Critical Regimes of Coal Ignition

In a normal operation of the coal fired power plant, critical regimes exist, where the particles cannot be ignited either in the gas mode or in the heterogeneous mode due to excessive heat loss. Following thermal theories of ignition, sufficient conditions for the extinction sizes for quenching gas phase combustion are presented along with critical limits for the gas phase and heterogeneous mode of ignition of coal particles. Universal plots are given to present the critical particle sizes of both modes of ignition. Terms of cabin and physico-chemical data of any coal/char particle. Quantitative results for the critical size and oxygen concentration of brown coal particles estimated from the plots are found to check with the iterative numerical results carried out elsewhere. Such sizes and oxygen concentrations may serve as igniteability indices of different coal particles.

1 Introduction

When pulverized coal particles encompassing a size variation (65 percent to 75 μm) are loaded into a hot furnace (about 7 kg/s), the particles undergo rapid heating (10^4 to 10^5°C/s), partial pyrolysis (40–50 percent high volatile coal gets gasified), ignition either in the gas phase or on the surface, combustion of volatiles and char (combustion intensity around 400 kJ/m^3 atm) [1–3] and finally rejection of ash and unburnt carbon through slag and exhaust. When these particles are injected with a swirl motion along with the primary air, the larger particles are thrown to the edge while the smaller ones are trapped in the center. Large particles (100–200 μm) mainly burn under diffusion control following familiar diameter square law [1, 4]. Smaller particles, on the other hand, burn under finite chemical kinetics [5, 6]. Very small particles unable to make up the heat loss, even take external heat input (from larger particles) to equilibrate with the ambient thermal condition. Sometimes the required temperature for ignition of small particles may be so high that raising the furnace temperature for ignition may melt the ash to form a slag around the particle thus preventing further erosion of carbon. Such slag coverage is not uncommon in a typical power plant [7]. Also, the calculations of the burning particle temperatures show that the temperature difference between the particle and the surroundings decreases to a very small value for smaller particles (∼ 15 K for a semi-Anthracite particle of 22 μm [8]) which result in negligible radiative transfer to the water banks, thus increasing the heat loss through exhaust gas. Not only is it an indication of decreased heat contribution from smaller particles, but it also poses a problem of ignition of such small particles (such as unburnt solid carbon particles which are analogous to unburnt hydrocarbons). Thus from the point of view of ignitability, the smaller the particles and the lesser the oxidant available for the attack, for given size of the furnace the unburnt losses are larger either through rejection via slag/ash (carbon content rejected in ash could be as high as 30–50 percent) or via exhaust gas (size of emitted particulate matter ranges from 10 μm–400 μm). Also, smaller particles are less amenable to rapid gas phase oxidation of CO unless intense recirculation is maintained [9]. Recently, attention has also been drawn to the problem of unburnt carbon not only from the point of view of combustible loss (about 1 percent) and the environmental hazards but also the difficulties they pose to the proper maintenance of the plant equipment [10].

The smaller particles, on the other hand, exhibit rapid heating (thus more pyrolysis may be available [11] which may ease ignition problem) and hence less time to attain the furnace temperature. If the particle is heated both by radiation from furnace walls at \( T = T_F \) and by conduction, the heating history \( T_w \) versus \( t \) of a particle of dia \( d_c \) is governed by the following equation:

\[
\frac{d_te_{C_D}}{6} \frac{dT_w}{dt} \approx \epsilon(4T_F^4 - T_w^4) + \frac{\Delta T}{T_F - T_w}
\]

where \( \epsilon \) is the emissivity, \( \sigma \) is Stefan-Boltzmann constant and other symbols are described in the nomenclature. The result of integration of equation (1) with initial condition \( T_w = T_{w0} \) at \( t = 0 \) is shown in Fig. 1. Thus when particle size is small, convective heating dominates the heat up time \( t = d_c^2 \) while at a larger size radiation is significant \( t = d_c \). For complete burning, the burning time \( t_b = d_c^2 \) under a diffusion control, \( t_b = d_c \) under chemically controlled rate and \( t_b \) is independent for size for volume reaction. Thus a 25 μm particle takes only about 1 ms to heat up to a temperature of 1000 K, while at the same temperature \( t_b \sim 100 \) ms. Thus dominant mechanisms of heating, ignition and burning shift depending upon the mode of heating, size and degree of reactivity of the particle. Also, for smaller particles, oxygen could diffuse through the porous interior, thus offering increased surface area of oxidation per unit volume and pro-

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1 Carbon is capable of reacting with NO (e.g., fluidized beds) to reduce NOx pollution while trace amounts could also increase radiative heat transfer to water tubes. Though soot may also be carbon particles, normally they refer to those particles occurring via gas phase fuel pyrolysis reactions.
moting burning at constant density (e.g., Semi-Anthracite [8]). Thus there exists a spectrum of optimum size and size distribution for the particles constrained by the differing requirements of environmental standards, maximum thermal efficiency in a smaller volume and optimum power production per unit mass of the fuel injected. One such constraint is imposed by the ignitability condition of coal/carbon. The parameters of interest are: 1) overall extinction limits for solid fuel-air mixture, 2) particle size, and 3) oxygen concentration. Overall extinction limits of a solid fuel-air mixture can be determined from laminar velocity experiments. An estimate of these limits can be given as follows.

Consider a long combustion chamber where there is a stationary flame front. The flame front is being supplied by a mixture of solid fuel particles and air at \( T = T_{fl} \). Extinction is assumed to occur when the flame temperature \( T_f \) falls below a critical value \( T_f = T_{crit} \). If the mixture is lean all the fuel is burnt and if rich all the oxygen in the incoming mixture is consumed. Neglecting heat losses to the chamber, the heat balance across the flame front yields the lean limit as

\[
\frac{\rho_{f}v_{f}}{\rho_{a}} = \frac{1}{\left[ \frac{Q}{C_{p,a}(T_{f, crit} - T_{a})} - 1 \right]}
\]

and the rich limit as

\[
\frac{\rho_{f}v_{f}}{\rho_{a}} = \left[ \frac{Q}{C_{p,a}(T_{f, crit} - T_{a})} \frac{C_{p,a}}{C_{p,o}} \left( 1 + \frac{v_{o}}{v_{a}} \right) + 1 \right] \frac{\Phi_{a}}{\Phi_{o}}
\]

where \( \rho_{a} \) is the density of air.

Letting \( T_{f, crit} = 1500 \text{ K} \), \( T_{a} = 300 \text{ K} \), \( Q = 3.1 \times 10^{6} \text{ J/kg} \), \( C_{p,a} = 1121 \text{ J/kg K} \), \( C_{p,o} = 1507 \text{ J/kg K} \), \( \rho_{o} = 1 \text{ kg/m}^{3} \) the lean limit is estimated to be 70 g/m³ while the recent experimental results of Smoot et al. [12] give the result as 80–200 g/m³. This lean limit can be reached by supplying a large number of smaller sized particles or by a smaller number of large sized particles. In lightening up and stabilizing a coal fired furnace, one needs to have the ignition of coal particles to occur at a lower temperature (i.e., firing) and to have an appreciate heat feedback from the ignited particles to stabilize the fire. In combustion theory we call the initiation of flaming as initial flaming and stabilization of flaming as ignition [13]. In the direction ignition analysis of individual coal particles is useful.

An ignition study on brown coal particles has been numerically carried out by Thomas, et al. with the assumption of quasi-steady-state and heterogeneous mode of ignition [14].

For example, consider the oxidation of a carbon particle (Fig. 2). The heat liberation rate for the heterogeneous oxidation is exponentially increasing with surface temperature while heat loss is increasing only linearly. According to thermal theory, at the time of ignition, the heat generation rate is equal to heat loss rate and rate of change of generation with temperature is equal to the rate of change of heat loss with temperature. Thus there are two solutions as given by points B and C. When surface temperature is slightly above the value given by point B, then the particle temperature runs away to a value corresponding to the point C. Then \( T_{o} < T_{o, c} \) is called the temperature jump. Critical condition for heterogeneous ignition is said to exist when the slope of heat loss curve is equal to the maximum slope of heat liberation curve (e.g., point D in Fig. 2). It is apparent that carbon (a nonsustaining fuel) ignites on the surface. On the other
hand, a liquid fuel like benzene (totally gasifying fuel) gasifies first and ignition occurs in the gas phase. However, coal is a partially gasifying fuel in that during pyrolysis gases like CH₄, CO, and H₂ are released and remaining substrate remains mainly as carbon. Thus ignition can occur either in gas phase or on the surface depending upon the particle size, oxygen concentration, etc. [15]. In the present paper, both gas phase [15] and heterogeneous ignition modes of coal particles are considered to investigate the existence of ignitability limits (analogous in some sense to the flammability limits of gaseous mixtures). The simplifications carried out in the present paper, without great loss of accuracy, are intended mainly to present the results in terms of general physico-chemical parameters of the coal-air system.

2 Definitions of Critical Regimes

For the purpose of analysis, the following definitions are applicable:

1. The spherical coal particle does not ignite in the gas phase at such a condition when no longer the pyrolysis evolution from the coal particle is sufficiently high enough to keep the flame away from the endothermic quenching coal surface.

2. The spherical coal particle does not heterogeneously ignite at a time when the chemical heat liberation rate is no longer sufficient to balance the heat loss rate to the surroundings and if any perturbation around this joint of thermal equilibration fails to produce a temperature jump for a steady-state problem (e.g., point D in Fig. 2).

3 Critical Regimes for Gas Phase Ignition

3.1 Formulations and Solutions. Consider a strongly pyrolysing spherical coal particle. The pyrolysis gases evolve from the interior or surface of coal, either under the control of competitive chemical kinetics of production and reverse char formation [16] or through the control of pore diffusion through the outer char layer. The fuel gases diffuse into the hot ambient atmosphere, mix with the diffusing oxygen and react in a finite region whose boundaries are defined by the combustible limit mixture corresponding to the local temperature [17]. The products along with the unreacted pyrolysis diffuse into the hot ambient atmosphere. Several ignition criteria are available in the literature which are tabulated in [17]. In general, selection of a particular criterion is based upon the physics of the problem, availability of necessary physicochemical data, the simplicity with which the results may be correlated and the extent to which further information could be meaningfully extracted. According to an adiabatic ignition criterion which is invoked in the present analysis, the ignition occurs at a temperature when the heat liberated in the gas phase regime is just sufficient to supply the endothermic heat of the pyrolysis at the coal surface and to heat the pyrolysisate to the ignition temperature. Hence, the conservation equations are formulated for the principal species (which in the present case is oxidant), products, pyrolyszate, and all other species and energy. For gas phase reaction, a Dirac-delta approximation is introduced for the constitutive Arrhenius reaction rate law in order to linearize the second order ordinary differential equation for oxygen mass fraction, Y₂, and to obtain simplified explicit approximate solutions. Such an approximation is carried out at a location where there is a stoichiometric combustible mixture and at the same time the volumetric nature of such a reaction is maintained by carrying out the step function approximation in a physically meaningful coordinate [18] (unlike the procedure followed in previous works) [19–21]. Then, imposing an adiabatic ignition criterion, an approximate but simple solution for the ignition temperature is obtained. The details of derivation are shown in [15] and [22]. For the sake of clarity, the steps are summarized below.

Energy:

\[
\mathbf{\rho} \mathbf{u} \cdot \frac{d\mathbf{T}}{dr} = \frac{1}{r^2} \left( r^2 \mathbf{D} \frac{d\mathbf{T}}{dr} \right) - \mathbf{w}_i' \cdot \mathbf{Q}_l / r_i \quad (5)
\]

Species:

\[
\rho_i \frac{dY_i}{dr} = \frac{d}{dr} \left( r^2 \rho_i \frac{dY_i}{dr} \right) + \mathbf{w}_i' \cdot \mathbf{Y}_i, \quad i = p, O, P \quad (6)
\]

Chemical Reaction at the Surface:

coal (c) → pyrolyszate (p) + char

\[
\begin{align*}
\mathbf{m}_p &= A_P \mathbf{r}_P \left( \frac{1}{6} \pi d_i^3 \right) \mathbf{Y}_{p,0} \exp \left[ -E_P / R \mathbf{T} \right] \quad (7a) \\
\mathbf{m}_p &= A_P \mathbf{r}_P \left( \frac{1}{6} \pi d_i^3 \right) \mathbf{Y}_{p,0} \exp \left[ -E_P / R \mathbf{T} \right] \quad (7b)
\end{align*}
\]

Chemical Reaction in Gas Phase:

pyrolyszate (p) + Oxygen (O) → Product (P)

\[
\mathbf{w}_p' \cdot \mathbf{Y}_p \mathbf{Y}_0 \mathbf{Y} \mathbf{Y}_0 \exp \left[ -E_p / R \mathbf{T} \right] \quad (7c)
\]

As \( r \rightarrow r_w \)

\[
\begin{align*}
K \frac{dT}{dr} &= \bar{m} \bar{Q}_f \quad (7e) \\
m &= m_p \quad (7f)
\end{align*}
\]

As \( r \rightarrow \infty \)

\[
\begin{align*}
\mathbf{Y}_0 &= \mathbf{Y}_{0,w} \quad (7g) \\
\mathbf{Y}_p &= \mathbf{O} \quad (7h)
\end{align*}
\]

With \( \xi = \bar{m} / 2 \pi \rho D d_i \) and \( \bar{m} = \bar{Q}_f \) in equation (6)

\[
\begin{align*}
d\mathbf{Y}/d\xi &= \mathbf{Y} \quad (8)
\end{align*}
\]

where the flux fraction \( \mathbf{Y}_0 \) is given by

\[
\begin{align*}
\mathbf{Y}_0 &= \mathbf{dY}_0/d\xi + \mathbf{Y}_0 \quad (9a)
\end{align*}
\]

and

\[
\begin{align*}
\mathbf{Y} &= D_{m,0} \mathbf{r} \mathbf{Y}_{0} \mathbf{Y}_0 \mathbf{Y}_0 \exp \left[ -1/\bar{\mathbf{m}} \right] \quad (9b)
\end{align*}
\]

where

\[
\begin{align*}
\bar{\mathbf{m}} &= T / (E_p / R) \quad (9c)
\end{align*}
\]

\[
\begin{align*}
D_{m,0} &= (A_P \mathbf{r}_P / 4 \pi \mathbf{D}(P/E_p))^2 \quad (9d)
\end{align*}
\]

With \( i = p \) in equation (6) one can solve for \( \mathbf{Y}_p \) and using equation (5) one can solve for \( \mathbf{H}_f \). Equation (8) may then be solved by using numerical methods and profiles \( \mathbf{Y}_0(d) \), \( \mathbf{H}_f(d) \) and \( \mathbf{Y}(d) \) in the gas phase can be obtained. With \( \Delta T = \mathbf{c}_p c_p T \) the temperature profile \( T(\xi) \) is known for given \( \mathbf{c}_p \). In order to obtain approximate explicit expression for gas phase ignition temperature the integration of equation (8) is carried by approximating the source term \( \psi \) by a step function. If the activation energy for gas phase oxidation is high (say 150 KJ/mole) then reaction occurs in such a narrow temperature region (e.g., the
Table 1  Definitions of $a$, $x$ and $M$ for critical parameters of gas phase ignition, equation $x^2M = a \ln x^2$

<table>
<thead>
<tr>
<th>The Problem</th>
<th>$x$</th>
<th>$M$</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Size</td>
<td>$m \neq 0$</td>
<td>$\left( \frac{D_{H2O}}{\xi^*} \right)^{1/2} \left[ \frac{1/E_p}{s} + \frac{2}{m} \right]$</td>
<td>$\left( \frac{D_{H2O}}{\xi^*} \right)^{1/2} \left[ \frac{1/E_p}{s} + \frac{2}{m} \right]$</td>
</tr>
<tr>
<td></td>
<td>$m = 0$</td>
<td>$1$</td>
<td>$1.0$</td>
</tr>
<tr>
<td>2) Volatile content</td>
<td>(see 1a)</td>
<td>$1/sE_p$</td>
<td></td>
</tr>
<tr>
<td>3) Oxygen mass fraction</td>
<td>(see 1a)</td>
<td>$(n - 2 + 1/E_p)/s$</td>
<td></td>
</tr>
</tbody>
</table>

Table 2  Chemical kinetics data for pyrolysis of some coals

<table>
<thead>
<tr>
<th>Coal No.</th>
<th>Coal Type</th>
<th>$A_p$</th>
<th>$E_p$</th>
<th>$Y_{p,c}$</th>
<th>$D_{H2O}$</th>
<th>References</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>Bituminous</td>
<td>$8.4 \times 10^5$</td>
<td>74.1</td>
<td>0.31</td>
<td>260.0</td>
<td>[24]</td>
<td>Heating rate 2.5 to 4.0 $\times 10^{14}$C/s</td>
</tr>
<tr>
<td>12</td>
<td>Bituminous</td>
<td>$1.14 \times 10^6$</td>
<td>74.1</td>
<td>0.35</td>
<td>400.0</td>
<td>[24]</td>
<td>Same</td>
</tr>
<tr>
<td>13</td>
<td>Bituminous</td>
<td>$2.81 \times 10^6$</td>
<td>74.1</td>
<td>0.367</td>
<td>1025.0</td>
<td>[24]</td>
<td>Same</td>
</tr>
<tr>
<td>14</td>
<td>Bituminous</td>
<td>$1.34 \times 10^6$</td>
<td>74.1</td>
<td>0.35</td>
<td>470.0</td>
<td>[24]</td>
<td>Same</td>
</tr>
<tr>
<td>15</td>
<td>Bituminous</td>
<td>$706$</td>
<td>49.4</td>
<td>0.298</td>
<td>2.80</td>
<td>[16]</td>
<td>Based on single reaction model 10$^6$C/s</td>
</tr>
<tr>
<td>21</td>
<td>Lignite</td>
<td>$277$</td>
<td>46.5</td>
<td>0.374</td>
<td>1.05</td>
<td>[16]</td>
<td>Same</td>
</tr>
<tr>
<td>31</td>
<td>Anthracite</td>
<td>$1.79 \times 10^7$</td>
<td>117.6</td>
<td>0.114</td>
<td>1015.0</td>
<td>[24]</td>
<td>Heating rate 2.5 to 4.0 $\times 10^{14}$C/s</td>
</tr>
</tbody>
</table>

Equations (3) and (4) will be used to derive the critical limits of the gas phase ignition of coal particles.

3.2 Results and Discussions. There are four main parameters of interest in the present problem: (1) particle size, (2) volatile content, (3) ambient oxygen concentration, (4) pressure.

Writing the solution of one critical parameter in terms of known physicochemical data and the other parameters, one can generalize the results of equations (13) and (14) in the following form.

$$x^{2M} = a \ln x^2$$

where $x$, $a$ and $M$ are defined in Table 1 for several problems of interest. Figs. 3(a) and 3(b) show the general solution of $x$ as a function of $a$ with positive and negative values for $M$. As an example, the critical limits are evaluated for the bituminous, anthracite and lignite coal particles and are listed in Table 3, while Table 2 lists the necessary kinetic data for different types of coal particles. For gas phase oxidation the following properties were used: $A_p = 2.5 \times 10^{12}$g/mole-s, $E_p = 156000$ J/mole, $n_0 = 1.4$, $T = -4^\circ$, $Q_0 = 5160$ J/mole (for methane), and $D_{H2O} = 588.0$. Referring to Fig. 3, it is observed that for values of $M > 0$ there are two values of $x$ for given $a$ and there is a limiting minimum value of $a$ below which there is no solution for $x$; this limit could be obtained from equation (15) as $x^2M = a \ln x^2$. 

#### Table 3  Critical limits of coal particles for gas phase ignition (flame on particle surface)

<table>
<thead>
<tr>
<th>Coal No.</th>
<th>Coal Type</th>
<th>Critical Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>Bituminous</td>
<td>44</td>
</tr>
<tr>
<td>12</td>
<td>Bituminous</td>
<td>30</td>
</tr>
<tr>
<td>13</td>
<td>Bituminous</td>
<td>12</td>
</tr>
<tr>
<td>15</td>
<td>Bituminous</td>
<td>24</td>
</tr>
<tr>
<td>21</td>
<td>Lignite</td>
<td>360</td>
</tr>
</tbody>
</table>

**Note:** This technique is found to work well with burning of heated carbon spheres in cold atmosphere where CO oxidizes in the gas phase.
\[ \alpha_{\text{min}} = \epsilon M \]  
(16a)

\[ x = e^{-1/2M} \]  
(16b)

Fig. 3(c) shows the limiting values of \( \alpha_{\text{min}} \) for given \( x \) (line CD) and the corresponding nondimensional temperature (line AB).

A brief discussion is appropriate. Mathematically, it is clear from equation (15) that for given \( M > 0 \), the ratio (\( \ln x^2/2M \)) \( \rightarrow 0 \) as \( x \rightarrow 1 \) and \( x \rightarrow \infty \); thus the quantity (1/\( \alpha \)) passes through a maximum which is given by equation (16). On the other hand, for \( M < 0 \), the ratio (\( \ln x^2/2M \)) is a monotonically increasing function with increase in \( x \).

For any change in size or volatile content of coal particle, the change in ignition temperature at the critical condition depends upon the following factors: 1) activation energy of pyrolysis, 2) activation energy for gas phase oxidation and 3) density dependence of above two reactions. In general, a large positive value of \( M \) is an indication of strong control of ignition by gas phase oxidation on the surface and a negative value of \( M \), on the other hand, represents the influence of pyrolysis on the ignition process. Thus for positive values of \( M \), one can attribute the two solutions \( x_1 \) (lower curve) and \( x_2 \) (upper curve) due to density dependence of gas phase oxidation. Those temperatures (corresponding to \( x_1 \)) are not of interest to us since we are interested in estimating the minimum temperatures required for ignition which are given by upper solutions of \( x \) (say \( x_2 \)).

Also, looking at Figs. 3(a) and 3(b), it can be observed that the values of \( x \) tend to unity for large values of \( \alpha \) which mean that either the gas phase Damkohler number is very large (fast kinetics, diffusion control in gas phase) or the Damkohler number for the pyrolysis is very small (fast kinetics of pyrolysis, see Table 1); also, when \( x \rightarrow 1 \), the required ignition temperature is of large magnitude. Thus one can formulate a sufficient condition that there is a definite extinction for an already established flame if

\[ \frac{D_H}{\xi} \rightarrow 1.0 \]  
(16c)

With \( Y_{0.5} = 0.23 \) and \( \nu = 4.0 \), a calculation for coal No. 15 shows that for a particle size below about 142 \( \mu m \) there cannot be any gas phase combustion. Howard and Essenhigh [28] assumed a diffusion controlled burning of volatiles released from coal under finite pyrolysis rate and also used their experimental data for the pyrolysis rate to establish a critical particle size of 15 \( \mu m \) below which there can only be burning of volatiles along with heterogeneous oxidation of carbon. Equation (16c) is consistent with this assumption and hence the agreement.

4 Critical Regimes for Heterogeneous Ignition

4.1 Formulations and Solutions. Semanov's thermal theory of ignition is applied for this problem. Assume that gas phase reaction is absent, surface reaction produces arbitrary species and radiation heat transfer at the time of ignition is small (only 20 percent of total heat transfer is contributed by radiation at the instant of ignition)\(^3\).

The oxygen concentration profile and temperature for frozen gas phase reaction is solved from equation (6) with \( i = 0 \) and \( \omega^w = 0 \) and then with \( i = h_1 \):

\[ Y_{0} - Y_{0.5} = \theta_h - \theta_w = 1 - \exp[-\xi] \]

\[ Y_{0.5} - Y_{0.5} = \theta_w - \theta_w - 1 - \exp[-\xi] \]  
(17a)

At the surface, due to stoichiometry, oxygen flux fraction is given as

\[ (\dot{m}_H/\dot{m}_O) = \epsilon = \frac{dY_O}{d\xi} + Y_{0.5} = -\nu \]  
(17b)

\(^3\) Radiation effects can still be included by replacing \( dD \) in the definition of \( (D_H - h)_c \) by \( dD \) \( + 2(\nu \rho) \sqrt{\pi} \) \( dD \).

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Transactions of the ASME
and the oxygen flux is consumed by coal oxidation

$$n_{o} = \rho_{a} A_{w} \frac{P}{RT} \exp(-E_{w}/RT) Y_{O, w}$$  \hspace{1cm} (17c)

Using equations (17a, 17b), and the definition of Damköhler number, the mass fraction $Y_{O, w}$ is obtained. From the heat balance condition at the interface

$$\left( \frac{d\theta_{h}}{dz} \right) = Q_{o, w} + \varepsilon $$  \hspace{1cm} (17d)

Equations (17a–17d) then lead to the following set of algebraic equations:

*The rate of burning of carbon/coal:

$$\varepsilon = (D_{m, w})_{h} \frac{\exp(-1/\theta_{w})}{\theta_{w}} \frac{Y_{O, w}}{\theta_{i}} \exp(-\xi_{h}) \cdot 1 - 1 - \exp(-\xi_{h})$$  \hspace{1cm} (18a)

*Heat Loss:

$$\theta_{w} - \theta_{h} = (\exp[\varepsilon_{h}] - 1) Q_{o, w} + \varepsilon $$  \hspace{1cm} (18b)

*Rate of Change of Heat Loss:

$$1 = \exp[\varepsilon_{h}] \frac{d\varepsilon_{h}}{d\theta_{w}} Q_{o, w} + \varepsilon $$  \hspace{1cm} (18c)

In order to present the solution in terms of generalized physico-chemical parameter, the following approximation is introduced. When the gasification reaction rate is low, prior to and at the time of ignition, ($m \ll 2 \pi \Delta d_{c}$)

$$\exp[\pm \varepsilon_{h}] \approx 1 \pm \varepsilon_{h}$$  \hspace{1cm} (18d)

At the critical point, equating the maximum rate of change of the heat liberation curve with the heat loss curve,

$$\left( \frac{d}{d\theta_{w}} (\varepsilon_{h} Q_{o, w} + \varepsilon_{h}) \right)_{max} = 1.0$$  \hspace{1cm} (19)

the following polynomial equation is obtained for $\theta_{w, h} (= \theta_{w, crit}$ at critical point)

$$a_{1} \sum_{j=0}^{n} a_{j} \theta_{w, crit}^{j} = 0$$  \hspace{1cm} (20)

The coefficients are $a_{0} = 0.25 R$, $a_{1} = 2.5 R$, $a_{2} = 1 - 1.5 R$, $a_{3} = 0.5 R - 4$, $a_{4} = 6$, $a_{5} = -4$ and $a_{6} = 1$. The term $R$ is a non-dimensional heat generation per unit mass of products and is given as follows:

$$R = Q_{o, w} + (Y_{O, w}/\rho_{i})/(1 + Y_{O, w}/\rho_{i})$$  \hspace{1cm} (21)

Using equation (18c) at critical point,

$$Z \exp(-1/\theta_{w, crit}) \left[ (1/\theta_{w, crit}) - (1/\theta_{w, crit}) \right]/\theta_{w, crit} = 1.0$$  \hspace{1cm} (22a)

where

$$Z = (D_{m, w})_{h} \rho_{i} (1 + Y_{O, w}/\rho_{i})$$  \hspace{1cm} (22b)

and $\theta_{w, crit}$ is the solution of equation (20). Equations (20) and (22a) provide the critical parameters (e.g., critical size, oxygen concentration, etc.). The required ambient temperatures to maintain this incipient combustion is given as

$$\theta_{h, crit} = \theta_{w, crit} \left( \theta_{w, crit} - 2 \theta_{w, crit} \right) \left( 1 - \theta_{w, crit} \right)$$  \hspace{1cm} (25)

4.2 Results and Discussion. As observed from equations (20) and (22a), there are three general variables, viz., the modified Damköhler number ($D_{m, w}h\rho_{i}$), the stoichiometric parameter $Y_{O, w}/\rho_{i}$ and the non-dimensional heat of reaction $Q_{o, w}$. Fig. 4 shows the universal plots for the critical heterogeneous conditions for arbitrary set of physico-chemical parameters. Fig. 5 plots the particle temperature versus the heat generation parameter $R$. The dotted line shows the ambient temperatures required to maintain the incipient combustion.

Numerical values of critical particle sizes at given oxygen concentration (say $Y_{O, w} = 0.23$) and critical oxygen concentration at a given particle size (say 100 μm) are of further interest. Table 4 lists the kinetic data collected from the literature for coals and chars. Using Table 4 and Figs. 4 and 5, the critical conditions for heterogeneous ignition of some coals and chars are tabulated in Table 5.

For brown coal the estimates from the plots give the critical size as 24 μm at $Y_{O, w} = 0.23$ and critical oxygen concentration as .12 at $d_{c} = 100$ μm, while the iterative numerical calculations carried out by Thomas et al. [4] including the radiative effects and the transient decrease in the particle size give the respective values as 20 μm at $Y_{O, w} = 0.23$ and .11 at $d_{c} = 100$ μm. Hence, present plots though approximate are still sufficiently accurate enough for the meaningful esti-
Table 4: Chemical kinetics data for heterogeneous oxidation of some coals

<table>
<thead>
<tr>
<th>Coal No.</th>
<th>Coal Type</th>
<th>Q_b[J/g]</th>
<th>E_a[KJ/mole]</th>
<th>A_{a,b}[^\dagger]</th>
<th>(D_{1/2})[^\dagger]</th>
<th>\tau</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Bituminous</td>
<td>20842</td>
<td>124.0</td>
<td>61.0 x 10^6</td>
<td>380.0</td>
<td>1.72</td>
<td>[25]</td>
</tr>
<tr>
<td>2</td>
<td>Lignite</td>
<td>10468</td>
<td>83.7</td>
<td>9.2 x 10^6</td>
<td>13.8</td>
<td>0.885</td>
<td>[25]</td>
</tr>
<tr>
<td>3</td>
<td>Anthracite</td>
<td>25164</td>
<td>140.2</td>
<td>76 x 10^6</td>
<td>418.0</td>
<td>1.885</td>
<td>[25]</td>
</tr>
<tr>
<td>4</td>
<td>Brown</td>
<td>9492[^*]</td>
<td>56.7</td>
<td>3.2 x 10^6</td>
<td>43.0</td>
<td>1.333</td>
<td>[14]</td>
</tr>
<tr>
<td>5</td>
<td>Petroleum Coke</td>
<td>9492[^*]</td>
<td>76.2</td>
<td>2.3 x 10^6</td>
<td>23.0</td>
<td>1.333</td>
<td>[8]</td>
</tr>
<tr>
<td>6</td>
<td>Anthracite Char</td>
<td>9492[^*]</td>
<td>69.6</td>
<td>1.2 x 10^6</td>
<td>13.0</td>
<td>1.333</td>
<td>[8]</td>
</tr>
<tr>
<td>7</td>
<td>Bituminous Char</td>
<td>9492[^*]</td>
<td>67.0</td>
<td>1.0 x 10^6</td>
<td>11.0</td>
<td>1.333</td>
<td>[8]</td>
</tr>
<tr>
<td>8</td>
<td>Brown Coal Char</td>
<td>9492[^*]</td>
<td>67.8</td>
<td>1.1 x 10^6</td>
<td>12.6</td>
<td>1.333</td>
<td>[8]</td>
</tr>
</tbody>
</table>

[^*] assumed that CO is the only product of oxidation.
[^\dagger] The kinetic schemes for heterogeneous oxidations differ as far as the dependence on oxygen concentration is concerned. The schemes were brought to the following format:

\[
m^* = A_{a,b} \frac{P}{RT_w} \exp(-E_a/RT_w)Y_{O_2}
\]

Then the pre-exponent factors A_{a,b} were computed.

Table 5: Critical parameters for heterogeneous ignition

<table>
<thead>
<tr>
<th>Coal No.</th>
<th>Coal/Chars</th>
<th>Critical Conditions at ( Y_{O_2} = 0.23 )</th>
<th>Critical Conditions at ( d_c = 100 \mu m )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>( d_c[\mu m] )</td>
<td>( T_w[K] )</td>
</tr>
<tr>
<td>1</td>
<td>Bituminous Coal</td>
<td>3.3</td>
<td>2540</td>
</tr>
<tr>
<td>2</td>
<td>Lignite</td>
<td>20.2</td>
<td>1750</td>
</tr>
<tr>
<td>3</td>
<td>Anthracite Coal</td>
<td>3.0</td>
<td>2700</td>
</tr>
<tr>
<td>4</td>
<td>Brown Coal</td>
<td>24.9</td>
<td>1190</td>
</tr>
<tr>
<td>5</td>
<td>Petroleum Coke</td>
<td>73.2</td>
<td>1480</td>
</tr>
<tr>
<td>6</td>
<td>Anthracite Char</td>
<td>129.0</td>
<td>1175</td>
</tr>
<tr>
<td>7</td>
<td>Bituminous Char</td>
<td>129.0</td>
<td>1160</td>
</tr>
<tr>
<td>8</td>
<td>Brown Coal Char</td>
<td>115.0</td>
<td>1170</td>
</tr>
</tbody>
</table>

5 Summary

1. Critical conditions exist both for the gas ignition and heterogeneous ignition modes. There exists a sufficient condition for extinction size of coal particle for quenching gas phase volatile combustion. However, even at much higher diameters of coal particles, gas phase ignition could not be obtained.

2. Universal plots are given to predict the critical condition of heterogeneous ignition mode where ignition no longer occurs with a "finite jump" in the temperature, a characteristic of Semenov's thermal theory. Approximate solution for critical conditions are found to be sufficiently accurate after comparison with numerical calculations for brown coal particles. Thus very small particles may not be efficiently burnt for given furnace conditions.

Acknowledgments

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References


14. Thomas, G. R., Harris, J. J., and Evans, D. G., "Ignition of Coal Particles
The diffusional rate of oxygen to the particle surface is given as

\[ \dot{m}_D = 4\pi PD \frac{\eta}{2} Y_{O_2} \]

where \( \eta = \frac{d_c}{D} \)

\[ D = \frac{1}{3} \lambda \mu \]

\[ p = n M \]

When \( n \) = no. of molecules per unit volume, \( M \) = mass of molecule

\( \lambda \), mean free path, \( \mu \), mean molecular velocity

Similarly from kinetic theory one can show that

the reaction rate or the conversion of colliding oxygen molecules into products is given as [Bradley]

\[ \dot{m}_R = \frac{1}{4} \pi \mu \frac{1}{3} Y_{O_2} \approx \frac{1}{4} \pi \mu \frac{1}{3} n^2 Y_{O_2} M \]

where collisional frequency is given to be \( \frac{1}{3} \pi \mu \). Thus

difusional rates and reaction rates are comparable when

\[ \left( \frac{M}{\lambda} \right) \approx 1.0 \]

When radius \( R < \lambda/\beta \), the reaction rate dominates.

Similarly, one can show that the temperature difference between particles and ambient \( \Delta T \) is given as

\[ \Delta T \sim \frac{Q_{with} Y_{O_2} \pi R^2}{\lambda} \]

Thus as particle size or oxygen concentration is reduced, \( \Delta T \) drops down, and smaller particles while reacting equilibrate with the ambient gas. Fig. 4 is consistent with isoplethted with \( \frac{Q_{with} Y_{O_2}}{\pi R^2} \), vs \( \frac{50}{Y_{O_2}} \), may be a straight line.
Small Particle vs Large Particle

\[ n = \frac{m}{\sqrt{\frac{2}{\pi}} \frac{\hbar^3}{\epsilon}} \]

Total energy even: \[ n \cdot \frac{\hbar^3}{4 \sqrt{\pi} \epsilon} \epsilon \sim \left(\frac{P}{m} - \frac{\hbar}{m} \right) \]

Total energy even: \[ \left(\frac{3m}{4\epsilon} \right) \epsilon \sim \left(\frac{P^2}{m^2} - \frac{\hbar^2}{m^2} \right) \]

\[ T = f(n) \]

\[ \frac{3m}{4\epsilon} \sim \left(\frac{T_p^0 - T_q}{\epsilon} \right) \]

\[ T_p - T_q \sim \epsilon \tau \]  

\[ T_p^0 - T_q^0 \sim \left(\frac{P}{m} - \frac{\hbar}{m} \right) \sim \frac{2\hbar}{m} \left(1 - \exp\left(-\frac{\hbar}{kT} \right) \right) T_p^0 \]

\[ \frac{3m}{4\epsilon} \sim \left(4\epsilon T_q T_p^3 + T_q^3 T_p \right) \]

\[ \frac{3m}{4\epsilon} \sim \left(4\epsilon T_q T_p^0 + T_q^0 T_p \right) \]
with \[ \frac{3m}{4GpL_0} \] and the probability ratio \[ T_p \rightarrow T_{ap} \]

\[ \frac{3m}{4GpL_0} \begin{array}{c} \varepsilon \left( \frac{T_0 + \varepsilon}{T_0 + \varepsilon - T_2} \right) \\
\varepsilon \left( \frac{T_0 + \varepsilon}{T_0 + \varepsilon - T_2} \right) \end{array} \]

Comparison relations

\[ \frac{T_{ap}}{T_{ap}} = \frac{T_p - T_0}{T_p - T_2} \left( \frac{T_p - T_0}{T_p - T_2} \right)^{\frac{1}{2}} \]

\[ \frac{1}{\left( \frac{T_p}{T_{ap}} \right)^{\frac{1}{2}}} \left( \frac{T_p - T_0}{T_p - T_2} + 1 \right) \left( 1 - \left( \frac{T_p}{T_{ap}} \right)^{\frac{1}{2}} \right) \]

\[ T_{ap} = T_{ap} \]

\[ \varepsilon = \frac{6}{5} \frac{\varepsilon}{\varepsilon} \]

\[ \varepsilon = \frac{16 - \varepsilon}{1 - \varepsilon} \]

\[ \varepsilon \left( 1 - \frac{\varepsilon}{\varepsilon} \right) = 16 \times \varepsilon \frac{1}{\varepsilon} \frac{1}{2} = \frac{16}{2} \]
Governing Equations

\[ \dot{q}_r = n \frac{Nu K}{n} \frac{\text{ln} n}{\text{ln} (n - 1)} (T_p - T_g) \]

For multi-term

\[ \dot{q}_r = \frac{Nu K}{\text{ln} n} \frac{n}{n - 1} (T_p - T_g) \]

\[ \dot{q}_r = \frac{3Nu K}{\text{ln} n} \frac{n}{n - 1} (T_p - T_g) \]

Total loss: \[ \{ \dot{q}_{in} + \dot{q}_{out} \} \]