VARIATION IN COAL COMPOSITION

A computational approach to study the mineral composition of individual coal particles

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Mineral matter transformations, and therefore fly ash evolution, during pulverized coal combustion depend on the amount, composition and spatial distribution of the inorganic matter within individual pulverized coal particles. Thus, it is necessary to have information on the mineral composition of individual particles, as well as that of the raw pulverized coal. A model has been developed to predict the variation of individual coal particle compositions. It uses CCSEM data for a given raw coal as input and randomly distributes the mineral inclusions in the coal volume. By random selection of monosize coal particles, it is possible to generate distributions of mineral content for any particle size distribution of coal. The model has been checked by comparing computed results with data on the compositional variations of narrowly size and density classified fractions of an Upper Freeport bituminous coal. The results for individual coal particle compositions are used to generate information on the variability of the composition of the fly ash generated during combustion.

1. INTRODUCTION

Understanding the processes that govern the size distribution and chemical composition of the ash within and at the exit of a pulverized coal fired combustor is important because the ash influences fouling, slagging, and heat transfer in boilers, as well as the downstream particulate control equipment. This understanding begins with not only a knowledge of the amount, composition, and spatial distribution of the mineral matter in the coal particles, but also with some knowledge of the variability of the mineral content of the coal particles.

In this paper a model is presented for calculating the distribution of mineral inclusions in pulverized coal of different size and density fractions from knowledge of the mineral inclusions in the parent coal. A test of the validity of the model is provided by comparing the model predictions of the variations in the composition of different size and density fractions of an Upper Freeport coal with computer controlled scanning electron microscopy (CCSEM) measurements of the mineral distributions. The results obtained for the Upper Freeport coal show good agreement between the CCSEM data and the model results, and also give information on the variation of individual coal particle compositions.

This study is part of a broader program on mineral matter transformations being funded by the DOE and coordinated by Physical Sciences Inc. The coal classification was done by Foster Wheeler and the CCSEM analysis by Huffman and Huggins at the University of Kentucky. The results of this study will be used as input into a model of char combustion which allows for coalescence of the mineral inclusions and fragmentation of the char in order to predict the composition and size of the fly ash.

2. EXPERIMENTAL

CCSEM analysis was performed on the Upper Freeport raw coal and several size and density fractions (63-105 μm , and less than 1.3, 1.3 - 1.8 , 1.8 - 2.85 , and greater than 2.85 g/cm^3) by Huffman and Huggins at the University of Kentucky. The CCSEM analysis provides the content and size distribution of each of the mineral species listed in Table 1. For details on the CCSEM analysis used to obtain these data, one can consult the publications of these two specialists [2][3][4], as well as other authors [5][6].

The main mineral species in the Upper Freeport raw coal are, by decreasing amount, Illite, Mixed silicates, Pyrite, Quartz and Kaolinite. All the other species occur in concentrations less than 2 wt%. The CCSEM gives the mineral inclusion size distribution for these five main mineral types and for the total minerals (Table 1). For the latter, all the sizes are equally represented in the range from 10 to 15%, except the largest size (greater than 40 µm) which reaches 36%.

The CCSEM data obtained for the Upper Freeport raw coal were used as input to the model. The CCSEM data obtained for the four size and density classified samples were compared with computed values in order to validate the model.

3. MODEL

The model has two objectives : first, it must simulate a raw coal volume with different types and sizes of mineral inclusions inside, and second, it must produce coal particles from this computed raw coal volume, sort them by density, and perform statistics on them. To accomplish these objectives two Fortran programs were created : Pr1 and Pr2.

The major difficulty in simulating the raw coal volume is storing the information about the mineral inclusions (type, size, location...) and about the coal particles (mineral composition, density...) during the run. In the case of the Upper Freeport coal, greater than five million inclusions must be stored in order to get at least one mineral inclusion for each type and size. Only a super computer has sufficient memory to handle all of this information. We used an IBM 3090-600E with 512 megabytes of real memory and 512 megabytes of expended storage.

3.1 Raw coal volume simulation (Pr1)

3.1.1 Definitions

The raw coal volume is cubic and divided into a cubic matrix with unit length of one micron. The mineral inclusions are assumed to be cubic and are assigned to occupy sites within the raw coal matrix. Eventually the coal matrix is divided into smaller cubes which are coal particles.

The model assumes 6 different possible mineral inclusion sizes, one average size for each size range given by the CCSEM analysis. These sizes are defined using an integer number I from 1 to 6 and the D (I) values are, respectively, 1, 4, 8, 16, 30, and 60 µm.

The model accounts for the five main mineral species of the Upper Freeport raw coal as defined by the CCSEM analysis [4] (see Table 1), and identifies them by an integer number J. To achieve a mineral mass balance, a sixth kind of mineral, called "Other", is defined. The "other" content, composition and size distribution are calculated to fit the total mineral inclusion analysis given by the CCSEM data :

$$f_m(6) = 1 - \sum_{J=1}^{5} f_m(J) \quad \text{and}$$

$$f_{m,s}(6,I) = 1/f_m(6) \cdot \left[f_{m,s}(\text{All mineral}, I) - \sum_{J=1}^{5} f_m(J) \cdot f_{m,s}(J,I) \right] \quad \text{with}$$

$$f_{m,s}(\text{All mineral}, I) = \sum_{J=1}^{6} f_{m,s}(J,I)$$

where $f_m(J)$ is the mass fraction of the mineral J in all mineral
and $f_{m,s}(J,I)$ is the mass fraction of the size I for mineral J.

The last species to be defined is the mineral free coal (J=0). The density of this last species is an input data for the model and depends on the raw coal studied. A value of 1.2 g/cm^3 was assumed for the Upper Freeport coal.

3.1.2 Random location of the mineral inclusions

An inclusion is defined by the location (X_i, Y_i, Z_i) of its closest point to the origin of the raw coal volume, and by its size D (I). X_i, Y_i, Z_i are randomly computed between 0 and L - D (I), where L is the size of the simulated raw coal cube.

In order to avoid overlap between two mineral inclusions, all of the sites used by a mineral inclusion are recorded. Then if a latter inclusion needs to use one of these recorded sites for its location, its location is randomly computed again. This test is necessary to avoid inclusion overlap, particulary for the Upper Freeport (20.5 wt% of mineral matter) where almost 10% of its sites are mineral sites, but at a cost of a significant increase in run time and memory requirement.

3.1.3 Mineral inclusion attribution to a coal particle

Knowing L, X_i, Y_i, Z_i, D (I) and the coal particle size (Nspart) which is to be created from the raw coal volume, it is possible to attribute a given mineral inclusion to a coal particle. The coal particles and mineral inclusions are identified as a function of their location in the raw coal cube by a characteristic integer given as :

$$\mathrm{Num} = \left[\sum_{k=1}^{3} \mathrm{INT}\, \{ (\mathrm{Loc}(k) + D(I)/2) / \mathrm{Nspart} \} \, . \, \mathrm{Nstep}^{k} \right] + 1$$

where Loc (k) for k=1 to 3 are X_i, Y_i, and Z_i, respectively,
L = Nstep · Nspart,
and INT (value) is the integer part of value.

All the inclusions within a coal particle will have the same identifying integer, Num, as the coal particle. A coal particle will be allowed to contain a mineral inclusion if its size is greater than the inclusion size , if it contains the gravity center of the inclusion, and if there is enough remaining space for the additional inclusion. If a mineral inclusion is not in a coal particle, it is a pure mineral particle, keeping the former inclusion size; however, this case was never encountered for the 84 µm Upper Freeport coal.

3.1.4 Running Pr1

All of the illustrations in this presentation are given for the Upper Freeport raw coal and its four well classified samples, previously described. Because the model is at this time only able to produce a monosize coal sample, the results from the model will be given for the size 84 µm, which is an average value for the experimental sample size range 63 - 105 µm. The input file for a run consists of the CCSEM data for a given raw coal, chosen coal particle size and chosen particle number. Typically, the Pr1 run time was 14'27" CPU, and 350 megabytes of virtual memory was used to produce 5 100 981 mineral inclusions randomly distributed in a raw coal volume 840 µm large. As shown in Table 2, for a small number of biggest inclusions (only 2 for the quartz) we obtain an increasing number of inclusions when the inclusion size decreases, to finally reach 4 994 227 inclusions of 1 µm (98% of the total number). This is a problem with this computation : i.e., the biggest mineral inclusion size is not statistically well-defined, and we are too close to the maximum of memory available, to increase the number of inclusions.

The number of inclusion (Ninc) for a given mineral type J and a size I is calculated as follows :

$$\mathrm{Ninc}(J, I) = \mathrm{INT}\left[(V(J, I) / D(I)^{3}) + 0.5 \right]$$

where V (J , I) is the volume used in the raw coal cube by the mineral J, calculated from the CCSEM data. In this way the difference between the computed and the measured coal sample mineral composition is always less than 0.1 wt% and the total mineral content is exactly the desired value of 20.5 wt%.

3.2 Coal particle characterization (Pr2)

Each individual coal particle is identified by an integer number, Num. Pr2 then calculates, for all the computed inclusions, the amount of mineral inclusion J with the size I which falls in the coal particle Num. All this information is stored and used to calculate the mineral content and composition, mass or density of every individual coal particle. A density classification is achieved and any kind of statistical analysis is possible for the whole computed coal sample or any well classified size and density fraction.

The mineral inclusion listing and a parameter listing (L, Nstep, Npart, D (I)...) generated by Pr1 are the two input files necessary to run Pr2. Typically the run time was 2'15" CPU and 160 megabytes of virtual memory was used to produce 1000 particles of 84 μm.

4 Results

4.1 Model validation

Comparison of experimental CCSEM data for density classified Upper Freeport coal to model predictions is shown in Figure 1. Figure 1 shows good agreement for the mass distribution between the four density ranges and for the total mineral content in each density range. The fourth density range, where .2 wt% of the whole sample and a total mineral content of 91.6 wt% was calculated, does not give satisfactry agreement, but the reason becomes clear from an examination of the particle statistics in each density range. Whereas 516, 399, and 84 coal particles were obtained in the first, second and third density ranges, respectively, only one ended up in the fourth density range. Thus, the current model is limited by the large amount of memory necessary for a run and the fourth density range sample is too small to give representative results.

Good agreement for the mineral composition in the first two density ranges was also obtained (Figure 1), but for the same reason the last two ranges show disagreements. Even though the agreement is not good in the last two density ranges, the results do agree with the CCSEM data that the pyrite is the main mineral in particle greater than 2.85 g/cm^3. The mineral composition cannot be statistically well determined because the sample size of the simulated biggest mineral inclusions is too small.

A new statistical approach is currently under development to reduce the representation of the smallest inclusion size (currently 98 % of the memory used by Pr1).

4.2 Individual coal particle information

Assuming the model is validated, we can study the mineral composition variation in individual coal particles. The results, obtained for the Upper Freeport, show as expected that the density classification provides coal samples with small variations in the total mineral content of individual particles (Figure 2). From the whole sample, which contains 18.08 wt% mineral matter per particle with a standard deviation of 15.20 wt%, we obtain four density classified samples, which contain 10.16, 18.40, 64.40 and 91.60 wt% of mineral matter per particle but with a standard deviation always less than 5 wt% (only 1.47 % for the first density range).

From an examination of the mineral composition of an individual coal particle (Figure 3), it appears that the fraction of a given mineral varies greatly even through the mean value does not (32 wt% for illite); the standard deviation, more over increases when the particle density increases (8.93, 18.90, and 49.5 wt% for the first, second and third density ranges, respectively). Denser coal particles contain larger inclusions, which because of their size they represent most of the mineral mass of that coal particle. This is why the mineral composition approaches the limit of either 0 or 100 wt% for a given mineral, when the particle density increases. Table 3 shows variations in compositions of a given mineral in individual particles. For the first and second density ranges the variation ranges are around 40 and 70%, respectively.

We also observed that the classified sample that is most representative of the whole coal sample is in the second density range (1.3 to 1.8 g/cm^3).

5 conclusion

This new computational approach allows information to be obtained information on the mineral composition variation in individual coal particles, which can be useful for predicting the mineral transformations and the final fly ash size distribution during pulverized coal combustion. Without using sophisticated and expensive experiments, it is possible to obtain data on any classified samples and to compare them with fly ash composition. This information will be used as input to a model of coal particle combustion. This model can also be used to design a process for preparation of a well classified coal sample with a given mineral composition.

A future improvement of the model will be to develop a new statistical approach in which will increase the number of simulated big inclusions and reduced the memory required. This will allow for the characterization of the large particle composition variations as well.

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Table 1 : CCSEM data from J. Huffman and F. Huggins for the Upper Freeport raw coal

mineral	Wt% mineral matter	Size distribution (wt%)					
		<2.5μm	2.5-5μm	5-10μm	10-20μm	20-40μm	>40μm
Quartz	10	8	14	26	20	26	6
Kaolinite	7	15	9	15	25	19	16
Illite	35	10	10	13	11	12	44
Mix.il.	19	12	16	15	21	12	23
Pyrite	18	4	2	13	13	14	54
All mine.	100	9	10	15	15	14	36

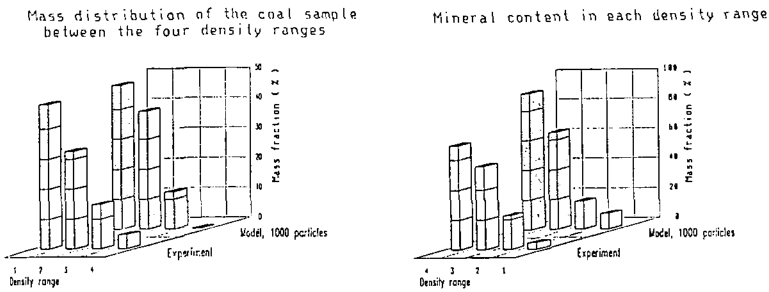
Table 2 : Number of mineral inclusion in 1 mm^3 of the raw Upper Freeport coal based on an average size, in each CCSEM analysis size range

Mineral	Number of inclusions					
	1 μm	4 μm	8 μm	16 μm	30 μm	60 μm
Quartz	503988	13781	3199	308	61	2
Kaolinite	604460	5667	1181	246	28	3
Illite	2014867	31482	5116	541	90	41
Mix. sil.	1268790	26433	3098	542	47	12
Pyrite	240402	1878	1526	191	31	15
Others	361720	9304	1750	145	22	14

Table 3 : Particle by particle mineral composition variations for two density classified samples of an 84 μm Upper Freeport coal (wt%)

	Range 1 : less than 1.3 g/cm^3				Range 2 : 1.3 to 1.8 g/cm^3			
	Mean	St. dev.	Min.	Max.	Mean	St. dev.	Min.	Max.
Particle number	516	-	-	-	399	-	-	-
Total mineral content	10.2	1.5	6.3	13.0	18.41	4.85	12.1	38.2
Mineral composition								
Quartz	14.8	7.3	3.2	46.8	15.1	16.0	1.5	69.5
Kaolinite	9.1	6.8	2.2	38.8	9.1	12.4	0.5	76.4
Illite	32.1	8.9	12.9	59.1	30.8	18.9	5.3	79.4
Mixed silicates	25.5	9.3	7.2	57.6	21.9	16.7	3.2	75.3
Pyrite	9.4	7.2	1.3	38.9	14.7	17.2	0.5	82.0
Others	9.1	5.5	1.8	32.9	8.4	11.4	0.9	64.0

Figure 1 : Comparison between experimental data and model results for an 84 μm Upper Freeport raw coal sample



Density ranges (g/cm^3)

1 : less than 1.3
2 : 1.3 to 1.8
3 : 1.8 to 2.85
4 : greater than 2.85

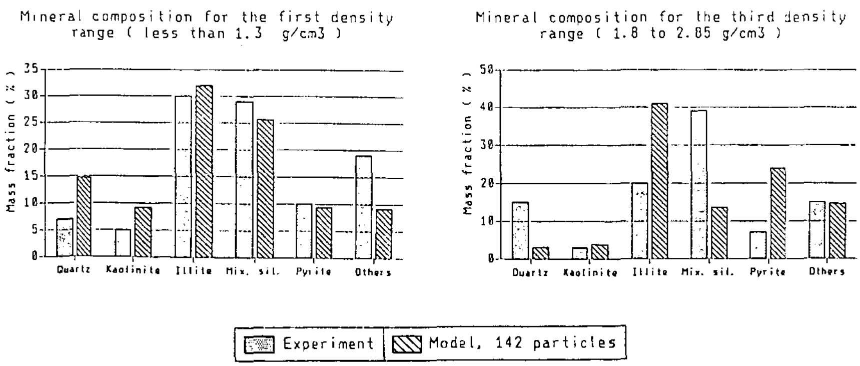


Figure 2 : Model predictions of the total mineral content in different density classes for na 84 µm Upper Freeport coal sample

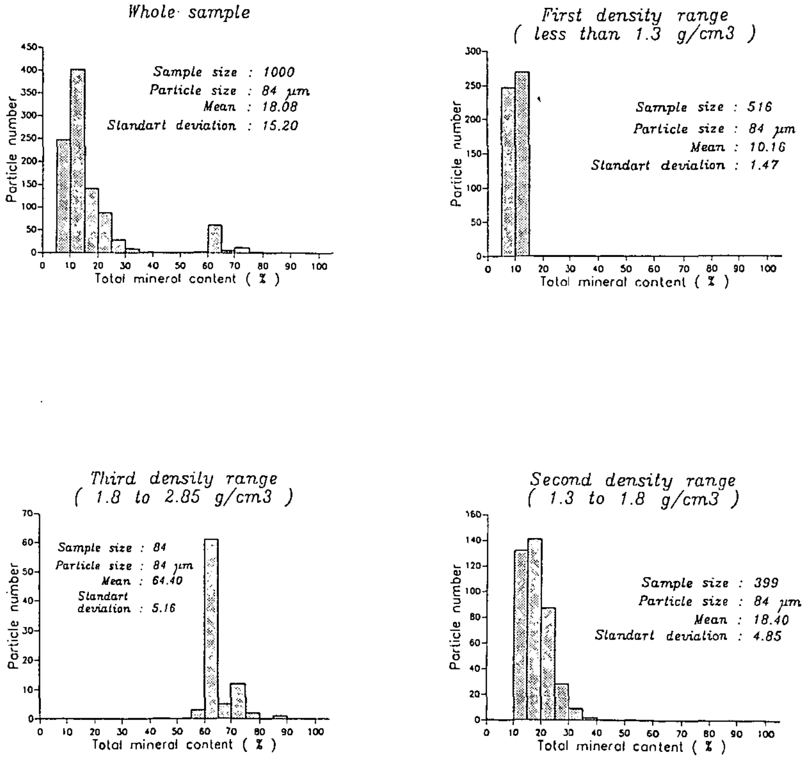


Figure 3 : Model predictions of the illite content in different density classes for an 84 μm Upper Freeport coal sample