EFFECT OF HEATING RATE ON THE THERMODYNAMIC PROPERTIES OF
PULVERIZED COAL

Semi-Annual Progress Report

For the Period September 24, 1998 to March 23, 1999

Ramanathan Sampath (Principal Investigator)

April 1999

Grant No. DE-FG22-96PC96224--05

For

AAD Document Control
U.S. Department of Energy
Federal Energy Technology Center
P.O. Box 10940, MS 921-143
Pittsburgh, PA 15236-0940

By

Department of Engineering
Clark Atlanta University
Atlanta, GA 30314

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ABSTRACT

This semi-annual technical progress report describes work performed under DOE Grant No. DE-FG22-96PC96224 during the period September 24, 1998 to March 23, 1999 which covers the fifth six months of the project. Devolatilization is an important initial step in virtually all commercial fossil fuel applications such as combustion, gasification, and liquefaction. Characterization of the temperature history of pulverized coal particles under high heating rates, representative of coal combustors, is critical to the understanding of devolatilization. During this reporting period, characterization experiments were continued from the previous reporting period and completed to a total of 28 single coal particles. These particles were caught in the electrodynamic balance and their volume, external surface area, mass, and density were measured. The same single particles were then heated bidirectionally with a pulsed (10 ms pulse width) Nd:YAG laser beams of equal intensity with heating rates (10^4 - 10^7 K/s) representative of coal combustors. The temporal power variation in the laser pulse was monitored for use in the heat transfer analysis by an ultra-fast fiber optic uv light transmitter included in the beam path and coupled to a silicon photodiode. Transient surface temperatures of the particles were measured using a single-color pyrometer. Dynamics of volatile evolution and particle swelling were recorded using well established time-resolved high-speed cinematography. Presently, extraction of devolatilization time-scales and temperature data at these time-scales running the high-speed films taken during the experiments employing a 16mm movie projector are in progress. Heat transfer analyses for the devolatilization time-scales, and temperature measurements (and hence an understanding of the effect of heating rates on coal thermal properties) are also in progress. Shipment of the donated heated grid system components from our industrial partner, United Technologies Research Center (UTRC), CT to CAU was complete during the previous reporting period. Testing of the heated grid system components at CAU and sensitivity analyses of the heated grid heat transfer calculations are also in progress.

TABLE OF CONTENTS

	page
ABSTRACT.....	ii
EXECUTIVE SUMMARY.....	1
INTRODUCTION.....	2
PROGRESS TO DATE	2
OUTCOMES TO DATE.....	4
WORK PERFORMED DURING THIS PERIOD.....	5
PLANS FOR THE NEXT REPORTING PERIOD.....	6
SUMMARY AND CONCLUSIONS.....	6
ACKNOWLEDGMENTS.....	7
REFERENCES.....	7

EXECUTIVE SUMMARY

In this semi-annual report, the work performed under DOE Grant No. DE-FG22-96PC96224 during the period September 24, 1998 to March 23, 1999 is described and the major accomplishments are highlighted summarizing the most important research results.

In all major coal conversion processes, coal undergoes a devolatilization stage while it is heated to the reaction temperature. The recent experimental studies of devolatilization of pulverized coal at rapid heating rates representative of coal combustors have greatly improved our general understanding of this process. But the heat transfer analysis with commonly-applied thermal properties developed from slow heating rate experiments did not predict either the early heating or the latter stages of heating. Knowledge of the role of heating rate on coal thermal properties is essential to progress in advanced coal utilization technology.

The objectives of this project are to understand the effect of heating rate on thermal properties of pulverized coal particles. The specific objectives are to subject coal particles into a broad range of heating rates, measure temperature histories, and develop thermal property (heat capacity and thermal conductivity) data that predict the measured temperature histories.

Experiments and modeling are being carried out to meet the project objectives. The successful accomplishment of the above goals will enhance our understanding of coal thermal properties and hence progress towards advanced combustion modeling.

During this reporting period, laser heating experiments were continued from the previous reporting period and completed to a total of 28 single coal particles. These particles were caught in the electrodynamic balance and their volume, external surface area, mass, and density were measured. The same single particles were then heated bidirectionally with a pulsed (10 ms pulse width) Nd:YAG laser beams of equal intensity with a range of heating rates (10^4 - 10^7 K/s) representative of coal combustors. The temporal power variation in the laser pulse was monitored for use in the heat transfer analysis by an ultra-fast fiber optic uv light transmitter included in the beam path and coupled to a silicon photodiode. Transient surface temperatures of the particles were measured using a single-color pyrometer. Dynamics of volatile evolution and particle swelling were recorded using well established time-resolved high-speed cinematography. Presently, extraction of devolatilization time-scales and temperature data at these time-scales from the high-speed films obtained during the experiments (employing a 16mm movie projector) are in progress. Heat transfer analyses for the devolatilization time-scales, and temperature histories are also in progress for comparison purposes. Shipment of the donated heated grid system components from our industrial partner, United Technologies Research Center (UTRC), CT to CAU was complete during the previous reporting period. Testing of the heated grid system components at CAU and sensitivity analyses of the heated grid heat transfer calculations are also in progress.

INTRODUCTION

This semi-annual technical progress report describes work performed under DOE Grant No. DE-FG22-96PC96224 during the period September 24, 1998 to March 23, 1999 which covers the fifth six months of the project.

In all major coal conversion processes, coal undergoes a devolatilization stage while it is heated to the reaction temperature. Recent experimental studies of devolatilization of pulverized coal at rapid heating rates representative of coal combustors have greatly improved our general understanding of this process [1-18]. But the heat transfer analysis with commonly-applied thermal properties developed from slow heating rate experiments did not predict either the early heating or the latter stages of heating [1-3,18-19]. Design of coal combustion and conversion processes require knowledge of thermal properties to construct an energy balance. It is accepted that there are uncertainties in the heat capacity of coal especially for the high heating rate studies [2,6]. It is also accepted that the large thermal gradients within the particle (due to thermal conductivity of coal) make prediction of the temperature difficult during the early heating in these studies [6]. However, there has been no independent study conducted to investigate the effect of heating rate on the thermal properties of coal particles. Knowledge of the role of heating rate on coal thermal properties is essential to progress in advanced coal utilization technology.

The objectives of this proposal are to understand the effect of heating rate on thermal properties of pulverized coal particles. The specific objectives are:

- 1) Subject coal particles into a broad range of heating rates and extract heat capacity information for high heating rate applications.
- 2) Also develop thermal conductivity information for coal particles subjected to rapid heating rates representative of coal combustors.

Experiments and modeling are being carried out to meet the project objectives. The successful accomplishment of the above goals will provide better understanding of coal thermal properties in high heating rate applications and hence improved combustion modeling.

PROGRESS TO DATE

Literature articles [1-45] were reviewed to understand the effect of heating rate on various parameters of a coal particle. The role of heating rate on the onset of volatile evolution, volatile yield, product composition to a lesser extent, coal type and particle size were found to be well established. As heating becomes more rapid, the onset of devolatilization shifts to much smaller time scales and to much higher surface temperatures [2,18-19]. However, the role of heating rate on coal thermal properties was not found to be well understood. Previous results clearly demonstrated that particle temperature-dependent thermal property assumptions routinely applied in coal combustion models result in large errors (up to 100 percent) in calculated temperature histories [2,18-19].

Remote access from CAU to the VAX/VMS system at FETC/Morgantown was established through telnet. Several modifications to the existing Single Particle Heat Transfer code were made that include option for various input and/or combinations of input for thermal properties such as constant, temperature-dependent, heating rate dependent, and time dependent values. Many sensitivity analyses were employed to evaluate and quantify the impact of several heat transfer parameters for coal such as thermal properties and heat transfer coefficient, geometry related properties such as shape, mass, and density, and chemical properties such as devolatilization kinetic coefficients on rapid heating. This work improved the model performance of the present work, and also aided in several publications [46-50]. Approval for physical access to the Single Particle Laboratory at FETC/Morgantown from Morgantown facility was obtained. This required completion of several laboratory safety courses by CAU researchers including the PI at the Morgantown site.

Several polystyrene spheres were caught in the electrodynamic balance system at FETC/Morgantown and the operation of the associated system components such as video-based imaging systems, diode-array imaging system, dc and ac power supply, particle position control, and GE tungsten strip lamp & lens systems for pyrometer were tested and found to be performing well. Completed calibration of several components of the balance measurement system including imaging systems and particle position control system. Also completed was the alignment and calibration of the heating laser to heat coal particles, and the single-color pyrometer to measure particle temperature histories.

Approvals from FETC/Pittsburgh, CAU, and UTRC for performing the heated grid work at Clark Atlanta University (CAU), GA, that was originally planned at United Technologies Research Center (UTRC), CT, were obtained. More recently, donation agreement for the heated grid measurement system from UTRC was obtained, and the shipment of the grid components from UTRC to CAU was complete in the last reporting period. Purchase of several instrumentation that were not available in the package from UTRC that include power supply, data acquisition interface, and spot welder was made by CAU. Inspection and testing of the heated grid system components at CAU and sensitivity analyses of the heated grid heat transfer calculations are also in progress.

Existing laser heating set-up at the Single Particle Laboratory, Federal Energy Technology Center, Morgantown, WV would work only in the range of 10^4 to 10^5 K/s. Appropriate changes were made to heat particles in the range of 10^4 to 10^7 K/s. For this, power attenuator and the charge voltage of the heating laser system were carefully adjusted, beam path reconfigured and aligned, and the laser power characterized to obtain optimum spatial and temporal distribution.

Dr. Sampath, PI of this project, was at FETC/Morgantown in several visits during the preceding reporting periods. He was involved in the alignment and setting up of the pyrometry system. Dr. Sampath is also involved in the reduction of experimental data, modeling activities including sensitivity analyses, comparison with data, and heat transfer analyses. Dr. Esmail Monazam who has coauthored with the PI in a number of publications in the subject matter is working as a part-time research associate in this project and is stationed at FETC/Morgantown. Dr. Monazam was involved in the experimental activities discussed below.

Calibration for all the components of the electrodynamic balance measurement system including single-color pyrometer and heating laser was successfully completed in the last reporting period. Following the calibration, a few coal particles were injected into the balance and by application of ac and dc potentials to the ring and endcap electrodes, a single particle that had a higher charge-to-mass ratio was confined at the null position of the balance. Following the approach of Maloney et al. [21-23], the particle volume, external surface area, mass, and density were measured. The same particle was then heated bidirectionally with a pulsed (10 ms pulse width) Nd:YAG laser beams of equal intensity. Using the approach of Sampath [18-19], the temporal power variation in the laser pulse was monitored for use in the heat transfer analysis by an ultra-fast fiber optic uv light transmitter included in the beam path and coupled to a silicon photodiode. Measurements of changes in particle size that accompanied rapid heating was made by means of the high-speed diode array imaging system. Dynamics of volatile evolution and particle swelling was recorded using well established [2,5,18] time-resolved high-speed cinematography. Measurements of the radiant emissive power from the heated and cooled (when the laser was turned off) particles was made using the single-color pyrometer. Particle experimental temperatures was calculated from the measurements of particle size and radiant emissive power by applying the Wein approximation to Plank's law.

Joie C. Taylor, an undergraduate student in Engineering, was partially supported and trained in the subject matter.

Several theoretical analyses were conducted to improve the model performance of the present work and the results were compared with data available from our previous studies. These activities resulted in one journal publication [47], four conference presentations [46,49-51], and one symposium presentation [48] to date.

OUTCOMES TO DATE

1. Sampath, R., Monazam, E. R., Maloney, D. J., and Zondlo, J. W., Development of Improved Coal Combustion Modeling: Analysis of Coal Particle Irregularity and Thermal Properties on Temperature Predictions, Fifth Annual HBCU conference organized by FETC/DOE at Southern University and A&M College, LA, March 1997.
2. Sampath, R., Maloney, D. J., and Monazam, E. R., Effect of Heating Rate on the Thermodynamic Properties of Pulverized Coal, Contractors Review Meeting, Fifth Annual HBCU conference organized by FETC/DOE at Southern University and A&M College, LA, March 1997.
3. Taylor, J. C., Sampath, R., Maloney, D. J., Zondlo, J. W., and Monazam, E. R., Transport Phenomena of Irregularly-Shaped Solid Particles in an Electrodynamic Balance, Poster Paper, Fifth Annual DOE/HBCU conference, Southern University and A&M College, LA, March 1997.
4. Sampath, R., Maloney, D. J., Zondlo, J. W., and Monazam, E. R., Temperature Histories for Single Coal Particles Prior to Devolatilization, Central States Technical Meeting, Combustion Institute, April 1997, Point Clear, AL.

5. Taylor, J. C., Sampath, R., and Maloney, D. J., Characterization of Small Single Particles in an Electrodynamic Balance, Annual Student Scientific Research Symposium, April 15, 1997, Clark Atlanta University, Atlanta, GA.
6. Sampath, R., Maloney, D. J., Zondlo, J. W., and Monazam, E. R., Evaluation of Errors Resulting From Nusselt Number Assumptions in Coal Combustion Modeling, Paper No. DETC97/CIE-4519, 1997 ASME Design Engineering Technical Conferences, September 14-17, 1997, Sacramento, CA.
7. Sampath, R., Maloney, D. J., and Proscia, W., Thermal Property Data for Coal Particles for Use in Rapid Devolatilization Models, Technology Transfer Session, Historically Black Colleges/Universities and Other Minority Institutions Sixth Annual Symposium, April 28-29, 1998, Ocean City, MD.
8. Taylor, J., Sampath, R., Maloney, D. J., and Proscia, W., Rapid Devolatilization Studies for Coal Particles in an Electrodynamic Balance and in a Heated Grid Reactor, Technology Transfer Session, Historically Black Colleges/Universities and Other Minority Institutions Sixth Annual Symposium, April 28-29, 1998, Ocean City, MD.
9. Sampath, R., Maloney, D. J., and Zondlo, J. W., Measurements of Surface Area and Volume for Irregularly-Shaped Coal Particles, Central States Technical Meeting, Combustion Institute, 31 May - 2 June, 1998, Lexington, KY.
10. Sampath, R., Maloney, D. J., and Zondlo, J. W., Evaluation of Thermophysical and Thermochemical Heat Requirements for Coals at Combustion Level Heat Fluxes, 27th International Symposium on Combustion, August 2-7, 1998, Boulder, CO.
11. Maloney, D. J., Sampath, R., and Zondlo, J. W., Heat Capacity and Thermal Conductivity Considerations for Coal Particles During the Early Stages of Rapid Heating, Combustion and Flame 116:94-104 (1999).
12. Sampath, R., Monazam, E. R., and Maloney, D. J., Devolatilization Temperature Histories for Coal Particles Subjected to Combustion Level Heat Fluxes, Technology Transfer Session, Historically Black Colleges/Universities and Other Minority Institutions Seventh Annual Symposium, April 1999, Miami, FL.

WORK PERFORMED DURING THIS REPORTING PERIOD

Raw size and intensity data for 15 coal particles were collected during the previous reporting period. The above experiments were continued and completed to a total of 28 single coal particles during this reporting period. Raw size and intensity data for the 28 coal particles tested are presented in Table 1.

Table 1. Raw Data for the Laser Heating Experiments

Particle		Rotaional	Rotational	Rotatioal	Rotational	Laser Det.	Side	Side	Side	Top	Top	Top
#	Cd/m	Area	Volume	Dp(area)	Dp(vol)	Power	Dp(area)	Dp(#line)	Dp(#width)	Dp(Area)	Dp(#line)	Dp(#Width)
1	49	26841	326542	93	85	0.629	85	84.8	88.4	77	93.8	70.8
2	52	33015	449444	103	95	0.652	74	115.3	57.4	82	65.9	113.2
3	31	34713	537058	105	101	0.632	95	113.6	84.5	91	77.8	103.8
4	32	36345	543636	108	101	0.638	106	100.1	112.3	107	113.6	99.0
5	22.5	47664	805956	123	115	0.639	123	164.5	93.9	99	105.6	101.5
6	80	75865	1533570	155	143	0.655	144	170.1	142.0	130	126.9	151.5
7	28	41374	691213	115	110	0.651	118	114.2	139.0	103	134.4	75.8
8	35	31006	408401	99	92	0.654	102	159.4	80.4	82	79.7	91.6
9	27	49500	798314	126	115	0.645	100	131.0	82.6	105	84.9	153.0
10	32	34096	518157	104	100	0.662	105	114.9	91.4	81	78.4	95.7
11	36	34933	515043	105	99	0.329	110	100.7	125.9	101	115.4	94.6
12	29	40315	660464	113	108	0.329	125	135.4	138.2	96	134.0	80.0
13	34	33469	464040	103	96	0.4	101	94.6	116.1	96	115.3	90.2
14	27	62815	970536	141	123	0.399	124	104.7	165.9	120	162.3	94.4
15	30	51816	828580	129	117	0.324	109	144.2	88.9	107	93.4	122.9
16	33.5	33664	480307	104	97	0.329	96	101.2	105.8	91	105.9	82.5
17	28	32877	467752	102	96	0.328	101	104.4	95.1	78	87.6	86.2
18	24	48124	859429	124	118	0.599	124	123.8	128.5	107	118.0	106.6
19	33	32180	440987	101	94	0.643	101	97.8	108.9	97	105.9	85.8
20	28	35640	522754	107	100	0.645	109	141.9	102.2	94	105.7	86.4
21	30	36476	559378	108	102	0.567	115	123.8	108.3	94	106.8	77.9
22	23	54042	1013520	134	125	0.569	138	115.1	166.5	138	172.2	113.8
23	28	37595	613923	109	106	0.561	122	111.1	130.2	99	133.1	68.2
24	40	23720	302077	87	83	0.464	84	81.8	96.3	82	96.7	80.4
25	25	49992	820358	126	116	0.473	116	112.2	121.9	139	134.4	143.6
26	26	42853	719152	117	111	0.592	106	137.4	103.6	91	103.5	90.8
27	27.5	39220	619320	112	106	0.652	109	111.8	105.2	106	105.4	111.3
28	26	49225	853388	125	118	0.592	115	140.3	96.7	111	107.2	120.4

A paper [51] was presented describing the experimental activities and the data collected at the Technology Transfer Session, Historically Black Colleges/Universities and Other Minority Institutions Seventh Annual Symposium, April 1999, Miami, FL. Data reduction, and numerical analysis for the effect of thermal properties on the temperature histories are in progress.

PLANS FOR THE NEXT REPORTING PERIOD

In the near future, data reduction and numerical analyses will be completed and the effect of heating rates on coal thermal properties evaluated.

SUMMARY AND CONCLUSIONS

Modification of the laser heating system at the Single Particle Laboratory, FETC, Morgantown to heat coal particles at very high heat fluxes with heating rates on the order of 10^4 -

10⁷ K/s was completed. Calibration activities for various instruments of the laser heating system were successfully completed. Temperature measurements on a large number of coal particles subjected to very high heating rates were made. Data reduction and analysis are in progress. Donation agreement for the donation of several components of the heated-grid system from UTRC, our industrial collaborator in this project, was obtained. Shipment of donated components from UTRC to CAU was complete in the previous reporting period. Testing of the heated grid system components at CAU and sensitivity analyses of the heated grid heat transfer calculations are also in progress.

ACKNOWLEDGMENTS

The project is supported by FETC/Pittsburgh under Grant No. DE-FG22-96PC96224. Assistance provided by Dr. Daniel J. Maloney, Single Particle Laboratory, FETC/Morgantown, during this reporting period is appreciated. Technical discussions provided by Dr. Mildred B. Perry are also gratefully appreciated.

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