Task 3.11 - Fuel Quality Advisor

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SUBTASK 3.11 - FUEL QUALITY ADVISOR

1.0 INTRODUCTION

The objective of the Fuel Quality Advisor (FQA) project is to create a generalized software package capable of advising operations, purchasing, environmental, and maintenance personnel in making decisions related to the use of coal in electricity generation facilities. The specific goals for this years work include the following:

- Develop a standardized computer shell to integrate existing and future algorithms
- Develop a strategy for integrating the shell with future databases and boiler models
- Integrate the current ash transformations and deposition algorithms into the shell
- Generate algorithms for coal handleability through experimentation and integrate them into the code
- Enhance the current ash transformation algorithms for low-NO_x and entrained gasification through laboratory experimentation and integrate available full-scale results into the code

The program is divided into three primary thrust areas: development of computerized shell and interface, development of coal handleability advisor, and enhancement of ash formation algorithms. The progress in each of these three areas over the last 6 months is described in detail below.

2.0 DEVELOPMENT OF COMPUTERIZED SHELL AND INTERFACE

The purpose of the software shell and interface is to bundle several existing computer models with a Windows graphical user interface. This interface will control entry into each of the existing and developing models and provide a unified and efficient interface to aid users in moving around among different segments of the FQA. The following features and advantages have been outlined for the creation of the advisor:

- A single executable user interface that can start all models without regard to program location
- A consistent visual display for ease of learning and using the computer models
- A Help facility that can describe each model along with the requirements for that model
- Shortcuts such as hot keys to improve the speed and acceptance for advanced users
- Tool bar icons that will give the user a set of tools for running the models
- A packaging system for the creation of both DOS and Windows programs

Also included within this task is the incorporation of existing algorithms into the FQA shell. The two existing algorithms to be added include the ash fouling model and the ash transformations code.

2.1 Construction of Shell/Interface

The main work thrust has been designing the overall structure of the system. This system is introduced by a splash screen containing a graphical image of the FQA title and Energy & Environmental Research Center (EERC) logo. A splash screen is a screen that remains visible for only a few seconds. The FQA main screen (Figure 1) will appear with bitmapped buttons for the selection of a model to be executed. The screen has been developed, but the actual bitmaps have not been selected. After a model has been selected either by the bitmapped buttons or through the pull-down menu, the program will enter the execution of that model. The Help system, which is being developed concurrently with the graphical system, will explain the details needed to execute each model. Context-sensitive Help (by specific topic) is being implemented with the development of each screen. Help buttons have been added to screens with links into the proper position in the system.

Figure 1. Initial "About" splash screen being incorporated into the user interface.

The following aspects of the user interface have been tested separately under a simplified GUI (graphical user interface):

- Bitmapped control buttons
- Context-sensitive Help buttons
- Menu-controlled jumps to models
- "About" dialogs
- Addition/removal of items in the menu bar
- Addition of items to the tool bar with unique tool buttons
- Splash screen functionality
- Updating status line
- Use/modification of the standard open/save dialog boxes
- Control transfer from FQA to model
- Adding bitmaps to main/dialog windows

Each of the items listed above has been implemented in the simplest form possible in order to determine the feasibility of using that feature in the final interface. The following features are being tested and will be combined in the overall interface:

- Execution monitor (time and percentage status of the current execution)
- Addition/removal of item in the menu bar during execution
- Automated search of the Help systems
- Control from model back to FQA
- Memory management of models
- Database execution

2.2 Ash Fouling Algorithm

A series of ash deposition algorithms have been developed at the EERC over the last 5 years. These algorithms are in various forms and at various levels of sophistication. The various codes have been combined into a single ash deposition algorithm for use in all aspects of ash fouling. The combined algorithm will utilize the ash formation algorithm discussed in Section 2.3. The overall structure of the algorithm is not new and will not be discussed in detail here. The general algorithm combines four fundamental principles of deposition: 1) deposit growth, 2) strength development, 3) thermal properties, and 4) deposit removal. Each of these principles is discussed below with respect to its implementation in the code.

2.2.1 Deposit Growth

The first function of the deposit growth submodel is to organize the ash by size into three ash categories. The code will utilize the data produced from the ash formation algorithms as discussed later. The particle-size and composition distribution (PSCD) of the ash is divided into six size and seven composition bins, for a total of 42 different bins of ash particles. The first ash category includes ash particles less than 5 microns in diameter, which makes up the initial layer. All ash particles less than 10 microns are included in the second category used in modeling the downstream deposit. Downstream deposits are formed by impaction from the recirculation eddies passing around the heat-exchange tubes. As the gas stream passes around the tube, those particles that do

not inertially impact (generally less than 10 microns) get caught in the recirculation eddies of the gas stream and are impacted into the downstream side of the tube surface, as shown in Figure 2. The last ash category forming the upstream deposit includes all the size and composition bins.

EERC SA11802.CDR

Figure 2. Downstream deposition.

As discussed previously, the three primary modes of fouling deposit growth are inertial and eddy impaction; vapor-phase and small-particle diffusion; and thermophoresis/electrophoresis. The inner layer, formed by small-particle diffusion and thermophoretic/electrophoretic forces, comprises primarily vapors and particles less than 5 microns that traverse through the boundary layer surrounding the tube and deposit. Which particles actually deposit depends upon the flow characteristics around the heat-exchange tubes. At higher temperatures and faster gas velocities, the inner layer is enriched in vapor-phase species and remains loosely bound, while at lower temperatures and lower velocities, the enrichment tends to shift to particles in the less-than-5-micron range. In both cases, the inner layer plays a role in the eventual formation of massive upstream deposits.

Both the downstream and inner layer deposition rates (DR_t), where t is the type of deposit layer—downstream (d) or initial (i), are calculated from the following equation:

$$DR_t = \frac{V_g^2}{T_g} \times R_r \times M_{ash} \times \frac{\delta}{A_d} \quad [1]$$

Potential deposition mass is the fraction of total mass in the respective ash categories described previously for initial and downstream deposition. Total ash is the total mass of ash passing through the convective pass.

The massive upstream deposits form primarily by inertial impaction onto the surface of the deposit. The deposit surface can be captive or noncaptive. The larger particles become separated from the gas stream as it flows around the tubes. The particles impact the surface and either stick or deflect off, depending upon their sticking ability and the captive surface of the tube. As massive deposits grow, the surface temperature of the deposit increases, developing a highly captive surface that will capture most of the impacting particles. As the deposit grows, it commonly becomes more aerodynamic, thus minimizing the amount of ash that impacts the surface.

The upstream deposition function is separated into three subfunctions, as shown in Figure 3. The sticking fraction subfunction determines the deposit potential, which is the fraction of the total ash in the path of the heat-transfer surface that sticks. A cutoff particle viscosity is calculated by using the values from the inertial impaction subfunction (IEF). If the particle viscosity is less than the cutoff viscosity, Equation 2, that particle is added to the sticking fraction.

Figure 3. Components of the deposit growth model.

$$DP = \alpha \times \frac{M_p}{100} \times IEF \quad [2]$$

The impact efficiency value is a combination of two values: the impact efficiency strike (IES) and the impact efficiency velocity (IEV). The IES value (0 to 1) is the fraction of ash that will strike the tube, and the IEV value (0 to 1) is used to determine whether the particle has sufficient kinetic energy to rebound off or stick to the tube surface. The upstream deposition function goes through each ash particle-size fraction using the gas stream temperature and

determines the impaction efficiency value for each size fraction and the cutoff particle viscosity. Summing all of the size bins, a cumulative sticking fraction (SF) value (0 to 1) can be determined. The cumulative sticking fraction is then used in Equation 3 to determine the upstream deposition rate.

$$DR_u = \frac{M_{ash}}{A_b} \times SF \times 2 \times Rad_{t_o} \quad [3]$$

2.2.2 Strength Development

Strength development is generally the result of one of two sintering mechanisms: silicate- or sulfate-based. The low viscosities necessary for silicate-based sintering are commonly attributed to higher temperatures and lower-melting-point phases such as sodium aluminosilicates. Some of the reduction in melting point happens after deposition, when interaction of the deposited material and gas-phase species forms low-melting-point phases. Sintering develops over time as low-viscosity material flows and fills the pores of a deposit. Decreasing the numbers or size of the pores in the deposit increases strength. The larger the quantity of liquid phase, the higher the potential for sintering and generating hard deposits.

Sulfate-based sintering is attributed to the filling of deposit pores by sulfation of the alkaline and alkaline-earth components in the deposit. Sulfates are generally unstable and decompose above 1850°F (1000°C), but form very rapidly at temperatures slightly below this decomposition temperature. The crossover temperature range from rapid sulfation to decomposition is narrow and can be crossed in some areas of the boiler as a result of load swings.

Both silicate- and sulfate-based strengths are determined for each deposit. The silicate strengths are a function of the viscosity and particle size of the deposited materials and the time duration of deposition. Equation 4 determines a silicate variable that is a function of the deposit potential, particle diameter, and particle viscosity.

$$Sil_v = DP \times D_p \times \mu_p \quad [4]$$

The silicate variable is summed for all of the particle-size bins for that particular deposit type. For example, using Equation 5, the silicate variable for a downstream deposit strength would sum the ash size bins less than 10 microns.

$$\overline{Sil_v} = \frac{\Sigma Sil_v}{\Sigma DP} \quad [5]$$

The cumulative silicate variable is divided by the total deposit potential, producing a weighted average silicate variable. The average silicate variable is the unitless time needed to achieve a completely sintered deposit. The silicate strength of the deposit at that time interval is determined using Equation 6.

$$\text{Str}_{\text{sil}} = 1 - \left(\frac{1}{(t+1)^{\text{sil}_v}} \right)^{S_{\pi}} \quad [6]$$

The silicate strength is summed over all of the deposit layers present. The longer a deposit has time to sinter, the higher the silicate strength. The weighted average silicate strength (Str_{sil}), Equation 7, is the sum of each deposit layer strength multiplied by that deposit layer's respective mass, divided by the total deposit mass. The weighted average silicate strength is an index value, from 0 to 1, with 1 being the maximum silicate strength.

$$\overline{\text{Str}_{\text{sil}}} = \frac{\sum(\text{Str}_{\text{sil}} \times M_L)}{M_{\text{dep}}} \quad [7]$$

The sulfate strength, Equation 8, is a function of composition and is assumed to reach maximum strength immediately. The PC factors 1 and 2 in the equation are calibration numbers the EERC has obtained from previous projects. Sulfation strengths are set to zero if the temperature is above the sulfate decomposition temperature.

$$\text{Str}_{\text{sulf}} = \frac{\frac{\text{Na}_2\text{O} + \text{MgO} + \text{K}_2\text{O} + \text{CaO}}{\text{Si}_2\text{O}} \times \text{PCF}_1 - \text{PCF}_2}{C_{\text{sulf}}} \quad [8]$$

The sulfate strength is divided by a constant to produce a sulfate strength index number, from 0 to 1. Both sulfate and silicate strength mechanisms can occur at the same location. Figure 4 shows how the sulfate and silicate strength curves may intersect. The greatest strength determined from the two functions is chosen as the strength for that deposit layer (Str_{depl}) at that time interval. An average deposit strength ($\text{Str}_{\text{depavg}}$) can be determined by summing the strength multiplied by the deposit layer mass and divided by the total deposit mass.

2.2.3 Thermal Properties

The thermal properties submodel is a collection of functions that support the other submodels. The thermal properties of the deposits depend upon the thickness, temperature, and physical sintered state of the deposit. Because of the changing temperature and sintered state throughout the thickness of a deposit, as well as its growth and removal, the thermal properties are not constant and require multiple iterations throughout the running of the FOULER model. Since the deposition rates and compositions of the upstream and downstream deposit are different, the thermal property calculations are considered separately for each half of the heat-exchange tube.

Figure 4. Strength development curve.

The main thermal property submodel is the heat-transfer function, which is responsible for the determination of the heat-transfer value through the deposit. The change in heat transfer is due to the convection and conduction through the gas stream, deposit, tube, and steam. Figure 5 shows

Figure 5. Heat transfer through deposit.

the components of the heat-transfer function, along with a relative temperature drop through an upstream deposit. The forced convection heat-transfer rate, q''_{conv} , occurs at the boundary layer between the gas stream and the deposit surface. The forced convection value is dependent upon surface geometry and flow conditions and several fluid properties, which include density, viscosity, thermal conductivity, and specific heat. The thermal property submodel contains several fluid property functions, which are documented in the FOULER code. Once the fluid parameters are determined, a subfunction determines whether the flow at the boundary layer is turbulent or laminar. Depending upon the flow characteristics and average convection coefficient, h_{conv} , q''_{conv} is determined. The conductive heat-transfer rate, q''_{cond} , through the deposit and tube is dependent upon thermal conductivity, temperature, and thickness of each layer. Determination at the convection heat-transfer rate through the steam is similar to solving the forced convection of the gas stream. The heat equation for the heat-transfer through the deposit is given in Equation 9.

$$q = \frac{T_{\text{gas}} - T_{\text{steam}}}{\frac{1}{2\pi \text{Rad}_{t_i} L h_{st}} + \frac{\ln\left(\frac{\text{Rad}_{t_o}}{\text{Rad}_{t_i}}\right)}{2\pi L K_t} + \sum \frac{\ln\left(\frac{\text{Rad}_{dn}}{\text{Rad}_{dn-1}}\right)}{2\pi L K_{dn}} + \frac{1}{2\pi \text{Rad}_{ds} L h_g}} \quad [9]$$

The deposit thermal conductivity is based on laboratory measurements of ash thermal conductivity. The conductivity of ash is nearly independent of the chemical composition, but is strongly dependent on the degree of sintering. Further, the ash conductivity exhibits hysteresis: once heated to a point where sintering occurs, the ash on cooling has a higher thermal conductivity than the original unsintered ash.

2.2.4 Deposit Removal

The deposit removal algorithm accounts for thermal shedding, sootblowing, and gravity shedding. The removal characteristics of the deposit are calculated based on the deposit growth and strength development. The removal indices have a value from 0 to 1, with 1 being complete removal. The sootblowing and load drop models are applied only at the time intervals supplied by the input data. The largest removal index is selected for each time interval.

Thermal shedding occurs when a utility drops load, resulting in a temperature change in the boiler. Because of the different thermal expansion value of the ash deposit and the steam tube, the result is shear fracture in the deposit. The difference in thermal expansion can be correlated to density of the deposit. The change in temperature and the strength of the deposit are the main variables in determining the thermal shedding index.

Gravity shedding is common in the backpass regions of a utility boiler where strength development is low, but deposition is high. This form of deposit removal is correlated to the strength:mass ratio of the deposit. The gravity-shedding index is a function of the deposit strength and weight. Unlike load shedding and sootblowing, gravity shedding is possible at every time interval, since shedding occurs as the weight of the deposit becomes greater than the strength.

The amount of removal due to sootblowing is calculated by comparing the strength of the deposit with the shear stress applied to the deposit by a retractable sootblower as a function of the blowing medium, pressure, nozzle angle, and spacing between sootblowers.

2.3 Ash Formation Algorithm

The ash formation algorithms are currently being completed under various projects at the EERC. Upon completion they will be added to the program shell and included in the interface.

3.0 DEVELOPMENT OF COAL HANDLEABILITY ADVISOR

The low-rank coal (LRC) upgrading technologies under development include evaporative and nonevaporative drying and mild pyrolysis and gasification. An obstacle affecting their development is the stability of the product with regard to dusting, moisture reabsorption, and spontaneous combustion. Because stability phenomena are often given only minor attention, devising improved stability-testing methods has been deemed a necessary and complementary component in the successful demonstration of upgrading technologies (1). Previous efforts to determine stability on a laboratory scale include various test methods such as the tumble, drop-shatter, and dust box tests. However, no single test has been available to address the quality of coals from attrition, coal weathering (slacking), shattering, and dusting properties of the fuel. The need for a system to address each of these categories exists, since one of the most common plant retrofits is that of coal receiving and handling for fuel switching and blending with western coals.

Friability, as measured by either the American Society for Testing and Materials (ASTM) drop-shatter test or tumbler test, has determined the LRCs to be the least friable. Table 1

TABLE 1

Average Friability Values of Various Coal Ranks	
Coal Type	Friability, %
Anthracite	33
Low- and Medium-Volatile Bituminous	70
High-Volatile Bituminous	43
Subbituminous A	30
Subbituminous B	20
Lignite	12

summarizes friability indices for various ranks of coal measured after tumbling the coal for 3 hours (2, 3). Even though LRCs are reported to be less friable, they show a pronounced tendency to disintegrate on exposure to the weathering conditions that are not simulated in ASTM procedures. This effect was first reported by Parry in 1941 when a sample of subbituminous coal was air-dried in a coal bin (4). The results show an increase of 34% in friability after air drying 10 days and a further increase to a total of a 138% increase after 20 days of air-drying. As these results indicate, slacking, like the handling of a friable coal, causes the formation of an excessive amount of fine

material at the expense of the coarser sizes, thus decreasing the value of the coal for most uses. Slacking indices of 5% or less characterize bituminous coals, whereas values for lignite approach 100% (5).

The EERC, in an effort to establish new standards for dried products, has used various known methods and developed new ones to evaluate the propensity of lump western coals, raw and dried, to produce dust in relation to coal-handling problems (6, 7). A conveyor test loop was designed to assess the friability and dust issues associated with handling solid fuels. Various time interval samples can be run through the system to simulate a specific transfer distance and loadout. The conveyor system offers a method to continuously monitor dust emissions and assess various dust suppression additives without conducting a full-scale field test. Establishing this system will provide an important link between research and commercial applications and extend EERC capabilities to better evaluate product integrity of upgraded fuel products.

3.1 Objectives

Program objectives are to establish indices for dust-handling characteristics for various coal types and how they are impacted by current dust suppression methods (e.g., containment methods, stockpiling, dust collection devices, or suppression additives). If successful, the results from the test program will be integrated into the overall FQA algorithm. The near-term objectives are as follows:

- To continue to develop improved methods for evaluating the physical stability of raw and dried coal samples
- To continue to correlate ASTM with modified procedures and understand their relationship or their appropriateness to real-world applications

3.2 Experimental Procedures – Maceral Analysis

Various size-classified coal samples were prepared and analyzed by The Pennsylvania State University (Penn State) and EERC to determine their macerals contents. Coal samples were collected and sized from tumbling tests reported in the previous semiannual report. Each of the coals samples were then ground to -50 mesh and distributed to the appropriate laboratories. Maceral analysis was performed on two lignite samples at the EERC based on experience with classifying lignitic characteristics. Two coals were evaluated, Knife River (lignite) and Illinois No. 6 (bituminous). Preliminary inspection indicated that samples were sized well below that required for an ASTM (D2799) analysis and that the sample surfaces would require a fresh polish. Owing to the particle size (averaging $< 50 \mu\text{m}$) and dispersion of coal particles within the briquettes, the procedure used for maceral analysis was modified. The maceral analysis performed at Penn State was based on a point count of 1000 points, 500 from each of two freshly polished surfaces. Thus, the samples were polished, 500 readings taken, and a new surface ground and polished for a second set of 500 readings. Also, identification of macerals that are dependent on relative differences in reflectance (i.e., vitrinite, semifusinite, and fusinite) was made more difficult by the particle size and could contribute some minor variation in the results. Results are reported on a mineral-matter-free basis.

3.3 Accomplishments - Maceral Analysis

Tables 2 and 3 summarize the Knife River lignite maceral analysis obtained from Penn State and the EERC. According to Penn State scientists, lignitic coals are normally evaluated using procedures developed for brown coals. The particle size made an accurate distinction between different huminite macerals impractical; consequently, Table 2 contains only a total huminite value. The as-received Knife River sample had less total huminite and more inertinite and liptinite group macerals than the tumbled sample. The results indicate that upon tumbling, the total reactive components are concentrated from 95.7% to 98.1%, and the total inert components are reduced from 4.3% to 1.9%. The total inertinite content does not show an increase in the tumbled samples until the -50-mesh fraction listed in Table 3. This correlates well with other results, which have indicated that the inertinite maceral is one of the most friable and is concentrated in the dust (7). For the samples in Table 2, qualitative analysis indicated the principal huminite maceral was ulminite, with lesser concentrations, in decreasing order, of humodetrinite, corpohuminite and gelenite. The minerals observed during analysis were mostly clays, intimately mixed with the organic fraction, rutulated quartz, and minor pyrite. The analysis from Penn State did not include mineral analysis, but the EERC results in Table 3 show the minerals are concentrated in the fine fraction, as expected.

Tables 4 and 5 contain maceral analysis performed at Penn State on four Illinois No. 6 samples. The maceral composition for the samples were fairly consistent. The vitrinite maceral, the most abundant component, remained relatively unchanged from the tumbling, ranging between 88.7% and 87.5% among all samples. Table 4 indicates the fusinite was reduced as a result of tumbling. For the as-received sample, particles of clay minerals, pyrite, and carbonates were observed as individual particles and intimately mixed with the organic fraction. The - 1/2 in. x 3/8 in. tumbled sample showed the most variation in maceral composition within the set, having slightly more liptinite (sporinite, resinite, and cutinite) and less inertinite than the other samples. In addition, clays and carbonates were observed in more relative abundance than pyrite, both as individual particles and mixed with the organic fraction.

3.4 Conclusions

Maceral analysis performed on lignite samples indicated that fusinite, sporinite, and micrinite were reduced in particle size as a result of tumbling the coal sample. Pyrite other mineral forms were also reduced in size.

Maceral analysis performed on Illinois No. 6 samples indicated that fusinite and sporinite were reduced in particle size as a result of tumbling the coal sample.

4.0 ENHANCEMENT OF ASH FORMATION ALGORITHMS

4.1 Introduction

The effects of combustion conditions on coal ash formation and deposition characteristics were investigated using a drop-tube furnace. A North Dakota Beulah lignite coal, Black Thunder

TABLE 2

Knife River Maceral Analysis, vol%, mineral-matter-free			
Analysis Report: Knife River, -½ in. × ⅜ in. as-received sample			
Reactive			
Huminite			
Total Huminite			92.9
Reactive Semifusinite	0.7		
Sporinite	1.6		
Resinite	0.4		
Cutinite	0.1		
Total Reactive Components			95.7
Inert			
Fusinite	1.3		
Inert Semifusinite	1.3		
Macrinite	0.0		
Micrinite	1.7		
Inertodetrinite	0.0		
Sclerotinite	0.0		
Mineral Matter	ND ¹		
Total Inert Components			4.3
	Total		100.0
Analysis Report: Knife River, -½ in. × ⅜ in. tumbled sample			
Reactive			
Huminite			
Total Huminite			96.5
Reactive Semifusinite	0.2		
Sporinite	0.9		
Resinite	0.5		
Cutinite	0.0		
Total Reactive Components			98.1
Inert			
Fusinite	0.4		
Inert Semifusinite	0.3		
Macrinite	0.0		
Micrinite	1.0		
Inertodetrinite	0.0		
Sclerotinite	0.2		
Mineral Matter	ND ¹		
Total Inert Components			1.9
	Total		100.00

¹ Not determined.

TABLE 3

Knife River EERC Maceral Analysis Report

Macerals	-50-mesh, tumbled		$\frac{3}{8}$ in. $\times$ 50-mesh, tumbled	
	Counts	Volume %	Counts	Volume %
Humotelinite	201	38.0	255	48.2
Humodetrinite/Humocollinite	237	44.8	179	33.8
Total Huminite	438	82.8	434	82.0
Sporinite	1	0.2	0	0.0
Cutinite	0	0.0	0	0.0
Resinite	2	0.4	0	0.0
Liptodetrinite	0	0.0	0	0.0
Total Liptinite	3	0.6	0	0.0
Fusinite	2	0.4	4	0.8
Semifusinite	12	2.3	4	0.8
Sclerotinite	0	0.0	0	0.0
Inertodetrinite	10	1.9	2	0.4
Total Inertinite	24	4.5	10	1.9
Pyrite	3	0.6	1	0.2
Other Minerals	67	12.7	7	1.3
Total Minerals	70	13.2	8	1.5
Total	535	101.1	452	85.4

subbituminous coal, and Illinois No. 6 bituminous coal were burned under conventional and low- NO_x combustion conditions. The resulting entrained ash and fouling deposits were sampled and analyzed to characterize their physical and chemical properties. The information from these tests and analyses was used to compare the ash formation and fouling deposition characteristics produced from the conventional and low- NO_x combustion of coals of varying rank. The results of these comparisons will be used for modeling ash transformations.

4.2 Experimental

The three test coals (Beulah lignite, Black Thunder subbituminous, and Illinois No. 6 bituminous) were pulverized to a particle-size distribution consistent with standard utility boiler practice (i.e., 70%–80% of the coal particles <200 mesh). Ash formation and deposition tests were conducted in an optical drop-tube furnace (ODTF), depicted in Figure 6, using conventional

TABLE 4

Illinois No. 6 Maceral Analysis, vol%, mineral-matter-free			
Analysis Report: Illinois No. 6, -½ in. × ⅜ in. as-received sample			
Reactive			
Vitrinite			
Total Vitrinite			88.0
Reactive Semifusinite	1.3		
Sporinite	2.3		
Resinite	0.3		
Cutinite	0.1		
Total Reactive Components			92.0
Inert			
Fusinite	3.6		
Inert Semifusinite	2.7		
Macrinite	0.0		
Micrinite	1.3		
Inertodetrinite	0.4		
Sclerotinite	0.0		
Mineral Matter	ND ¹		
Total Inert Components			8.0
	Total		100.0
Analysis Report: Illinois No. 6, -½ in. × ⅜ in. tumbled sample			
Reactive			
Vitrinite			
Total Vitrinite			88.8
Reactive Semifusinite	1.1		
Sporinite	4.0		
Resinite	0.3		
Cutinite	0.1		
Total Reactive Components			94.2
Inert			
Fusinite	1.6		
Inert Semifusinite	2.3		
Macrinite	0.0		
Micrinite	1.7		
Inertodetrinite	0.2		
Sclerotinite	0.0		
Mineral Matter	ND ¹		
Total Inert Components			5.8
	Total		100.0

¹ Not determined.

TABLE 5

Illinois No. 6 Maceral Analysis, vol%, mineral-matter-free			
Analysis Report: Illinois No. 6, - $\frac{3}{8}$ in. $\times$ 50 mesh tumbled sample			
Reactive			
Vitrinite			
Total Vitrinite			87.5
Reactive Semifusinite	1.1		
Sporinite	2.9		
Resinite	0.3		
Cutinite	0.3		
Total Reactive Components			92.1
Inert			
Fusinite	3.1		
Inert Semifusinite	2.3		
Macrinite	0.0		
Micrinite	1.5		
Inertodetrinite	1.0		
Sclerotinite	0.0		
Mineral Matter	ND ¹		
Total Inert Components			7.9
Total			100.0
Analysis Report: Illinois No. 6, -50 mesh tumbled sample			
Reactive			
Vitrinite			
Total Vitrinite			88.3
Reactive Semifusinite	1.3		
Sporinite	2.3		
Resinite	0.3		
Cutinite	0.0		
Total Reactive Components			92.2
Inert			
Fusinite	3.9		
Inert Semifusinite	2.6		
Macrinite	0.0		
Micrinite	0.8		
Inertodetrinite	0.5		
Sclerotinite	0.0		
Mineral Matter	ND ¹		
Total Inert Components			7.8
Total			100.0

¹ Not determined.

and staged low- NO_x combustion conditions. During the conventional combustion tests, coals were fed with about 50% excess air and heated to an initial temperature of 1530°C before passing through a cooler temperature regime of 1200°C . To simulate low- NO_x conditions, the coals were fed into the furnace using a N_2 primary gas and an air- N_2 secondary gas and heated to an initial temperature of 1330°C before passing through a maximum temperature regime of 1430°C and a final, lower-temperature regime of 1200°C . The lower temperature and slower mixing of fuel and air extended the burning time and significantly reduced both the thermal and fuel NO_x , while maintaining an acceptable level of carbon burnout. Compared in Figure 7 are the furnace temperature profiles and gas flows for conventional and low- NO_x combustion conditions.

A quenching probe shown in Figure 8 was attached to the bottom of the ODTF to cool the fly ash before collection. A filter assembly was attached to the exit of the quench probe to collect bulk particulate samples. Samples of size-fractionated ash were collected using an U.S. Environmental Protection Agency Southern Research Institute five-stage multicyclone (EPAFSC). During several tests, the EPAFSC was used in conjunction with a scanning mobility particle sizer in an attempt to determine the size distribution of the submicron ash fraction. Baseline tests, however, indicated that the concentration of contaminate submicron particles was too great to obtain reliable results. Most of the contaminate particles, >70% by volume, were $<0.1\ \mu\text{m}$ in diameter. As an alternative, several samples of bulk ash were mounted on vitreous carbon substrates using a modified version of a freeze-dry dispersion method (9) and then analyzed using computer-controlled scanning electron microscopy (CCSEM) to determine the size and chemical composition of individual microparticles ranging from 0.1 to $100\ \mu\text{m}$ in average diameter. Approximately 1000 particles were analyzed in selected samples using CCSEM.

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Figure 6. Schematic of the ODTF.

Figure 7. Comparison of gas flows and temperature profiles used in the ODTF to simulate conventional and staged low- NO_x combustion conditions.

Figure 8. Schematic of the fly ash quenching probe.

Deposits were formed in the ODTF on a deposition probe that simulates an actual boiler tube. Expendable sample coupons were attached to the probe and maintained at temperatures corresponding to boiler heat-transfer surfaces, 350° to 540°C. An insulating refractory constrictor was used to accelerate the gas flow and entrained ash onto the deposit probe. The crushing strengths of the deposits were determined. The resulting deposits were also analyzed using a scanning electron microscope point count method (SEMPC) described by Galbreath et al. (10).

4.3 Results

4.3.1 Ash Formation Tests

The ash formation test matrix and ODTF operating conditions are summarized in Table 6. Entrained ash was produced using relatively long residence times ranging from 3.9 to 5.2 seconds. Several tests at shorter residence times of 0.2 and 0.5 seconds were also conducted on the Black Thunder coal. The simulated low-NO_x combustion conditions reduced NO_x by about 50% relative to conventional combustion while maintaining a relatively high degree of gas carbon conversion (Table 6).

Presented in Figure 9 are the multicyclone ash collection results for the ODTF tests. These results indicate that the Black Thunder coal produced the coarsest ash. In addition, combustion conditions most significantly affected the size distribution of the Black Thunder ash, whereby the ash produced under low-NO_x conditions was coarser relative to the ash generated during conventional combustion. The particle-size distributions of the Beulah and Illinois No. 6 coal ashes are similar, and combustion conditions appear to have had very little effect.

The fine-particle fractions (0.1- to 10- μ m diameter) of the ashes were investigated in detail using CCSEM. Particle-size distributions presented in Figure 10 indicate that combustion conditions greatly affected the formation of fine ash for the lower-rank Beulah and Black Thunder coals, but not for the Illinois No. 6 bituminous coal. The morphology of particles in the fine ash fractions was examined using scanning electron microscopy. The ashes produced from the conventional combustion of coal consist primarily of discrete spherical particles, as exemplified in Figure 11. Particle agglomerates, however, are characteristic of the low-NO_x Beulah and Black Thunder fine ashes, as illustrated in Figure 12. The agglomeration is the result of sintering between individual ash particles. Apparently the lower oxygen fugacity and extended combustion duration associated with low-NO_x test conditions enhance the sintering propensity of individual fine ash particles in the lower-rank coals. The fine ash fractions of the Beulah and Black Thunder coals produced using the low-NO_x combustion conditions are coarser because of the agglomeration, as indicated in Figure 10. The predominant particle morphology was similar for the conventional and low-NO_x Illinois No. 6 fine ash fractions, that is, individual spherical particles.

Chemical analysis of individual ash particles indicates that the fine ash fractions are composed of very diverse particle-type assemblages, as shown in Table 7. The Beulah fine ash fraction is composed primarily of sodium and calcium aluminosilicate (Na-Al-Si and Ca-Al-Si) phases, which is consistent with the high concentrations of organically bound sodium and calcium

TABLE 6
Operating Parameters for Drop-Tube Furnace Ash Formation Tests

Coal	Conditions	Furnace Temperatures, °C				Residence Time, s	Excess Air, %	Gas Carbon Conversion, %	Initial Thermal NO _x , ppm	Total NO _x , ppm
		Furnace 1	Furnace 2	Furnace 3	Furnace 4					
Black Thunder	Conventional	1100	1530	1450	1230	3.9	53	NA ¹	34.6	143.4
Black Thunder	Conventional	1100	1530	1450	1230	3.9	53	NA	34.3	147.4
Black Thunder	Low-NO _x	800	1330	1430	1230	4.1	52	99.3	2.2	97.1
Black Thunder	Low-NO _x	800	1330	1430	1230	4.1	53	NA	7.7	97.9
Black Thunder	Conventional	1100	1530	1450	1230	0.2	50	62.5	17.1	55.6
Black Thunder	Conventional	1100	1530	1450	1230	0.5	54	82.2	15.9	64.5
Black Thunder	Low-NO _x	800	1330	1430	1230	0.2	51	91.2	3.0	10.0
Black Thunder	Low-NO _x	800	1330	1430	1230	0.5	50	61.1	2.4	36.6
Black Thunder	Conventional	1000	1530	1450	1200	5.0	51	NA	NA	NA
Black Thunder	Low-NO _x	800	1330	1430	1200	5.2	51	NA	NA	NA
Illinois No. 6	Conventional	1100	1530	1450	1230	3.9	49	96.0	34.5	175.9
Illinois No. 6	Conventional	1100	1530	1450	1230	3.9	52	85.0	14.3	158.7
Illinois No. 6	Low-NO _x	800	1330	1430	1230	4.1	50	93.0	2.9	112.7
Illinois No. 6	Low-NO _x	800	1330	1430	1230	4.1	64	91.3	3.2	116.6
Illinois No. 6	Conventional	1000	1530	1450	1200	5.0	52	84.4	16.8	139.3
Illinois No. 6	Conventional	1000	1530	1450	1200	5.0	52	NA	NA	NA
Illinois No. 6	Low-NO _x	800	1330	1430	1200	5.2	52	90.1	3.43	108.7
Illinois No. 6	Low-NO _x	800	1330	1430	1200	5.2	52	NA	NA	NA
Beulah	Conventional	1100	1530	1450	1230	3.9	53	92.5	32.0	121.0
Beulah	Conventional	1100	1530	1450	1230	3.9	58	100.8	32.9	122.3
Beulah	Low-NO _x	800	1330	1430	1230	4.1	54	89.8	3.7	71.7
Beulah	Low-NO _x	800	1330	1430	1230	4.1	54	100.5	4.0	85.4
Beulah	Conventional	1000	1530	1450	1200	5.0	50	88.3	16.2	103.8
Beulah	Conventional	1000	1530	1450	1200	5.0	50	NA	NA	NA
Beulah	Low-NO _x	800	1330	1430	1200	5.2	50	91.3	3.65	77.3
Beulah	Low-NO _x	800	1330	1430	1200	5.2	50	NA	NA	NA

¹ Not analyzed.

Figure 9. Comparison of particle-size distributions for the Black Thunder, Illinois No. 6, and Beulah ND lignite ashes produced using conventional and low-NO_x combustion conditions.

Figure 10. Comparison of particle-size distributions for the Black Thunder, Illinois No. 6, and Beulah ND lignite fine ash fractions produced using conventional and low- NO_x combustion conditions.

Figure 11. Secondary electron image of the Beulah fine ash fraction produced using conventional combustion conditions.

that is available in ND lignite coals to react with clays during combustion. Likewise, the predominance of calcium aluminosilicate (Ca-Al-Si), calcium aluminate (Ca-Al), and calcium carbonate, hydroxide, or oxide [(Ca)CO₃, OH, or O] phases in the Black Thunder fine ash is consistent with the relatively high concentrations of organically bound calcium that is available in Powder River Basin subbituminous coals to react with mixed clays and kaolinite during combustion or to vaporize and condense. The Illinois No. 6 fine ash is composed largely of aluminosilicate (Al-Si), sodium aluminosilicate (Na-Al-Si), and mixed aluminosilicate [(Ca, Mg, Fe)-Al-Si] particle types. The different combustion conditions (conventional and low-NO_x) used to produce the fine ash fractions appear to have had a negligible effect on phase proportions.

4.3.2 Ash Deposition Tests

Deposits were produced in the ODTF under conventional and low-NO_x fouling conditions. The operating parameters used during the ash deposition tests are presented in Table 8. The deposits are largely amorphous. However, small crystals with chemical compositions consistent with the minerals clinopyroxene, melilite, plagioclase, and quartz have been identified. A total of 250 randomly selected locations on each of the deposit samples were chemically analyzed using a scanning electron microscope to assess compositional homogeneity. In addition, the crushing strengths of the deposits were determined. The analysis data are currently being reduced and results will be presented in the project final report.

Figure 12. Secondary electron images of the Black Thunder fine ash fraction produced under low- NO_x combustion conditions.

TABLE 7

Fine-Ash-Phase Proportions, ¹ frequency %			
	Beulah	Black Thunder	Illinois No. 6
SiO ₂	1.7 3.2¹	5.3 5.1	6.4 8.1
Na-Al-Si	11.8 17.4	ND ² ND	17.6 14.2
Ca-Al-Si	24.0 19.1	19.6 20.8	1.8 1.7
K-Al-Si	ND ND	ND ND	2.4 2.2
Fe-Al-Si	ND ND	ND ND	1.2 1.3
(Ca,Mg,Fe)-Al-Si	3.5 1.8	4.5 8.7	17.5 13.3
Al-Si	0.4 ND	25.1 19.9	31.6 27.6
Na-Si	ND ND	ND 0.9	ND ND
Ca-Si	0.5 0.2	ND ND	0.1 ND
Fe-Si	0.1 ND	0.8 ND	0.1 0.2
Si-Rich	1.7 2.0	3.6 6.6	5.2 4.5
Ca-Al	0.2 0.6	16.5 9.6	ND ND
(Ca,Mg,Fe)CO ₃ , OH, or O	1.1 2.6	23.4 16.6	1.1 0.8
Al ₂ O ₃	0.3 ND	ND ND	ND 0.1
Fe _x O _x	0.2 0.3	0.6 0.3	0.1 0.1
Na ₂ SO ₄	ND ND	ND 2.1	ND ND
CaSO ₄	0.3 0.4	ND 3.0	1.4 0.1
S-Rich	3.7 3.8	0.6 0.6	1.8 4.1
(Na,K)Cl	ND ND	ND ND	ND 0.1
Cl-Rich	0.3 1.1	ND 3.0	0.1 0.2
P-Rich	0.2 0.4	ND 0.3	ND ND
Na-Rich	ND ND	ND 2.4	ND ND
Unclassified	50.0 48.9	0.0 0.0	11.6 21.4

¹ Values in bold type correspond to low-NO_x combustion conditions² Not detected.

TABLE 8

Operating Parameters for Drop-Tube Furnace Fouling Tests

Coal	Conditions	Furnace Temperatures, °C				Residence Time, s	Excess Air, %
		Furnace 1	Furnace 2	Furnace 3	Furnace 4		
Beulah	Conventional	1000	1530	1450	1200	3.5	50
Beulah	Low-NO _x	800	1330	1430	1200	3.6	50
Illinois No. 6	Conventional	1000	1530	1450	1200	3.5	51
Illinois No. 6	Low-NO _x	800	1330	1430	1200	3.6	52

4.4 Conclusions

An important finding from the tests is that the fine ash fraction ($< 10 \mu\text{m}$) produced by burning the lower-rank Beulah ND lignite and Black Thunder subbituminous coals under low-NO_x conditions is coarser than the corresponding ash produced under conventional combustion conditions. The lower partial pressure of oxygen and extended combustion duration associated with the low-NO_x combustion conditions promotes the sintering of individual ash particles to form agglomerates. This agglomeration effect was insignificant for the Illinois No. 6 bituminous ash.

5.0 FUTURE WORK

The work for the remainder of this project is summarized below.

5.1 Shell/Interface

- Complete construction of interface and shell
- Complete inclusion of ash formation and ash deposition algorithms

5.2 Coal Handling

- Evaluate results and applicability to computer algorithm

5.3 Ash and Fouling Deposit Formation

- Incorporate the effects of combustion conditions on the particle-size distribution of ash produced from low-rank coals into ash transformation models
- Assess the effects of combustion conditions on ash deposition and fouling deposit formation

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APPENDIX A

VARIABLE DEFINITION LIST

VARIABLE DEFINITION LIST

A_d	=	Total cross-sectional area available for ash deposition, ft^2
A_t	=	Cross-sectional area of the convective pass, ft^2
C_{sulf}	=	Sulfate constant
D_p	=	Particle diameter, microns
DP	=	Deposit potential mass of ash that sticks to the tube, lb
DR_t	=	Low-temperature deposition rate, $\text{lb}/(\text{ft}^2 \text{ hr})$
DR_u	=	Upstream deposition rate, $\text{lb}/(\text{ft}^2 \text{ hr})$
h_{conv}	=	Average convection coefficient, $\text{Btu}/(\text{ft}^2 \text{ hr} \cdot ^\circ\text{F})$
h_g	=	Heat-transfer coefficient of the gas, $\text{Btu}/(\text{ft}^2 \text{ hr} \cdot ^\circ\text{F})$
h_{st}	=	Heat-transfer coefficient of the steam, $\text{Btu}/(\text{ft}^2 \text{ hr} \cdot ^\circ\text{F})$
IEF	=	Inertial impaction subfunction—fraction of ash that will strike the tube
K_{down}	=	Average downstream deposit thermal conductivity
K_{dn}	=	Thermal conductivity of deposit layer, $\text{Btu}/(\text{ft}^2 \text{ hr} \cdot ^\circ\text{F})$
K_t	=	Thermal conductivity of tube, $\text{Btu}/(\text{ft}^2 \text{ hr} \cdot ^\circ\text{F})$
K_{up}	=	Average upstream deposit thermal conductivity
L	=	Unit length of 1 ft
M_{ash}	=	Total ash, lb/hr
M_{dep}	=	Total deposit mass
M_L	=	Deposit layer mass
M_p	=	Mass percent for a specific particle size
PCF_1	=	PC Sulfate Factor 1
PCF_2	=	PC Sulfate Factor 2
q	=	Heat-transfer rate, Btu/hr
q''_{cond}	=	Conductive heat-transfer rate
q''_{conv}	=	Forced convection heat-transfer rate
Rad_{ds}	=	Outer deposit radius
Rad_{max}	=	Maximum radius of ellipse, in.
Rad_{min}	=	Minimum radius of ellipse, in.
Rad_t	=	Outside radius of tube, ft
Rad_i	=	Inside radius of tube, ft
R_{dn}	=	Deposit layer radius n, ft
$R_{\text{dn-1}}$	=	Next deposit layer radius n-1, ft
R_{dt}	=	Total deposit radius
SF	=	Cumulative sticking fraction, 0 to 1
Sil_v	=	Silicate variable
S_{rc}	=	Silicate reference constant
$\text{Str}_{\text{depavg}}$	=	Average deposit strength
Str_{depL}	=	Strength of individual deposit layer
Str_{sil}	=	Silicate strength
Str_{sulf}	=	Sulfate strength
T_g	=	Gas temperature stream, R
T_{gas}	=	Temperature of the gas stream, $^\circ\text{F}$
T_{dn}	=	Deposit layer temperature, $^\circ\text{F}$
$T_{\text{dn-1}}$	=	Next deposit layer temperature, $^\circ\text{F}$
T_{douter}	=	Temperature of outermost deposit layer

T_{steam}	=	Temperature of the steam, °F
V_g	=	Gas velocity, ft/s
α	=	Angle factor
δ	=	Potential deposition mass fraction
μ_p	=	Particle viscosity, poise