HIGH PRESSURE COAL COMBUSTION KINETICS PROJECT

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FOR

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1. Abstract

NEA completed the CFD simulations for all NBFZ tests. SRI resumed work on HPBO experiments and conducted preliminary tests using the UCONN impactor. UCONN prepared several samples of char for cross-sectional analysis by SEM and characterization is underway. BU completed the NBFZ char characterization program. CBK model had been implemented into Fluent.

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2. Executive Summary

NEA developed the computer programs to apply NEA's ChemNet™ CFD post-processing to the CFD simulations for all NBFZ tests. All the NBFZ datasets have been simulated within useful quantitative tolerances. It is most interesting that the detailed chemistry depicts all the features in the measured N-species data, including the persistence of HCN for stoichiometric ratios S. R. values that are much greater than unity at 3.0 MPa only.

NEA began developing a NO_x production submodel to reproduce the performance of the full chemical reaction mechanism in interpreting the NBFZ datasets.

SRI conducted tests on PRB coal at 2 and 20 atm and a total furnace length of 89 cm (using 2 added Kanthal heater stages), continuing earlier tests with the induction furnace only (L = 16 cm) and one Kanthal stage (56 cm). Preliminary tests using the UCONN impactor were conducted with the impactor mounted in its conventional vertical orientation at the end of a sidearm off the centripeter housing.

BU completed the tap density measurements on Illinois #6 NBFZ chars, essentially completing the NBFZ char characterization program.

UCONN also prepared several samples of char for cross-sectional analysis by SEM. These samples included Pittsburgh #8 (SRI sample 51), Illinois #6 (SRI samples 82 and 99), and the PRB coal (SRI sample 101). An optical microscope was used for a preliminary characterization. SEM characterization is still underway. UCONN also conducted preliminary SEM characterization of ash samples generated in HPBO experiments utilizing the PRB coal at a pressure of 2 atm. .

FW performed the ASPEN PPCC and the Fluent PPCC simulation of the Vision 21 plant. Detailed results of the simulation were presented at the project review meeting in Morgantown.

During the project review meeting the team discussed the implementation of sub-models into ASPEN and Fluent. In June AAL have received the CBK sub-model and its complete documentation from Prof. Hurt. AAL has also received the additional files from Foster Wheeler to run their Aspen Plus Advanced Power Plant simulation.

AAL and Fluent received the ash formation code from UCONN.

CBK model had been implemented into Fluent. Thermal annealing and ash effects are included in the CBK version that had been implemented in Fluent.

3. Experimental

SRI added a third stage of Kanthal heaters to increase the furnace length to 120 cm and the nominal residence time to 2.7 seconds at 2 atm. There was no apparent improvement in the results, with the impactor solids again dominated by soot deposits.

4. Results and Discussions

Task 0 Planning

Completed

Task 1.0 Submodels for Pollutant Formation

Task 1.4 Fuel-N Conversion Mechanism Development

NEA developed the computer programs to apply NEA's ChemNet™ CFD post-processing to the CFD simulations for all NBFZ tests, and completed the first sweep of calculations for all tests with Pit. #8 at 10 atm in April. The method first develops an equivalent network of reactors that match the residence time distributions, thermal histories, and entrainment rates among the regions in the flow. Then the reactor network is used to evaluate the chemical conversion based on complete elementary reaction mechanisms for all stages of the process.

Two plug flow reactors in parallel represent the bulk flow patterns in all NBFZ tests. One series represents the stream near the reactor wall that contains from 70 to 95 % of the fuel particles and the other represent the core flow, which is significantly cooler. Oxygen is entrained from the core stream into the boundary layer stream. Nevertheless, the abundance of particles in the boundary layer stream maintains stoichiometric ratios (S. R.) that are much richer than the nominal values for the entire flow. This relatively rich stream is responsible for the coexistence of O₂ and CO in the exhaust that is evident in the datasets for all coals at all pressures. The equilibrium calculations indicated that CO, hydrocarbons, and HCN for tests with S. R. greater than 0.5 would have vanished without any segregation of particles near the walls of the reactor tube, at odds with the data. NEA also verified this finding with simulations based on full chemical reaction mechanisms and uniform particle dispersion across the reactor tube. However, when the particles were segregated to match the dispersion patterns in the CFD simulations, the detailed chemistry calculations correctly predicted an abundance of CO and also HCN for even the leanest operating conditions, in accord with the measured values.

In May, all the NBFZ datasets have been simulated within useful quantitative tolerances and the figures below represent our best interpretations for the NBFZ data. Hence, task 1.4 is now complete. It is most interesting that the detailed chemistry depicts all the features in the measured N-species data, including the persistence of HCN for S. R. values that are much greater than unity at 3.0 MPa only.

Task 1.5 NO_x production submodels

NEA began developing a NO_x production submodel to reproduce the performance of the full chemical reaction mechanism in interpreting the NBFZ datasets. The submodel will be suitable for deployment in Fluent. NEA initially focused on generating a baseline set of predictions with Fluent's current NO_x submodel for CFD post-processing. Fluent arranged to provide NEA a copy of Fluent v.6.1 for this project, which enables NEA to use the latest version as baseline reference condition. All the primary CFD simulations for post-processing with the NO_x production submodel were previously developed under Tasks 1.3 and 1.4.

Task 2.0 Submodels for Char Oxidation

Task 2.1-2.5

SRI conducted tests on PRB coal at 2 and 20 atm and a total furnace length of 89 cm (using 2 added Kanthal heater stages), continuing earlier tests with the induction furnace only (L = 16 cm) and one Kanthal stage (56 cm). Coal suspension loadings and oxygen concentrations were varied widely in an attempt to find conditions where the flowtube survived the test and yet complete burnout was achieved.

Preliminary tests using the UCONN impactor were conducted with the impactor mounted in its conventional vertical orientation at the end of a sidearm off the centripeter housing. These tests showed that large particles failed to convect into the sidearm and then to the impactor, and so a large number (15 to date) of subsequent impactor tests have been made with the centripeter removed and the impactor mounted in an inverted orientation directly at the exit of the flowtube. These tests show that the large particles now collect primarily in the first stage of the impactor, but it appears that smaller particles are captured on the various stages without significant influence of gravity.

The impactor tests show the ongoing difficulty of achieving complete burnout conditions. Thus far, we find that at 2 atm and 10% coal suspension loading, an oxygen level of about 40% (stoichiometric ratio $SR = 2$) is required to achieve burnout, while at 20 atm and 2.25% suspension loading an oxygen level of 14% ($SR = 3$) is required. These stoichiometric ratios are in contrast to a typical operating value of $SR = 1.15$ used in atmospheric pressure reactors.

Complete burnout is defined when the solids (ash) captured on the impactor stages or in the centripeter are light in color (varying from beige to light grey). In the majority of runs, the solids are dominated by soot, which is low density, fluffy, sticking to all surfaces, and very black. It is probable that the soot amounts to no more than 1% of the fed coal amount, but its relatively large volume obscures the ash and presumably precludes useful analyses.

In the NBFZ experiments, SRI used argon as the carrier gas instead of N₂ in order to achieve higher gas temperatures, leading to earlier and more extensive combustion. Initial HPBO tests were conducted with N₂ carrier, and we have seen some evidence of

differences in the HCN/NH₃/NO yields due to thermal NO_x processes. Nevertheless, SRI recently reverted back to argon carrier in an attempt to achieve burnout at lower stoichiometries. Thus far, there doesn't seem to be a significant effect of this change on soot burnout.

The nominal residence times (i.e., furnace length/entrance carrier gas velocity) for the 89-cm long furnace are 1.9 seconds at 2 atm and 3.0 seconds at 20 atm. In most recent test, SRI added a third stage of Kanthal heaters to increase the furnace length to 120 cm and the nominal residence time to 2.7 seconds at 2 atm. There was no apparent improvement in the results, with the impactor solids again dominated by soot deposits. Ash samples from the 2 atm tests of PRB coal that showed complete burnout were sent to UCONN for analysis.

Results of our complete program efforts through May 15th were presented at the Project Review Meeting on May 16th, 2003.

During April BU completed the tap density measurements on Illinois #6 NBFZ chars, essentially completing the NBFZ char characterization program.

During April, UCONN experimented with different epoxy resins that could be used to prepare polished cross-sections of char particles and ultimately prepared a successful cross-sectioned sample of Pittsburgh #8 (sample 51) with EPO-TEK - 353 ND epoxy resin. Subsequent SEM characterization of the sample, done both at UCONN and in conjunction with Prof. Hurt's group at Brown, showed two different types of char wall structure, one with a wall thickness of less than 5 mm and another type that is less porous (see Figure 1).

Figure 1. Cross-sectioned SEM of Pittsburgh #8, sample 51.

BU worked on the analysis and interpretation of the SRI NBFZ char characterization. Discussions about swelling and annealing effects were held with both Steve Niksa, and outside the project with Prof. Tom Fletcher, who's laboratory has also done a lot of work on swelling and heating rate effects. To aid in the interpretation of the data BU asked NEA for calculated particle temperature histories, and they provided a detailed set from their recent simulations.

Task 3.0 Submodels for Flyash and Fumes

Task 3.1-3.4

UCONN received the results of the analysis of the Pittsburgh #8 ash chemical composition from an external laboratory. The mineral content determined by ASTM D3174 was 12.3 weight percent, which corresponds to the value determined in UCONN in-house analysis last December. These values differ from the level calculated from the CCSEM analysis of the coal minerals reported previously (25.6%). A comparison of the chemical composition resulting from bulk ash analysis and calculated from the CCSEM mineral analysis is reported in Table 1.

Table 1. Comparison of the results from CCSEM and ASTM D3682 for Pittsburgh #8

Compound	Calculated from CCSEM results	ASTM D3682 results
SiO ₂	43	31
Al ₂ O ₃	17	16
Fe ₂ O ₃	32	47
TiO ₂	0.6	0.6
P ₂ O ₅	1	0.3
CaO	4	3
MgO	0.6	0.5
Na ₂ O	0.6	0.5
K ₂ O	2	2

UCONN also prepared several samples of char for cross-sectional analysis by SEM. These samples included Pittsburgh #8 (SRI sample 51), Illinois #6 (SRI samples 82 and 99), and the PRB coal (SRI sample 101). An optical microscope was used for a preliminary characterization. SEM characterization is now underway.

UCONN also conducted preliminary SEM characterization of ash samples generated in HPBO experiments utilizing the PRB coal at a pressure of 2 atm. Samples examined were the size segregated samples collected on the stages of the low pressure cascade impactor. Examples of these SEM micrographs are shown in Figures 2 and 3. These micrographs show no presence of char residue.

Figure 2. SEM of PRB 139 ash – Stage 7

Figure 3. SEM of PRB 139 ash – Stage 11

Task 4.0 Deployment in Design Codes

Task 4.1-4.2

During the project review meeting at NETL the team members discussed the implementation of sub-models into ASPEN.

AAL have received the CBK sub-model and its complete documentation from Prof. Hurt. AAL has also received the additional files from Foster Wheeler to run their Aspen Plus Advanced Power Plant simulation.

AAL and Fluent received the ash formation code from UCONN.

Task 4.4

CBK model had been implemented into Fluent starting from the User defined function that had been created in Q4 2001. The model includes effects of thermal annealing and ash inhibition on the char combustion. The implementation had been tested on a 2 dimensional coal combustion test case. The GUI Graphical user interface for the CBK input had been completed.

Fluent received the ash formation code from UCONN .

Task 5.0 Vision 21 Design Analysis

Task 5.2 Conceptual Design of Vision 21 Process

FW performed the ASPEN PPCC and the Fluent PPCC simulation of the Vision 21 plant. Minor inconsistencies between the ASPEN PPCC simulation and the Fluent PPCC model inputs were eliminated . Overall performance is summarized in the Table presented below.

<u>Results at Outlet</u>		ASPEN	Fluent
Burnout	%	99.50	100.00
FEGT	F	1778	1752
Wall Heat Absorption	MM Btu/hr	631	624

During the project review meeting FW presented the Vision 21 plant simulation and detailed results of the three dimensional CFD simulation of the PPCC furnace.

Task 5.4 (Component Level Analysis)

No significant work in this area was performed.

Task 6.0 Reporting

Task 6.1 Program/Project Management Plans

Monthly emails will be sent to Kamalendu Das (NETL).

Task 6.2 Technical Reports

The second quarterly report for 2003 is being prepared.

Task 7.0 Project Management

Monthly phone conferences are being conducted with full participation from each of the HPCCCK team members.

The HPCCCK Project Review meeting was held on May 16th in Morgantown.

5. Conclusion

Work plans for the next quarter are summarized below.

Task 1 Submodels for Pollutant Formation

Task 1.2 NBFZ Tests

Continue HPBO experiments .

Task 1.5 Fuel-N Conversion Development

Continue model development.

Task 2 Submodels for Char Oxidation

HPBO experiments on Pittsburgh No. 8 coal at 2, 10, 20, and 30 atm will be conducted.

Task 3 Submodels for Flyash and Fumes

Continue model development.

Task 4 Deployment in Design Codes

AAL will run CBK model as a stand-alone code and become familiar with it and to have a good idea about its capabilities and limitations and begin the implementation into ASPEN

Task 4.4 Incorporate submodels in Fluent

Begin to incorporate ash formation submodels into Fluent.

Task 5 Vision 21 Process Design Analysis

Task 6 Reporting

Task 6.1-6.5

Continue reporting as required

6. References

None to report for this report.

7. Personnel and Affiliation, List of Abbreviations

<u>Personnel Name</u>	<u>Affiliation</u>
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Verna Bungay	Fluent
Soung Cho	FWC
Lewis Collins	Fluent
Don Ekstrom	SRI
Joe Helble	UCONN
Bob Hurt	BU
Usman Ghani	AAL
Chris Guenther	Fluent
Ovidiu Marin	AAL
Steve Niksa	NEA
John Rockey	NETL
Stefano Orsino	Fluent

<u>Name</u>	<u>Description</u>
AAL	American Air Liquide
BU	Brown University
CBK	Carbon Burnout Kinetics Model
CFD	Computational Fluid Dynamics
ECT	Electric Charge Transfer Device
FWC	Foster Wheeler Corporation
HPBO	High Pressure Burnout Testing Mode

HPCKK	High Pressure Coal Combustion Kinetics
NBFZ	Near-Burner Flame Zone Testing Mode
NEA	Niksa Energy Associates
NETL	National Energy Technology Laboratory
PRB	Powder River Basin
SRI	SRI International
SRT-RCFR	Short Residence Time Radiant Coal Flow Reactor
UConn	University of Connecticut

8. Appendix A: Project Milestone Chart (Update 12-26-01)

	Lead	Year 1				Year 2				Year 3			
		Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4
Task 0. Planning	Fluent												
Task 1. Submodels for Pollutant Formation													
1.1 NBFZ Test Characterization	SRI												
1.2 NBFZ Tests	SRI												
1.3 RCFR Simulations for NBFZ Tests	NEA												
1.4 Fuel-N Conversion Development	NEA												
1.5 NOx Production Submodel	NEA												
1.6 Hg Transformations	NEA												
Task 2. Submodels for Char Oxidation													
2.1 HPBO Test Characterization	SRI												
2.2 HPBO Tests	SRI												
2.3 HPBO Char Analyses	BU												
2.4 RCFR Simulations for HPBO Tests	NEA												
2.5 Char Oxidation Mechanism	BU												
2.6 Char Oxidation Submodel	NEA												
Task 3. Submodels for Flyash and Fumes													
3.1 HPBO Tests	UConn												
3.2 NBFZ Tests	UConn												
3.3 PPC Ash Mechanism Development	UConn												
3.4 Flyash Formation Submodel	UConn												
Task 4. Deployment in Design Codes													
4.1 Couple PC Coal Lab® and ASPEN Plus	AL												
4.2 Incorporate submodels in ASPEN Plus	AL												
4.3 Couple PC Coal Lab® and FLUENT	Fluent												
4.4 Incorporate submodels in FLUENT	Fluent												
Task 5. Vision 21 Process Design Analysis													
5.1 Advisory Review	FWC												
5.2 Conceptual Design of Vision 21 Process	FWC												
5.3 System-Level Analysis	AL												
5.4 Component-Level Analysis	FWC												
Task 6. Reporting													
6.1 Program/Project Management Plans	Fluent	1	2	1	2	1	2	1	2	1	2	1	1
6.2 Technical Reports	NEA												
6.3 Environmental Reports	SRI	4											4
6.4 Property Reports	Fluent												5
6.5 Exception Reports	Fluent												6
Task 7. Project Management	Fluent												