DEVELOPMENT OF TECHNOLOGIES AND ANALYTICAL CAPABILITIES FOR VISION 21 ENERGY PLANTS

COOPERATIVE AGREEMENT NO DE-FC26-00NT40954

QUARTERLY REPORT FOR JANUARY-MARCH 2001

FOR

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1. Executive Summary

The project management plan was finalized during a project kick off meeting held on January 16, 2001 in Lebanon, NH, which was attended by all project participants. The project management plan was submitted to DOE and was revised based on comments from DOE (Task 1.0). A survey of the potential users of the integrated software was conducted. A web-based survey form was developed and was announced in the *ProcessCity* discussion forum and in AspenTech's e-mail digest *Aspen e-Flash*. Several Fluent clients were individually contacted. A user requirements document was written (Task 2.2). As a prototype of AspenPlus-Fluent integration, the flowsheet for allyl alcohol production via the isomerization of propylene oxide was developed. A stirred tank reactor in the flowsheet for converting the byproduct acetone into n-propyl propionate was modeled with Fluent, version 5.4. The convergence of the AspenPlus-Fluent integrated model was demonstrated, and a list of data exchanges required between AspenPlus and Fluent was developed (Task 2.6). As the first demonstration case, the RP&L power plant was selected. A planning meeting was held on February 13, 2001 in Cambridge, MA to discuss this demonstration case. It was decided that the steam-side of the power plant would be modeled with AspenPlus and the gas-side, with the ALSTOM Power in-house code INDVU. A flowsheet model of the power plant was developed (Task 3.1). Three positive responses were received for the invitation to join the project Advisory Board. It was decided to expand the membership on the Advisory Board to include other industrial users interested in integrating AspenPlus and Fluent. Additional invitations were sent out (Task 5.0). Integraph's role in the project was restructured based on discussions among the project participants. Fluent hired Dr. Maxwell Osawe to work on the project. Dr. Osawe brings to the project a unique combination of skills (expertise in CFD and object-oriented design and programming) required for the software integration task (Task 7.0).

2. Technical Accomplishments

Task 1.0 Project planning:
<u>Task 1.1 Project Planning</u>

The project kickoff meeting was held at the Fluent headquarters in Lebanon, NH on January 16,2001. The meeting was attended by **ALSTOM Power (**Woody Fiveland, John Marion, and Dave Sloan), **Aspen Tech (**Steve Zitney), **CERC/WVU** (Joe Cleetus and Igor Lapshin), **Fluent** (Lewis Collins, Dipankar Choudhury, Kumar Dhanasekharan, Paul Felix, Barb Hutchings, Peter Runstadler, and M. Syamlal) and **Intergraph** (Bob Fisher). The topics discussed at the meeting are given in Appendix A. The team members reviewed the project plans and finalized the Project Management Plan and also discussed technical strategies. The project management plan was submitted to DOE on January 23, 2001. A revised plan incorporating DOE comments was submitted on February 28, 2001.

Task 2.0 Software Integration
<u>Task 2.2 User survey</u>
SEZ posted a note on the ProcessCity CFD discussion forum inviting people to complete the web-based survey (http://www.fluent.com/vision21/survey.htm) on requirements for integrating CFD and process simulations. SEZ submitted a write-up for inclusion in the February issue of AspenTech's email digest, Aspen eFlash (http://www.aspentech.com/index.asp?menuchoice=ef1_0201). The write-up briefly described the DOE Vision 21 project and invited people to complete the web-based survey (http://www.fluent.com/vision21/survey.htm) on requirements for integrating CFD and process simulations.

The user survey was sent to several key clients of Fluent, which produced two responses. There were no responses from the web-based survey. Nevertheless, a number of good ideas have emerged from the discussions within the project group. By demonstrating a version of the software that implements those ideas, we expect to be able to elicit a better response from the potential users.

Based on the user survey responses and ideas generated within the project group KJC wrote a User Requirements Document (URD) and circulated it within the group for comments. SEZ reviewed and proposed changes to the URD. SEZ, KJC, IBL, and MXS participated in a URD review meeting held at Fluent in Morgantown on March 28, 2001 and arrived at a clarification of SEZ's extensive comments on the URD. Most especially on the CFD Database, which will have a hierarchy of models, some Pre-configured Generic models with only the Case files (mesh generated), and some with Case and Data files, i.e., Pre-computed with results available.

Task 2.6 Software Design

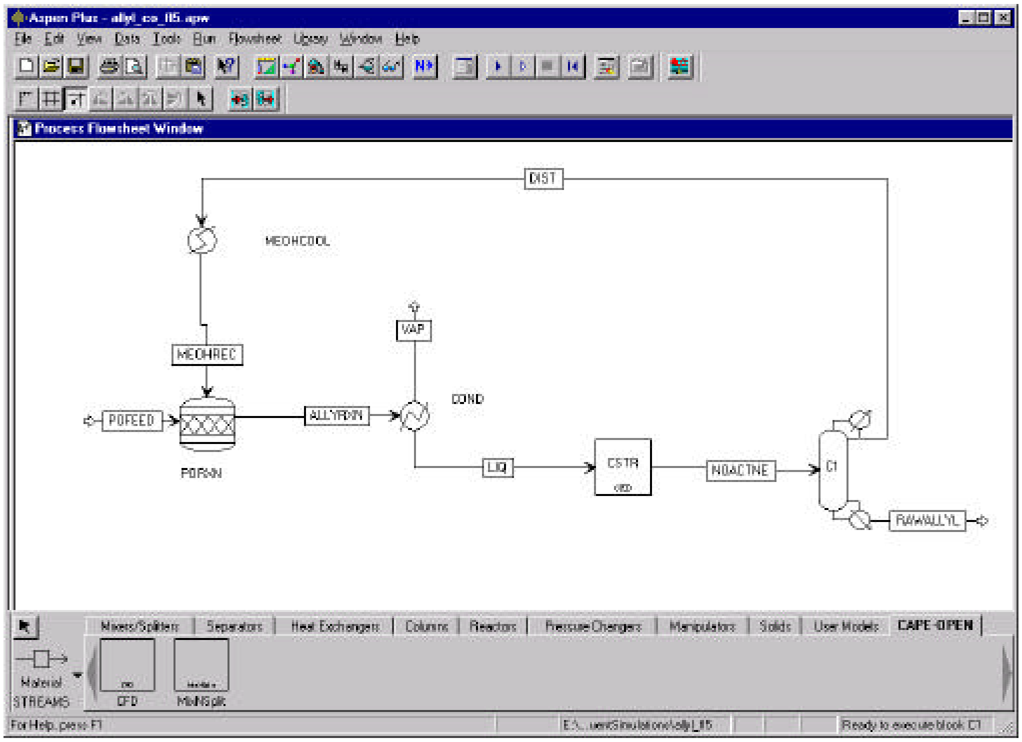
SEZ made several enhancements to the Fluent-AspenPlus Integration prototype:

- The AspenPlus installation was upgraded with AspenPlus 10.2 Service Pack 1 (SP1) in order to exploit recent Cape-Open updates in the Vision 21 prototype. As a result, SP1 is now required to run the latest version of the prototype. Vision 21 developers will have to update their AspenPlus 10.2 installations (See Appendix B).

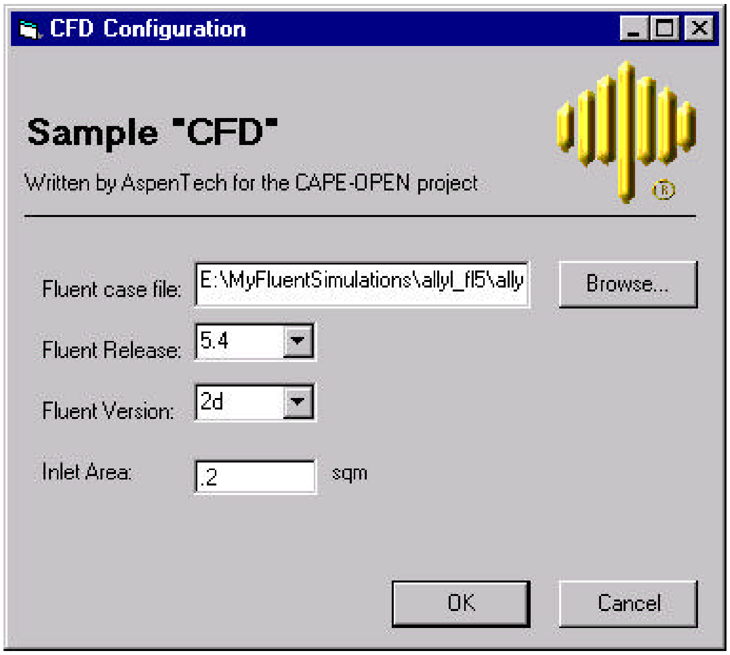
- The Cape-Open VB Controller code was updated with changes made to the Mixer-Splitter template in AspenPlus 10.2 SP1. Some of the modifications were related to the use of the CAPE-OPEN type library vs. AspenCapeTypeLib. AspenCapeTypeLib includes all the CAPE-OPEN definitions and some AspenTech extensions. In the Vision 21 CFD prototype, SEZ changed all AspenCapeTypeLib definitions to CAPE-OPEN definitions, except for those that use the ATCapeXDiagnostic interface to write diagnostics to the AspenPlus history file.

- Diagnostics was added to the ICapeUnit_Calculate method, particularly around the Cape-Open physical property calls.

- SEZ extended the flowsheet from a single unit operation to an entire AspenPlus flowsheet for the production of allyl alcohol. In this process, propylene oxide is converted to allyl alcohol via a liquid phase isomerization, using methanol as a solvent. This reaction is carried out in a stoichiometric reactor (PORXN) based on fractional conversion. Acetone is produced as a byproduct and must be separated from the mixture prior to distillation so as to remove it from the methanol recycle to the isomerization reactor. For this purpose, acetone is converted to n-propyl-propionate by catalytic reaction with allyl alcohol in a CSTR (Fluent CFD reactor). Two additional by-products are produced in the CSTR. The mixture is then stripped of



methanol that is cooled and recycled back to the isomerization reactor.



- The Fluent CFD model was converted from version 4.5 (structured mesh) to version 5.4 (unstructured mesh). A user-defined function was written to specify the impeller velocity profile. A parameter was added to scale the velocity profile as a function of the impeller speed. This Cape-Open CFD reactor model in the allyl alcohol flowsheet was modified to use Fluent 5.4. This required modifying many of the Fluent text input commands used to exchange data to and from AspenPlus.

- The following Aspen stream data are now automatically communicated to Fluent: Number of chemical species, Species names, Molecular weights, Mass fractions. The Cape-Open VB Controller prototype was enhanced with additional CAPE-OPEN thermo routine calls and Fluent text input commands so that the following Aspen Properties data are now automatically communicated to Fluent at each flowsheet iteration: Density, Viscosity, Heat capacity, and Thermal conductivity.

- SEZ added combo boxes to the Cape-Open VB Controller GUI for the user to specify the Fluent release (i.e., 5.3, 5.4, 5.5) and version (i.e., 2d, 2ddp, 3d, 3ddp) in addition to the Fluent case file name.

- The Fluent CFD model is executed at each iteration of the AspenPlus flowsheet, which converges in several iterations.

- SEZ worked with Michael Halloran (AspenTech UK) to prepare an installation kit for the CAPE-OPEN CSTR prototype.

IBL evaluated the pros and cons of using Java or C++ as the language for developing the Vision21 Controller. Based on that evaluation C++ was selected for Vision 21 Controller development because of the ease with which COM connections can be made to AspenPlus. The project staff has more experience in C++ than in Java, which also makes C++ the best choice. Work on a high-level software design has been started.

Task 2.14 Step Five

ALSTOM Power sought the release of the INDVU source code from one of their business units and obtained the permission. Porting of the INDVU code from the UNIX platform to the PC is being scheduled.

Task 3.0 Select Demonstration Cases

SEZ worked with WAF and DGS (ALSTOM Power) and hosted a Vision 21 Meeting at AspenTech in Cambridge, MA on February 13, 2001. The goals of the meeting included accelerating the Richmond Power & Light (RP&L) cycle analysis, aligning the controller specifications with the requirements for the ALSTOM Power in-house codes, outlining the desired contents of the DOE presentation in November, and discussing the Cape-Open formulation and usage strategies. The meeting participants included WAF, DGS, and Paul Hansen (ALSTOM Power); SEZ, Randy Field, Michael Halloran, and Mark Jarvis (Aspen Tech); IBL (CERC/WVU); and MXS and PEF (Fluent). Mark Jarvis and Michael Halloran were invited to the meeting because of their expertise in certain areas. Mark used to work for the DOE and has experience using AspenPlus and other software packages to model power plants. Michael is the developer of the Cape-Open (CO) interfaces in AspenPlus and gave valuable insight to PEF and IBL.

SEZ gave a demonstration of the CSTR prototype to integrate Fluent and AspenPlus via CO unit operation interfaces. The inputs/outputs for the INDVU program and specifications for the Vision21 Controller were discussed at the meeting. During the meeting it was decided that the INDVU program would be integrated with AspenPlus flowsheet model of the RP&L plant.

AspenPlus was installed at ALSTOM Power. Paul Hansen constructed a skeletal flow sheet model with the proper connectivities, using the AspenPlus library modules, although the cycle analysis does not yet incorporate the RP&L design parameters. The cycle analysis now incorporates the requisite RP&L design parameters, and runs with an EXCEL interface in one of the three modes: (a) once through, (b) single design spec, and (c) sensitivity block. FORTRAN coding was added to help the cycle run as an *off-design* model. More sophisticated upgrades will be made to the cycle as additional information becomes available and as circumstances dictate.

The blueprints and data for the RP&L units were obtained. A survey of all of the data and information available within ALSTOM Power on the RP&L unit revealed that key pieces of information were still lacking. A contact was established at RP&L to help get additional information. RP&L is in the process of sending ALSTOM Power the requested blueprints of their unit.

SEZ read a number of papers and web pages on using AspenPlus to model power plants (see Appendix C) and sent the first two papers to Vision 21 participants.

Task 5.0 Advisory Board Activities

A limited number of responses were received from prospective advisory board members with respect to the original invitation to be panel participants. Letters were sent to the remaining invitees, reminding them to respond to the original solicitation. Positive responses have been received from Diane Madden, Ed Ruben, and Eugene Baxter. Several negative responses have been received; the others are pending. The names of additional individuals that may be invited are being sought.

Task 7.0 Project management

Much progress was made in defining the role of Integraph in the project. The software integration accomplished through this project will assist the modularized design of the Vision 21 power plants. It is desired that the integration must ultimately consider the data and models used to represent the process and physical domains. The present project, however, focuses only on the integration of models of different design granularity in the process domain (CFD, proprietary design codes and flowsheet models). In a follow on project (perhaps lead by Intergraph) integration across the physical and process domains will be accomplished. With the limited funding available in the present project, Intergraph will demonstrate how such integration will help future designers. This demonstration will help the current project to define what factors need to be considered in our current software integration methodology so that the future integration across the physical and process domains is not constrained. The restructuring of Intergraph's contribution to the project will add much value to the project without additional cost. Subcontract negotiations are ongoing with Intergraph and a revised subcontract is expected to be executed any day now.

Fluent has hired a developer to work full time on the project. Dr. Maxwell Osawe is a Ph.D. in Computational Fluid Dynamics at Queen Mary, University of London, UK. Maxwell brings to the project a unique combination of skills: expertise in CFD, object-oriented design, and C++ programming.

3. Issues and Resolution:

- Task 2.2 User Survey. Only very few responses were received from the User Survey. It appears that without having a working prototype it will be difficult for the potential users to define the requirements for the integrated software. So the user requirements document (URD) is based mainly on information generated from discussions within the project group, by developing and testing the AspenPlus-Fluent prototype, and from publications and presentations on the integration of flowsheet simulator with CFD. We plan to update the URD as additional information is gathered from Advisory Board meetings and other meetings. This will not impact the project schedule or deliverables because we have sufficient information to develop the early versions of the software.

- Task 3.1 Demo Case 1. The documentation that constitutes the deliverable for Task 3.1, concerning the selection of the RP&L facility that will serve as Case 1, was due by 1-31-01. RP&L has provided the required blueprints to ALSTOM Power. The blueprints are being reviewed by Lorraine Miemiec to ensure that sufficient information is available to construct and INDVU case. Sufficient information should now be available to complete the Task 3.1 deliverable. The formal completion of the deliverable is expected by May 15, 2001.

- Task 5.0 Advisory Board Activities. Because of the number of negative responses that have been received to date, additional individuals from industry, that were not on the original list of potential advisory board members, are being contacted and invited to serve on the advisory board. This has delayed the scheduling of the first advisory board meeting. The current plan is to hold the first advisory board meeting during the Fluent Users Group Meeting in June 2001.

4. Progress forecast for the next quarter

- Task 2.3
  - Write Software Requirements Specifications

- Task 2.4

  - Define the APIs for communication between Vision21 Controller and Fluent.

- Task 2.6:
  - Continue to work on prototype of a Fluent CFD model running in AspenPlus via the Cape Open unit interface.
  - Write software design document

- Task 2.7
  - Write software development plan
  - Develop Vision21 controller version 0.1

- Task 2.14
  - Investigate linkage of INDVU program with AspenPlus via USER2 block and assess whether steam flowrate can be controlled using a design spec.
  - Complete the porting of the INDVU program to the PC platform.
  - Complete stand-alone INDVU case for RP&L unit.

- Task 3.1:
  - Continue to gather additional information from RP&L personnel and complete the deliverable.
  - Complete basic flow sheet of RP&L plant using library modules and incorporate RP&L design parameters.

- Task 5.0:
  - Complete Advisory Board formation
  - Schedule the first advisory board meeting

- Task 7.0:
  - Complete subcontracts to Intergraph
  - Complete project web site

5. Project Milestones

Task Number	Milestone/Deliverables	Completion Date		
		Original	Revised	Actual
1.0	Project Management Plan	1-30-01		1-23-01
2.2	User Requirements Document (URD)	3-15-01		3-28-01
2.3	Software Requirements Specifications (SRS)	4-15-01		
2.6	Software Design Documentation	5-15-01		
2.7	Software Development Plan	6-30-01		
2.7	Working Test Case 1	6-30-01		
2.10	Working Test Case 2	9-30-01		
2.12	Working Test Case 3	1-15-02		
2.13	Working Test Case 4	3-30-02		
2.14	Working Test Case 5	1-1-02		
2.15	Working Test Case 6	6-15-02		
2.17	Working Test Case 7	9-15-02		
2.17	Beta version of Controller	9-15-02		
2.18	User documentation for Controller	12-30-02		
2.20	Integrated Software suite and demonstration	6-30-03		
3.1	Demonstration Case 1 selection	1-31-01	5-15-01	
3.2	Demonstration Case 2 selection	8-30-01		
4.1	Demonstration Case 1 simulation completed	6-30-02		
4.2	Demonstration Case 2 simulation completed	6-30-03		
4.3	Report on Demonstration Case simulations	7-30-03		
5.1	Advisory Board Meeting	3-31-01		
5.2	Advisory Board Meeting	9-30-01		
5.3	Advisory Board Meeting	3-31-02		
5.4	Advisory Board Meeting	9-30-02		
5.5	Advisory Board Meeting	3-31-03		
5.6	Advisory Board Meeting	7-30-03		
7.0	Quarterly reports to DOE	Every quarter		
7.0	Final project report	12-31-03		

6. Personnel initials, List of Abbreviations and Glossary

Personnel Name	Affiliation	Initials
Woodrow Fiveland	ALSTOM Power	WAF
John L. Marion	ALSTOM Power	JLM
David G. Sloan	ALSTOM Power	DGS
Herb Britt	AspenTech	HB
Randy Field	AspenTech	RF
Steve Zitney	AspenTech	SEZ
Joe Cleetus	CERC	KJC
Igor Lapshin	CERC	IBL
Lewis Collins	Fluent	RLC
Paul Felix	Fluent	PEF
Ahmad Haidari	Fluent	AH
Barb Hutchings	Fluent	BJH
Lanre Oshinowo	Fluent	OSH
Madhava Syamlal	Fluent	MXS
Bob Fisher	Intergraph	RJF

Name	Description
ActiveX	A Microsoft technology built on top of COM that extends the basic capabilities of OLE to allow components to be embedded in Web sites.
API	Application Programming Interface.
C++	C++ programming language.
CERC	Concurrent Engineering Research Center, WVU
CFD	Computational Fluid Dynamics
CAPE-OPEN	Computer Aided Process Engineering – Open Simulation Environment Interface definitions for exchanging information with process simulation software. (www.quantisci.co.uk/Cape-Open).
COM	Component Object Model – Refers to both a specification and implementation developed by Microsoft Corporation that provides a framework for integrating software components.
CORBA	The Common Object Request Broker Architecture is a specification of a standard architecture for object request brokers (ORBs). A standard architecture allows vendors to develop ORB products that support application portability and interoperability across different programming languages, hardware platforms, operating systems, and ORB implementations. (www.omg.org)
CSTR	Continuous Stirred Tank Reactor
DCOM	Distributed Component Object Model – An extension of COM that allows software components to be distributed over a network.
GUI	Graphical User Interface
IDL	Interface definition language, which is used for defining the communications between software components linked through a middleware.
INDVU	ALSTOM Power in-house code for the analysis and design of the gas side of a powerplant.
Java	Java programming language.

Middleware	Connectivity software that consists of a set of enabling services that allow multiple processes running on one or more machines to interact across a network.
OLE	Object Linking and Embedding. Builds on COM to provide services such as object "linking" and "embedding" that are used in the creation of compound documents (documents generated from multiple tool sources).
PFD	Process Flow Diagram
Python	Python programming language
RP&L	Richmond Power and Light power plant.
Swing	A Java GUI tool kit.
URD	User Requirements Document
Visual Basic	Visual Basic programming language
WVU	West Virginia University
XML	Extensible Markup Language: A metalanguage -- a language for describing other languages -- which lets one create their own markup language for exchanging information in their domain (music, chemistry, electronics, hill-walking, finance, surfing, CFD, process simulation).

Appendix A: Kick off meeting agenda

Goal:
1. Review the project plans and progress for all project participants and the management representatives. Sign off on the project management plan to be submitted to DOE.
2. Discuss expectations of the organizations involved.
3. Provide an opportunity for project participants to meet in person and discuss project-related issues and next steps.

9:00 – 9:25 a.m.	Introductions	All
9:25 – 9:30 a.m.	Welcome	Barb Hutchings (Fluent)
9:30 – 9:45 a.m.	Project Overview	M. Syamlal (Fluent)
9:45 – 10:00 a.m.	Current status of AspenPlus and Fluent Integration	Steve Zitney (AspenTech)
10:00 – 10:15 a.m.	User Requirements	Joe Cleetus (CERC)
10:15 – 10:45 a.m.	Overview of the proposed Software Architecture	Paul Felix (Fluent) and Igor Lapshin (CERC)
10:45 – 11:15 a.m.	Software applications and Advisory Board activities	Woody Fiveland and David Sloan (ALSTOMPower)
11:15 – 11:30 a.m.	Intergraph Capabilities	Bob Fisher (Intergraph)
11:30 – 12:15 p.m.	Lunch (boxed lunch provided)	
12:15 – 12:30 p.m.	Administrative topics	Lewis Collins (Fluent)
12:30 – 3:00 p.m.	Open discussion of project-related issues	Moderated by Peter Runstadler (Fluent)
3:00 p.m.	Meeting adjourned	

Appendix B: Notes on Fluent-AspenPlus Prototype

- Nonconventional (NC) solid substreams are often used when modeling coal processing facilities with AspenPlus. Nonconventional solids are materials characterized in terms of empirical factors called component attributes. Component attributes represent component composition by one or more constituents. Nonconventional solids never participate in phase or chemical equilibrium calculations. AspenPlus always assigns substreams of type NC to nonconventional solids. The current Cape-Open implementation works with a single mixed substream. The Cape-Open interfaces are being extended to support electrolytes and petroleum fractions, but not solids and polymers. It is not clear whether or not the extensions will map onto AspenPlus stream structure. We may be able to treat coal as a conventional component using various workarounds.

- Vision 21 developers will have to update their AspenPlus 10.2 installations to use AspenPlus 10.2 Service Pack 1 (SP1). The AES 10.2 SP1 will be downloadable from AspenTech's Technical Support Center on the web. Vision 21 developers should register on-line at http://support.aspentech.com.

- In the Cape-Open CSTR prototype, the area was determined from the geometry of the model inlet and hard coded to compute the appropriate velocity inlet boundary condition. This is a limitation of FLUENT 4 only having velocity inlets. Since AspenPlus passes the mass flow, FLUENT 5 can use a mass flow rate boundary condition directly (or compute the area for the inlet surface and specify a velocity inlet). This is preferred to reduce the dependency on having to specify the area explicitly.

- In the Cape-Open CSTR prototype, the density of the inlet stream was chosen arbitrarily. As the definition of physical properties in AspenPlus and in FLUENT are different, the properties were set up twice in the USER2 demo and in the initial Cape-Open prototype discussed at the Vision 21 Kickoff Meeting. However, the ideal scenario is one in which the property data is passed to FLUENT from AspenPlus. SEZ has now done this for component (species) molecular weights. This needs to be done for other physical properties.

- The current Cape-Open interfaces do not support the use of reaction information (reaction rates and stoichiometric information). Thus, it is not possible to specify reaction information in AspenPlus and get it into Fluent. Global-Cape-Open Task 2-2 is studying the feasibility of introducing a Reaction Manager for kinetic reactions.

- For multiple species, FLUENT 5 requires a mixture template to be set up. This template contains the list of components, the reaction models to be used, and the calculation methods for the mixture properties. This template can be created along with the custom components and loaded into FLUENT during the problem setup. In this way the properties of the individual components are passed to FLUENT and FLUENT is responsible for computing the mixture properties using the available methods. One idea is to generate a function to write out the AspenPlus component data and reactions in the FLUENT material property database format. The user would specify the reaction models for use in FLUENT.

Appendix C: List of papers on the usage of AspenPlus for modeling powerplants

- Ong'iro, A. O., V. I. Ugursal, and A. M. Al Taweel, Simulation of Combined Cycle Power Plants using the AspenPlus Shell, Heat Recovery Systems & CHP, 15(2), pp. 105-113 (1995)
- Solantausta, Y., T. Makinen, E. Kurkela, and K. Sipila, New Alternatives for Electricity Production, Part 4. Performance of peat-fuelled air gasification combined-cycle power plants, Technical Research Centre of Finland, VTT Research Notes 1451 (1993)
- Ong'iro, A. O., V. I. Ugursal, and A. M. Al Taweel, Using AspenPlus for Power Plant Simulation and Process Integration, Presented at the CSChE 2000 Conference, Montreal, Canada, October (2000)
- Ree, R., van, A.B.J. Oudhuis, A. Faaij, A. Curvers, Modelling of a biomass integrated gasifier/combined cycle (BIG/CC) system with the flowsheet simulation programme ASPENPLUS, Netherlands Energy Research Foundation, Department of Science Technology and Society, Utrecht University, Report ECN-CX-94-057, May 1995.
- Elseviers, W.F., Van Mierlo, T., Van de Voorde, M.J.F. and Verelst, H. Thermodynamic Simulations of Lignite-Fired IGCC-Cycles with Desulphurization and CO2 Capture. IGCC Simulations. Fuel, 1996. http://wwwtw.vub.ac.be/ond/chis/dep/research/r_joule2.htm
- Ruth, L. A. and S. M. Klara, Process Simulation in the U.S. Department of Energy's Combustion 2000 Program, U.S. Department of Energy Pittsburgh Energy Technology Center Pittsburgh, PA 15236-0940 http://www.osc.edu/pcrm/Ruth.html