TITLE: MECHANISMS AND OPTIMIZATION OF COAL COMBUSTION

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ABSTRACT

OBJECTIVE

This project aims to:

(1) elucidate the fundamental pyrolysis and combustion mechanisms and quantify the effect of several important process conditions on the combustion behavior of chars;

(2) measure some key structural parameters of coals and chars needed for the optimal design of coal combustors;

(3) develop and test models that can predict particle ignitions and calculate the bum-off times of coal and char particles; and

(4) propose process modifications that will improve combustion efficiency and lower the emission levels of atmospheric pollutants.

One of the novelties of the proposed research involves the application of video microscopy and digital image analysis to study (a) the transient particle swelling during pyrolysis and (b) particle ignitions during coal and char combustion.

ACCOMPLISHMENTS TO DATE

A new technique combining video microscopy, image processing and thermogravimetry was developed to detect ignitions of char and coal particles. Chars were prepared at heating rates ranging from 0.1 EC/s to 1,000 EC/s using two reactor systems. The f'u'st system used was a TGA/VMI reactor that is built around a thermogravimetric analyzer and is equipped with a sophisticated video microscopy system. Heating rates up to 20 EC/s could be achieved with this reactor. A captive sample reactor was used to produce chars at high pyrolysis heating rates. This reactor was also equipped with a video microscopy system and could achieve heating rates as high as 1,000 EC/s with good reproducibility.

Chars produced from Illinois #6 and Pocahontas coals were then reacted with oxygen at ambient temperatures ranging from 400 to 750 EC. The multiple-particle combustion experiments were recorded and the video tapes were processed with the help of a digital image analysis system to obtain time-resolved light intensity traces for *each* of the reacting char particles. By analyzing the light intensity

traces and the simultaneously collected thermogravimetric data, we were able to accurately detect thermal particle ignitions. While isolated ignitions could be detected by either thermogravimetry or video microscopy alone, multiple ignitions occurring over a short period of time could only be detected through video microscopy. This is because the reactivity peaks caused by the sudden increase in the combustion rates of ignited particles overlapped when these ignitions occurred within a short time interval, leading to a broad maximum in the reactivity pattern. On the other hand, thermogravimetric data allowed us to detect faint ignitions where the rise in the char particle temperature was not high enough to produce bright light emissions. Our video microscopy setup also enabled us to observe that some char particles ignited multiple times in the same combustion run. These secondary ignitions commonly occurred at high combustion temperatures and high oxygen concentrations. Secondary ignitions could produce a separate reactivity peak, if there was a sufficiently long delay between the primary and secondary ignitions. In many cases, however, the secondary ignitions occurred very soon after the primary ignitions and video microscopy was the only means of detection.

The combination of video microscopy with digital image processing gave us a powerful tool for detecting ignitions occurring in ensembles of reacting char particles. By allowing detailed characterization of the ignition behavior of *individual particles* in an ensemble, the new technique provides information that previously could be obtained only with single particle experiments. Thus, we expect that the new ignition detection technique will be particularly useful for studying particle interactions, which play an important role in coal combustion. Video microscopy was also very useful in identifying the ignition mechanism of reacting char particles. Our results showed that the ignition of char particles typically occurs heterogeneously. Other transient phenomena (such as multiple ignitions of a single particle) were also detected.

We have also studied coal combustion using an experimental procedure that attempts to simulate more closely the sequence of pyrolysis and combustion steps occurring in industrial combustors. The new technique was used to investigate the effect of heating rate on the overall reactivity of coal particle and the time required to reach 98% conversion. When reaction took place in the regime of diffusional limitations, particles heated at the intermediate rate of 1 EC/s exhibited the highest reactivity and shortest burn-off times. This is because pyrolysis at this heating rate produced chars that have more open macropore structures than chars produced at either 0.1 or 10 EC/s. We observed, however, that the differences in reactivity and burn-off times measured for the various heating rates became smaller as the combustion temperature increased. This is because diffusional limitations in both the micropores and the macropores of the coal particles became more severe as the combustion temperature increased.

SIGNIFICANCE TO THE FOSSIL ENERGY PROGRAM

The macropore structure of chars is a major factor in determining their reactivity during the gasification stage. Our studies aim at quantifying through *direct measurements* (a) the effect of pyrolysis conditions of the macropore structure of chars, and (b) the effect of the macropore structure on the char reactivity pattern observed during gasification at high temperatures where intraparticle diffusional limitations are rate-controlling. These studies will provide essential parameters for the optimal design of coal combustion processes.

PLANS FOR THE COMING YEAR

Our plans for the last year of this grant are to complete the development of a theoretical model that can explain the observed effects of pyrolysis heating rates, char macropore structure, and combustion conditions on the reactivity and burn-off times of coal particles. This comprehensive model will consider a bimodal pore size distribution and will describe the diffusion-reaction problem both at the microscopic (micropore) scale and the macroscopic (coal particle) scale.

ARTICLES, PRESENTATIONS AND STUDENT SUPPORT

Journal Articles

D.S. Perkins and K. Zygourakis, "Detection of Coal and Char Particle Ignitions," *Industrial & Engineering Chemistry Research*, submitted.

, A. Ismail, D. S. Perkins and K. Zygourakis,"The Effect of Pyrolysis Conditions on Coal Particle Swelling and D evolatilization Rates," to be submitted.

- A. Ism ail, D. S. Perkins and K. Zygourakis,"A Mathematical Modei for the Ignition of Devolatilized Char Particles," to be submitted.
- Y.W. Cai and K. Zygourakis, "Effect of Combustion Conditions of Burn-off Times of Coal Particles," in preparation.

Presentations

- D.S. Perkins and K. Zygourakis, "Ignition and Reactivity of Coal and Char Particles," presented at the 1996 Annual MeetingoftheAIChE,Chicago, IL, November 1996.
- D.S. Perkins and K. Zygourakis, presented at the 1997 Annual Meeting of the AIChE, Los Angeles, CA, November 1997.
- K. Zygourakis, "Mechanisms and Optimization of Coal Combustion," University Coal Research Contractors Review Meeting, Pittsburgh, PA, June 1998.
- Y. Cai and K. Zygourakis, "Effect of Combustion Conditions of Burn-off Times of Coal Particles," to be presented at the 1999 A nnu al A IC hE Meeting, D alias, TX, N ovem ber 1999.

Students Supported Under this Grant

- D. Samuel Perkins, graduate (Ph.D.) student in chemical engineering, Rice University.
- Y.W. Cai, graduate (Ph.D.) student in chemical engineering, Rice University.