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North Carolina A&T State University

A Distributed Activation Energy Model of Heterogeneous Coal Ignition

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Introduction

It is well known that coal is a highly inhomogeneous fuel made up of mostly carbon by mass. Usually, it also contains a substantial amount of mineral matter. These facts lead to the expectation, borne out by experimental observations, that in any single batch of pulverized coal, both chemical and thermophysical properties vary widely from particle to particle. It is also obvious that in any sample batch, there exists a wide distribution of particle sizes (diameters) — even after the sample is sized through standard wire-mesh sieves — and densities.

Experiments designed to measure kinetic rate constants of ignition of pulverized coals showed clearly that, for single particles or dilute suspensions, particle-to-particle variations due to reactivity and/or thermophysical properties are important. There exists ample evidence that the most important factor in interpreting these data is the existence of a variation in chemical reactivity in the sample. It is surprising, therefore, to note that all previous studies presumed that a single (average) activation energy is adequate to describe the ignition process. The equations formulated using this presumption are then correlated to the experimental measurements to infer the kinetic rate constants of ignition.

Our major objectives are to develop a model of heterogeneous ignition which allows for a *distribution of activation energies*, and to implement this model to interpret previously published data. It is our hypothesis that variations in chemical reactivity account for the experimental trends observed. Another objective of this project is to examine the effects of variations in thermodynamic and physical properties (e.g. specific heat, particle diameter, density) on data interpretation from previous ignition experiments.

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Objectives

Our objectives for this project are:

1. To acquire a computer workstation on which to conduct this study;
2. Develop the Distributed Activation Energy Model of Heterogeneous Ignition;
3. Identify and gather all previous studies of coal ignition studies, and tabulate those ignition data deemed reliable and useful;
4. Apply our model to analyze previous data and determine ignition rate parameters;
5. Communicate our findings to the research community.

Accomplishments in This Quarter

Personnel

We were unsuccessful in recruiting undergraduate students to work on this project. However, a student has committed to working on this project during the summer months.

Research

During this reporting period, we have completed all equipment purchases for this project, and have received all items.

We have also made significant progress in formulation of our Distributed Activation Energy Model of Coal Ignition. Some initial calculations were performed and the results accurately model the experimental data reported by various researchers. Our results to date have been compiled and it will be presented in April at the Contractors' Review Meeting in Atlanta, Georgia. A copy of the presentation is included as part of this report.

During the next quarter, we will begin to apply the model to previously published data in the literature in order to determine kinetic rate constants. All of the relevant data were listed as references in our previous Technical Progress Report. We will also begin to write a paper, for submission to a journal, describing these efforts.

Goals for Next Quarter

During the next quarter, we expect to:

1. perform computations using the model;

2. tabulate previous ignition data (from references listed in the previous Technical Progress Report) for comparison;
3. extract kinetic rate constants from previously published data in the literature;
4. prepare a paper for journal publication.

North Carolina A&T State University

A Distributed Activation Energy Model of Coal Ignition

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Conventional Ignition Experiment

Experiment Conditions

- hot, still gas in furnace
- controlled O_2 concentration
- T_g is independent variable
- several runs under same condition

Heterogeneous Ignition Theory

$$\text{heat generation} = Q_g = H_c \cdot \chi_{O_2}^n \cdot A_o \cdot \exp \left[\frac{-E}{RT_p} \right]$$

$$\text{heat loss} = Q_l = \frac{2k}{D}(T_p - T_g) + \varepsilon\sigma(T_p^4 - T_g^4)$$

AT CRITICAL IGNITION:

$$Q_g = Q_l$$

$$\frac{dQ_g}{dT_p} = \frac{dQ_l}{dT_p}$$

Experimental Results:

conventional experiment

Experimental Results:

laser-ignition experiment

bituminous coal

■ 96 μm in 100% O₂

● 136 μm in 100% O₂

▲ 96 μm in 51% O₂

anthracite coal

▼ 136 μm in 100% O₂

Distributed Activation Energy Model (DAEM)

$$f(E) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(E - E_0)^2}{2\sigma^2}\right]$$

Model Assumptions

- particles in sample have *activation energies* described by Gaussian distribution
- ignition or non-ignition determined by particle with highest reactivity (lowest E)

DAEM of Ignition Experiments

Simulation Conditions

- initial sample contains 10^5 particles, with energy distribution given by Gaussian distribution
- each 'run' of experiment consists of 100 randomly chosen particles
- total of 20 'runs' at each gas temperature
- ignition or non-ignition determined by particle with lowest activation energy (highest reactivity)

Model Results:

Two Simulations of Identical Conditions

Simulation Input

- $E_o = 120$ kJ/mol
- $\sigma = 16$ kJ/mol
- $A_o = 500$ kg/(m² s)
- $H_c = 9210$ kJ/kg
- $\chi_{O_2} = 1.00$
- $n = 1.0$

Model Results: Effect of E_o

Simulation Input

- $E_o = 110$ kJ/mol
- $E_o = 120$ kJ/mol
- $\sigma = 16$ kJ/mol
- $A_o = 500$ kg/(m² s)
- $H_c = 9210$ kJ/kg
- $\chi_{O_2} = 1.00$
- $n = 1.0$

Model Results: Effect of σ

Simulation Input

- $E_o = 120 \text{ kJ/mol}$
- $\sigma = 20 \text{ kJ/mol}$
- $\sigma = 12 \text{ kJ/mol}$
- $A_o = 500 \text{ kg/(m}^2 \text{ s)}$
- $H_c = 9210 \text{ kJ/kg}$
- $\chi_{O_2} = 1.00$
- $n = 1.0$

Did We Get Everything Right?

"We had a little problem with the decimal point."

Experimental Results:

effect of χ_{O_2}

What's Left Out?

product of reaction of C with O₂

measurements show product depends on T_p

$$y = \frac{\text{moles CO}}{\text{moles CO}_2} = A \cdot \exp \left[\frac{-E}{RT_p} \right] \Rightarrow H_c = y(9210) + (1-y)(32790)$$