# STRUCTURE BASED PREDICTIVE MODEL FOR COAL CHAR COMBUSTION

Technical Progress Report for the Period: July 1, 2000 - September 30, 2000.


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Report Issue Date: June 15, 2001

DOE Award Number: DE-FG22-96PC96249



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## Disclaimer

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## EXECUTIVE SUMMARY

This report is part on the ongoing effort at Brown University and Ohio State University to develop structure based models of coal combustion. A very fundamental approach is taken to the description of coal chars and their reaction processes, and the results are therefore expected to have broad applicability to the spectrum of carbon materials of interest in energy technologies.

This quarter, the project was in a period no-cost extension and discussions were held about the end phase of the project and possible continuations. The technical tasks were essentially dormant this period, but presentations of results were made, and plans were formulated for renewed activity in the fiscal year 2001.

## PROJECT DESCRIPTION

The problem of excessive unburned carbon in fly ash could be better managed if designers and users of combustion systems could determine the reactivity of a given char from basic coal properties, avoiding the need to resort to expensive full-scale testing. Establishing a mechanistic link between coal properties and fuel behavior has long been a goal of the coal research community, as such a capability would find numerous uses in predictive tools and optimization tools for coal technologies. Such a predictive capability will not likely be achieved through incremental improvements to current models — new, more fundamental approaches are needed such as the structure-based approach, which we believe has the long term potential to make the required mechanistic links between coal properties and char behaviors.

The overall objective of this project is to carry out the fundamental research needed to develop a first-generation, structure-based model of coal char combustion. The project involves combustion experimentation at a variety of scales, theoretical treatments of surface chemistry, and the development and refinement of advanced modeling techniques describing solid-state transformations in coal chars. The fundamental modeling approaches taken here may also produce auxiliary benefits for other coal technologies, including cokemaking, liquefaction, activated carbon production and use, and carbon materials manufacture (fibers, composites, graphite, etc.). The crystalline structure of carbons and its evolution during processing plays an important role in each of these diverse applications.

This combined experimental and theoretical approach will result in a first-generation, structure-based model that is a significant improvement over empirical models in its ability to:

- predict the rank-dependence of char reactivity
- predict the dependence of char reactivity on heat treatment conditions
- describe reaction kinetics in a wide variety of combustion environments

### Task Structure

This Project consists of the following three interrelated tasks:

*Task 1. Project Management*

This task involves reporting, documentation, coordination of effort at the three participating universities, and interactions with the advisory board.

*Task 2. Development of Structure-Based Models*

The objective of this is the development of new models that describe the combustion process on a more fundamental basis. Dynamic models will be formulated that describe the evolution of char crystal structures in flames, and fundamental computational treatments of oxidative attack on model PAH and graphitic structures will be carried out. This task also includes laboratory-scale

experiments designed to establish link between char structure and oxidation reactivity, and a direct investigation of carbon crystalline rearrangements by in- situ, hot-stage HRTEM.

*Task 3. Experiments in Practical Combustion Systems*

This represents a parallel effort to investigate and document the importance of thermal history effects on char structure and reactivity in well-controlled and characterized coal flames. Comparative experiments will be carried out on two reactor facilities with widely varying flame type and the properties and reactivities of the chars characterized.

**Project Team**

The project involves three universities (Brown, Ohio State, and Boston University), in order to couple engineering experts in coal combustion and carbon science (at Brown and Ohio State) with research groups in the pure sciences specializing in modern computational chemistry (OSU) and in solid state physics (BU). The multidisciplinary team will apply modern scientific tools to the challenging technological problem of linking char combustion behavior with coal properties and processing conditions.

The project is supported by an advisory panel assembled from industry, academia, and the national laboratories with a wide range of expertise. The panel members are:

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|---|---|
| Hamid Farzan | Babcock and Wilcox Co |
| Alan Kerstein | Sandia National Laboratories |
| Harry Marsh | University of Alicante |
| Arun Mehta | Electric Power Research Institute |
| Richard McCreery | Ohio State University |
| Nsakala Nsakala | ABB Combustion Engineering |
| Stuart Daw | Oak Ridge National Labs |

## PROGRESS THIS PERIOD

### Brief Summary of Activities

In July, PIs Hurt and Calo attended the World Carbon Conference and presented results derived in part from the current project. The two main references are given below:

1. Hu, Y., Hurt, R.H., "A Comprehensive Thermodynamic Model of Carbonaceous Mesophase," *Proceedings of Eurocarbon 2000: The First World Conference on Carbon*, Berlin, July, 2000.

2. Shim, H-S., Hurt, R.H., Crawford, G., Woodward, C., and Bernstein, S. "Investigation of Surface Anchoring in Mesophase Pitch by In Situ and Ex Situ Optical Microscopy" *Proceedings of Eurocarbon 2000: The First World Conference on Carbon*, Berlin, July, 2000.

Laboratory work was essentially dormant this period as plans were made for a final continuation phase into the fiscal year 2001. These plans include the continuation of work on the memory loss phenomena, additional work on computations chemistry of aromatic oxidation, and new studies on liquid crystal surface anchoring in mesophase pitch.