HIGH PRESSURE COAL COMBUSTION KINETICS PROJECT

COOPERATIVE AGREEMENT NO DE-FC26-01NT40777

QUARTERLY REPORT FOR JUNE-AUGUST, 2001

FOR

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DISCLAIMER

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1. Executive Summary

The HPCCK project was initiated with a kickoff meeting held on June 12, 2001 in Morgantown, WV, which was attended by all project participants. SRI's existing g-RCFR reactor was reconfigured to a SRT-RCFR geometry (Task 1.1).
This new design is suitable for performing the NBFZ experiments of Task 1.2. It was decided that the SRT_RCFR apparatus could be modified and used for the HPBO experiments. The purchase, assembly, and testing of required instrumentation and hardware is nearly complete (Task 1.1 and 1.2). Initial samples of PBR coal have been shipped from FWC to SRI (Task 1.1). The ECT device for coal flow measurements used at FWC will not be used in the SRI apparatus and a screw type feeder has been suggested instead (Task 5.1). NEA has completed a upgrade of an existing Fluent simulator for SRI's RCFR to a version that is suitable for interpreting results from tests in the NBFZ configuration (Task 1.3) this upgrade includes finite-rate submodels for devolatilization , secondary volatiles pyrolysis, volatiles combustion, and char oxidation. Plans for an enhanced version of CBK have been discussed and development of this enhanced version has begun (Task 2.5). A developmental framework for implementing pressure and oxygen effects on ash formation in an ash formation model (Task 3.3) has begun.

2. Technical Accomplishments

Task 0 Planning

The HPCCK project kickoff meeting was held at NETL in Morgantown, WV on June 12, 2001. The meeting was attended by John Rockey (NETL), Bill Rogers and Lewis Collins (Fluent), Soung Cho (Foster Wheeler Development Corporation), Don Eckstrom (SRI), Steve Niksa (Niksa Energy Associates), Bob Hurt (Brown Universty), Joe Helble (University of Connecticut), and Usman Ghani (American Air Liquide). Discussion topics from the meeting are given in Appendix A. Contract negotiations with each of the subcontractors has proceeded throughout this quarter. Contracts are in place or waiting for appropriate signatures with the exception of Brown University. Brown University strongly objects to the wording (review and approval all documents) in Attachment B (Federal Assistance Reporting Requirements) Section 16 page B-8.

Task 1.0 Submodels for Pollutant Formation

<u>Task 1.1 NBFZ Characteristics</u>
FWC has prepared and delivered 168 grams of 75-90 micron PRB coal samples to SRI for the NBFZ experiments. Larger quantities of the PRB coal is needed for the entire NBFZ experiments and it was agreed by team members that all of the PRB coal should be prepared and shipped before any experiments begin to avoid modeling errors. SRI is in the process of determining the total quantity of PRB coal needed to complete the NBFZ experiments.

It was determined that the g-RCFR would be modified to handle both the NBFZ and HPBO experiments. The g-RCFR was reconfigured to a SRT-RCFR geometry. The purchase, installation, testing, and calibration for the instrumentation and hardware for SRI's existing g-RCFR reactor reconfigured to a SRT-RCFR geometry is nearly complete.

SRI has provided NEA a detailed description of the NBFZ experiment to support their modeling task.

Task 1.3 RCFR Simulations for NBFZ Tests

A previously Fluent simulator has been upgraded to a version suitable for interpreting results from tests in the NBFZ configuration. The upgrade included (1) Re-vamping two in-house programs that determine the radiant heat flux and wall temperature profiles along the SRI furnace, so that the model can be run on any modern PC; (2) Converting user-defined subroutines developed for Fluent 4.4 to Fluent 5.5; (3) Re-formulating the Fluent simulator of SRI's test facility under NEA's current license.

The current upgraded Fluent simulator for two-dimensional analysis of the SRI facility includes finite-rate submodels for devolatilization, secondary volatiles pyrolysis, volatiles combustion, and char oxidation. The simulations have shown:

(1) The actual flow is upward because, in a downflow configuration at elevated pressure, buoyancy causes recirculation patterns to develop near the walls, which disperse particles into the walls, causing deposits to grow without limit. These simulations show that buoyancy is often problematic in upflow configurations as well, although not in any prohibitive ways. In this system, the entrainment gas heats by convection through the flow tube walls, and by convection from the coal particles. Wall convection dominates, so very steep gradients form adjacent to the walls. The buoyancy flow patterns driven by these gradients are strong enough to divert enough gas from the central core to decelerate the centerline gas velocity, and to move particles toward the walls. The patterns get stronger for progressively higher pressures, as expected

(2) SRI had planned to use N_2/O_2 mixtures instead of Argon for the NBFZ tests. Current simulations showed that these suspensions could not be heated enough to ignite either volatiles or char to the flame burning condition for the maximum furnace operating temperature and for a reasonable reactor length. Switching the entrainment gas to Ar yielded the desired performance, because Ar has a significantly lower heat capacity than the other gases. Argon is also preferable because it enables N-species balances to be formulated in terms of the monitored stable reaction species.

Task 2.0 Submodels for Char Oxidation

Task 2.1 HPBO Test Characterization

It was determined that the g-RCFR would be modified to handle both the NBFZ and HPBO experiments. The purchase, installation, testing, and calibration for the instrumentation and hardware for SRI's existing g-RCFR reactor reconfigured to a SRT-RCFR geometry is nearly complete.

Task 2.5 Char Oxidation Mechanism

The latest version of CBK model (CBK8) will be upgraded for the HPCCK project. The current version (CBK8) has been delivered to Fluent Inc. Discussions were held with other researchers on their experience implementing burnout submodels. Based on these discussions a developmental framework for an enhanced version of CBK is being prepared. From these discussions a reduced version of CBK specifically design for CFD applications is under consideration. This reduced version would allow users more flexibility with the model and easier implementation into existing CFD codes. In particular many CFD codes already contain their own particle size distribution and particle energy balance models and a reduced version of CBK would significantly reduce to amount of work needed to implement CBK. The development of the enhanced version of CBK is proceeding by using a intrinsic rate and a generalized (mechanism independent) Thiele modulus evaluated at the particle surface and used to estimate the effectiveness factor within the particle. In addition to this approach a single ODE reduced thermal annealing expression was also identified and tested.

Task 3.0 Submodels for Flyash and Fumes

Task 3.1-3.4

The development of the framework for implementing pressure and oxygen effects on ash formation in an ash formation model and a literature search on the effects of high pressure on ash formation are being conducted.

Task 4.0 Deployment in Design Codes

Task 4.1-4.2

PC Coal Lab, Version 2.2 User Guide and Tutorial have been delivered to Fluent Inc. and AAL. License agreements have been finalized between Fluent Inc., NEA, and AAL and software is being shipped to Fluent Inc. and AAL.

Task 5.0 Vision 21 Design Analysis

Task 5.1 Advisory Review

Discussions between FWC and SRI on measuring devices for the coal flow rate were conducted. The ECT device for coal flow measurements was suggested to SRI, but due to the low flow rates involved in the experiments a screw type feeder has been adopted.

Task 5.2 Conceptual Design of Vision 21 Process

FWC current Vision 21 plant concept has been reviewed.

Task 6.0 Reporting

Task 6.1 Program/Project Management Plans
Monthly emails are being sent to John Rockey (NETL) as requested to support Fluent Inc. invoices and summarize monthly technical progress.

Task 6.2 Technical Reports
The first quarterly report is being prepared.

Task 6.3 Environmental Reports
The hazardous substance plan has been completed and delivered.

Task 7.0 Project Management
Considerable effort has been spent in organizing communication links between NETL, Fluent Inc. and each of the subcontractors. Monthly emails are being sent to John Rockey (NETL) in support of each monthly invoice from Fluent Inc. As requested by John Rockey these emails breakdown the invoice at the task level and track percent completion of both labor and job completion for the first year of the HPCCK project. Monthly phone conferences are being conducted with full participation from each of the HPCCK team members. These calls give each of the team members a chance to summarize their recent work and forecast the next months activities. These calls are not only useful for project management issues but allow team members to discuss current technical issues and plan together for future work. Finally, a web site for the HPCCK project has been built by Fluent web services. This site is password protected and serves as a central location for information, announcements, papers, data, modeling results, reports, etc.

3. Issues and Resolutions

Since SRI's reconfigured SRT-RCFR is going to be used for both the NBFZ and HPBO experiments, team members talked about running a large number of NBFZ before any HPBO experiments are conducted. The actual number of NBFZ experiments has not yet been determined but the goal is to run NBFZ experiments as soon as possible so other team members can begin analyzing the experimental results. Should the need for HPBO experiments become important SRI can run some HPBO experiments if needed.

SRI had planned on using a mixture of N_2/O_2 rather than Argon for the carrier gas in the NBFZ experiments. Simulations by NEA have shown that such a mixture can not be heated enough to ignite either volatiles or char under the existing experimental operating conditions. This was not a problem when the carry gas was Argon. However, using Argon as the carry gas would make amonia and O_2 measurements difficult. Discussions and further simulations are underway to try and resolve this issue.

Instrumentation used for measuring particle residence times and particle temperatures at the exit are not fully ready. To avoid any delays team members decided to go ahead with initial NBFZ experiments without these instruments fully in place.

Due to the small coal feed rates used in the experiments at SRI the ECT device used at FWC was not adopted for the measurement of coal flow rates. Instead, a screw type feeder will be used to measure coal flow rates.

SRI is going to provide FWC with the total amount of PRB coal needed for the NBFZ experiments and the initial shipment of PRB coal will be used to test the SRT-RCFR. Once the entire quantity of PRB coal is received SRI will begin the NBFZ experiments.

Fluent simulations by NEA of SRI's SRT-RCFR showed buoyancy flow patterns driven by strong temperature gradients near the wall divert gas from the central core decelerating the centerline gas velocity moving particles towards the wall. This is behavior is amplified under higher pressure. Further simulations are being conducted to try and counteract this tendency.

Contract negotiations have proceeded with all subcontractors with final signatures expected before the end of September. However, negotiations with Brown University have slowed due to the phrase "The recipient shall submit to DOE for review and approval all documents generated by the recipient, …" found in Attachment B, Section 16, page B-8 in the contract between Fluent Inc. and DOE and passed down to each of the subcontractors of the HPCCK project. Brown University would like a "softer" version which would replace the wording review and approval with review and recommend changes. Negotiations with Brown University and DOE will continue in the second quarter.

4. Progress Forecast for the Next Quarter

Task 0 Planning

Obtain signed subcontract agreements from SRI and FWC. Continue contract negotiations with Brown University.

Task 1 Submodels for Pollutant Formation

Task 1.1 NBFZ Test Characterization
Design optical probe system for measuring residence times and particle temperatures and order components.

Task 1.2 NBFZ Tests
FWC will ship the required PRB coal for all the NBFZ experiments to SRI. NBFZ experiments will begin immediately upon receiving the shipment. Initial PRB coal already received by SRI will be used to test the SRT-RCFR configuration.

Task 1.3 RCFR Simulations for NBFZ Tests

Complete the upgrade of existing RCFR simulator for NBFZ test conditions. Validate SRT-RCFR simulations with measured suspension temperatures.

Task 1.4 Fuel-N Conversion Development
Begin Simulations of the NBFZ test conditions.

Task 2 Submodels for Char Oxidation

Task 2.5 Char Oxidation Mechanism
Continue working on the enhanced version of CBK and begin code development.

Task 2.6 Char Oxidation Submodel
Continue working on the internal reaction and diffusion submodel and compare this approach with existing models in CBK. Continue working on incorporating a thermal annealing expression into the model.

Task 3 Submodels for Flyash and Fumes

Task 3.2 NBFZ Tests
Begin analyzing selected NBFZ char and ash samples from PRB coal under all operating conditions.

Task 3.4 Flyash Formation Submodel
Continue development of the framework for implementation of pressure and oxygen effects on ash formation in an ash formation model.

Task 4 Deployment in Design Codes

Task 4.1 Couple PC Coal Lab and ASPEN Plus
Begin reviewing PC Coal Lab documentation and receive software from NEA. Begin development framework for implementing PC Coal Lab in ASPEN Plus.

Task 4.4 Incorporate submodels in Fluent
Develop a framework for implementing submodels into Fluent. Begin implementing existing version of CBK in Fluent.

Task 5 Vision 21 Process Design Analysis

Task 5.1 Advisory Review
Begin working with BU and UCONN on recommendations on implementing CBK and ash formation models into Fluent.

Task 6 Reporting

Task 6.1-6.5
Continue reporting as required

5. Personnel and Affiliation, List of Abbreviations

Personnel Name	Affiliation
Al Alhuwalia	FWC
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
Bill Rogers	Fluent

Name	Description
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
HPCCK	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

6. Appendix A: Kickoff Meeting Agenda

9:00-9:15	Introductions and project overview	NETL
9:15-9:45	Project overview & CFD use in combuster design	Fluent

9:45-10:00	Advanced high pressure combustion system concept	FWC
10:00-11:45	Experimental and Data Analysis	
10:00-10:30	Facilities	SRI/NEA
10:30-10:45	Break	
10:45-11:00	Devolitilization	NEA
11:00-11:15	Pollutant Formation	NEA
11:15-11:30	Char Burnout	BU
11:30-11:45	Ash Characterization	UCONN
11:45-12:30	Lunch	
12:30-12:50	CFD Modeling	Fluent
12:50-1:15	ASPEN PLUS	AAL
1:15-1:30	Administration Issues	Fluent
1:30-	Discussion of Technical Issues	

7. Appendix B: Project Milestone Chart

	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											8,9	
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											10	
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						11						
4.3 Couple PC Coal Lab® and FLUENT	Fluent												
4.4 Incorporate submodels in FLUENT	Fluent												12
Task 5. Vision 21 Process Design Analysis													
5.1 Advisory Review	FWC												
5.2 Conceptual Design of Vision 21 Process	FWC				7								
5.3 System-Level Analysis	AL												
5.4 Component-Level Analysis	FWC												
Task 6. Reporting													
6.1 Program/Project Management Plans	Fluent	1	1	1	1	1	1	1	1	1	1	1	1
6.2 Technical Reports	NEA		2		2		2		2		2		3
6.3 Environmental Reports	SRI	4											4
6.4 Property Reports	Fluent												5
6.5 Exception Reports	Fluent												6
Task 7. Project Management	Fluent												