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SHORT COMMUNICATION

On Internal Temperature Gradients in a Pyrolysing Coal Particle

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Abstract—This paper stresses the point that, contrary to common notion, temperature gradients do exist in pulverized coal particles, and that such gradients may or may not be important, depending on the coal thermal properties. Such properties are not routinely measured and are not well documented. In general a particle heats up by an inward moving "heat wave" which is followed by a "pyrolysis wave". The pyrolysis rate is a function of time and position as described by an "onion peel" model.

The prevailing assumption that no temperature gradients exist inside a pulverized coal particle heated in a high intensity combustion system is to be examined. Such particles are reported to undergo rapid heating at rates up to 10^6 or 10^7 K/s (Essenhigh, 1976). Recent experimental evidence indicates that under certain conditions during rapid heating and volatiles release, the particles are being propelled in an ordered motion which implies the existence of a temperature gradient. Witte *et al.* (1980) have used a laser beam to heat particles and have observed the particles to move in the direction of the beam, Figure 1. When the particles were heated from two opposing sides, this behavior was not observed. This observed "rocketing" effect may be created by preferential heating and nonuniform expulsion of gases. Since if the particles cannot sustain a temperature gradient, then the probability of volatiles expulsion from random directions would prevent such an ordered motion.

That a temperature gradient can exist in a particle can be seen from the solution to the transient heat conduction equation. For instance, the temperature distribution in a sphere subject to a constant heat flux is given in closed-form by Carslaw and Yaeger (1959) and VanSant (1980). The temperature history at the particle surface and at the center is shown in Figure 2, taken from the latter reference. From the figure it is seen that the temperature gradient is established within about 0.2 of the thermal characteristic time (τ), and is as high as 0.5 of the reference temperature (T_R). The definition of these quantities and the values of the physical properties used to calculate these quantities are given in the Nomenclature. T_R is calculated for a 35 μm (radius) coal particle at two heat flux levels, 1000 and 2000 W/cm^2, and two values of the thermal conductivity as given in the Nomenclature. The reference temperature at the two respective flux levels are 1020 K and 2040 K for the high value of K_p, and 2786 K and 5573 K for the low value of K_p. These numbers show that a significant gradient may exist in such a particle, and that the temperature difference between the center and the surface is a strong function of the thermal properties; in particular the thermal conductivity. The importance of this observation is directly related to the fact that the thermal properties of coal are not well

FIGURE 1 Pulverized coal particles carried downwards in a nitrogen stream through a transverse laser beam. Beam direction is from left to right and the heated particles are "rocketing" in the direction of the beam.

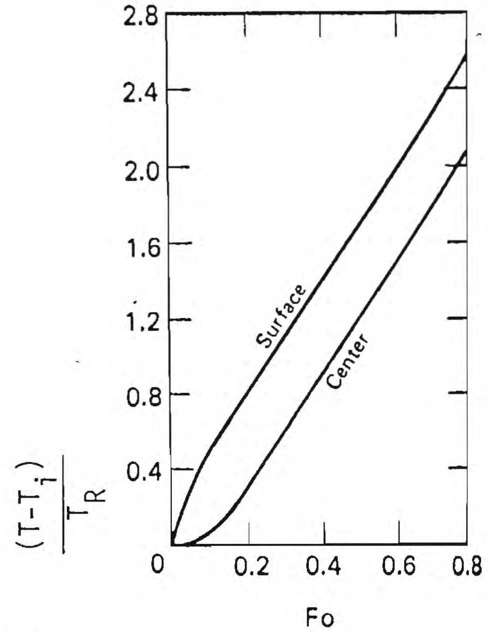

FIGURE 2 Temperature rise in a sphere caused by a steady surface heat flux.

documented and, as shown above, a factor of roughly 3 in the thermal conductivity makes a big difference.

The simplified thermal analysis above does not take into account radiation heat loss from the surface, or other effects which may moderate the temperature gradient. Before making such corrections, Figure 2 is again used to estimate the heat flux crossing the particle's boundary when the heating rate is specified. The slope of the curve in Figure 2 is roughly $2.6/0.8=3.25$, and it can be shown that the required heat flux is:

$$q = \rho\times C_p\times R\times \dot{T}/3.25. \tag{1}$$

For a heating rate of, say, 2×10^5 K/s, and an $R=35$ μm particle, the required heat flux is about 1170 W/cm^2. It makes no difference what the mechanism of heat transfer is (radiation or convection); that heat flux must cross the particle's boundary in order to maintain the specified heating rate.

An additional analysis which accounts for the radiation heat loss and for some chemistry is performed to investigate the effect of such temperature gradients on the pyrolysis of a coal particle. A numerical calculation was performed of the heat diffusion into a 35 μm particle which is subject to 12 ms of uniform external heating and then quenched in a room temperature environment. Mass loss due to pyrolysis was also incorporated. Two parallel pyrolysis reactions are assumed which proceed at a rate dependent on the local temperature (an "onion peel" model). The mass transfer is neglected however (*i.e.*, assumed instantaneous). Particle density, like the temperature, is therefore a function of time and radial position.

The temperature distribution is obtained by integration in time of the energy equation across the particle radius. The boundary conditions at the particle surface allow for heat flux (convection from the surrounding gas, thermal radiation, and radiative heating such as by laser beam). The pyrolysis reactions in the calculation may be turned on or off by specifying either a finite reaction rate or a zero rate, respectively. Similarly, heating may be accomplished either by radiation, convection, or both, by specifying the appropriate boundary conditions. The pyrolysis reaction rate constants are taken from Gat *et al.* (1983). The latent heat of pyrolysis (which theoretically could be calculated from the heats of formations of the reactants and the products, but in practice is unknown) is obtained from Lee *et al.* (1977), and the radiative heat flux is $q=2000$ W/cm^2 (this high heat flux is required since convective and radiative cooling reduce the effective heat flux). This heat flux produces a rapid heating at a rate near 2×10^5 K/s.

Shown in Figures 3 and 4 are (1) the calculated temperature map of the particle (T, in deg K, as a function of time and radial position), (2) the particle surface and center temperature-histories, (3) the normalized density map of the particle, and (4) the normalized total mass-history of the particle. The figures are for the high and the low thermal conductivity particles, respectively. Internal temperature gradients as high as 300 K and 600 K (across the particle radius) are indicated for the high and the low thermal conductivity coals, respectively. Consequently, the density profiles are affected by these temperature profiles, and in the case of the low thermal conductivity the extent of pyrolysis is much greater near the particle surface than near the center because the temperature near the surface is higher than in the high K_p particle. Turning the chemical reaction off does not affect noticeably the temperature map, only the density map.

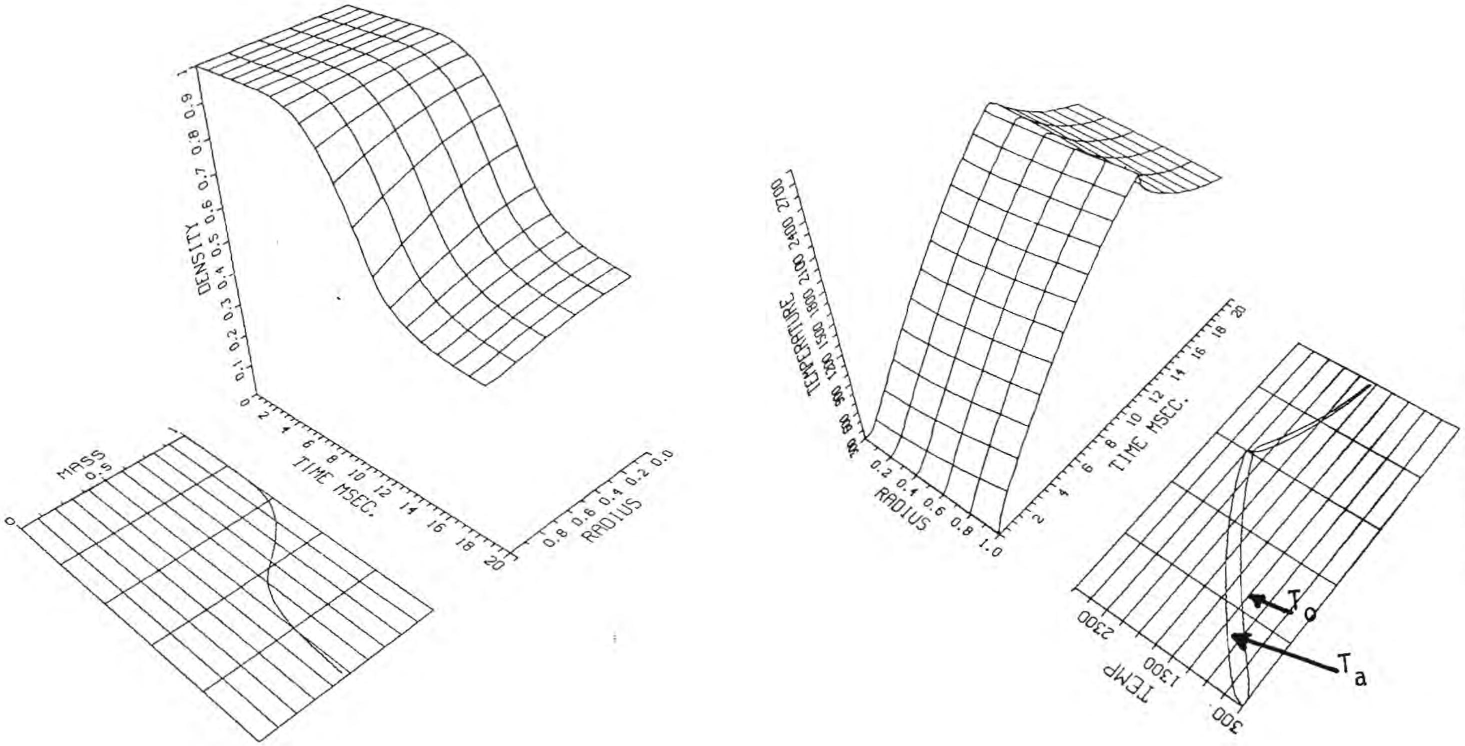

FIGURE 3 Temperature gradients and density map for a 70 μm diameter particle, $K_p = 0.3433$ W/m-K.

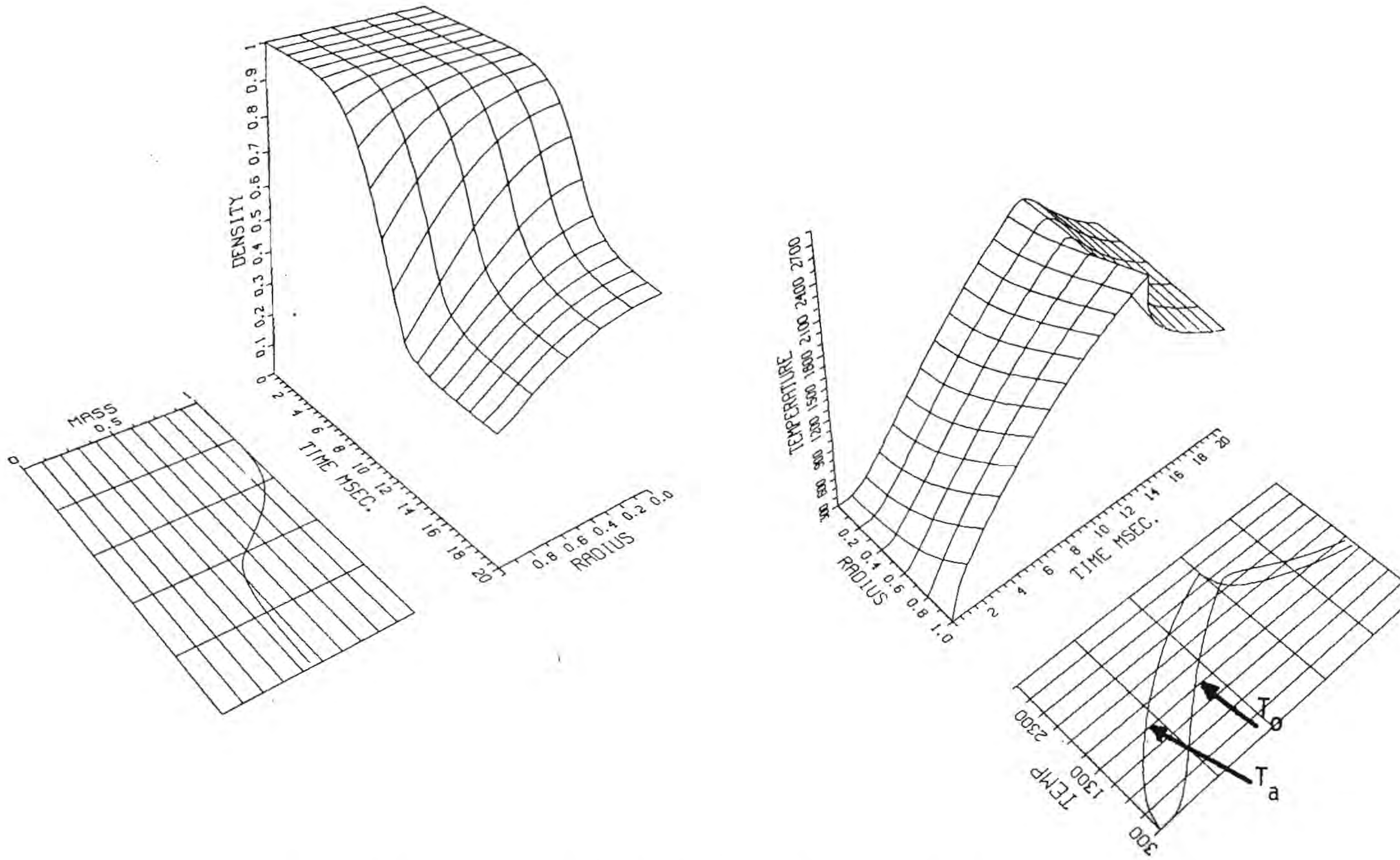

FIGURE 4 Temperature gradients and density map for a 70 μm diameter particle, $K_p=0.1256$ W/m-K.

CONCLUSIONS

1) The extent of a temperature difference between the particle surface and the center, or a temperature gradient, depends on the thermal diffusivity of the coal. And since for most cases the thermal conductivity is unknown (even a factor of three may be significant), the assumption of a uniform temperature profile cannot always be made. The internal heating of a particle is more accurately described by an inward motion of a "heat wave".

2) The pyrolysis reaction rate is a function of time as well as of radius (an "onion peel" model), and a "pyrolysis wave" propagates from the surface toward the center. The activation energy for the pyrolysis reaction determines the location of the pyrolysis wave front relative to the heat wave front. For the range of thermal conductivities of coal, neither a constant diameter (infinite thermal conductivity) nor a constant density (zero thermal conductivity) model describes the process accurately enough.

3) At the high heating rate, the heat absorbed by the endothermic pyrolysis reaction is negligible compared with the heat flux to the particle, so that the temperature history is only marginally affected by the pyrolysis reaction.

4) For the range of thermal conductivities for coal, the rate of pyrolysis during rapid heating is not limited by heat transfer but by the chemical rate.

NOMENCLATURE (and numerical data)

(Values of α and τ are given for the two values of K_p)

A_1, A_2	pre-exponential factors (2.25×10^4 and $2.85\times10^5\ s^{-1}$)
E_1, E_2	activation energies in rate equation $k=A\exp(-E/T)$ (14,000 and 16,814 K)
C_p	specific heat (4187 J/kg-K)
F_0	Fourier modulus $=t/\tau$
K_p	thermal conductivity (0.3433 and 0.1256 W/m-K)
L_v	latent heat (125.6 J/gm)
q	heat flux
R	particle radius
T	temperature
$\dot{T}$	heating rate
T_a	surface temperature
T_0	temperature at center
T_i	initial temperature
T_R	reference temperature $=qR/K_p$

Greek Symbols

α	thermal diffusivity $=K_p/C_p\rho$ (6.31×10^{-4} and 2.31×10^{-4} cm^2/s)
ρ	density (1.3×10^3 kg/m^3)
τ	characteristic time $=R^2/\alpha$ (19.4 and 53.0 ms)

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