R & D NOTES

A Model for Simultaneous Heating and Devolatilization of a Single Coal Particle in a Hot Gas Stream in the Presence of a Thermal Radiative Field

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The devolatilization of coal is a complex process (Lowry, 1963; Kobayashi et al., 1977). A simple approach has been employed to develop a theoretical model required for the prediction of simultaneous heating and devolatilization of a single coal particle entrained in a hot inert gas stream in the presence of a thermal radiative field. Reidelbach and Algermissen (1978) have described a single coal particle heating model that predicts the temperature of the particle as a function of time. Their model, however, does not account for the effect of loss of mass of the coal solid phase on the particle temperature during devolatilization. The model described in this note accounts for this deficiency.

THE MODEL

A single coal particle is flowing with an inert hot gas stream with zero slip velocity in a duct with the black-body surface temperature of T_r (Figure 1). The free hot gas stream and the duct surface temperatures are assumed to be constant with regard to time and spatial coordinates. Heat is transported to the particle from the hot gas through the fluid thermal boundary layer surrounding the particle and by thermal radiative heat transfer from the interior surface of the duct. Thermal radiation exchange between the particle and the hot gas is assumed to be negligible. Some of the thermal energy received by the particle is utilized for thermal decomposition of solid coal matter to yield volatile matter. The solid phase of the coal particle loses some of its sensible thermal energy because of solid phase transformation to gas phase at the solid phase temperature. Net thermal energy remaining increases the sensible energy content of the solid phase of the coal particle.

It is stated that the transport of heat to the particle from the surrounding hot gas during rapid pyrolysis of coal is a complex process. Jets of volatile matter would likely be issued from the particle with sufficient jet momenta to violently disturb the surrounding boundary layer. The thermal energy transport to the particle takes place through the disturbed boundary layer. Jets of volatile matter convect thermal energy away from the particle. A formulation accounting for such processes is needed for the determination of heat transfer rate to the particle under rapid pyrolysis conditions. Such a formulation is a complex one. In the absence of such a formulation, and to keep mathematics associated with the devolatilization model tractable, a Nusselt number, Nu, of 2 has been assumed in the preliminary investigation presented here. For a $Nu = 2$, heat transfer through the boundary layer surrounding the coal particle is considered to be slow relative to the thermal conduction inside the particle. Therefore, the thermal conduction inside the particle is neglected and spatial temperature uniformity inside the particle is assumed.

In their discussion of the combustion behavior of two British coals (Rawdon and Ackton Hall), which represent extremes in swelling behavior, Baum and Street (1971) have reported that swelling ceased with the end of devolatilization. The ratio of the average coal particle diameter after swelling to the average initial diameter was 1.04 for the Rawdon coal and 1.10 for the Acton Hall coal. These data indicate that the effect of coal swelling on the particle diameter should be taken into account in the development of a devolatilization model, especially for the high-swelling bituminous coals. This feature has not yet been incorporated in the elementary model being presented here, where the particle diameter is assumed constant during devolatilization. The particle surface is also assumed to be gray.

At any instant of time, t, conduction heat transfer flux to the particle surface is

$$q_c = \frac{2k}{d_a}(T_\infty - T_a),\ \mathrm{kJ/(m^2 \cdot s)} \tag{1}$$

Net thermal radiative heat flux to the particle surface from the duct interior surface is

$$q_r = F\epsilon\sigma(T_r^4 - T_a^4),\ \mathrm{kJ/m^2 \cdot s} \tag{2}$$

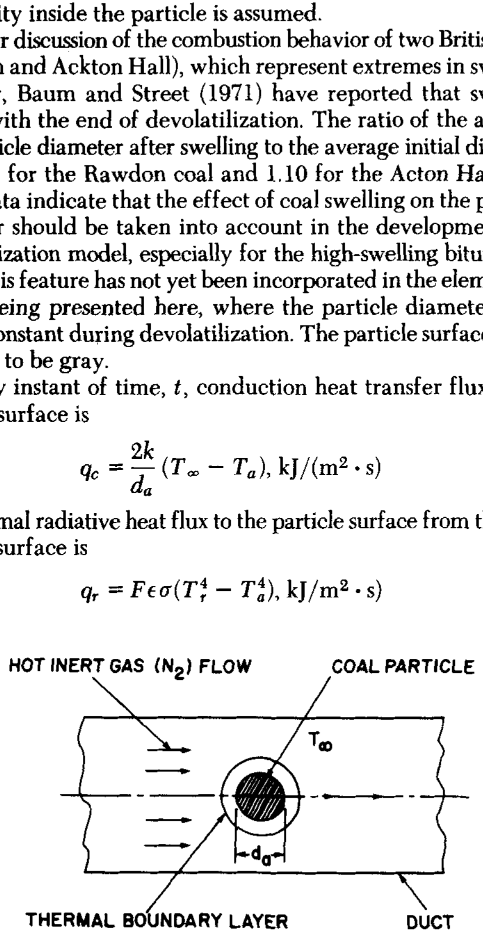

Figure 1. Schematic of the physical model.

For a relatively short diameter and long tube devolatilization reactor, such as a laboratory-scale reactor, the view factor, F, can be considered to be equal to unity. Assuming first-order chemical devolatilization kinetics with respect to mass of volatile matter remaining in the coal particle, the rate of decrease of the particle mass is

$$\frac{-dm}{dt} = A_0 \exp[-E/(RT_a)](m - m_+), \text{ kg/s} \tag{3}$$

The rate of thermal energy utilized for decomposition of solid phase to gas phase is

$$\frac{-dm}{dt}(\Delta\overline{H}_d), \text{ kJ/s} \tag{4}$$

The rate of thermal energy leaving the solid phase because of solid phase transformation to gas phase at temperature, T_a, is (Jenson and Jeffreys, 1963)

$$\left(-\frac{dm}{dt}\right) C_{pc}(T_a - T_i) \tag{5}$$

Thermal energy balance over the solid phase of the particle is

Rate of change of the sensible energy content of the particle =

[(1) + (2)] × (Particle exterior surface area) − (4)–(5) (6)

$$\frac{d}{dt}[mC_{pc}(T_a - T_i)] = (q_c + q_r)(\pi d_a^2) - \left(\frac{-dm}{dt}\right)(\Delta\overline{H}_d) - \left(\frac{-dm}{dt}\right) C_{pc}(T_a - T_i) \tag{7}$$

Taking C_{pc} as constant

$$C_{pc} m \frac{d}{dt}[T_a - T_i] + C_{pc}\left(\frac{dm}{dt}\right)(T_a - T_i) = (q_c + q_r)(\pi d_a^2) - \left(\frac{-dm}{dt}\right)(\Delta\overline{H}_d) + \left(\frac{dm}{dt}\right) C_{pc}(T_a - T_i) \tag{8}$$

On simplification, Eq. 8 reduces to

$$\frac{dT_a}{dt} = (q_c + q_r)\frac{\pi d_a^2}{mC_{pc}} - \left(\frac{-dm}{dt}\right)\frac{\Delta\overline{H}_d}{mC_{pc}} \tag{9}$$

On substitution for q_c and q_r, Eq. 9 reduces to

$$\frac{dT_a}{dt} = \left[\frac{2k}{d_a}(T_\infty - T_a) + F\epsilon\sigma(T_r^4 - T_a^4)\right]\frac{\pi d_a^2}{mC_{pc}} - \left(\frac{-dm}{dt}\right)\frac{\Delta\overline{H}_d}{mC_{pc}} \tag{10}$$

To find the relationship between particle mass and temperature, Eq. 10 is divided by $(-dm/dt)$

$$\frac{-dT_a}{dm} = \frac{1}{mC_{pc}}\left\{\frac{\left[\frac{2k}{d_a}(T_\infty - T_a) + F\epsilon\sigma(T_r^4 - T_a^4)\right](\pi d_a^2)}{(-dm/dt)} - \Delta\overline{H}_d\right\} \tag{11}$$

Equation 11 can be interpreted as

$$\frac{-dT_a}{dm} = \frac{1}{mC_{pc}} \times \left[\begin{pmatrix}\text{Heat supplied to the particle per}\\ \text{unit mass of volatile matter evolved}\end{pmatrix} - \begin{pmatrix}\text{Heat required per}\\ \text{unit mass of}\\ \text{volatile matter}\\ \text{evolved}\end{pmatrix}\right] \tag{12}$$

On substitution for $(-dm/dt)$ from Eq. 3 into Eq. 11, a relationship between the particle temperature, T_a, and its mass, m, at any instant of time is obtained.

$$\frac{dT_a}{dm} = -\frac{1}{mC_{pc}}\left\{\left[\frac{2k}{d_a}(T_\infty - T_a) + F\epsilon\sigma(T_r^4 - T_a^4)\right] \times \left[\frac{\pi d_a^2}{(m - m_+)}\right]\left[\frac{\exp(E/(RT_a))}{A_0}\right] - \Delta\overline{H}_d\right\} \tag{13}$$

Equation 3 is integrated to determine the time required for simultaneous sensible heating and devolatilization of the particle.

$$\Delta t_d = \frac{1}{A_0}\int_{m=m}^{m=m_0}\left\{\frac{\exp[E/(RT_a)]}{(m - m_+)}\right\} dm \tag{14}$$

Initial mass of the coal particle, m_o, is calculated from the following equation:

$$m_o = (\pi/6) d_a^3 \rho_c \tag{15}$$

DATA COMPUTATION

Equations 3 and 10 have been solved using the Euler method. The particle mass and temperature and their rates of change are shown in Figure 2 as functions of time for three diameters of a coal particle. In the computational scheme a time step of 0.5 ms has been used. To carry out the sample calculations the suitable property data were acquired from Kreith and Black (1980) and others (see Notation and Literature Cited).

To compute the data it was necessary to select values for the temperature of the start of the devolatilization process and the kinetic parameters. The temperature at which the evolution of volatile matters begins could vary from one coal to another. Although "active" devolatilization begins between approximately 623 and 673 K, thermal decomposition actually begins at much lower temperatures (Berkowitz, 1979). Baum and Street (1971) have used 600 K as the temperature of the start of the evolution of volatile matter for their investigation. We have chosen 573 K as the initial particle temperature. The apparent activation energy for the devolatilization process is reported to vary from 4.18 × 10^4 to 33.47 × 10^4 kJ/kmol, depending on the coal type and temperature of pyrolysis (Kobayashi et al., 1977). Our preliminary calculations indicated that the major fraction of volatile matter evolved above about 1,000 K for all the coal particle diameters studied. The research work by Kobayashi et al. on the devolatilization of a lignite and a bituminous coal, carried out in the temperature range 1,000–2,100 K, reported an apparent activation energy value of 10.46 × 10^4 kJ/mol and a corresponding frequency factor of 6.6 × 10^4 s^{-1} for first-order devolatilization kinetics. Therefore, selection of these kinetic parameter values was an appropriate one for the sample calculations presented in this note.

RESULTS AND DISCUSSION

Figure 2 shows the plots of particle mass, temperature, and percent volatile matter evolved vs. time for three particle diameter

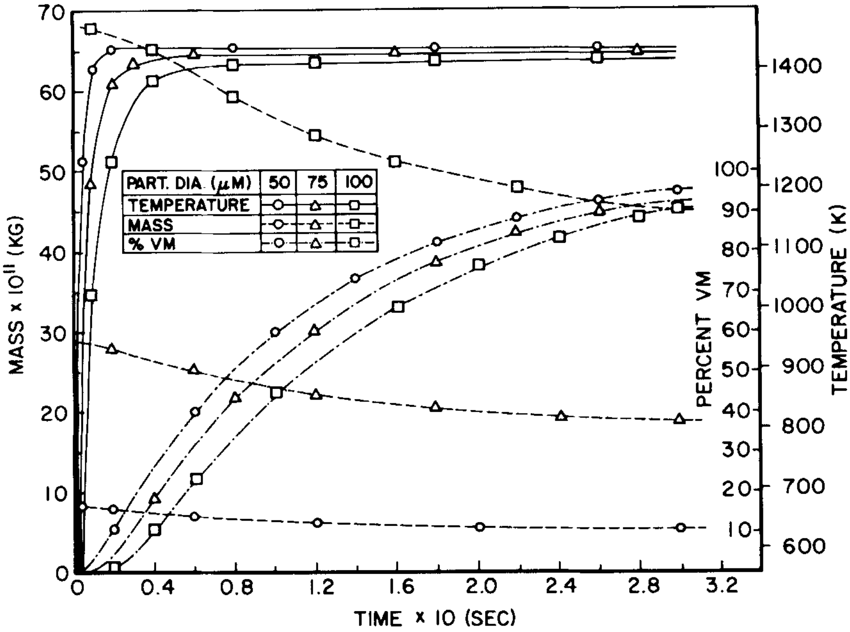

Figure 2. Plots of particle temperature, mass, and percent volatile matter vs. time.

(50, 75, and 100 μm). It is apparent that:

- The smaller the particle, the shorter the time duration in which it reaches its maximum temperature.
- The maximum temperature is higher for a smaller particle relative to a larger particle.
- The 50 μm dia. particle attains a temperature of 1,433 K in 20 ms, whereas a particle of 100 μm dia. is heated to a temperature of 1,400 K in 60 ms. In the case of the 50 μm particle the temperature plateau is reached in about 20 ms, with volatile matter evolution of only 11%. The particle mass decrease as a function of time is also evident. Evolution of the major fraction of volatile matter takes place at almost constant temperature. A delay time of about 12 ms is observed for the start of volatile matter evolution for the 100 μm dia. particle. During this period, the particle temperature reaches 1,060 K. Time periods for the evolution of 90% of volatile matter are 233, 266, and 300 ms for the particle diameters of 50, 75, and 100 μm, respectively. Figure 3 shows particle mass decrease and temperature rise rates plotted vs. time for the 100 μm dia. particle. A sharp decrease in temperature rise rate is observed, whereas mass decrease rate first rises to its maximum value and then decreases. The particle mass decrease rate first increases because of the rise in its temperature. The curve following the peak indicates the effect of depletion of volatile matter for an almost constant temperature condition of the particle.

CONCLUSION

The model predicts particle mass, temperature, percent volatile matter evolved, temperature rise, and mass decrease rates as functions of time. The predicted time periods for evolution of 90% of volatile matter for a simulated coal are 233, 266, and 300 ms for particle diameters of 50, 75 and 100 μm, respectively.

NOTATION

A_o = frequency factor, 6.6×10^4 s^{-1} (Kobayashi et al., 1977)
C_{pc} = specific heat of coal, 1.05 kJ/(kg · K)(Berkowitz, 1979)
d_a = coal particle diameter, m, E activation energy, 10.46×10^4 kJ/kmol (Kobayashi et al., 1977)
F = view factor for radiative heat exchange between the coal particle and the interior surface of the duct
$\Delta \overline{H}_d$ = enthalpy of coal devolatilization, 627.6 kJ/kg (Baum and Street, 1971)
k = thermal conductivity of fluid for transport of heat through thermal boundary layer surrounding the coal particle, 6.84×10^{-5} kJ/(m · s · K) (Kreith and Black, 1980)
m = mass of the coal particle at any instant of time, kg; m_o, initial mass of the coal particle
Nu = Nusselt number
m_+ = mass of the coal particle on complete devolatilization, kg ($m_+ = 0.63\, m_o$)
P_∞ = system pressure, 1 atm. (101.3 kPa)
R = universal gas law constant, 8.28 kJ/(kmol · K)
T_∞ = free stream or bulk temperature of hot inert gas, 1,473 K
T_a = instantaneous temperature of the coal particle, K

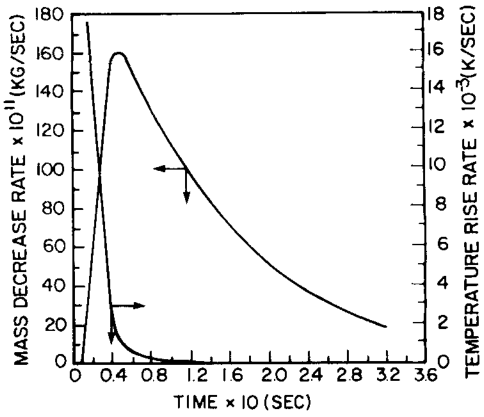

Figure 3. Plots of particle temperature rise and mass decrease rates vs. time for 100 μm dia. particle.

T_i = injection temperature of the coal particle, chosen as a convenient reference temperature

$T_{a,i}$ = temperature at which devolatilization is assumed to begin, 573 K

T_r = black-body temperature of the interior surface of the refractory lined duct, 1,283 K

ϵ = emissivity of the coal particle surface, assumed 1; ρ_c coal density, 1,300 kg/m^3

σ = Stefan-Boltzmann constant, 5.677×10^{-11} kJ/(m$^2 \cdot$ s $\cdot$ K^4)

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