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The Role of Pore Structure on Char Reactivity

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Quarterly Progress Report

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Introduction

Studies of the role of pore structure on the reactivity of coal chars are being conducted using an electrodynamic balance. Correlations of the kinetically limited reactivity of chars with their micro-, meso-, and macro-porosities will be used to guide the refinements of models of char reactivity. The adequacy of the models will be tested by their ability to reproduce the burning history of char particles over a wide temperature range, from ignition to above 25000 K.

Progress Report

The projet has had a slow start because of the delays in enrolling a student, which has been recently accomplished. In the interim the literature was reviewed and organized for a presentation as an invited lecture at an International Workshop on Heterogeneous Combustion at the Dead Sea in January. In addition, preliminary work on preparing char samples for use in the electrodynamic balance has been conducted.

The Wyoming lignite raw coal was size classified to 38-45 μm, first by air-classification to remove the fine particles, and then by sieving with a standard Ro-tap sieving machine. The size-classified Wyoming lignite was then pyrolyzed in a laboratory-scale laminar flow furnace at 1650K, 100% N_2. About one gram of pyrolyzed char was collected with Millipore membrane filters (teflon/polyethylene).

The char sample thus collected was carefully poured into an cylindrical mold filled with epoxy resin and thoroughly mixed with epoxy resin. In order to remove the air bubbles trapped during mixing in the mixture, the sample-filled mold was placed in a dessicator connected to a vacuum pump. By periodically evacuating the dessicator, trapped air bubbles could be removed. The mold with the char sample and epoxy resin was placed in a cool area for 24 hours until it hardened. One end of the hardened cylindrical plug was carefully polished with alumina paste so that char particles embedded could also be cross-sectioned.

The polished end of the sample plug thus prepared was observed under a Wetzlar optical microscope with a built-in camera. Pictures of fifty cross-sections of char particles were taken. The magnification was in the range of ×100 and ×650. Figure 1 shows cross-sections of char particles shown in black and white images. (The carbonaceous matrix is shown in black.)

Characterization of the pore structure of the char was carried out by digital image processing on cross-sections of the char particles. Pictures of cross-sections were scanned in, digitized in 600×512–pixel, 256-grayscale images using an Apple Scanner. Grayscale images were first converted to binary black-and-white images by setting a grayscale threshold that gives the best images of pores and char. Editing, i.e., sharpening and noise reduction, was performed to the binary images using *Image* v 1.17, a public domain

Figure 1. Cross-sections of 38-45 μm Wyoming lignite char particles

program. In *Image*, the area of the cross-sectioned char (including pores) was measured as well as the areas of pores in the char. Area measurement was done by counting the number of pixels a feature occupies.

A stereological analysis was then performed to obtain the three-dimensional pore size distribution from two-dimensional data. Assumptions were made that pores are spherical in shape and do not overlap with each other. When spheres of random radius, r, between 0 and r_m, distributed randomly in a three-dimensional space with N(r) as its corresponding probability density function are intersected by a plane of random orientation, a collection of circles is generated on the plane with their respective radius, ρ, randomly distributed between 0 and r_m, and with a probability density function, n(ρ). The two probability density functions N(r) and n(ρ) are related to each other as follows (Wicksell, 1925).

$$n(\rho)\, d\rho = \int_{\rho}^{r_m} \frac{2\, N(r)\, \rho\, d\rho\, dr}{\sqrt{r^2 - \rho^2}}$$

The integral equation was converted into a set of linear equations by discretizing it and employing a trapezoidal integration rule (Zygourakis and Glass, 1988). The details of the procedure is found elsewhere (Kang, 1991).

The size distribution of pores greater than 1 μm that are of interest in the present study were generated by the digital imaging process described earlier. The macroporosities of the char were obtained by taking the ratio of the measured cross-sectional area of pores and that of char matrix. The average porosity of the lignite char was 0.732 ± 0.097. Fifty particles were examined.

The cumulative pore volume distribution obtained from the stereological analysis is shown in Fig. 2. The log mean radius of the pores of the char calculated by the volume weighting was 15.3 μm.

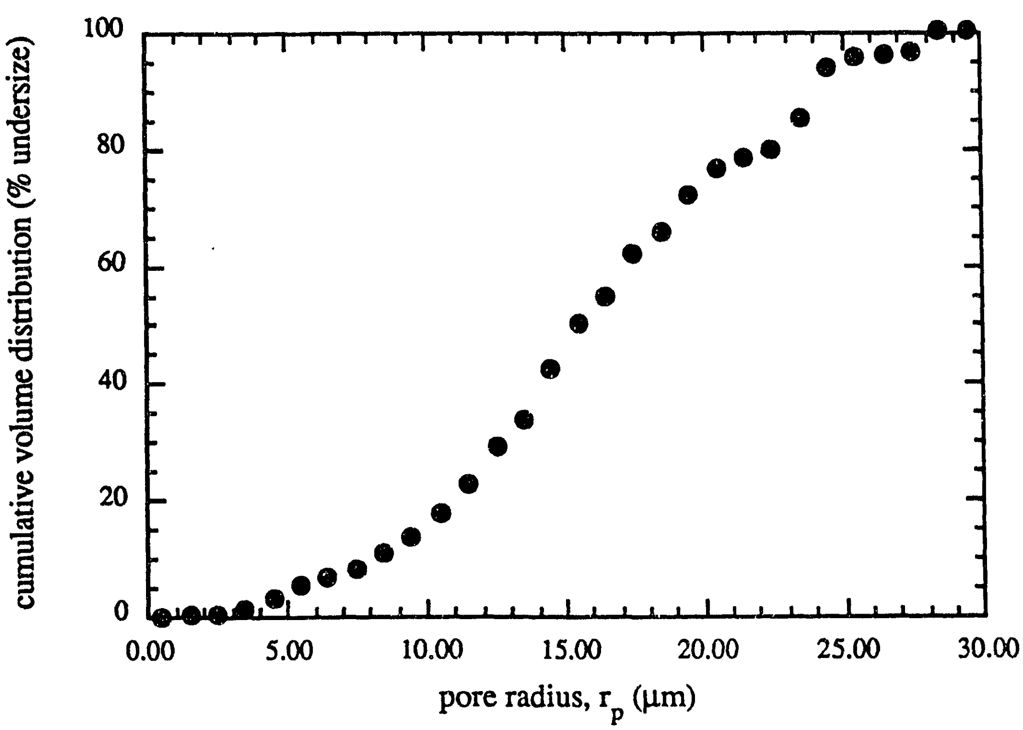

Figure 2. Cumulative pore size distribution of Wyoming lignite

References

Kang, S.G. (1991), PhD Thesis, Department of Chemical Engineering, MIT.
Kang, S.G. and Sarofim, A.F. (1992), submitted to Combustion Science and Technology
Wicksell, D.D. (1925), Biometrica, **17**, 84.
Zygourakis, K., and Glass, M. (1988), Chem. Eng. Comm., **70**, 39.

Publications

With M. D'Amore and L. Tognotti, "Oxidation Rates of a Single Char Particle in an Electrodynamic Balance", presented at "International Workshop on Heterogeneous Combustion", Jan 5-9, 1992, submitted for publication in Combustion and Flame. (Result of collaboration between P.I. and colleagues in Italy on modeling of role of pore structure).

Future Plans

No research will be carried out over the summer while the Sc.D. student is away. Program will be reinitiated on his return 9/1/92.

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