, *PREKIN*, a kinetic preprocessor was developed that includes processes such as

- devolatilization;
- intrinsic kinetics of char oxidation/gasification;
- thermal annealing;
- ash encapsulation; and
- pore diffusion.

PREKIN generates kinetic parameters for a given range of temperatures and pressures that can be used directly in our process and CFD-based gasifier models. Preliminary results from the application of the *PREKIN*-generated kinetics emphasize the importance of the accurate description of the heterogeneous kinetics in a gasifier. The preprocessor uses standard fuel (coal) properties, intrinsic kinetics data and an optimization routine to generate the global kinetics used by the REI models. Development of *PREKIN* involved collaboration with Prof. Terry Wall and Dr. David Harris of the Collaborative Research Center for Coal and Sustainable Development (CCSD) in Australia. The CCSD has an internal project to obtain intrinsic kinetic data for coal

gasification from a pilot-scale gasifier system. Through our Memo of Understanding (MOU) with the CCSD, REI has worked with the CCSD to benchmark our models against data being collected by the CCSD.

Please note that this Appendix is intended to be a standalone document. Hence, all figures, tables and literature citations refer to information contained in this appendix.

In the remainder of this Appendix, we present, in order, the following material:

- an overview of relevant reaction mechanisms;
- a literature survey on oxidation/gasification kinetics including devolatilization and relevant features in determining the rates;
- a description of *PREKIN*, a coal gasification kinetics preprocessor developed within this project;
- a description of the GUI for operating *PREKIN*;
- concluding remarks; and
- literature references (for this appendix only).

Reaction Mechanism

Reaction mechanisms controlling char oxidation/gasification rates consist of three regimes – chemical kinetics, pore diffusion, and external mass transfer-controlled regimes – and their transitional regimes. There is an extensive study on the char reaction under pulverized-coal (pc) conditions. The role of heterogeneous chemical kinetics under gasification conditions can be understood using simple scaling laws to extend our knowledge of atmospheric pc systems to higher pressures. The relative importance of chemical kinetics is governed by the dimensionless ratio of the maximum diffusion rate to the reaction rate based on conditions in the bulk fluid: $k_m P_{ox} / k P_{ox}^n$, using global nth order rate expression, where k is a global reaction rate constant and k_m a mass transfer coefficient.

$$k = k_o \cdot \exp\left(-\frac{E}{R \cdot T}\right) \quad (G.1)$$

$$k_m = \frac{Sh \cdot D}{d_p} \quad (G.2)$$

where Sh is the Sherwood number, D the diffusivity, E the activation energy, R the universal gas constant, T the temperature, and d_p the particle diameter. The ratio is a measure of resistances of all internal processes (chemical reaction and pore diffusion). Substituting ShD/d_p for k_m and recognizing that the diffusivity (D) is inversely proportional to pressure, one obtains the following scaling relation:

$$\text{Extent of chemical kinetic control} \sim \frac{Sh \cdot x_{ox}^{1-n}}{d_p \cdot k \cdot P^n} \quad (G.3)$$

where P is the total pressure and x_{ox} is the oxygen mole fraction.

This indicates that high total pressure shifts the reaction toward the diffusion-limited regime, but that both enhanced oxygen concentration (x_{ox}) and small particle size (both inherent features of high-pressure suspension firing) shift the reaction back toward the kinetically limited regime (for n less than 1). Based on experience with atmospheric systems, it is expected that the oxygen reaction will be governed by the combined effects of boundary layer transport and surface chemical reaction.

Gasification reactions are believed to be strongly influenced by chemical kinetics under IGCC conditions for a variety of reasons. First the H_2O and CO_2 reactions are intrinsically much slower than the O_2 reaction (much smaller k in the scaling law above), therefore they are much more likely to be chemically limited under identical conditions. Further, volatile matter, leaving the less reactive gasification agents to consume the final char — the slowest stage of the overall gasification process, consumes much of the oxygen. Finally, peak temperatures in oxygen-blown IGCC can be very high, leading to low reactivity chars in the late stages of burning. All of these factors conspire to make intrinsic chemical kinetics of the carbon/ H_2O and carbon/ CO_2 reactions particularly important in gasifiers.

The scaling laws for intra-particle processes clearly show the importance of pore diffusion under some of the reaction conditions of interest (particularly for oxygen and for larger particles).

Because of the mixed reaction modes, detailed coupled kinetic and transport models are needed to describe the combustion process in advanced process control systems.

In the following, we present, in order, a literature survey on oxidation/gasification kinetics including devolatilization, relevant features in determining the rates, and a kinetic preprocessor (*PREKIN*) developed during this program.

Literature Survey & Assessment of Kinetics Database

There is extensive literature on the kinetics of devolatilization and gasification. Much of it is directed at the early moving bed and fluidized bed gasifiers and therefore is not directly relevant to entrained flow gasifiers that involve higher temperatures and shorter residence times than packed and fluidized bed gasifiers. The literature on entrained flow gasification is limited; furthermore, some of the gasification kinetics at high pressures have been carried out on char samples generated at atmospheric pressure or slow heating conditions and that are therefore not representative of chars present in entrained flow gasifiers. In the current work, we built a kinetics database from literature to gain an insight to assist in understanding and modeling devolatilization, oxidation, and gasification behaviors relevant to gasifiers. This includes data from an ongoing effort on gasification kinetics being carried out in Australia under the directions of Dr. David Harris at the CSIRO and Prof. Terry Wall at the University of Newcastle. The Australian data constitute one of the best sources of information.

Devolatilization

Thermal decomposition kinetics is fast at entrained gasification temperatures and is not a strong function of pressure. Volatile yields are suppressed because volatile transport out of coal particles is inhibited as the pressure is increased. Many models have been developed for devolatilization, which give the rate and volatile yield. Some models provide the capability of predicting the composition of the products, which is also important in devolatilization. The two components of interest are the tar, that is the precursor to soot, and methane. The two-step Kobayashi/Ubayachar correlation [Kobayashi et al., 1977],[Ubhayakar et al., 1977] has been widely used in a devolatilization modeling for a CFD model due to its simplicity, but the two-step model does not provide the composition of the products as well as a pressure dependence. The three most widely used models are the Functional-Group, Depolymerization, Vaporization, Cross-linking (FG-DVC) model developed by Solomon and co-workers (1988,1992), FLASHCHAIN by Niksa and Kerstein (1991), and the Chemical Percolation Devolatilization (CPD) model by Fletcher et al. (1990). The models yield relatively comparable results. We have chosen the CPD model of Fletcher and Pugmire to provide information of importance to gasification such as tar yields, since it is in the public domain. The model also provides the effect of pressure on volatile yields. The results from the Fletcher and Pugmire model on the effect of pressure on volatile yields are compared in Figure G.1 with data and correlations from a number of different investigations [Fletcher et al., 1990] [Wen and Chaung, 1979], [Beath, 1996], [Okumura et al., 2001], [Gibbins and Kandiyoti, 1989], [Griffin et al., 1994], [Suuberg et al., 1978], [Anthony and Howard, 1976], [Arendt and van Heek, 1981], [Harris et al., 2002].

Figure G.1. Comparison of model prediction of volatile yields [Fletcher et al., 1990], [Wen et al., 1979], [Beath et al., 1996], [Okumura et al., 2001], [Gibbins et al., 1989], [Griffin et al., 1994], [Suuberg et al., 1978], [Anthony and Howard., 1976], [Arendt et al., 1981], [Harris et al., 2002].

The effects of pressure show a large variation among the investigators. The CPD model tends to under-predict the decrease in volatile yields with increasing pressure, over a range of pressure from 1 to 30 atm, using a variety of coals. Another correlation, by Beath (1996), significantly over-predicts the effect of pressure on volatile yields compared to the other correlations. The volatile yield correlation by Wen and Chaung (1979), based on the data of Anthony and Howard. (1976) over the range of 0.1 to 50 atm has the form:

$$\frac{V_p}{V_{p=1}} = 1 - 0.066 \ln P_t \quad (\text{G.4})$$

where P_t is the total pressure in atmospheres, V_p the volatile yield at a given pressure, and $V_{p=1}$ the volatile yield at one atmosphere. Our approach is to use the correlation from Wen et al. (1979) as a reference value for the pressure dependence of volatile yields, since it passes through the middle of the widely varied correlations among the investigators as shown in Figure G.1. Therefore, re-calculation of the correlation based on CPD results and Wen et al. (1979) correlation leads to the following correction form:

$$\frac{V_p}{V_{CPD,p}} = 1 - 0.101082 \cdot \ln P \quad (\text{G.5})$$

where $V_{CPD,p}$ is the volatile yield calculated by CPD at pressure P .

Char Morphology

The more important effect of total pressure on devolatilization is that on the morphology and reactivity of the product char. Because of the inhibition of volatile transport out of particles during devolatilization, the particles produced at high pressures have a higher percentage of particles with more macropores but with fewer micropores. The chars produced at high pressures contain a high percentage of cenospheric particles, classified as Group I by Wall et al. (2002). They developed a correlation for the effect of pressure on the fraction of particles forming cenospheres, f_{ce} . It is

$$f_{ce} = 0.006P_t + 0.0053vitr + 0.37 \quad (G.6)$$

where P_t is the total pressure in atmospheres and *vitr* is the volume percentage of vitrinite content of coal. Vitrinite concentration in coal can be obtained from readily available Department of Energy Coal Sample (DECS) Bank maintained by Penn State University for a suite of 56 coals [Coal and Organic Petrology Laboratories]. Collection of DECS samples is a continuing effort that begun in 1989. An example DOE Sample data sheet is shown in Table G.1. For a gasifier operated at 25 atmospheres with a bituminous coal having 80% vitrinite, all of the particles are predicted to be present as cenospheres. For a lower vitrinite content of 50%, again at 25 atmospheres, 75% of the particles are predicted to be present as cenospheres. The increase in cenosphere content with increasing pressure increases the char fragmentation during gasification with an attendant increase on char reaction rates [Benfell et al., 2000] and a decrease in the particle size of ash produced [Wu et al., 2000].

The microporosity and therefore total surface area of the char is also impacted by the increase in total pressure. These changes in surface area and porosity will also influence the high-pressure reactivity of the chars [Benfell et al., 2000]. A further complication on structure is provided by the annealing and deactivation of the carbon structure with increased exposure to high temperatures [Hurt et al., 1998], [Seneca et al., 1998]. Such deactivation needs to be considered at the longer residence times in the two-stage gasifier and potentially for the char that is recycled.

Table G.1. Example Department of Energy Coal Sample Bank.

Sample	Seam	ASTM Rank	Sample Type	State	County	Year	Ash, dry	S, dry	Btu/lb, dmmf	C, dmmf	H, dmmf	V.M., dmmf	Vit. %	VRo %
DECS-1	Bottom	subC	Chan-Seam	TX	Freestone	1989	15.8	0.99	13239	75.9	5.8	55.5	78	0.36
DECS-2	Illinois #6	hvcB	Chan-Seam	IL	Randolph	1989	16.2	4.52	14556	81.8	5.7	43.8	87	0.52
DECS-3	Coal Basin M	mvb	Chan-Seam	CO	Gunnison	1990	5.4	0.65	15831	88.1	5.9	28.2	94	1.28
DECS-4	Blue	hvcB	Chan-Seam	NM	McKinley	1990	6.2	0.46	13951	78.9	5.8	48.1	88	0.51
DECS-5	Hiawatha	hvcB	Chan-Work	UT	Sevier	1990	8.5	0.56	14073	80.4	5.5	43.6	66	0.59
DECS-6	Blind Canyon	hvaB	Chan-Work	UT	Emery	1990	5.8	0.40	14874	81.9	6.3	46.9	69	0.66
DECS-7	Adaville #1	hvcB	Chan-Seam	WY	Lincoln	1990	4.2	0.98	13710	77.8	5.6	47.8	95	0.45
DECS-8	Smith-Roland	subC	ROM	WY	Campbell	1990	13.8	0.73	13148	75.8	5.3	51.8	79	0.37
DECS-9	Dietz	subB	Drill-Seam	MT	Bighorn	1990	6.4	0.41	13251	76.1	5.2	47.1	88	0.38
DECS-10	Rosebud	subB	Chan-Work	MT	Rosebud	1990	12.6	1.16	13378	79.7	4.3	46.9	74	0.42
DECS-11	Beulah	ligA	Chan-Seam	ND	Mercer	1990	9.6	0.74	12350	74.1	4.5	61.6	74	0.35
DECS-12	Pittsburgh	hvaB	Chan-Seam	PA	Greene	1990	10.3	1.12	15259	84.7	5.8	39.4	83	0.87
DECS-13	Sewell	mvb	Chan-Seam	WV	Greenbrier	1990	4.2	0.62	15604	88.8	5.0	25.7	77	1.35
DECS-14	Upper Kittanning	hvaB	Chan-Work	WV	Barbour	1990	10.5	1.80	15503	87.0	5.6	35.4	89	1.07
DECS-15	Lower Sunnyside	hvaB	Chan-Seam	UT	Carbon	1991	10.1	1.67	14967	84.3	5.7	41.3	77	0.80
DECS-16	Blind Canyon	hvaB	Chan-Work	UT	Emery	1991	13.9	0.47	14749	82.4	6.0	47.3	77	0.64
DECS-17	Blind Canyon	hvaB	Chan-Sect	UT	Emery	1991	6.6	0.44	14897	82.3	6.3	49.7	80	0.59
DECS-18	Kentucky #9	hvbB	Chan-Seam	KY	Union	1991	12.3	4.21	14773	82.2	6.0	45.6	86	0.56
DECS-19	Pocahontas #3	lvb	Chan-Seam	VA	Buchanan	1991	4.6	0.74	15819	90.6	4.9	18.7	89	1.71
DECS-20	Elkhorn #3	hvaB	Chan-Seam	KY	Floyd	1991	5.5	0.97	15173	85.0	5.9	39.2	78	0.87
DECS-21	Lykens Valley #2	an	Chan-Seam	PA	Columbia	1992	11.2	0.50	15122	91.5	4.1	3.9	87	5.19
DECS-22	Upper Kittanning	hvaB	Chan-Lith	PA	Armstrong	1993	23.3	1.71	15827	87.8	6.1	37.8	30	0.77
DECS-23	Pittsburgh	hvaB	Chan-Seam	PA	Washington	1994	9.4	3.87	15307	84.6	5.8	42.3	79	0.73
DECS-24	Illinois #6	hvcB	Chan-Seam	IL	Macoupin	1994	13.4	5.53	14407	80.1	5.6	45.5	90	0.49
DECS-25	Pust	ligA	Chan-Seam	MT	Richland	1994	11.9	0.72	12569	75.8	5.3	46.9	74	0.23
DECS-26	Wyodak	subB	ROM	WY	Campbell	1994	7.6	0.43	13237	76.2	6.2	48.1	86	0.29
DECS-27	Deadman	subA	Drill-Seam	WY	Sweetwater	1994	13.9	0.72	13757	79.2	5.4	40.6	74	0.46
DECS-28	Green	hvcB	Chan-Seam	AZ	Nauvajo	1994	6.1	0.40	13648	77.8	5.5	47.9	76	0.43
DECS-29	Upper Banner #3	hvaB	Chan-Seam	VA	Dickenson	1995	6.4	0.59	15638	87.4	5.6	36.2	71	1.00
DECS-30	Splash Dam	mvb	Chan-Seam	VA	Buchanan	1995	3.9	0.79	15751	88.5	5.4	30.9	77	1.16
DECS-31	Pond Creek	hvaB	Chan-Seam	KY	Pike	1995	10.9	0.60	15538	86.8	5.5	36.6	73	0.99
DECS-32	Stockton-Lewiston	hvaB	Chan-Seam	WV	Kanawha	1995	20.3	0.73	15213	85.4	5.8	38.2	68	0.90
DECS-33	Ohio #4A	hvbB	Chan-Seam	OH	Meigs	1995	12.0	3.74	14630	81.8	6.0	47.8	77	0.51

Sample	Seam	ASTM Rank	Sample Type	State	County	Year	Ash, dry	S, dry	Btu/lb, dmmf	C, dmmf	H, dmmf	V.M., dmmf	Vit. %	VRo %
PSOC-1442	Darco	ligA	Chan-Seam	TX	Harrison	1985	11.3	0.78	12970	74.9	4.6	75.7	83	0.47
PSOC-1443	unnamed	ligA	Chan-Seam	TX	Titus	1985	21.4	0.74	12878	74.4	5.4	78.2	90	0.44
PSOC-1446	New Mexico #8	hvcB	Chan-Seam	NM	San Juan	1985	20.8	0.85	14142	79.4	5.1	46.4	85	0.59
PSOC-1448	York Canyon	hvaB	Chan-Seam	NM	Colfax	1985	11.4	0.46	15380	85.2	6.1	40.8	85	0.71
PSOC-1468	Buck Mountain	an	ROM	PA	Luzerne	1985	6.8	0.49	14860	96.2	1.4	3.2	86	5.45
PSOC-1470	Pratt	hvbB	Chan-Seam	AL	Walker	1985	20.6	2.50	15031	83.9	5.8	39.6	84	0.89
PSOC-1471	Fee Wee	hvaB	Chan-Seam	TN	Morgan	1985	8.0	1.04	15046	84.0	5.6	39.4	76	0.94
PSOC-1482	Hagel	ligA	Chan-Seam	ND	Oliver	1985	8.5	0.72	12254	72.2	4.6	46.5	88	0.39
PSOC-1486	Big Dirty	subB	Chan-Seam	WA	Lewis	1985	19.4	0.94	13234	75.2	6.1	52.5	90	0.38
PSOC-1490	Brazil Block	hvcB	Chan-Seam	IN	Greene	1985	5.3	0.73	14830	83.4	4.5	39.8	70	0.45
PSOC-1491	Indiana #6	hvcB	Chan-Seam	IN	Sullivan	1985	15.2	2.85	14817	82.4	5.1	43.3	89	0.43
PSOC-1492	Illinois #5	hvcB	Chan-Seam	IL	Perry	1985	10.5	4.35	14490	81.4	5.4	43.6	88	0.62
PSOC-1498	Wadge	hvcB	Chan-Seam	CO	Routt	1985	7.1	0.52	13837	78.2	5.5	44.8	89	0.60
PSOC-1501	Juanita C	hvbB	Chan-Work	CO	Gunnison	1985	5.6	0.64	14465	81.2	5.3	42.7	92	0.73
PSOC-1515	Penna. Semian. C	sa	Chan-Seam	PA	Sullivan	1986	29.2	0.58	15567	91.5	4.1	8.6	91	2.80
PSOC-1516	Lower Kittanning	lvb	Chan-Seam	PA	Somerset	1986	10.3	1.40	15841	90.4	4.8	18.6	90	1.73
PSOC-1517	Ohio #5	hvbB	Chan-Seam	OH	Mahoning	1986	4.8	1.92	15105	84.0	5.5	39.3	87	0.86
PSOC-1521	Lower Hartshorne	lvb	Chan-Seam	AR	Sebastian	1986	11.2	0.80	15510	90.5	4.7	21.1	89	1.61
PSOC-1523	W. Va. #5 Block	hvbB	Chan-Seam	WV	Kanawha	1986	16.1	0.71	15061	85.4	5.5	37.0	62	0.92
PSOC-1532	#4	subC	Chan-Seam	AK	Koy.-Mid. Y.	1987	9.5	0.22	12108	70.6	5.3	58.9	79	0.33
PSOC-1533	#3	ligA	Chan-Work	AK	Koy.-Mid. Y.	1987	8.3	0.16	11665	69.6	5.0	58.4	84	0.35
PSOC-1534	Waterfall	subC	Chan-Work	AK	Kenai-Ck. I.	1987	11.1	0.15	12592	71.7	5.8	49.7	87	0.28
PSOC-1535	Deadfall Syn. #4	subA	Chan-Work	AK	Bar.-Pt. Hp.	1987	3.3	1.46	12586	75.6	4.3	37.5	86	0.73

Oxidation and Gasification Rates

Rate Expression

Having the correct combustion/gasification kinetics is critical for any gasifier model. Kinetics is needed to size the gasifier/combustor and determine the char combustion efficiency and possible char recycle requirements. The three reactants of importance are O_2 , H_2O , and CO_2 , with the possible addition of H_2 which can contribute to the formation of CH_4 at high pressures. The kinetics are determined by three resistances, that of external diffusion of the gas phase reactants to the particle surface and diffusion of the reactants from the surface, diffusion through the porous structure of the char, and reaction at the internal (mostly) and external char surface.

The rate of external diffusion is given by [Smith, 1982],

$$R_D = 0.75D_i \left(\frac{P_0}{P_i} \right) \left(\frac{T_m}{T_0} \right)^{1.75} \frac{(C_i - C_s)}{d_p} \quad (\text{G.7})$$

where the diffusion rate, R_D is in $\text{kg/m}^2\text{s}$, T_m is the average temperature of the boundary layer around the particle, and the subscript 0 denotes the reference conditions. For $P_0 = 1$ bar and $T_0 = 1500$ K, $D_i = 3.1 \times 10^{-4}$ m^2/s for O_2 . C_i , C_s , and d_p in the above equation are the reactant concentrations in the gas phase and particle surface and the particle diameter, respectively.

Intrinsic kinetics, a reaction rate based on internal char surface area, is a more fundamental property of the char as it permits the calculation of the effects on the total reaction of changing char structure and surface area.

$$R_{\text{int}} = k_{\text{int } o} \cdot \exp\left(-\frac{E_{\text{int } o}}{R \cdot T_p}\right) \cdot (P_{\text{si}})^{n_{io}} \quad (\text{G.8})$$

where R_{int} is the intrinsic reactivity, $k_{\text{int } o}$ the intrinsic reactivity coefficient, $E_{\text{int } o}$ the true activation energy, T_p particle temperature, P_{si} partial pressure, and n_{io} the true reaction order. Values for the intrinsic rate for a range of pressures is given by the Australian researchers [Benfell et al., 2000], [Roberts and Harris, 2000], together with models on how the rates can be converted to the effective surface rate [Liu et al., 2000]. One of the advantages of the more fundamental rate expression is that it can permit the determination of the effect of the change in internal pore structure with conversion. Such models have been used to determine the change of reactivity with changing conversion, where there is an initial increase in rate with conversion as the result of the increase in surface area as pores enlarge, followed by a decrease as pores overlap [Liu et al., 2000].

The intrinsic kinetics that needs to be used in gasification rate expression is complicated by the adsorption/desorption kinetics at sites with a range of activities. The Langmuir-Hinshelwood model is found to provide a simple representation of the competition of different reactants as well as products with the surface. For the CO_2 -char reaction, for example, it provides the following relationship for the reaction rate

$$R_c = \frac{k_1 P_{\text{CO}_2}}{1 + k_2 P_{\text{CO}} + k_3 P_{\text{CO}_2}} \quad (\text{G.9})$$

where k_1 , k_2 , and k_3 are kinetic reaction rate constants, and P_{CO_2} and P_{CO} are the partial pressures of CO_2 and CO .

The denominator represents the inhibition of the reaction as a result of adsorption on reactive surface sites by reactants and products. The fractional order rate law (or n th order power law), which is often used in representing the reaction rate, includes reactant inhibition but does not include product inhibition. Therefore, the Langmuir-Hinshelwood type kinetics may be suitable for describing gasification behavior including the inhibition effect. The importance of the inhibition effect is further described later. The number of terms in the denominator of the Langmuir-Hinshelwood model will increase in a product mixture containing other species that can be adsorbed on surface sites, such as H_2O . As a consequence of the inhibiting factor of adsorbed species, the order of the reaction between CO_2 and carbon decreases with increasing

pressure [Roberts et al., 2001]. This is a reason, additional to the changes in char morphology with pressure, that it is difficult to extrapolate kinetics from atmospheric to higher pressures.

The intrinsic kinetics can be combined with pore diffusion models to obtain the reaction of a particle or to derive reactivity per unit external surface area of a particle, the so-called apparent reactivity. Data obtained on particles are often correlated in terms of the apparent reactivity. A commonly used correlation used for chemical kinetics is the fractional order kinetics (or n th order power-law kinetics) as shown in the following:

$$R_s = k_g P_{si}^{n_g} e^{-E_g / RT} \quad (G.10)$$

where the rate constant k_g , the activation energy E_g , and the reaction order n_g includes the complexity of the internal diffusion and therefore may vary with extent of reaction, and the exponent n_g includes the effects of partial pressures P_{si} of other species at the particle surface and therefore also applies only over a limited range of pressures and gas concentrations. Examples of the dependence of the reaction order on pressure are given for the case of the H_2O /carbon and CO_2 /carbon reactions in Figure G.2. The reaction orders are seen to decrease from around 0.7 at one atmosphere to less than 0.2 at 30 atmospheres. The open symbols represent predictions of n_g for CO_2 and H_2O based on a model of the saturation of surface sites [Roberts et al., 2001].

Figure G.2. The effect of pressure of gasification gas on the parent order n_g for CO_2 and H_2O [Roberts et al., 2001]. Comparison of theoretical values (open triangles) with data (closed triangles).

Effectiveness Factor

The effectiveness factor is defined as the ratio of the actual reaction rate to that which would occur if all of the surface throughout the inside of the particle were exposed to reactant of the same concentration and temperature as that existing at the outside surface of the particle. The factor is a measure of the effects of mass transfer within a porous structure on observed reaction characteristics [Roberts and Satterfield, 1965] and is used to describe global reaction rate in conjunction with intrinsic kinetics. The effectiveness factor can be estimated for Langmuir-Hinshelwood type kinetics as described in [Roberts and Satterfield, 1965]. Figure G.3 shows the

estimated effectiveness factor for a particle of 100 μm in diameter at pressures of 1 and 30 atm. The initial CO_2 mole fraction was fixed to 0.09. Calculation was performed under two CO/CO_2 ratios, 0.1 and 10, respectively. Mühlen et al.'s (1985) kinetics was used in the calculation. It is estimated that chemical kinetics controls a reaction at 1500K or lower temperatures. At temperatures higher than 1500K, pore diffusion starts to play a role in determining the rate. At higher pressures, CO/CO_2 ratio also affects the effectiveness factor. High CO/CO_2 ratio shifts the point where pore diffusion starts to control to a higher temperature. Typical gasifier temperatures can be from 1200K to 1900K and the pressure can reach up to 80 atm. Under these widely varied conditions, Figure G.3 implies that pore diffusion or external mass diffusion in addition to intrinsic chemical kinetics should be well addressed in determining the rates in a model.

Figure G.3. Estimated effectiveness factor using Roberts and Satterfield's formulation [Roberts and Satterfield, 1965].

Oxidation Rates in Literature

The literature on char oxidation is enormous and the references in Table G.2 were selected because the authors had applied the correlations in the modeling of gasifiers.

Table G.2. Selected Kinetics for Char Oxidation with O₂.

Authors	E, J/mol	k	n
Banin et al. (1997)	51048	40 kg/m ² ·s	-
Joutsenoja et al. (1999)	82368	1903 m/s	1
Monson et al. (1995)	f(P _t)	F(P _t)	0.5
Lupa and Kliesch (1979)	100483	1404 kg/m ² ·s·atm	1
Otaka et al. (2001)	105000*	95000 1/atm ⁿ	0.75
Benyon (2002)	223000	5.81×10 ⁻¹⁰ - 1.02×10 ⁻¹¹ kg/m ² ·s·atm ⁿ	0.83
Roberts and Harris (2000)			

* E in Otaka et al.'s (2001) paper is given as 105,000 J/kmol but this gives too small a temperature dependence. The value was interpreted as being J/mol to bring it into line with the other measurements.

The intrinsic reaction rates of oxygen with carbon can be 10³ to 10⁵ greater than those of H₂O and CO₂ [Harris and Smith, 1990], [Roberts and Harris, 2000], but these differences decrease to factors less than ten at the higher temperatures in oxygen-blown gasifiers since the activation energies for CO₂ and H₂O are higher (i.e. higher temperature dependence) than those of O₂ (see Figure G.5 and Figure G.6). When allowance is made for diffusion within pores and in the particle boundary layer, the differences between the rates of the exothermic O₂/C reaction and the endothermic CO₂/C and H₂O/C become much smaller. But it is usually the case that the reaction of oxygen with carbon precedes those of CO₂ and H₂O.

The importance of a chemical kinetics, R_s with the surface concentration P_{si} equated to the bulk concentration, is compared in Figure G.4 with a mass transfer-controlled rate, R_D with C_{si} for the case of reactions at 18 atmospheres with oxygen having a mole fraction of 0.2. There are wide differences in the rates among the different investigators at low temperatures but the data spread is much smaller at the higher temperatures. Most of the correlations show the higher reaction rates, at the temperatures of interest for oxidation in either a single-stage or the first stage of a two-stage gasifier (≥ 2000K), that equal or exceed the mass transfer resistance (with the exception of the results of Monson et al. (1995) indicating that the reaction occurs under mass diffusion-controlled regime. As the temperature drops, however, the chemical kinetic rate becomes controlling, underlying the importance of finding good kinetic data on char oxidation.

Figure G.4. Comparison for a mole fraction of 0.2 oxygen at 18 atm of the apparent kinetic reaction rates from different correlations in the literature along with the mass transfer-controlled rate.

Gasification Rates in Literature

Fractional Order Gasification Kinetics

The CO_2 and H_2O gasification rates are compared in Figure G.5 and Figure G.6 along with O_2 oxidation rates for the kinetics correlations of Lupa and Kliesch (1979) and Roberts and Harris (2000), at total pressures of 18 and 70 atmospheres. The mole fractions of each oxidation or gasification agent were set to 0.2. Both correlations show that the oxidation rates are greater than CO_2 and H_2O gasification rates by two to ten orders of magnitude over the temperature range of 1000 to 3000 K with the large differences being at the lower temperatures. Kinetics from Lupa and Kliesch (1979) shows that, at the high temperature end of the gasifier (over 2500 K), the CO_2 and H_2O gasification rates are approaching that of O_2 and can exceed the mass transfer limit implying that the gasification occurs under mass diffusion-controlled regime. The oxidation rate is limited by external mass diffusion at temperatures over 1150 K. At the low temperatures of the second stage of a two-stage gasifier (1200 – 2000 K), the rates of the reactions of gasification with CO_2 and H_2O are much slower than that of O_2 . On the other hand, Roberts et al.'s kinetics show that both oxidation and gasification occurs under chemical kinetics-controlled regime when the temperature is lower than 2200 K. At temperatures over 2200 K, gasification still occurs under chemical kinetics control, while oxidation is limited by mass diffusion. Similar trends are found at high pressure (see Figure G.6).

The temperature range in a gasifier can vary from 1200 to 3000 K so that the gasification reaction rate can be controlled by chemical kinetics, external mass diffusion, or both. The kinetics model to describe oxidation/gasification in a gasifier should allow for a smooth transition from the two limiting reaction regimes including pore diffusion-controlled regime in between.

Figure G.5. Comparison of the rates at 18 atmospheres from Lupa and Kliesch (1979) and Roberts and Harris (2000) for the apparent reaction rates of O_2 , CO_2 , and H_2O (each with a mole fraction of 0.2) with the mass transfer-controlled rate for oxygen (also with a mole fraction of 0.2)

Figure G.6. Comparison of the rates at 70 atmospheres from Lupa and Kliesch (1979) and Roberts and Harris (2000) for the apparent reaction rates of O₂, CO₂, and H₂O (each with a mole fraction of 0.2) with the mass transfer-controlled rate for oxygen (also with a mole fraction of 0.2)

Langmuir-Hinshelwood Gasification Kinetics

Reactant and product inhibition effects can be significant in determining gasification rates. For example, the fractional order kinetics for CO₂ takes care of the CO₂ inhibition but not the CO inhibition. Therefore, a Langmuir-Hinshelwood formulation was adopted as it explicitly places the product inhibition effect in the denominator as shown in the following equation for CO₂ gasification:

$$r_s \left(\frac{g}{g \text{ min}} \right) = \frac{k_1 P_{CO_2}}{1 + k_2 P_{CO} + k_3 P_{CO_2}} \quad (\text{G.11})$$

where

$$k_1 = k_{10} \cdot \exp \left(-\frac{E_1}{RT} \right) \quad (\text{G.12})$$

$$k_2 = k_{20} \cdot \exp \left(-\frac{E_2}{RT} \right) \quad (\text{G.13})$$

$$k_3 = k_{30} \cdot \exp \left(-\frac{E_3}{RT} \right) \quad (\text{G.14})$$

Selected Langmuir-Hinshelwood CO₂ gasification rates used in this study are shown in Table G.3.

Mühlen et al. (1985) used more complicated formulation for gasifications including the effects of conversion represented by the following equation:

$$r_s(\text{min}^{-1}) = \exp\left(-\frac{bX^2}{RT}\right) \frac{r_1 P_{\text{CO}_2} + r_8 P_{\text{CO}_2}^2 + r_9 P_{\text{H}_2\text{O}} + r_{11} P_{\text{H}_2\text{O}}^2 + r_{12} P_{\text{H}_2\text{O}} P_{\text{H}_2} + r_4 P_{\text{H}_2}^2}{1 + r_2 P_{\text{CO}_2} + r_3 P_{\text{CO}} + r_{10} P_{\text{H}_2\text{O}} + r_5 P_{\text{H}_2}} \quad (\text{G.15})$$

where

$$b(\text{kJ/mol}) = \frac{1245 - T}{1.56}, \quad (\text{G.16})$$

$$r_i = k_{i0} \cdot \exp\left(-\frac{E_i}{RT}\right), \quad (\text{G.17})$$

X is a conversion level, and $P_{\text{H}_2\text{O}}$ and P_{H_2} are the partial pressures of H_2O and H_2 . Rate constants, r_i are shown in Table G.4.

Table G.3. Selected CO₂ Gasification Rates Using Langmuir-Hinshelwood Formulation.

Investigators	Sample	k_{10} , bar-1min-1	k_{20} , bar-1	k_{30} , bar-1	E1, kJ/mol	E2, kJ/mol	E3, kJ/mol	Temp., °C	Pres.,atm
Wu et al. (1988)	Electrode Carbon	8.428E+06	2.166E-09	1.569E-01	205.2	-257.2	-30.1	871-1038	1.026
Gadsby et al. (1948)	Coconut shell cahrcoal	8.049E+09	1.276E-08	3.204E+06	246.2	-190.5	126.0	734-829	0.013-1.0
Wu (1949)	Coke	5.078E+08	4.034E-06	3.060E-02	258.3	-168.7	-25.5	816-1038	1.026
McBride (1947)	Coke	8.049E+05	1.276E-02	2.545E-01	200.5	-64.5	-26.8	802-1093	1
Strange et al. (1976)	SP-1 graphite	NA	NA	NA	414.5	-54.4	50.2	900-1007	0.013-0.197
Mentser et al. (1973)	Spheron 6	NA	NA	NA	221.9	-92.1	-20.9	900-1200	1
Biederman (1965)	SP-1 graphite	NA	NA	NA	433.3	29.3	129.8	960-1120	0.14
Ergun (1956)	Graphite and activated carbons							700-1400	1
von Fredersdorff et al. (1957)	Pitch Coke	8.866E+05	1.689E-10	0.000E+00	167.9	-230.7	0.0	800-1090	
Lewis et al. (1949)	Anthracite	1.858E+02	3.884E-04	1.520E-04	136.1	-70.8	-69.5	926-1150	
Harris et al. (2002)	Port Kembla-3	7.539E+17	1.814E+04	1.530E+18	510.0	89.0	461.0		
	Port Kembla-4	3.303E+07	1.925E-09	6.140E+21	250.0	-247.0	544.0		
	Port Kembla-5	4.884E+06	1.135E-05	6.485E+17	222.0	-155.0	452.0		
	Queensland B Coke-1	2.320E+18	1.753E+17	2.310E-23	495.0	368.0	-526.0		
	Queensland C Coke-1	3.030E+16	4.731E+01	4.256E+08	469.0	31.0	209.0		
	Queensland C Coke-3	3.253E+13	4.256E-01	1.135E+10	381.0	-45.0	238.0		

Table G.4. Rate Constants for Mühlen et al.'s (1985) Kinetics.

	k_{i0}	k_{i0} Unit	E_i , kJ/mol
r_1	2.710E+04	$\text{bar}^{-1}\text{min}^{-1}$	153.1
r_2	2.060E-02	bar^{-1}	-23.0
r_3	3.820E-02	bar^{-1}	-48.1
r_4	3.180E+07	$\text{bar}^{-2}\text{min}^{-1}$	237.4
r_5	1.530E-09	bar^{-1}	-209.2
r_8	1.220E-02	$\text{bar}^{-2}\text{min}^{-1}$	68.5
r_9	2.960E+05	$\text{bar}^{-1}\text{min}^{-1}$	154.0
r_{10}	1.110E+01	bar^{-1}	29.5
r_{11}	4.400E-03	$\text{bar}^{-2}\text{min}^{-1}$	80.3
r_{12}	6.140E-03	$\text{bar}^{-2}\text{min}^{-1}$	8.5
Temp., °C	800-950		
Pres., atm	39.48		

Product Inhibition Effect

Figure G.7 shows the CO inhibition effects by plotting the normalized CO₂ gasification rate from various literature references as a function of $P_{\text{CO}}/P_{\text{CO}_2}$ for two conditions: 1300 K/1atm and 1300 K/60atm. Calculations were performed under varying CO/CO₂ ratios keeping the sum of CO and CO₂ constant arbitrarily set to the total pressure. As seen in the figure, the inhibition effect can be quite significant and this effect should be addressed in any gasification rate formulation. Under typical operating conditions in various units as specified in the figure, the inhibition effects can cause a change of up to 4 orders of magnitude in the rate depending on which correlation is used. At the higher pressure (60 atm) and at the same temperature, the degree of rate reduction is even higher. At 1600 K, the variations in the rate reduction become small compared to those at 1300 K as shown in Figure G.8, however, increases with increasing pressure.

Figure G.7. Gasification rates normalized by the rates without CO inhibition as a function of CO/CO₂ ratio for CO₂ gasification at 1300 K / 1 atm and 1300 K / 60 atm.

Figure G.8. Gasification rates normalized by the rates without CO inhibition as a function of CO/CO₂ ratio for CO₂ gasification at 1600 K / 1 atm and 1600 K / 60 atm.

CO₂ Effect

Using the correlations of Mühlen et al. (1985) and Wu et al. (1988), CO₂ effect is studied in Figure G.9 and Figure G.10. Calculations were performed under a given CO₂ and varying CO. As CO₂ partial pressure increases, the CO inhibition effect also increases. In addition, with decreasing temperature and increasing pressure, the degree of CO inhibition increases. These results indicate that both reactant and product can be involved in the rate reduction.

Figure G.9. Effect of CO₂ under varying CO and CO₂ using the correlation of Mühlen et al. (1985).

Figure G.10. Effect of CO₂ concentrations for different ratios of CO and CO₂ using the correlation of Wu et al. (1988).

Comparison of CO₂ and H₂O Gasification Rates

For a typical gas composition in a gasifier, the importance of gasification is estimated using the correlation from Mühlen et al. (1985) (see Equations G.15-17).

Typical gas compositions in a gasifier are shown in Table G.5 for a dry and slurry feed.

Table G.5. Typical Gas Composition in a Gasifier for a Dry and Slurry Feed.

Mole Fraction	Dry Feed	Slurry Feed
CO	0.415	0.380
CO ₂	0.086	0.117
H ₂	0.290	0.269
H ₂ O	0.158	0.163
H ₂ S	0.008	0.008
CH ₄	0.032	0.052
COS	0.000	0.000
AR	0.011	0.011

The rate equation can be re-arranged as in the following to understand contributions to the overall rate from each composition:

$$r_s (\text{min}^{-1}) = \exp\left(-\frac{bX^2}{RT}\right) \frac{[C - \text{CO}_2] + [C - \text{H}_2\text{O}] + [C - (\text{H}_2\text{O}, \text{H}_2)] + [C - \text{H}_2]}{1 + r_2 P_{\text{CO}_2} + r_3 P_{\text{CO}} + r_{10} P_{\text{H}_2\text{O}} + r_5 P_{\text{H}_2}} \quad (\text{G.18})$$

where

$$[C - \text{CO}_2] = r_1 P_{\text{CO}_2} + r_8 P_{\text{CO}_2}^2 \quad (\text{G.19})$$

$$[C - \text{H}_2\text{O}] = r_9 P_{\text{H}_2\text{O}} + r_{11} P_{\text{H}_2\text{O}}^2 \quad (\text{G.20})$$

$$[C - (\text{H}_2\text{O}, \text{H}_2)] = r_{12} P_{\text{H}_2\text{O}} P_{\text{H}_2} \quad (\text{G.21})$$

$$[C - \text{H}_2] = r_4 P_{\text{H}_2}^2 \quad (\text{G.22})$$

Mass diffusion-limited gasification rates are also calculated for comparison. The diffusion coefficient for a mixture is calculated by the following equations based on the Chapman-Enskog kinetic theory [Chapman and Cowling, 1951].

$$D_{ik} = 0.0018583 \cdot T^{2/3} \cdot \frac{\left[\frac{1}{M_k} + \frac{1}{M_i}\right]^{1/2}}{P \cdot \sigma_{ik}^2 \cdot \Omega_d} \quad (\text{G.23})$$

where D_{ik} is a species diffusivity for i and k , Ω_d is a dimensionless function of the temperature and of the intermolecular potential field for one molecule of i and one of k , M_i and M_k are molecular weights for species i and k , respectively, and σ_{ik} is the Lennard-Jones parameters of species i and k .

Mixture diffusivity can be estimated by:

$$D_{im} = \frac{(1 - X_i)}{\sum_{k \neq i} \left(\frac{X_k}{D_{ik}}\right)} \quad (\text{G.24})$$

where D_{im} is the diffusivity for the i^{th} specie and X_i or X_k the mole fraction of species i and k .

Figure G.11 shows a degree of contribution from each of the gasification reactions. Gasification by H_2O and H_2 gasifying are much greater than that by CO_2 . With increasing temperature, the relative contributions from H_2O and H_2 gasifying agents are even greater. In addition, the total gasification rate approaches the mass transfer-limited rate at high temperatures.

Mass diffusion-limited (ML) rates were calculated assuming Sherwood number is 2, particle diameter 150 μm , and specific surface area 200 m^2/g

Figure G.11. Contributions by various gasifying agents to the total gasification rate as a function of temperature (K): A) dry feed and B) slurry feed

Figure G.12 shows measurements on the inhibition effects of H_2O and CO_2 gasifications [Muhlen et al., 1985]. The inhibition effect of H_2 in H_2O gasification is higher than that of CO in CO_2 gasification. For example, when $P(\text{H}_2 \text{ or } \text{CO})/P$ is equal to 0.2, CO_2 gasification is reduced by about 35% and H_2O gasification about 82% reduction in the rates. In addition, it shows that the H_2O rates are faster than CO_2 gasification rates. This is consistent with the estimation performed in Figure G.11.

Figure G.12. Influence of the product gases H_2 and CO on the steam and CO_2 gasification, respectively, Temperature, $900^\circ C$; pressure, 40 bar [Muhlen et al., 1985].

Catalytic Effect

Biomass is an attractive option to use in gasification for energy production. One of the important characteristics of biomass is highly dispersed inorganic matter resulting in high combustion rate. As an example, Figure G.13 shows gasification rates as a function of potassium loading in carbon (K/C) [Meijer et al., 1991]. With increasing K/C, the rate increased from a negligible rate at K/C=0. K/C values can vary depending on fuel; however, the importance of catalytic effect is clear as shown in the figure. Therefore, the effect of catalyst (e.g. alkali metal) on gasification rate should be well addressed in a model.

Figure G.13. Steady state reaction rates (r_n) for CO_2 ($\blacktriangle$) and H_2O (+) gasification at 1000K (at 25% burn-off) and r_{ox} (H_2O , CO) ($\bullet$) at 844K (after partial gasification in H_2O at 1000K to 25% burn-off) as a function of the K/C_i ratio of the sample [Meijer et al., 1991].

PREKIN

To account for all of the aforementioned solid fuel combustion/gasification behaviors, a model is required. The current heterogeneous reaction model in CFD uses global (or apparent) kinetics due to its simplicity. However, to estimate/study the effects of operational change such as varying total pressure in a system, a more mechanistically based model is required. Our strategy is to use a separate submodel to address the effects of operational change on kinetics and provide a global kinetics parameters based on the results from the submodel. This was accomplished by developing a kinetic preprocessor (*PREKIN*) that includes fundamental description of combustion/gasification processes including devolatilization, intrinsic rate, and pore/mass diffusion. Several models are available for each process in order for the user to choose a specific model to obtain kinetics for combustion/gasification. Figure G.14 illustrates how global kinetics parameters are obtained in *PREKIN*. Briefly, *PREKIN* calculates reaction rates based on inputs specified by the user and optimizes the global rate expression to fit the calculated rates by varying three parameters: A_G , E_G , and m . In the following subsections, various models implemented in *PREKIN* are described. Then, preliminary results are presented and compared with kinetics from Lupa and Kliesch (1979).

Figure G.14. Schematics of *PREKIN* algorithm.

Submodels

Devolatilization

The user can choose from two devolatilization models: the Two-step mechanism [Kobayashi et al., 1977] and the Chemical Percolation Devolatilization (CPD) model [Grant et al., 1989]. The user needs to input kinetic parameters to use the two-step mechanism. The CPD model needs

coal structure parameters from ^{13}C NMR measurements. The structure parameters can manually be typed in or *PREKIN* can generate the parameters based on the fuel compositions [Grant et al., 1989]. When the CPD model is selected and the total pressure is higher than 1 atm, the following correlation is used:

$$\frac{V_p}{V_{CPD,p}} = 1 - 0.101082 \cdot \ln P_t \quad (\text{G.25})$$

where V_p is the volatile yield at total pressure, P_t and $V_{CPD,p}$ is the volatile yield calculated by CPD at pressure, P .

Single-Film Char Oxidation

The single-film char oxidation model sets a foundation for the *PREKIN* model and consists of four aspects:

- 1) intrinsic n th (fractional) order kinetics or semi-global kinetics [Hurt and Calo, 2001];
- 2) film diffusion in the particle boundary layer;
- 3) heat generation and transfer; and
- 4) mode of burning expressions.

The model assumes that the particle is isothermal and oxygen is assumed to be the sole oxidizer; the intrinsic n th order rate equation is used to represent char oxidation rates:

$$q_{rxn} = \eta \cdot k_o \cdot \exp\left(-\frac{E}{R \cdot T_p}\right) \cdot \left(\frac{P_s}{R \cdot T_p}\right)^n \cdot s \cdot \sigma_A \cdot \gamma \quad (\text{G.26})$$

where q_{rxn} ($\text{gC}/\text{cm}^2\text{-s}$) is the rate of reaction (expressed per unit external area of solid), γ (cm) the characteristic dimension of the particle ($d/6$ for sphere and thickness/2 for flat plate), η the effectiveness factor, s (cm^2/gC) the specific surface area, σ_A (gC/cm^3) the carbon density in the particle, k_o ($\text{gC}/\text{s}\cdot\text{cm}^2\cdot(\text{mol}/\text{cm}^3)^n$) the intrinsic reactivity coefficient (or the pre-exponential factor in the Arrhenius form), P_s the partial pressure at the particle surface, and n the true reaction order.

In the semi-global kinetics[Hurt and Calo, 2001], the following mechanism was used for steady-state combustion:

1. $\text{C} + \text{O}_2 \rightarrow 2\text{C}(\text{O})$
2. $\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{CO}_2 + \text{C}(\text{O})$
3. $\text{C}(\text{O}) \rightarrow \text{CO}$

Then, intrinsic rate is expressed as:

$$q_{rxn,int} = \frac{k_1 k_2 P_{O_2} + k_1 k_3 P_{O_2}}{k_1 P_{O_2} + k_3 / 2} \quad (\text{G.27})$$

where k_1 , k_2 , and k_3 are reaction rate constants (dimensionless or bar^{-1}) and P_{O_2} is the partial pressure of O_2 .

This report will describe the oxidation submodel based on intrinsic n th order kinetics. Semi-global kinetics can be similarly derived.

Both CO and CO₂ are considered as primary products of the heterogeneous char oxidation reactions. The CO/CO₂ product ratio (MR) [Mitchell, 1992] is assumed to depend on particle temperature and is expressed as:

$$MR = \frac{CO}{CO_2} = A_C \cdot \exp\left(-\frac{E_C}{RT_p}\right) \quad (G.28)$$

The fraction of the carbon content of the particle converted to CO₂ is denoted as ψ and determined from the CO/CO₂ product ratio (MR):

$$\psi = \frac{1}{1 + MR} \quad (G.29)$$

The mass diffusion outside the particle is [Frank-Kamenetskii, 1969]:

$$q_{diff} = \frac{k_D P}{\gamma} \ln\left(\frac{1 - \gamma P_s / P}{1 - \gamma P_g / P}\right) \text{ where } \gamma \neq 0 \quad (G.30)$$

P_g is partial pressure of gas and P is total pressure.

$$q_{diff} = k_D (P_{og} - P_{os}) \text{ where } \gamma = 0 \quad (G.31)$$

and the mass transfer coefficient is given by:

$$k_D = \frac{M_C D_{ox} Sh}{d_p R' T_m v_o} \quad (G.32)$$

where M_c is molecular weight of carbon (gC/mol), D_{ox} oxygen diffusion coefficient (cm²/s), R' gas constant, and v_o and γ are given by:

$$v_o = \frac{1 + \psi}{2}, \quad (G.33)$$

$$\gamma = \frac{\psi - 1}{\psi + 1}. \quad (G.34)$$

Then, the quasi-steady state assumption leads to

$$q_{diff} = q_{rxn}. \quad (G.35)$$

If the particle temperature is known, the above equations can be used to determine the value of P_s (partial pressure at the char surface). Numerically, a value is guessed for P_s , the difference between q_{rxn} and q_{diff} is driven to zero by changing the value of P_s using the Newton-Raphson method.

A set of equations was derived to describe the evolution of particle size and density during combustion. The char particle is assumed to consist of two components: a combustible

component (w_c) whose density changes with burnoff and a noncombustible inorganic component (w_a) whose density is constant. The particle (or apparent) density is defined as:

$$\rho_P = \frac{\text{total weight of particle}}{\text{volume of particle}} = \frac{w_c + w_a}{V_p} \quad (\text{G.36})$$

where the particle volume, V_p , is the volume occupied by a sphere having a diameter of d_p . Rewriting this equation in terms of the apparent densities of the combustible material and the ash and the volumes they occupy yields:

$$\rho_P = \frac{w_c}{V_p} + \frac{w_a}{V_p} = \frac{v_c}{V_p} \cdot \frac{w_c}{v_c} + \frac{v_a}{V_p} \cdot \frac{w_a}{v_a} = \frac{v_c}{v_c + v_a} \cdot \rho_c + \frac{v_a}{v_c + v_a} \cdot \rho_a \quad (\text{G.37})$$

where v_c and v_a are the volumes of the combustible component and noncombustible inorganic component, respectively.

The weights of combustible material and ash in the particle can be expressed as:

$$w_a = x_a \cdot V_p \cdot \rho_P = v_a \cdot \rho_a \quad (\text{G.38})$$

and

$$w_c = (1 - x_a) \cdot V_p \cdot \rho_P = v_c \cdot \rho_c \quad (\text{G.39})$$

where x_a is ash mass fraction.

Then,

$$v_a = \frac{x_a \cdot V_p \cdot \rho_P}{\rho_a} \quad (\text{G.40})$$

and

$$v_c = \frac{(1 - x_a) \cdot V_p \cdot \rho_P}{\rho_c} \quad (\text{G.41})$$

Finally, total volume is defined as:

$$V_p = v_a + v_c = \frac{x_a \cdot V_p \cdot \rho_P}{\rho_a} + \frac{(1 - x_a) \cdot V_p \cdot \rho_P}{\rho_c} \quad (\text{G.42})$$

Utilizing the above equations to eliminate v_a and v_c yields the following relation for the apparent density of the coal char particle:

$$\rho_P = \frac{1}{\frac{x_a}{\rho_a} + \frac{(1 - x_a)}{\rho_c}} \quad (\text{G.43})$$

The change of parent carbon density is related to burnout by:

$$\frac{\rho_c}{\rho_{c,o}} = \left(\frac{m_c}{m_{c,o}} \right)^\alpha \quad (\text{G.44})$$

where m_c is the mass of combustible component (subscript “o” denotes properties of unreacted char) and α is the empirical mode of burning parameter [Hurt et al., 1998], [Mitchell et al., 1992]. The values of α were calculated from high-temperature char oxidation data [Mitchell et al., 1992] for ten US coals and were found to vary only modestly from char to char, and a mean value of 0.2 can be taken as an estimate for an unknown char. After calculating a new ρ_c , the equation above can be used to convert the ρ_c value into a ρ value, after which geometric considerations yield:

$$\frac{d_p}{d_{p,o}} = \left[\left(\frac{m}{m_o} \right) \left(\frac{\rho_o}{\rho} \right) \right]^{1/3} \quad (\text{G.45})$$

Pore Structure Model

The molecular diffusivity, D_M is estimated by the correlation developed for O_2 diffusion into N_2 [Mitchell, 1980]:

$$D_M = 1.523 \cdot 10^{-5} \cdot \frac{T_m^{1.67}}{P} \quad (\text{G.46})$$

where T_m is $(T_g + T_p)/2$ and P pressure.

A pore structure model is required to convert molecular diffusivity to effective diffusivity. Two pore models were implemented into *PREKIN*: the parallel pore model and the random pore model. The parallel model [Wheeler, 1951] uses the porosity and tortuosity to obtain effective diffusivity as in the following equation:

$$D_{effC} = \frac{D_M \cdot \theta_{CORE} \cdot f}{\tau} \quad (\text{G.47})$$

where θ_{CORE} is core porosity, f the fraction of the total porosity in feeder pores, and τ the tortuosity. In *PREKIN*, the intraparticle transport parameter (τ/f) is treated as a single empirical parameter (default value is 6). In the random pore model [Wakao and Smith, 1962], the effective diffusivity can be expressed as:

$$D_{effC} = \theta_{Macro}^2 D_{Macro} + \frac{(\theta - \theta_{Macro})^2 (1 + 3\theta_{Macro})}{1 - \theta_{Macro}} D_{micro} \quad (\text{G.48})$$

where

$$D_{Macro} = \frac{l}{\frac{l}{D_M} + \frac{l}{D_{K,Macro}}}, \quad (\text{G.49})$$

$$D_{micro} = \frac{1}{\frac{1}{D_M} + \frac{1}{D_{K,micro}}}, \quad (G.50)$$

$$D_{K,Macro} = 9.7 \times 10^3 r_{p,Macro} \left(\frac{T}{Mw_g} \right)^{0.5} \quad (G.51)$$

and

$$D_{K,micro} = 9.7 \times 10^3 r_{p,micro} \left(\frac{T}{Mw_g} \right)^{0.5} \quad (G.52)$$

where $r_{p,Macro}$ and $r_{p,micro}$ are the average macro- and micro-pore radii, respectively, θ porosity, θ_{Macro} macro porosity, and Mw_g molecular weight of reactant (32 for O_2).

Effectiveness Factor

An η is estimated by calculating Thiele modulus (M_T):

$$M_T = \gamma \cdot \sqrt{\frac{n+1}{2 \cdot D_{effC}} \cdot \left(\frac{P_S}{R \cdot T_P} \right)^{n-1} \cdot k_o s \cdot \exp\left(-\frac{E}{RT_P}\right) \cdot C_{incore} \cdot d_C} \quad (G.53)$$

where C_{incore} is the core carbon mass per unit volume (gC/cm^3) and is calculated by:

$$C_{incore} = \rho_{CORE} \cdot (1 - x_{ao}) \quad (G.54)$$

The effective diffusivity for transport to the particle interior is estimated as described in section entitled Pore Structure Model. For example, by utilizing the parallel pore model, the effective diffusivity is:

$$D_{effC} = \frac{D_M \cdot \theta_{CORE} \cdot f}{\tau} \quad (G.55)$$

where θ_{CORE} is core porosity, f the fraction of the total porosity in feeder pores, and τ the tortuosity. Porosity in core region (θ_{CORE}) is calculated by the following equations:

$$\theta_{CORE} = 1 - x_{ao} \cdot \left(\frac{\rho_{CORE}}{\rho_{at}} \right) - \frac{1}{2} \cdot \rho_{CORE} \cdot (1 - x_{ao}) \quad (G.56)$$

where x_{ao} is initial ash fraction, ρ_{at} true ash density, and ρ_{core} core density is calculated from particle diameters, d_p and d_c :

$$\rho_{CORE} = \rho_P \cdot \left(\frac{d_P}{d_C} \right)^3 \cdot (1 - x_a \cdot (1 - AshinCore)) \quad (G.57)$$

where $AshinCore$ is ash fraction in carbon-rich core region.

Then, η is calculated based on M_T value assuming a sphere:

$$M_T > 4 \quad \eta = \frac{1}{M_T} \quad (G.58)$$

$$M_T < 0.4 \quad \eta = 1 \quad (G.59)$$

$$0.4 < M_T < 4 \quad \eta = \frac{1}{3M_T} \cdot \left(\coth(3M_T) - \frac{1}{3M_T} \right) \quad (G.60)$$

Finally, the burning rate (q_{rxn} , gC/cm²-s) is calculated by the following equation:

$$q_{rxn} = \gamma \cdot \eta \cdot k_o s \cdot \left(\frac{P_s}{R \cdot T_p} \right)^n \cdot \exp\left(-\frac{E}{R \cdot T_p}\right) \cdot C_{incore} \quad (G.61)$$

Thermal Annealing

The thermal annealing submodel is a variation of the distributed activation energy formulation proposed by Suuberg (1991) and based on Hurt's Carbon Burnout Kinetics code [Hurt et al., 1998]. The thermal annealing model assumes that the intrinsic reactivity is proportional to the total number of active sites. The active sites are assumed to have identical oxidation kinetics, but to anneal at different rates. The number of active sites for a given type is assumed to be annealed by a first order thermal process:

$$\frac{d(N_E/N_o)}{dt} = -\left(\frac{N_E}{N_o}\right) A_d \exp\left(-\frac{E_d}{RT_p}\right) \quad (G.62)$$

where N_E is the number of active sites that share a common annealing activation energy E_d , N_o is the total number of active sites, and A_d and E_d are the empirical kinetic parameters. All active sites are assumed to share a common pre-exponential factor for annealing, A_d , but to be distributed with respect to E_d :

$$d(N_E/N_o) = f_E(t, E_d) dE_d \quad (G.63)$$

$$\frac{N(t)}{N_o} = \int_0^\infty f_E(t, E_d) dE_d \quad (G.64)$$

At time zero the function f_E is assumed to be a normalized log-normal distribution in E_d and integration yields a value of unity. In Zone I,

$$\frac{A(t)}{A_o} = \frac{N(t)}{N_o} = \int_0^\infty f_E(t, E_d) dE_d \quad (G.65)$$

In Zone II, classical Thiele theory leads to [Hurt et al., 1998]:

$$\frac{A(t)}{A_o} = \left[\frac{N(t)}{N_o} \right]^{1/2} = \left[\int_0^\infty f_E(t, E_d) dE_d \right]^{1/2} \quad (G.66)$$

The Ash Encapsulation

Mineral matter inhibits combustion in the late stages by one of several physical mechanisms. First, an ash film can pose an additional resistance to oxygen transport to the reacting surface; second, the existence of the inert ash layer outside the particle increases the diameter of the particle, reducing the global rate expressed on an external area basis.

The ash encapsulation submodel assumes the presence of a porous ash film surrounding a carbon-rich core as shown in Figure G.15. The core region is assumed to have a constant local mass fraction of mineral matter equal to the overall mineral mass fraction in the unreacted char. The following figure illustrates the particle and carbon-rich core diameters during burnoff.

Figure G.15. Diameters of particle and carbon-rich core region.

The core region has a constant local mass fraction of mineral matter equivalent to the overall mineral mass fraction in the unreacted char, $(M_a/V_p)_o$. A mass balance on the inorganic fraction yields:

$$M_a = \frac{\pi}{6} dc^3 \left(\frac{M_a}{V_p} \right)_o + \frac{\pi}{6} (d_p^3 - dc^3) \rho_{af} \quad (G.67)$$

where the first term accounts for ash in the carbon-rich core, and the second term accounts for ash in the outer film. Note that this expression neglects the effects of vaporization and inorganic reactions involving mass changes. $(M_a/V_p)_o$ can be expressed as:

$$\left(\frac{M_a}{V_p} \right)_o = \frac{M_a}{\left(\frac{M_{t,o}}{\rho_o} \right)} = x_{a,o} \rho_o \quad (G.68)$$

where the ash mass is:

$$M_a = x_a M_P = x_a \rho \left(\frac{\pi}{6} \right) d_P^3 \quad (G.69)$$

and the subscript “o” denotes properties of the unreacted char. The ash density can be expressed as:

$$\rho_{af} = \rho_{a,n} (1 - \theta_{af}) \quad (G.70)$$

where Θ_{af} is the porosity of the ash film, and $\rho_{a,n}$ is the density of nonporous ash.

The ash film thus has a volume determined by its mass, the nonporous ash density, $\rho_{a,n}$, and the porosity of the ash film, Θ_{af} . Using the above equations:

$$d_c = d_p \left[\frac{(X_a \rho - \rho_{a,n} (1 - \theta_{af}))}{(X_{ao} \rho_o - \rho_{a,n} (1 - \theta_{af}))} \right]^{1/3} \quad (G.71)$$

This result allows the calculation of the core diameter, d_c , knowing the constants $\rho_{a,n}$, Θ_{af} , $X_{a,o}$, ρ_o , the instantaneous overall particle diameter, d_p , and density, ρ . The latter two parameters can be calculated from the mode of burning equations.

The effective diffusivity through the ash film (D_{effa}) is estimated by the empirical correlation [Hampartsoumian et al., 1989]:

$$D_{effa} = D_M \cdot \theta_{af}^{2.5} \quad (G.72)$$

where D_M is the molecular diffusivity and θ_{af} the porosity of the ash film.

The overall mass diffusion coefficient representing the combined diffusional coefficient in the boundary layer and ash film can be expressed by:

$$k_{diff} = \frac{Sh \cdot D_M \cdot D_{effa} \cdot d_p}{R \cdot T_m \cdot v \cdot (Sh \cdot \Delta t \cdot D_M \cdot d_c + D_{effa} \cdot d_c^2)} \quad (G.73)$$

where Sh is a Sherwood number (default is 2.0), Δt ash film thickness, and v stoichiometric coefficient (molO₂/gC).

$$v = \frac{(1 + \psi)}{2} \frac{1}{m_c} \quad (G.74)$$

Mass-Weighted Rate

The mass-weighted rate for multiple particle sizes is calculated as in the following equation:

$$\bar{q}_{rxn} = \frac{\sum (q_{rxn,i} \cdot pmf_i)}{\sum pmf_i} \quad (G.75)$$

where $q_{rxn,i}$ is the oxidation/gasification rate for particle size, i , and pmf_i is the mass fraction of the particle size, i .

Gasification Kinetics

Approach

Two models are available in *PREKIN*; power-law (or fractional order rate law) and Langmuir-Hinshelwood kinetics. Power-law kinetics is similar to the one previously described for oxidation. Therefore, only Langmuir-Hinshelwood kinetics is described here.

For a given gasifier operation, rate is a function of P_{CO} and P_{CO_2} (or P_{H_2} and P_{H_2O}). Both the products of gasification (CO or H_2) and the ratio of the product (CO or H_2) to the reactant (CO_2 or H_2O) are a function of conversion (extent of reaction) as shown in Figure G.16. Then CO/CO_2 can be expressed as a function of CO_2 . Similarly, H_2/H_2O can be expressed as a function of H_2O .

$$CO/CO_2 = f(CO_2) \quad (G.76)$$

$$H_2/H_2O = f(H_2O) \quad (G.77)$$

Then, the calculated reaction rate can be fitted with the nth order global power-law expression with embedded inhibition effect of the product (including reactant) in gasification.

Figure G.16. Sum of CO and CO_2 as a function of extent of reaction.

Effectiveness Factor for Langmuir-Hinshelwood Kinetics

Generally, the Langmuir-Hinshelwood gasification rate is of the form:

$$r_{in} = \frac{k_1 C_{CO_2}}{1 + k_1 C_{CO} + k_3 C_{CO}} \quad (G.78)$$

or

$$r_{in} = \frac{k_1 C_{H_2O}}{1 + k_1 C_{H_2} + k_3 C_{H_2O}} \quad (G.79)$$

where C is the species concentration.

Then, according to Roberts and Satterfield (1965):

$$r_{in} = \frac{k \cdot C_{CO_2}}{1 + K \cdot C_{CO_2}} \quad (G.80)$$

or

$$r_{in} = \frac{k \cdot C_{H_2O}}{1 + K \cdot C_{H_2O}} \quad (G.81)$$

where

$$k = \frac{k_1}{w}, \quad (G.82)$$

$$K = \frac{\left[k_3 - \left(\frac{D_{CO_2}}{D_{CO}} \right) \cdot k_2 \cdot v_{CO} \right]}{w} \quad (G.83)$$

or

$$K = \frac{\left[k_3 - \left(\frac{D_{H_2O}}{D_{H_2}} \right) \cdot k_2 \cdot v_{H_2} \right]}{w}, \quad (G.84)$$

$$w = 1 + k_2 \cdot P_{CO_2,S} \cdot \left[\frac{P_{CO,S}}{P_{CO_2,S}} + v_{CO} \cdot \left(\frac{D_{CO_2}}{D_{CO}} \right) \right] \quad (G.85)$$

or

$$w = 1 + k_2 \cdot P_{H_2O,S} \cdot \left[\frac{P_{H_2,S}}{P_{H_2O,S}} + v_{H_2} \cdot \left(\frac{D_{H_2O}}{D_{H_2}} \right) \right] \quad (G.86)$$

where r_{in} is the intrinsic rate, v_i (i = product gas, CO or H₂) the stoichiometric coefficient for the products and D the diffusivity.

Then the observed rate would be:

$$r_{obs} = \eta \cdot r_{in} \quad (G.87)$$

where η is the effectiveness factor.

On the other hand, the global reaction rate can be expressed as:

$$r_{obs} = A \cdot C_s^n \quad (G.88)$$

where C_s is the reactant concentration (CO₂ or H₂O) at the surface.

A global or effective reaction order can be obtained by:

$$\frac{d \ln(r_{obs})}{d \ln(C_s)} = n_{eff} \quad (G.89)$$

Then, we can replace r_{obs} with the one from the Langmuir-Hinshelwood expression and obtain the effective reaction order:

$$\frac{d \ln(r_{obs})}{d \ln(C_s)} = \frac{d \ln \left(\eta \cdot \frac{k \cdot C_s}{1 + K \cdot C_s} \right)}{d \ln(C_s)} = \frac{1}{1 + K \cdot C_s} = n_{eff} \quad (G.90)$$

The Thiele modulus (M_T), then, can be expressed as:

$$M_T = \gamma \cdot \sqrt{\rho \cdot v_{C-CO_2} \frac{n_{eff} + 1}{2 \cdot D_{CO_2}} \cdot \frac{1}{C_{CO_2,S}} \cdot \frac{k \cdot C_{CO_2}}{1 + K \cdot C_{CO_2}}} \quad (G.91)$$

or

$$M_T = \gamma \cdot \sqrt{\rho \cdot v_{C-H_2O} \frac{n_{eff} + 1}{2 \cdot D_{H_2O}} \cdot \frac{1}{C_{H_2O,S}} \cdot \frac{k \cdot C_{H_2O}}{1 + K \cdot C_{H_2O}}} \quad (G.92)$$

where v_{C-CO_2} and v_{C-H_2O} are stoichiometric coefficients for CO_2 and H_2O gasification, respectively.

Then the effectiveness factor can be calculated for a sphere from:

$$M_T > 4 \quad \eta = \frac{1}{M_T} \quad (G.93)$$

$$M_T < 0.4 \quad \eta = 1 \quad (G.94)$$

$$0.4 < M_T < 4 \quad \eta = \frac{1}{3M_T} \cdot \left(\coth(3M_T) - \frac{1}{3M_T} \right) \quad (G.95)$$

Application of *PREKIN*

Global oxidation and gasification kinetics parameters were obtained by *PREKIN* for Pittsburgh No. 8 under 27.22 atm of total pressure based on the intrinsic expression of Mühlen et al. (1985). Properties of Pittsburgh No. 8 coal is shown in Table G.6. Figure G.17 shows *PREKIN* generated kinetics along with kinetics contained in [Lupa and Kliesch, 1979]. Lupa and Kliesch (1979) use the same kinetics for H_2O and CO_2 gasification that is based on Dobner's work (1976) performed at one atmosphere assuming it is meaningless to account for difference in gasification with inherent errors of extrapolation since combustion is more significant than gasification [Dobner, 1976]. The oxidation rate from Lupa and Kliesch (1979) shows about 3 orders of magnitude higher than those of gasification. *PREKIN*-generated oxidation rate is higher by a factor of 10 than kinetics from Lupa and Kliesch's (1979) at low temperature, but the difference becomes smaller as temperature increases. At the temperatures higher than 1600 K, the *PREKIN* rate is higher by a factor of 2 than the kinetics from Lupa and Kliesch (1979). *PREKIN* H_2O gasification rate, on the other hand, is higher than kinetics from Lupa and Kliesch (1979), while *PREKIN* CO_2 gasification rate is slower than CO_2 rate from Lupa and Kliesch (1979). In the *PREKIN* results, the H_2O gasification rate is higher than the CO_2 gasification rate by a factor of 10 at 1200 K. However, the difference becomes smaller with increasing

temperature and the rates are almost identical at temperatures higher than 1700 K. A faster rate H_2O gasification rate is consistent with the literature data (see Figure G.12) in which the H_2O rate is faster than CO_2 rate by a factor of 3 or 4 at one atmosphere. At a higher pressure, the difference is expected to be smaller, as the mass diffusion effect becomes more significant.

Table G.6. Pittsburgh No. 8 properties.

Proximate Analysis	As-Received (wt%)	size, μm	mass fraction
Moisture	4.74	5.44	0.04
Ash	7.88	8.95	0.06
Volatile Matter	-	12.30	0.08
Fixed Carbon	-	16.15	0.10
HHV (Btu/lb)	13290	21.19	0.13
Ultimate Analysis	As-Received (wt%)	29.20	0.18
Moisture	4.74	40.07	0.13
Carbon	73.76	52.53	0.10
Hydrogen	4.72	69.09	0.08
Nitrogen	1.39	95.33	0.06
Sulfur	2.45	168.72	0.04
Chlorine	0.10		
Ash	7.88		
Oxygen (by difference)	4.96		
TOTAL	100.00

Figure G.14. *PREKIN* generated kinetic parameters along with kinetics from Lupa and Kliesch (1979).

The kinetics was applied to REI's workbench process model that had been developed during the current project. Operating conditions were adapted from the Tampa Electric IGCC power plant configuration [Tampa Electric IGCC Project, 2000]. Briefly, the Tampa unit uses a single-stage, downward-firing, entrained flow coal reactor. The summary of operating conditions is shown in Table G.7.

Table G.7. Tampa Electric IGCC Power Plant Operating Conditions.

Gasifier Pressure	27.22 atm
Coal	Pittsburgh No. 8
Coal flow rate	23.10 kg/s
Oxidant flow rate	22.795 kg/s (95% O ₂ and 5% N ₂)
Slurry temperature	298K
Oxidant temperature	298K

Gas product distributions using two different kinetic sets: kinetic set from Lupa and Kliesch (1979) and *PREKIN* are compared in Figure G.18 along with the reported composition of cleaned syngas from the Tampa unit. The gas product distributions were estimated by assuming similar H₂O and H₂S compositions as in the reported composition. The CO/CO₂ ratio based on kinetics from Lupa and Kliesch (1979) is by a factor of 2 higher than that based on *PREKIN* kinetics, illustrating the impact of faster char oxidation rate in *PREKIN*. The reported CO/CO₂ is 3.0 while kinetics from Lupa and Kliesch (1979) and *PREKIN* kinetics show 4.6 and 2.1, respectively. *PREKIN* kinetics shows lower H₂ concentrations, while giving a similar N₂ level to the others. Further study is required to understand these differences; however, it is clear that the kinetics used in the model make a significant difference in product gas distribution, therefore, an accurate description of kinetics is required.

Figure G.18. Comparison of gasification products from Tampa IGCC power plant using kinetics from Lupa and Kliesch (1979) and *PREKIN* kinetics along with the reported composition of cleaned syngas.

PREKIN UI

The *PREKIN* tool is designed for easy use by engineers and scientists with an advanced level of understanding of the physics, chemistry and modeling methods used for high-pressure gasification kinetics. It is not intended for the casual user.

PREKIN requires numerous, detailed inputs for coal parameters (typically obtained from laboratory tests), reaction conditions within the gasifier and model parameters. The inputs are organized into five panels (see Figures G.19-G.23):

- general coal information;
- devolatilization kinetics;
- oxidation kinetics;
- char gasification kinetics; and
- reaction conditions in the gasifier.

In the following we provide a brief overview of the *PREKIN* input panels. For details see the discussions in the above sections within this Appendix for the corresponding topics. Illustrated in Figures G.19-G.23 are the input windows for *PREKIN*.

The screenshot shows the 'Prekin' window with the 'Coal' tab selected. The 'Coal Name' is 'Pittsburg_#8'. The 'Mode of Burning' is 0.2. The 'Linear Swelling Factor' is -1. The 'Initial Fuel Carbon Density, g/cm3' is -1. The 'Ash Film Porosity' is 0.17. The 'Ash Grain Size, um' is 5. The 'Ash Thermal Conductivity, cal/cm-s-deg' is 0.005. The 'Particle Size Distribution' section shows '% through 50 Mesh' as 97.4 and '% through 200 Mesh' as 73.4. The 'Pore Structure Model' section has 'Parallel Model' selected with 'T/f' as 6, and 'Random Pore Model' selected with 'Average Radii For Macropore, um' as 75, 'Average Radii For Micropore, um' as 0.1, 'Macroporosity' as 0.1, and 'Porosity' as 0.58. The bottom buttons are 'OK', 'Gen Profile', and 'Cancel'.

Figure G.19. *PREKIN* inputs for coal properties.

The screenshot shows the 'Prekin' window with the 'Devolatilization' tab selected. The 'Model Selector' section has 'Manual Input of Volatile Yield' selected with '120% of ASTM' and 'CPD' selected with 'Two-Step'. The 'HTVL (%) (0~100)' is -1. The 'CPD parameters' section shows a table of values: AB (2.602e+01), EB (55400), EBSIG (1800), AC (0.9), EC (0), AG (3e+015), EG (69000), EGSIG (8100), ACR (3e+015), ECR (65000), P0 (0.61), C0 (0), SIGP1 (4.6), MW (267), MDEL (29). The 'Two-Step parameters' section shows a table of values: A1,1/s (962000), E1,cal/mol (17579), Y1 (0.65), A2,1/s (1.5e+013), E2,cal/mol (59950), Y2 (1). The 'Devolatilization Conditions' section shows 'Heating Rates, deg/s' as 100000, 'Maximum Temp, K' as 2000, 'Total Residence Time, sec' as 0.1, '# of Grid Points: Heating' as 30, and '# of Grid Points: Isothermal' as 20. The bottom buttons are 'OK', 'Gen Profile', and 'Cancel'.

Figure G.20. *PREKIN* inputs for devolatilization.

Coal

This panel is used to enter general properties of the coal (see Figure G.19). Required items include the coal type (can select coal types contained in a database), coal swelling factor, ash characteristics, coal grind (mass of particles through 50 and 200 mesh), and pore structure information. More generic coal data such as ultimate and proximate analysis is accessed via the coal database capability within the framework.

Devolatilization

In this panel the user selects the devolatilization model to use (see Figure G.20). Options include manual input of volatile, 120% of ASTM volatile yield value determined in the ultimate/proximate analysis, CPD [Brown et al., 1998], or a two step model [Kobayashi, 1978]. These models and their corresponding parameters are described in more detail in the section entitled Devolatilization located above.

Oxidation

In this panel the user selects the oxidation model to use and enters corresponding numerical parameters (see Figure G.21). The available options include reuse of values from the char gasification model inputs, fractional order power-law, semi-global kinetic rates or specifying the CO:O₂ ratio. For additional detail on the different models and model parameters see the section entitled Oxidation located above.

Gasification

In this panel the user can select from different options on how to model the char gasification (see Figure G.22). Available models include using information from the oxidation model inputs, fractional order power law for CO₂ and/or H₂O, Langmuir-Hinshelwood kinetics or specifying the product/reactant ratio. Additional details on these models and their corresponding numerical parameters are provided above in the section entitled Gasification.

Reaction Conditions

This input panel is used to enter general conditions that are expected to occur within the gasifier as well as required numerical parameters (see Figure G.23).

The outputs from the model are gasification rates (numerical values) that can be used in most modeling tools intended for modeling coal combustion or gasification. Within the framework, the gasification rates computed by *PREKIN* are passed directly to the entrained flow models.

Prekin

Coal | Devolatilization | **Oxidation** | Gasification | Reaction Conditions

☒ **Gasification Page**

☐ Fractional Order Power Law

FOPL Parameters

☐ Mass-specific Intrinsic Reactivity

KoSo, gC/gC-s-(mol/m³)ⁿ -1

Ko, gC/m²-s-(mol/m³)ⁿ 1e+007

So, m²C/gC 500

Intrinsic Activation Energy, cal/mol 42000

Intrinsic Reaction Order 0.5

☐ Semi-global

Semi-global Parameters

K3o, 1/s -1 E1, cal/mol 6000

K2o/K3o 50000 E2, cal/mol 28000

K3o/K1o 1e-006 E3, cal/mol 32000

Intrinsic Reaction Order for Step 2 1

CO/CO2 Ratio

Aco 200 Eco, cal/mol 9000

OK Gen Profile Cancel

Figure G.21. *PREKIN* inputs for oxidation.

Prekin

Coal | Devolatilization | **Oxidation** | Gasification | Reaction Conditions

☐ **Oxidation Page**

☒ Fractional Order Power Law **PLK1**

☒ CO2 ☐ H2O

Ko, gC/m²-s-(mol/m³)ⁿ 324300

So, m²/gC 200

Intrinsic Activation Energy, cal/mol 41850

Intrinsic Reaction Order 1

☐ Langmuire-Hinshelwood Kinetics **LHK1**

☒ CO2 ☐ H2O

K1o, 1/atm-s 5000 E1, cal/mol 36782

K2o, 1/atm 1.55e-009 E2, cal/mol -49966.6

K3o, 1/atm 11.2 E3 7046

Product/Reactant Ratio

from 0.01 to 200 # of steps 20

OK Gen Profile Cancel

Figure G.22. *PREKIN* inputs for gasification.

Prekin

Coal | Devolatilization | Oxidation | Gasification | Reaction Conditions

Simulation Conditions

Mean Rxn Temp, K: 1900 +/- 15 # of Temp Steps: 6

Reactant Fractions: 0.02 to 0.99 # of Pressure Steps: 6

Total Pressure, atm: 27.22

Time Interval, sec: 0.5 # of Time Steps: 100000

Conversion Level, %: 90

Optimization

Starting Values :

kG, $\text{kgC/m}^2\text{-s-(Pa)}^m$: 0.01

EG, kcal/mol: 41.5

m: 0.8

Tolerance: 1e-030

Schema:

☒ Varying kG only ☐ Varying kG and m ☐ Varying All

Recommended Time Interval, sec

for oxidation : 0.01 sec

for gasification : ≥ 10 sec

OK Gen Profile Cancel

Figure G.23. *PREKIN* inputs for reaction coefficients.

Comparison to Niksa Model

An excellent review of the gasification literature by Liu and Niksa (2004) was published as this report was being prepared. In the following we compare the conversion rates predicted by *PREKIN* with those reported by Liu and Niksa (2004). This includes H_2O and CO_2 gasification for temperatures from 800 to 1500°C and pressures from atmospheric to 14.8 atm.

Figure G.24 shows the comparison of H_2O gasification conversions for a North Dakota lignite at 7.7 atm under 76% H_2O at various temperatures [Yang et al., 1986]. Although there are underpredictions at low temperature (especially at 800°C) and overpredictions at high temperatures (especially at 1100 and 1200°C), overall the agreement is good.

Figure G.24. Reported and predicted conversion changes as a function of time for North Dakota lignite char steam gasification at 7.7 atm under 76% H_2O at 800 (□), 900 (•), 1000 (▲), 1100 (◆), and 1200 °C (○) [Yang et al., 1986].

Figure G.25 shows char conversion histories for CO₂ gasification at temperatures of 1317, 1467, and 1497°C under 14.8 atm with 2.5% CO₂ [Moors, 1998]. At two high temperatures (1467 and 1497°C), the predicted curves are very similar to the reported data. At the lower temperature (1317°C), *PREKIN* under-predicts the conversion at longer time scales.

Figure G.25. Reported and predicted conversion changes as a function of time for El Cerejon bituminous char CO₂ gasification at 14.8 atm with 2.5% CO₂ at 1317 (□), 1467 (•), and 1497 °C (▲) [Moors, 1998].

Figure G.26 shows predicted and reported char conversion histories for Polish and Gottelborn chars at 0.99 atm with pure CO₂ at 1500°C [Moors, 1998]. Overall, the char conversion histories predicted by *PREKIN* show good agreement with the reported conversion histories from gasification.

Figure G.26. Reported and predicted char conversion changes as a function of time for Polish (▲) and Gottelborn (●) chars CO₂ gasification at 0.99 atm with pure CO₂ at 1500 °C [Moors, 1998].

Concluding Remarks

Kinetics is an important aspect in modeling a gasifier as it is needed to size the gasifier/combustor and determine the char combustion efficiency and possible char recycle requirements. In this study, a literature survey on coal devolatilization and char combustion/gasification was performed to provide guidelines in developing a kinetic package that can be interfaced with REI's process and CFD gasifier models.

The following summarizes the literature survey:

- Wide variations exist in the published kinetics on coal devolatilization, char combustion/gasification. The kinetics of choice were selected from the literature for a case where the model results were used to fit the burnout in an operating gasifier.
- Higher pressure suppresses volatile yield, which should be reflected in devolatilization kinetics for a gasifier. The three most widely used models that predict this behavior are FG-DVC, FLASHCHAIN, and CPD models, all of which predicted similar results. We recommend the publicly available CPD model, with a correction based on Wen and Chaung (1979) data.
- High pressure will increase the cenosphere content in the char with a subsequent increase in char reaction rates and a decrease in the particle size of ash produced. Wall et al. (2002) provide a correlation that describes the effect of pressure on the fraction of particles forming cenosphere based on vitrinite content of coal.
- Effectiveness factors estimated by using the kinetics from Mühlen et al. (1985) show that chemical kinetics is important at temperatures lower than 1500K and pore diffusion controls the reaction rate above 1500K. As typical gasifier temperatures range from 1200K to 3000K, both mechanisms should be included in a kinetic model.
- Comparison of the fractional order kinetics of char oxidation and gasification implies that both chemical kinetics and external mass transfer are important over the relatively wide range of temperature found in a gasifier (1200-3000K).
- Product inhibition effect can be significant, potentially reducing the rate by up to 4 orders of magnitude, under typical CO/CO₂ ratios for a real gasifier based on comparisons of various Langmuir-Hinshelwood kinetics available in the literatures.
- H₂O and H₂ make higher contributions than CO₂ to the overall gasification rate based on the calculation performed using Mühlen et al. (1985) kinetics.
- Catalytic effects of inorganic matter should be considered in a kinetic model. Literature survey shows that the gasification rates increase increased potassium-to-carbon ratio (K/C). This also applies to the oxidation rate.

Based on the literature survey and previous experience with char kinetics modeling, a kinetic preprocessor, *PREKIN*, was developed, which could be interfaced with the REI's process and CFD gasifier models. *PREKIN* includes a fundamental description of combustion/gasification processes including devolatilization, intrinsic rate expression, and pore/mass diffusion. Table G.8 shows the implemented models for each process. In addition, thermal annealing and ash inhibition effect are implemented.

Table G.8. Submodels Implemented into *PREKIN*.

Devolatilization	Manual input of volatile yield Two step model [Kobayashi et al., 1977] Modified CPD [Fletcher et al., 1990]
Oxidation	Fractional order power law Semi-global kinetics [Hurt and Calo, 2001]
Gasification	Fractional order power law Langmuir-Hinshelwood kinetics
Pore structure	Parallel model [Wheeler, 1951] Random pore model [Wakao and Smith, 1962]

Comparison of *PREKIN*-generated kinetics and kinetics from Lupa and Kliesch, (1979) resulted in a somewhat different gasifier product distribution. This emphasizes the need to have the correct kinetics. *PREKIN* provides a mechanistic approach in generating kinetics under typical operating conditions found in a gasifier and can be easily interfaced with REI's CFD and process engineering-based models of entrained flow gasifiers.

References

- Anthony D.B. and Howard J.B., Coal devolatilisation and hydrogasification, *AIChE J.*, 22, 625-656, 1976.
- Arendt P. and van Heek K.H., Comparative investigations of coal pyrolysis under inert gas and H₂ at low and high heating rates and pressures up to 10 MPa, *Fuel*, 60, 779-787, 1981.
- Banin et al., *Combustion and Flame*, 108, 1-8 (1997)
- Beath A.C., Mathematical modeling of entrained flow gasification, PhD thesis, University of Newcastle, Australia, 1996.
- Benfell, K. E., Liu, G.-S., Roberts, D. G., Harris, D. J., Lucas, J. A., Bailey, J. D., and Wall, T. F., *Proceedings of the Combustion Institute*, 28, 2233-2241 (2000)
- Benyon P.J., Computational modeling of entrained flow slagging gasifiers, PhD thesis, University of Sydney, Australia, 2002.
- Biederman DL "A study of the oxidation of graphite by carbon dioxide", PhD Thesis, Penn. State Univ., 1965.
- Brown AL, and Fletcher TH., *Energy Fuels*, 1998, 12, 745-757.
- Chapman S, Cowling TG "Mathematical Theory of Non-Uniform Gases", Second Edition, Cambridge University Press (1951), Chapters 10 and 14.
- Dobner S, Modeling of Entrained Bed Gasification: The Issues; LUPA AND KLIESCH (1979) Internal Report, 1/15/76.
- Ergun S J.*Phys.Chem.* 1956, 60,480.
- Fletcher T.H., Kerstein A.R., Pugmire R.J. and Grant D.M., *Energy & Fuels*, 4, 54, 1990.
- Frank-Kamenetskii DA, *Diffusion and Heat Transfer in Chemical Kinetics*, Plenum Press, New York (1969).
- Gadsby J, Long FJ, Sleightholm P, Sykes KW *Proc.Roy.Soc.(London)* 1948, A193, 357
- Gibbins J.R. and Kandiyoti R., The effect of variations in time-temperature history on product distribution from coal pyrolysis, *Fuel*, 68, 895-903, 1989.
- Grant, D. M., R. J. Pugmire, T. H. Fletcher, and A. R. Kerstein, "A Chemical Model of Coal Devolatilization Using Percolation Lattice Statistics," *Energy and Fuels*, 3, 175 (1989).
- Griffin T.P., Howard J.B. and Peters W.A., Pressure and temperature effects in bituminous coal pyrolysis: experimental observations and a transient lumped-parameter model, *Fuel*, 73, 591-601, 1994.

Harris D.J., Kelly M.D., Roberts D.G., Mill C.J., Stubington J.F. and Wall T.F., Determining coal reactivity parameters at elevated pressures using bench-scale techniques, 2002.

Harris, D. J., and Smith, I. W., Proceedings of the Combustion Institute, 23, 1185-1190 (1990)

Hurt RH, Calo JM Semi-Global Intrinsic Kinetics for Char Combustion Modeling Comb.Flame 125, 1138-1149 (2001).

Hurt RH, Sun JK, Lunden M, "A Kinetics Model of Carbon Burnout in Pulverized Coal Combustion," Combustion and Flame 113, 181 (1998).

Kobayashi H, Howard JB, Sarofim AF 16th Symp. (Int.) Comb., Combustion Inst., Pittsburgh, 411 (1977).

Joutsenoja et al., Energy and Fuels, 13, 130-145 (1999)

Lewis WK, Gilliland ER, McBride GT Jr., Ind.Eng.Chem. 31, 1213-26 (1949)

Liu, G., Benyon, P., Benfell, K.E., Bryant, G.W., Tate, A.G., Boyd, R. K., Harris, D.J., and Wall, T.F., Fuel, 79, 617-626 (2000)

Liu GS; Niksa S, Coal conversion submodels for design applications at elevated pressures. Part II. Char gasification, Prog Energy Combust Sci 2004; 30:679-717.

Lupa and Kliesch, "Simulation of a Texaco Gasifier, Vol.1 A Steady State Model", LUPA AND KLIESCH (1979) Report AF-1179, Vol. 1 Research Project 1037-1. Final Report, 1979

Meijer R, Sibeijn M, van Dillen MRB, Kapteijn F, Moulijn JA I&EC Research., 30(8), 1760-1770 (1991).

Mentser M, Ergun S, "A study of the carbon dioxide carbon reaction by oxygen exchange", Bull.US Bur.Mines No. 664, 1973.

Mitchell RE A Theoretical Model of Chemically reacting Recirculating Flows, Sandia Technical Report, SAND79-8236, Sandia National Laboratory, Livermore, CA (1980)

Mitchell RE, Hurt RH, Baxter LL, Hardesty DR Compilation of Sandia Coal Char Combustion Data and Kinetic Analyses: Milestone Report Sandia Technical Report, SAND92-8208, 1992.

Monson et al., Combustion and Flame, 100, 669-683 (1995)

Moors JHJ, Pulverized char combustion and gasification at high temperatures and pressures. PhD Dissertation, Eindhoven Tech. Univ., The Netherlands; 1998.

Mühlen H-J, van Heek KH, Jüntgen H "Kinetic studies of steam gasification of char in the presence of H₂, CO₂ and CO" Fuel, Vol 64, July, 944-949 (1985).

Niksa S. and Kerstein A.R., FLASHCHAIN theory for rapid coal devolatilization kinetics 1. Formulation, Energy & Fuels, 5, 673-683, 1991.

Okumura Y., Sugiyama Y. and Okazaki K., Evolution behavior of coal-nitrogen in high-pressure pyrolysis processes, Fuel Chemistry Division Preprints, 46, 141-143, 2001.

Otaka et al., 26th International Conference on Coal Utilization and Fuel Systems, Clearwater, FL, 2001

Roberts, D. G., and Harris, D. J., Energy & Fuels, 14, 483-489 (2000)

Roberts, D.G., Harris, D. J., and Wall, T. F. , "High-Pressure Intrinsic Char Gasification Kinetics: an Application of a modified nth-order rate equation", 18th Pittsburgh Coal Conference, Newcastle, Australia, 3-7 Dec, 2001.

Roberts GW, Satterfield CN, "Effectiveness Factor for Porous Catalysts", Ind. Eng. Chem. Fundamentals, Vol. 4, No. 3, 288 (1965)

Request forms, a booklet describing the entire Penn State Coal Sample Bank and Database, and assistance in acquiring samples and data can be obtained from:

Coal and Organic Petrology Laboratories
The Pennsylvania State University
105 Academic Projects Building
University Park, PA 16802-2300

Senneca, O., Salatino, P., Masi, S., Fuel, 77, 1483 (1998).

Smith I.W., The combustion rates of coal chars: a review, Proceedings of the Combustion Institute, 1045-1065 (1982)

Solomon P.R., Hamblen D.G., Carangelo R.M., Serio M.A. and Deshpande G.V., General model of coal devolatilization, Energy & Fuels, 2, 405, 1988.

Solomon P.R., Serio M.A. and Suuberg E.M., Coal pyrolysis: experiments, kinetic rates and mechanisms, Prog. Energy Combustion Sci., 18,m 133-220, 1992.

Strange JF, Walker PL Jr. Carbon 1976, 14, 345.

Suuberg EM, Fundamental Issues in Control of Carbon Gasification Reactivity, Kluwer Academic Publishers, Dordrecht (1991).

Hampartsoumian JE, Pourkashanian M, Williams A Journal of the Institute of Energy, March, p. 48 (1989)

Suuberg E.M., Peters W.A. and Howard J.B., Product compositions and formation kinetics in rapid pyrolysis of pulverised coal - implications for combustion, Proceedings of the Combustion Institute, 17, 117-128, 1978.

Tampa Electric Integrated Gasification Combined-Cycle Project, Clean Coal Technology Topical Report Number 19, July 2000.

Ubhayakar SK, Stickler DB, von Rosenberg CW, Gannon RE 16th Symp.(Int.) Comb., Combustion Inst., Pittsburgh, 427 (1977).

von Fredersdorff CG, Pyrcioch EJ, Pettyjohn ES Inst.Gas Technol., Research Bull., NO. 7, 71 (1957)

Wakao N, Smith JM, Diffusion in Catalyst Pellets, Chem. Eng. Sci., 17, 825 (1962).

Wall T.F., Liu G.-S., Wu H.-W., Roberts D.G., Benfell K.E., Lucas J.A. and Harris D.J., The effect of pressure on coal reactions during pulverized coal combustion and gasification, to be published, 2002.

Wen C.Y. and Chaung T.Z., Entrained coal gasification modeling, Ind. Eng. Chem. Process Des. Dev., 18, 684-695, 1979.

Wheeler A, Advances in Catalysis, Academic Press, New York (1951).

Wu, H., Bryant, G. W., and Wall, T. F., Energy and Fuels, 14, 745-750 (2000).

Wu PC "The kinetics of the reaction of carbon with carbon dioxide", ScD thesis Chem.Eng., Massachusetts Institute of Technology, 1949

Wu P-C, Lower WE, Hottel HC "Reaction kinetics of carbon dioxide with electrode carbon particles", Fuel, Vol 67, February, 205 (1988).

Yang RYK; Lee IC; Raghunathan K; Peng FF; Jiang WD, Kinetics of high temperature and pressure char-steam reaction in coal gasification. NTIS NO. DE87001088, Department of Chemical Engineering, University of West Virginia, Morgantown, WV; 1986.

Appendix H

Entrained Flow Gasifier – Soot and Tar Models

Note - All figures, tables and literature citations refer to information in this Appendix.

Introduction

The gasifier is a key element to any plant based on coal gasification because it converts a solid fossil fuel into a more environmentally attractive syngas. Within this project we have put significant effort into creating advanced gasifier models with capabilities not available in models described in the open literature.

A reducing environment within a gasifier can result in significant concentrations of sub-micron soot particles. The potential impacts of soot include increases in fine particulate emissions and opacity and gasifier heat imbalances due to enhanced local radiation. Likewise, soot formation imposes a lower limit on the oxygen-carbon ratios that can be used to operate a gasifier. Preliminary versions of the REI gasifier model calculated local soot concentrations from a correlation, and tar formation was not estimated. This soot model was subsequently replaced with the Brown and Fletcher model for predicting the generation and destruction of soot [Brown and Fletcher, 1998]. The Brown and Fletcher soot model is comprised of three transport equations for tar mass fraction, soot mass fraction, and soot number density. Coal-derived soot is assumed to form only from tar, the evolution of which is calculated from Lagrangian particle-phase equations that use the Chemical Percolation Devolatilization (CPD) model to determine devolatilization rates and tar yields. The CPD model describes the devolatilization behavior of a rapidly heated coal based on the chemical structure measured by ^{13}C NMR. The soot and tar submodels implemented into the gasifier model are based on submodels used in previous REI modeling projects focused on combustion (not gasification) [Shim et al., 2003].

In the following we provide further details on the models implemented into the entrained flow gasifier model to predict the generation and destruction of soot and tar. The description provided below assumes the submodels are to be implemented into a CFD based model. For inclusion in a process model, standard modeling methods are used to reformulate the model.

Soot Formation Mechanism

Brown and Fletcher's soot model [Brown & Fletcher, 1998] was implemented into REI's IGCC framework to account for soot evolution and its related heat transfer characteristics in a gasifier. In the model, coal-derived soot is assumed to form from tar as shown in Figure H.1 that illustrates the principal pathway for the formation of coal-derived soot. Coal particles go through devolatilization upon injection into a gasifier and form char, light gas, and tar. Tar yields vary with coal type, temperature, heating rate, and pressure and can be modeled by existing coal particle models based on measured characteristics for the coal. Tar produced from coal devolatilization can be oxidized, gasified to light gas, or converted to primary soot by dehydration. Then primary soot particles can be either oxidized or agglomerated. To accurately describe soot formation, the model should be able to describe both the transport of tar and conversion to soot. The detailed model is discussed in the following section.

Figure H.1. Soot formation mechanism assumed in the model.

Model Description

Conservation equations, source terms, and boundary conditions for 3D calculation of soot mass fraction (Y_C), soot particles per unit mass (N_C), and tar mass fraction (Y_T) are generated. The boundary conditions for soot mass fraction, tar mass fraction, and the soot particles per unit mass are similar to the boundary conditions for other flowfield variables in REI's IGCC-FCT framework, as shown in Table H.1.

Table H.1. Boundary Conditions for the Transport Equations.

Location	Soot Mass Fraction (Y_C)	Tar Mass Fraction (Y_T)	Soot Particles per Unit Mass (N_C)
Primary	0.0	0.0	0.0
Secondary	0.0	0.0	0.0
Walls	$d/dx_{\perp} = 0.0$	$d/dx_{\perp} = 0.0$	$d/dx_{\perp} = 0.0$
Outlet	Quadratic extrapolation	Quadratic extrapolation	Quadratic extrapolation
Symmetry Plane	$d/dx_{\perp} = 0.0$	$d/dx_{\perp} = 0.0$	$d/dx_{\perp} = 0.0$

The equations for conservation of the mass of soot (Y_C) and tar (Y_T), and the number of soot particles (N_C) are:

$$\vec{\nabla} \cdot (\rho_g \vec{u} X) = \vec{\nabla} \cdot \left(\frac{\mu}{\sigma} \vec{\nabla} X \right) + \rho_g S_Y, \quad (\text{H.1})$$

where

X = the conserved variables (Y_C , Y_T , or N_C),

S = the source terms (S_{Y_C} , S_{Y_T} , or S_{N_C}) for each transport equation,

μ = the turbulent viscosity,
 σ = the turbulent Schmidt number,
 ρ = the time-averaged density,
 u = the Favre-averaged velocity,
 and g and C subscripts refer to the gas and carbon, respectively.

Soot volume fraction ($f_{v,C}$) is assumed to be small (i.e. $\rho_{tot} \cong \rho_g$). Diffusivity is represented through the turbulent Schmidt number; standard values of the Schmidt number (700) are used for the transport equations for Y_C and N_C [Kennedy, et al., 1990; Fairweather, et al., 1992]. For the tar mass fraction equation (Y_T), 0.7 is assumed for the Schmidt number, which is the value commonly assumed for the gas-phase Schmidt number [Hill & Smoot, 1993]. Soot and tar source terms are derived based on the soot formation mechanism shown in Figure H.1. The source terms for the N_C equation are derived following Fairweather et al (1992). The N_C agglomeration term comes from the Smoluchowski particle rate equation, as described by Haynes (1991) and Ulrich (1971).

Source terms for the conservation equations are:

$$S_{Y_C} = \dot{r}_{FC} - \dot{r}_{OC}, \quad (H.2)$$

$$S_{Y_T} = \dot{r}_{FT} - \dot{r}_{FC} - \dot{r}_{GT} - \dot{r}_{OT}, \quad (H.3)$$

$$S_{N_C} = \left(\frac{N_a}{M_C C_{min}} \right) \dot{r}_{FC} - \dot{r}_{AN}, \quad (H.4)$$

where

$\dot{r}_{FT} = SP_{tar}$	Formation of Tar
$\dot{r}_{OT} = \rho_g Y_T Y_{O_2} A_{OT} e^{-E_{OT}/RT}$	Oxidation of Tar
$\dot{r}_{GT} = Y_T A_{GT} e^{-E_{GT}/RT}$	Gasification of Tar
$\dot{r}_{FC} = Y_T A_{FC} e^{-E_{FC}/RT}$	Formation of Soot
$\dot{r}_{OC} = \left(\frac{6}{\rho_c} \right)^{2/3} \left(\pi \frac{N_c}{Y_c} \right)^{1/3} \frac{X_{O_2}}{T^{1/2}} Y_c A_{OC} e^{-E_{OC}/RT}$	Oxidation of Soot
$\dot{r}_{AN} = 2C_a \left(\frac{6M_C}{\pi\rho_C} \right)^{1/6} \left(\frac{6kT}{\rho_C} \right)^{1/2} \left(\frac{\rho_g Y_C}{M_C} \right)^{1/6} (\rho_g N_C)^{11/6}$	Agglomeration of the particle per unit mass
N_a	Avogadro's Number
X_{O_2}	Oxygen mole fraction
C_{min}	Number of carbon atoms per incipient soot particle concentration (mol/m ³)
M_C	Molecular weight of Carbon

The average carbon soot density is assumed to be 1950 kg/m³, and the collision frequency constant (C_a) is assumed to be 3. Table H.2 gives Arrhenius parameters used in the model. Tar yields are calculated from the Lagrangian particle-phase equation which uses the CPD model [Fletcher, et al., 1992] to determine devolatilization rates and tar yields. When 13C NMR data are not available as input parameters for the CPD model, a correlation [Genetti & Fletcher, 1997] can be used to estimate 13C NMR parameters from the proximate and ultimate analysis.

Table H.2. Transport Equation Source Terms – Arrhenius Rate Parameters.

Term	A	E (kJ/gmol)	Source
$\dot{r}_{FT}$	NA	NA	Particle phase calculations
$\dot{r}_{OT}$	$1.87 \times 10^6 \text{ (m}^3\text{/(kg} \cdot \text{s))}$	52.3	Shaw et al.
$\dot{r}_{GT}$	$9.77 \times 10^{10} \text{ (1/s)}$	286.9	Ma
$\dot{r}_{FC}$	$5.02 \times 10^8 \text{ (1/s)}$	198.9	Ma
$\dot{r}_{OC}$	$1.09 \times 10^4 \text{ (K}^{1/2}\text{/s} \cdot \text{kg/m}^2\text{)}$	164.5	Lee et al.
$\dot{r}_{AN}$	NA	NA	Fairweather et al.

Y_C values calculated from the above equations can be used to calculate the soot volume fraction ($f_{v,C}$) using the following equation.

$$f_{v,C} = \left(\frac{\rho_g}{\rho_C} \right) Y_C, \quad (\text{H.5})$$

Correlation-Based Soot Model

In the alternate soot correlation model the soot volume fraction is calculated from the local equivalence ratio via the following equations:

$$f_v = \frac{0.1 C_2 b_c M_c}{\rho_{soot}}, \quad (\text{H.6})$$

where 0.1 is an experimentally based constant that represents the mass fraction of available volatile fuel carbon that forms soot, M_c is the molecular weight of carbon, b_c is the mass-atoms of carbon per mass of reactant mixture, and ρ_{soot} is the soot (carbon) density. The value for b_c is calculated as a function of the local gas density and mixture fraction and basically determines the amount of volatile fuel carbon which is available to form soot. The constant C_2 represents the fraction of soot formed which survives to radiate and is calculated from the relation

$$C_2 = \frac{\text{MAX}(0.0, \text{MIN}(E - E_{cr}, E_{inf} - E_{cr}))}{(E_{inf} - E_{cr})}, \quad (\text{H.7})$$

where E is the equivalence ratio, E_{cr} is the critical equivalence ratio where soot formation begins, E_{inf} is the equivalence ratio where all soot formed remains to radiate (i.e., no burnout), and MIN and MAX represent FORTRAN minimum and maximum functions, respectively. The critical equivalence ratio varies with fuel type and lame type, but for most lower order hydrocarbons, a

single value of 1.0 is sufficiently representative [Glassman, 1987]. A value of twice the critical equivalence ratio was use for E_{inf} .

Then for both models the soot volume fraction is used to determine the soot emissivity (ε_C):

$$\varepsilon_C = 1 - (1 + 350 f_{v,C} T L_e)^{-4}, \quad (H.8)$$

where T is the temperature (K) and L_e is the mean beam path length (m) [Sarofim and Hottel, 1978] .

The emissivity may be related to the absorption coefficient (κ) through Bouguer's Law

$$\kappa = -\left(\frac{1}{L_e}\right) \ln(1 - \varepsilon), \quad (H.9)$$

giving

$$\kappa_C = \left(\frac{4}{L_e}\right) \ln(1 + 350 f_{v,C} T L_e), \quad (H.10)$$

This absorption coefficient is then summed with the calculated absorption coefficient for the radiating gases (i.e., CO_2 and H_2O) to form a total absorption coefficient.

Implementation of the soot and tar submodels described above into a CFD-based combustion/gasification code is straightforward and has been completed. Likewise, the same submodels can be implemented into a process model of a gasifier with straightforward modifications.

References

- Brown AL, Fletcher TH., *Energy Fuels* ,1998, 12, 745-757.
- Fairweather M, Jones WP, Lindstedt RP, *Combustion and Flame*, 1992, 89, 45-63.
- Fletcher TH, Kerstein AR, Pugmire RJ, Solum MS, Grant DM, *Energy Fuels* ,1992, 6, 414-431.
- Genetti DB, Fletcher TH, *ACS Division of Fuel Chemistry*, 1997, 42, 194-198.
- Glassman, I., *Combustion*, Academic Press, Orlando, FL, 1987.
- Haynes BS, "Soot and Hydrocarbons in Combustion". In *Fossil Fuel Combustion*; Bartok W, Hill SC, Smoot LD, *Energy Fuels*, 1993, 7, 874-883.
- Kennedy IM, Kollmann W, Chen JY, *Combustion and Flame*, 1990, 81, 73-85.
- Lee, K.B., Thring, M.W., Beer, J.M., "On the Rate of Combustion of Soot in a Laminar Soot Flame," *Combustion and Flame*, 6, 3, Sep. 1962.
- Ma J, Fletcher, TH, Webb BW, *26th Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1996, pp 3161-3167.
- Sarofim AF, Hottel HC, *Heat Transfer-1978*, Hemisphere Publishing, Washington DC, 1978, pp 199-217.
- Shaw DW, Zhu X, Misra MK, Essenhigh, RH, *Twenty-Third Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1990; pp 1155-1162.
- Shim, H., Sarofim, A., Davis, K., Bockelie, M. "Modeling the Impacts of Soot From Low-NOx Combustion Systems", *Proceedings of The 28th International Technical Conference on Coal Utilization & Fuel Systems*, Clearwater, FL, March 2003.
- Ulrich GD, *Combustion Science and Technology*, 1971, 4, 47-57.

Appendix I

Modeling Of Gas Turbine Combustors

Note - All figures, tables and literature citations refer to information in this Appendix.

Preamble

The gas turbine in an IGCC plant has to be tailored to allow for differences in mass flow rate, combustion temperature, gas emissivity, and composition of the syngas supplied to the turbine. The changes in hardware are issues that the manufacturers are addressing. It was felt, however, important to have a model of the gas turbine combustor since the emissions from the turbine need to be quantified to ensure that the IGCC plant meets the goals set by DOE. Particular challenges in developing a gas turbine model is that the turbines meet the ultra-low NO_x levels projected for the next generation plants. For this purpose CFD model was developed by REI and RECOM for a combustor that would be representative of the type used in major manufacturer's mainframe gas turbines.

A DLN (dry Low-NO_x) combustor rig for the GE Frame 7 machine was selected for this purpose. The model results were compared with data from a rig combustor operated by the Power Systems, Mfg (PSM) of Jupiter, FL, the *only* after-market company with a viable DLN combustion system for the GE Frame 7 installed base. Another motivation for developing a combustor model, is that radiative heat transfer to the liner may become a problem with hydrogen, leading to de-rating of the gas turbine. The CFD model can be used to assess issues of NO_x and CO emissions and heat transfer. The CFD model of the combustor was executed in a “standalone” manner for this study, but a similar model could be incorporated into the framework.

The collaborative effort with PSM were performed under a MOU between REI, RECOM and PSM.

Modeling of Gas Turbine Combustors

A CFD model was developed of a rig combustor that would be representative of the type used in major manufacturer's designs for mainframe gas turbines. A DLN combustor RIG for the GE Frame 7 machine was selected for this purpose. In order to develop confidence that the model provided results in general agreement with industrial units, REI entered into an agreement with Power Systems, Mfg (PSM) of Jupiter, FL, the *only* after-market company with a viable DLN combustion system for the GE Frame 7 installed base. Under the agreement, PSM agreed to provide to REI, on a confidential basis, design drawings, combustion conditions, and measurements on NO_x and CO from their test burn. REI would be able to report the results, subject to review by PSM. The following sections discuss the basis of the DLN combustor design, the critical test of our combustion chemistry with data published by GE on premixed combustors operating in the range of interest to DLN combustors, and finally a comparison of model predictions and data for the PSM gas turbine combustor.

The basic concept of the DLN combustor is to operate with a fuel lean flame that can run at temperatures at which the fixation of atmospheric nitrogen is minimized. The total air to the combustor is determined by the maximum allowable temperature of the gases to the expansion turbine. The total air is supplied to the combustor through an inner swirler with the fuel and an outer swirler to cool the liner. The basic GE design consists of concentric counter-swirling annular flows. The constraints and challenges in implementing these concepts is discussed in a series of papers and research reports published by GE [Davis and Black; Correa, 1992; Leonard and Stegmaier, 1993; Joshi et al., 1994].

The NO is formed in the combustion products of the fuel and air supplied to the primary swirler. The lower limit of emissions is that achieved with perfect premixing of the fuel and air prior to combustion. The following section provides the results of modeling NO_x formation in premixed flames for the conditions of interest in gas turbines.

NO_x formation in Premixed Flames

Leonard and Stegmaier (1993) provide NO_x measurements in a premixed isothermal plug-flow flame reported at 15%O₂ dry, shown in Figure I.1. The data were taken for premixed flames stabilized with a variety of flame holders, for pressures of 1 to 30 bar, inlet air temperatures of 300 to 800K, and residence times of 2 to 100 milliseconds. The authors point out, that contrary to expectations from the classical Zeldovich kinetics for the thermal fixation of nitrogen:

- the amount of NO_x formed varies little with total pressure.
- the amount of NO_x formed is independent of residence time.

These data were used to test the validity of the REI kinetic model in the range of conditions of interest to DLN combustors. The REI kinetic model for the formation of nitrogen oxides in hydrocarbon flames was assembled from a number of references in the literature. The basic mechanism is that of Miller and Bowman (1991), with additions and revisions from Dean, Hanson, and Bowman (1991) from their article in J. Phys. Chem. on

nitrogen chemistry and Miller and Melius (1992) from their article on hydrocarbon chemistry. The mechanism consists of 66 species and 372 reactions.

Figure I.1. NO_x corrected to 15% O₂ dry for stabilized very well-mixed natural gas flames, for pressures of 1 to 30 bar, 300 to 800 K air inlet temperature, and 2 to 100 milliseconds residence time [Leonard and Stegmaier, 1993].

In order to apply the code it was first necessary to determine an adiabatic temperature for conditions relevant to gas turbines. This was accomplished by using an Equilibrium Code (Gaseq, <http://www.gaseq.co.uk/>). Air and natural gas were compressed reversibly and adiabatically to pressures of 5 to 30 atmospheres, mixed and burned for different ratios of methane to air to determine the adiabatic temperature as a function of equivalence ratio and pressure. The kinetic code was then used to calculate composition as a function of time at the computed adiabatic temperature. The results of NO versus time are shown in Figure I.2 for pressures of 5 and 30 atmospheres, and a combustion temperature of about 1760 K.

Figure I.2. NO_x corrected to 15% O₂ wet for a PFR as a function of residence time, for pressures of 5 and 30 atmosphere, and a temperature of about 1760K.

The results show that, in agreement with the data of Leonard and Stegmair, the effect of pressure is small and the NO_x concentration is relatively independent of residence time. The NO_x formation is dominated by a very rapid rise at early times, followed by a slower growth rate. Three factors contribute to this early growth [Turns, 2000]:

- Superequilibrium O atom concentrations in the Zeldovich reaction ($O + N_2 = NO + N$),
- the increased importance at lower temperatures of the N₂O pathway ($N_2 + O + M = N_2O + M$) relative to the Zeldovich reaction, and
- the so-called Fenimore or prompt NO mechanism. The first step in the Fenimore mechanism is $CH + N_2 = HCN + N$.

The prompt NO_x corresponds to the occurrence of spikes in the O and CH concentration versus time, with the amount of NO formed being proportional to the integral in those spikes. As the temperature increases beyond 1900K, the Zeldovich reaction becomes dominant, with the O atom concentration approaching its equilibrium value with O₂. The NO formation for the higher temperature regime ($T > 1900K$) is dependent on residence time and pressure. This is evident in Figures I.3 and I.4. The time resolved NO formation in Figure I.3, calculated for pressures of 5 and 30 atmospheres, show a pressure and time dependence at 1942 K but not at 1763K. The NO formed at pressures of 5, 17, and 30 atmospheres, shown as a function of temperature in Figure I.4 for a fixed residence time of 7 milliseconds, begins to show a significant pressure dependence as the temperature exceeds 1900K.

Figure I.3. NO_x uncorrected for a PFR as a function of residence time for temperatures of about 1760 and 1940 K.

Figure I.4. NO_x uncorrected as a function of combustion temperature in a PFR, for pressures of 5, 17, and 30 atm.

The above results indicate that the reaction model assembled by REI is able to reproduce the trends reported by Leonard and Stegmaier. Figure I.5 provides a comparison of the model predictions, for a fixed residence time of 7 milliseconds, with the least square correlation of the experimental results shown in Figure I.1. The agreement between the predictions and experiments indicates that the REI chemistry model is able to provide a good estimation of the absolute values as well as predicting the trends with temperature and pressure of the GE results.

Figure I.5. NO_x corrected to 15% O₂ wet as a function of temperature, comparison of results of Leonard and Stegmaier (1993) and values calculated using the code assembled by REI.

Importance of Mixing

The Leonard and Stegmaier (1993) reference emphasized that the results on the residence time and pressure independence of NO_x under gas turbine conditions were for “extremely well premixed flames operating at less than 1900 K”. They show how non-uniform fuel and air mixing influences NO_x formation. They provide in Figure I.6 results for “a nearly perfect premixer, well-designed premixer, and non-optimized premixer”. It is clear that the variations in composition and temperature in time and space for the non-ideal mixing conditions lead to significant increases in NO. They also indicate that reaction zone film cooling leads to early flame blowout and the formation of large quantities of CO and unburned hydrocarbons.

Figure I.6. Effect of mixing conditions on NO_x from stabilized premixed flames of natural gas [Leonard and Stegmaier, 1993].

The presence of amounts of NO_x that do not lie on the correlation of NO_x versus adiabatic flame temperature shown in Figure I.5 and are dependent on pressure or residence time, can therefore be used as a *measure of the unmixedness*. The GE publications underline the difficulty of designing fuel injectors that can achieve complete premixing very close to the inlet to the combustion zone.

Modeling of the PSM Combustor

PSM provided detailed drawings of the combustor and process conditions, including detailed characterizations of the flows to the inner and outer swirlers shown in Figure I.7. The temperature, equivalence/ratio, mass flow rates to the primary swirler and the air flow rate to the secondary swirler were provided. The combustor was modeled by RECOM Services using the *AIOLOS* code developed by IVD at the University of Stuttgart, Germany. The capabilities of the code are described at (http://www.ivd.uni-stuttgart.de/english/frame_ru/aiolos_e_ru.html). Briefly, they are:

- **General features**
 - 3D Finite Volume code for turbulent reactive flows
 - Cartesian, or cylindrical co-ordinates, body-fitted co-ordinates
 - Non-staggered, structured grid
 - SIMPLEC or PISO pressure correction scheme
 - Higher-order schemes for spatial discretization to minimize numerical diffusion
 - Temporal discretization by Euler Implicit
 - Hybrid parallelization strategy: Combined multiblock- and microtasking methodology for distributed and shared memory computer architectures
 - Solution algorithms: SOR, Stone, CG methods, Multigrid (under development), optimized for vector- and parallel processor computer systems

- Domain decomposition techniques: Individual choice of co-ordinate system and grid resolution, and of physical models and numerical methods in different sub-domains
- Installations in industry on various hardware platforms
- **Turbulent two-phase flow**
 - k,epsilon-model and Differential Reynolds Stress model
 - Eulerian approach (particle phase treated as a continuous phase)
 - Eulerian/Lagrangian two-phase flow description (fully coupled)
- **Heat transfer**
 - Discrete Ordinates Method
 - Semistochastic Monte Carlo radiation model
 - Moment Method
 - Finite Volume Method
 - Flux Method
 - Discrete Transfer Model
- **Reaction model**
 - Kinetic model using GRI Mech 3.0, advanced Eddy Dissipation Concept (EDC)
 - For pulverized-coal combustion (pyrolysis, tar formation and tar decomposition, char and volatile combustion). Consideration of particle-size distribution
 - Model for pollutant formation (fuel NO, thermal NO) for unstaged, air-staged, and fuel-staged (reburn) combustion systems. GRI-Mech 3.0 was used for the modeling of the gas turbine combustor.

The computations carried out by RECOM used two approaches: a 2D geometric axisymmetric configuration (see Figure I.7) and a 3D body-fitted coordinate system (see Figure I.8). For the 2D case the mixing-chemistry interaction was evaluated using full chemistry and the Eddy Dissipation Concept (EDC) with global kinetics. For the 3D case, only the global kinetics with the EDC was utilized. The agreement between the temperature and velocity fields for the 2D and 3D cases was sufficiently good that it was considered adequate, to save computational time, to include full chemistry only in the 2D cases.

Figure I.7. 2D axisymmetric grid of the gas turbine combustor with 25,000 cells.

Figure I.8. 3D body-fitted grid of the gas turbine combustor with 350,000 cells, including primary swirler.

Case Studies

The conditions provided by PSM were:

Premixer inlet

- Air Mass Flow 6.00 pps.
- Fuel Mass Flow = 0.2235 pps.
- Inlet Temperature (bulk) = 660.2°F

Outer Swirler inlet (note here that igniter leakage has been rolled into these values).

- Mass Flow 2.73 pps.
- Inlet Temperature = 660.2°F
- Air only

Fuel Composition (mol%):

CO₂ 1.6212%

N₂ 8.8313%

CH₄ 85.9352%

C₂H₆ 2.8797%

C₃H₈ 0.5251%

n-Butane 0.0752%

i-Butane 0.0633%

i-Pentane 0.0152%

neo-pentane 0.0035%

c6+ 0.037%

These conditions correspond to an equivalence ratio of 0.52 in the primary combustor, and 0.36 after mixing with the air through the secondary swirler. Two additional cases were suggested with higher equivalence ratios in both the primary combustor and in the well-mixed gases. The pair of equivalence ratios of the fuel/air mixture to the premixed swirler and after complete mixing with the air through the secondary swirler is shown in Table I.1 for all three cases. NO was also calculated using the REI kinetic model for premixed combustion for all three cases in order to provide limiting cases for perfect premixing in the primary combustor. For completeness the NO was also calculated assuming that the gases were quenched and reacted at the final mean equivalence ratio.

Table I.1. Equivalence Ratios in Primary and Final Mixed Products for Three Cases.

NO values calculated for premixed combustor run as a PSR for 7 milliseconds, corrected to 15%O₂, wet.

Case	ϕ , mean	ϕ , primary swirler	NO, ppm ϕ , mean	NO, ppm ϕ , primary swirler
1	0.36	0.52	0.126	1.58
2	0.52	0.76	1.58	125
3	0.66	0.97	20.5	1311

Selected concentration maps are shown for the temperature, oxygen, unburned hydrocarbons, CO, and NO in Figures I.9 through I.13, with concentrations reported for 15% O₂ dry. Examination of the profiles indicates that combustion occurs prior to significant premixing towards the end of the cylindrical duct, with some additional reaction at the interface between the primary and secondary swirling flows. More

detailed information, for comparison with the experimental results, is provided in the profiles of concentration at the sampling location for temperature (Figure I.14), O₂ (Figure I.15), CO (Figure I.16), and NO (Figure I.17).

Figure I.9. Temperature distribution calculated by RECOM with full kinetics for 2D axisymmetric case, detailed kinetics.

Figure I.10. Oxygen concentration distribution calculated by RECOM with full kinetics for 2D axisymmetric case, detailed kinetics.

Figure I.11. Hydrocarbon distribution calculated by RECOM with full kinetics for 2D axisymmetric case, detailed kinetics.

Figure I.12. Carbon monoxide distribution calculated by RECOM with full kinetics for 2D axisymmetric case, detailed kinetics

Figure I.13. Nitric oxide distribution calculated by RECOM with full kinetics for 2D axisymmetric case, detailed kinetics.

Figure I.14. Temperature distribution along measurement path for 2D simulation by RECOM, detailed kinetics.

Figure I.15. Oxygen distribution along measurement path for 2D simulation by RECOM, detailed kinetics.

Figure I.16. Carbon monoxide distribution along measurement path for 2D simulation by RECOM, detailed kinetics.

Figure I.17. Nitric oxide distribution along measurement path for 2D simulation by RECOM, detailed kinetics.

The average of the CO and NO at the sampling locations for the three case studies are provided in Table I.2. The final average concentrations for NO are intermediate to the limiting values in Table I.1, suggesting that significant mixing occurred before the combustion was completed. The mean and peak temperature in the calculated CO and temperature are also provided.

Table I.2. NO and CO Concentrations at the Sampling Plane. Mean and peak values with concentrations corrected to 15% wet.

Case	NO, ppm mean	CO, ppm mean	CO, ppm peak	T, K mean	T, K peak
1	1.2	750	9000	1393	1833
2	17.5	420	6400	1648	2283
3	118.0	220	5600	1818	2373

PSM provided mean concentrations measured at the sampling plane for case 1. The values are:

O₂ 13.53%

NO_x (15% O₂) 3.7 ppm (wet)

CO (15% O₂) 1305 ppm

UHC (15% O₂) 483 ppm

The values of CO and NO are in the general range of values calculated by RECOM. It should be noted that the calculations were performed prior to having access to the data, and no attempt has been made to tune the model to fit the data.

Clearly more comparisons are needed but the CFD model appears to have a sufficient predictive capability to be useful for making decisions on the impact of the changing fuel composition, changing scales, and changing operating conditions that may be encountered in IGCC plants.

References

- Davis, L. B., and Black, S. H., "Dry Low NO_x Power Systems", Report GER-3568G, GE Power Systems, Schenectady, NY
- Correa, M. C., "A Review of NO_x Formation Under Gas-Turbine Combustion Conditions", *Combust. Sci. and Tech.*, Vol. 87, pp. 329-362 (1992)
- Dean, A.J., Hanson, R.K., and Bowman, C.T., *J. Phys. Chem.* 95:3180-3189 (1991).
- Leonard, G., and Stegmaier, J., "Development of an Aeroderivative Gas Turbine Dry Low Emissions Combustion System", Paper 93-GT-288, ASME, 1993
- Joshi, N. D., Epstein, M. J., Durlak, S., Marakovits, S., and Sabla, P. E., "Development of a Fuel Air Premixer for Aeroderivative Dry Low Emissions Combustors", Paper 94-GT-253, ASME, 1994
- Miller, J.A., Bowman, C.T., *Int J. Chem. Kinet.* 23:289 (1991)
- Miller J.A., Melius C.F., *Combustion and Flame* 91:21-39 (1992)
- Turns, S., "An Introduction to Combustion: Concepts and Applications", 2nd Edition, pp. 559-561, McGraw Hill, 2000