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Elemental Analysis of Coal Combustion: Coal, Char, and Volatiles

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As the demand for modeling complex processes such as coal combustion in industrial coal applications increases, there is a greater need for sub-models that are both computationally simple and physically detailed. Many research codes rely heavily on simplified chemistry, or do not even include chemistry. The chemistry of the system can greatly affect the performance and accuracy of the simulations. This paper details an analysis of elemental compositions of various aspects of the coal combustion process. Experimental data were analyzed to find a correlation that predicts the elemental compositions of the devolatilization products (char and total volatiles) from the proximate and ultimate analyses of the parent coal. These predictions can inform chemistry and transport models in complex simulations, particularly char and soot reactions.

1. Introduction

The determination of chemical composition of combustion products is a standard in experimental work, and is also very important in emissions control. Combustion conditions influence which elements end up in different combustion products. The location of each of these elements can influence the NOx and SOx compositions of the combustion product exhaust [1].

Several variables affect pyrolysis behavior, and many of them likely affect the elemental composition of the pyrolysis products. Coal type significantly impacts the pyrolysis product yields [2]. Coal type influences the chemical and elemental composition of the parent coal. Parent coal chemistry can inform pyrolysis behavior in the way that bonds break during rapid heating. Pyrolysis temperature (or the temperature at which pyrolysis is performed) heavily affects the pyrolysis product yields [3]. A third possible variable to influence product compositions is the rate at which the particle is heated. This heating rate has been shown to affect the pyrolysis product yields, especially at high heating rates (on the order of 10^3 to 10^6 K/s) [4].

Experimental data was gathered from previously completed experiments. Sandia National Laboratories was heavily involved in collecting both devolatilization data [5] and char fragmentation data [6] from several types of coal and under several pyrolysis conditions. Liu, *et al.*, also experimented on parent coal and coal char formation, including the elemental composition of each [7]. Researchers at Argonne National Laboratories conducted extensive experiments and analyses on the Argonne Premium Coal Samples [8]. These references were the primary source of data for the completion of the elemental analysis; however, other sources of data were used as a verification for the elemental correlation. The verification sources do not have as complete of experimental data as the sources used for correlation regression. Holstein, *et al.* experimented on various coal types to determine if the geographic location of coal affects the pyrolysis behavior, specifically the tar and methane yields during pyrolysis [9].

The contents of this paper detail the progress toward this final correlation. It continues to be a work in progress.

2. Approach

Using the data from Sandia National Laboratories [5, 6], Liu [7], and Argonne National Laboratories [8], an extensive analysis was completed to determine a correlation of the elemental composition of the tar and char products of pyrolysis. Several variables were checked to ascertain any correlation between the variables and the elemental composition of the pyrolysis products. This was done to ensure that the final correlation would contain only the variables that affect the pyrolysis product elemental composition. After the variables affecting product elemental composition are determined, these variables will then be regressed to find a correlation or set of correlations. These correlations will then be tested and verified against the verification sources, including the data from Holstein, *et al* [9]. Further refinement of the correlations may be necessary as more experimental data is incorporated into the study.

3. Results and Discussion

The Sandia Devolatilization Milestone Report contains the data for several different coal types: North Dakota Beulah Zap (a lignite), New Mexico Blue (a subbituminous), Illinois #6 (a high volatile B bituminous), Pittsburgh #8 (a high volatile A bituminous), and West Virginia Pocahontas #3 (a low volatile bituminous). The proximate and ultimate analysis data for these coal types were evaluated at two different temperatures (1050 K and 1250 K) for both the parent coal and the char formed at these temperatures. The coal particles were allowed to pass through the experimental apparatus at different residence times (the longer the particle took to travel through the apparatus, the hotter the final temperature).

Starting with the char elemental composition, the correlation between particle residence time and the fraction of each element in the char samples was analyzed. The plots for carbon fraction, hydrogen fraction, oxygen fraction, and nitrogen fraction follow.

Figures 1-5 show the normalized mass percent of carbon, hydrogen, oxygen, nitrogen, and sulfur (respectively) in the char particles at different residence times. All mass percent values are normalized by dividing them by the parent coal elemental mass percent values. Parent coal mass percent values are included at a residence time of zero milliseconds. A residence time of zero milliseconds indicates the elemental composition of the parent coal, and higher residence times correlate to longer amounts of time in the reactor.

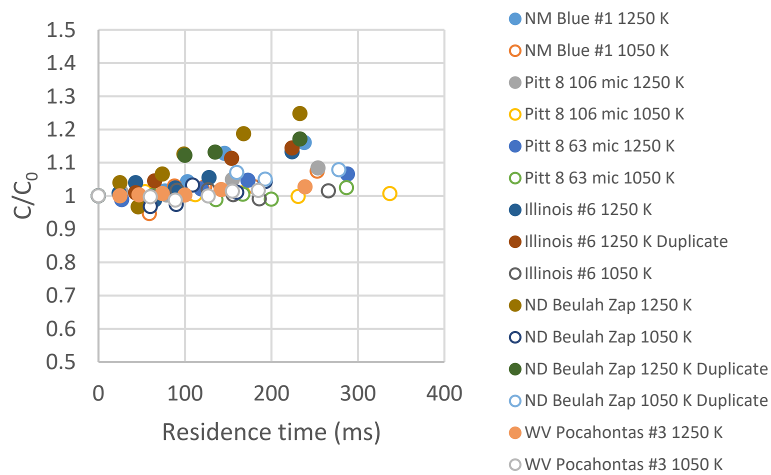

Figure 1: Shows the mass percent of carbon in the char particles at different residence times. Data was taken for a variety of coals at different hold temperatures (1050 K and 1250 K) and at different residence times

As shown in Figure 1, the normalized mass percent of carbon in the char particles generally increases with increasing residence time, with greater increases at higher temperatures.

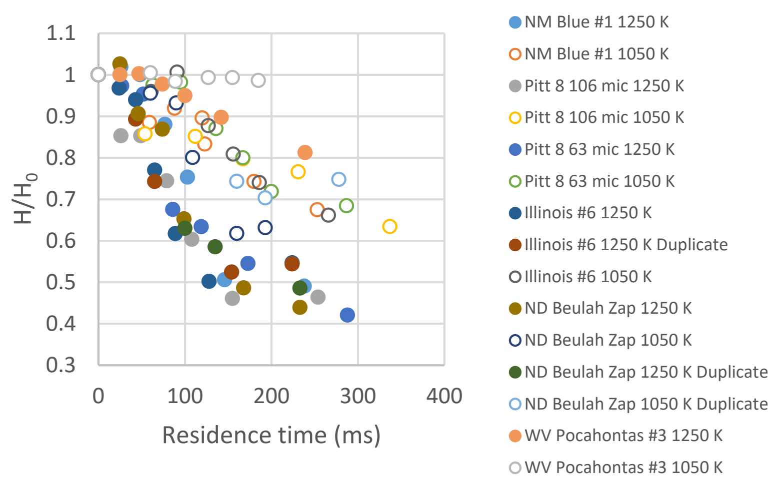

Figure 2: Shows the mass percent of hydrogen in the char particles at different residence times.

Figure 2 shows the mass percent of hydrogen in the char particles as a function of residence time. The normalized mass percent of hydrogen appears to decrease dramatically as residence time increases, particularly at higher temperatures. More analysis is necessary to determine if this is significant for the final correlation.

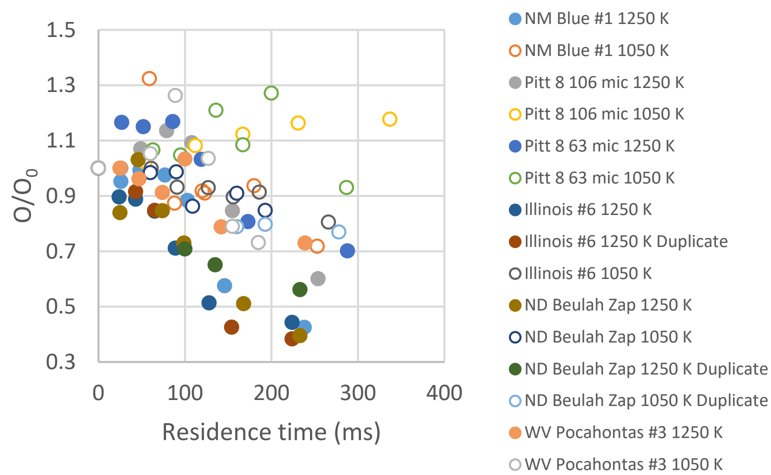

Figure 3: Shows the mass percent of oxygen in the char particles at different residence times.

As Figure 3 indicates, the normalized mass percent of oxygen in the char appears to decrease as residence time increases, however, there are some coal types that appear to increase the normalized mass percent of oxygen. As with the hydrogen mass percent, more analysis is necessary to determine if this is significant in the final correlation.

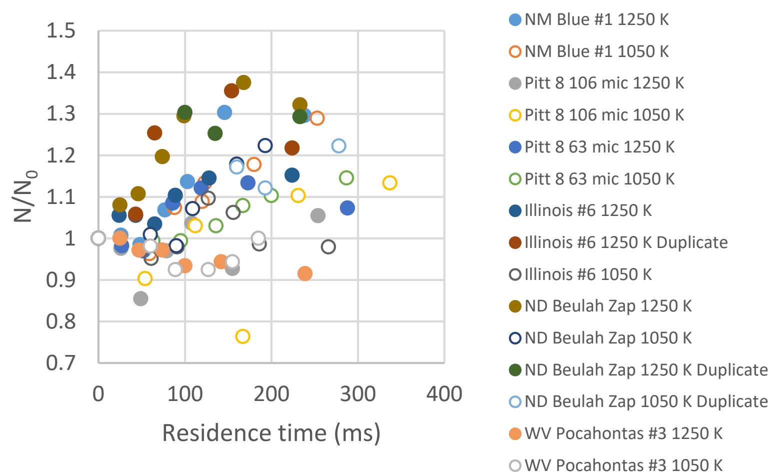

Figure 4: Shows the mass percent of nitrogen in the char particles at different residence times.

Figure 4 shows the normalized mass percent of nitrogen in char particles as a function of residence time. There appears to be a slight increase in the mass percent of nitrogen as residence time increases for some coal types, but not for others. More analysis is necessary to determine the statistical significance.

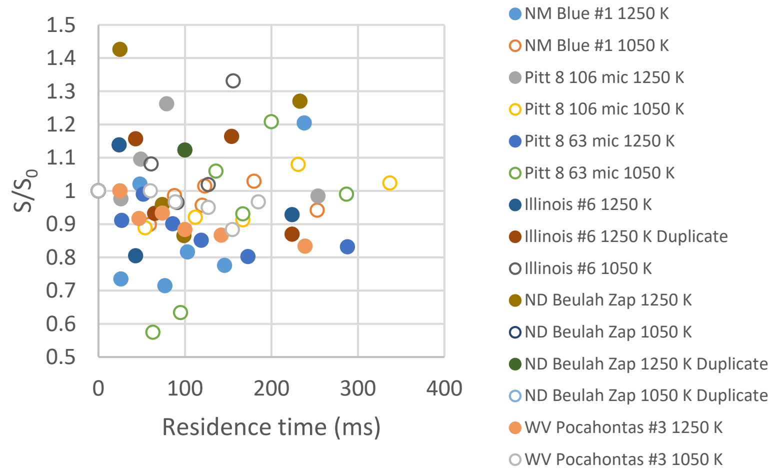

Figure 5: Shows the mass percent of sulfur in the char particles at different residence times.

Figure 5 shows the the normalized mass percent of sulfur in the char particles at different residence times. As with the other elements, a residence time of zero milliseconds corresponds to the parent coal composition. This figure seems to indicate a general decreasing trend of sulfur content as residence time increases at sufficiently high residence times. At low residence times, the sulfur content shows some interesting trends, greatly increasing or decreasing from the parent coal content depending on coal type and hold temperature.

As stated in the introduction, this material comprises the progress of this research up to this point. More analysis is needed to determine the remainder of the variables important for the final correlation.

4. Conclusions

As shown, there are some promising results toward the construction of a correlation to predict the elemental composition of the products of pyrolysis, primarily the char and tar compositions. The analysis indicates that the higher temperature experiments produced more extreme results than the lower temperature experiments. This means that the normalized mass percent of all elements increased or decreased more significantly at higher hold temperatures than at lower temperatures, indicating a need to focus more on temperature effects, including hold temperature and heating rate. More analysis is necessary to complete the correlation.

Acknowledgements

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