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Characterizing char particle fragmentation during pulverized coal combustion

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Abstract

A particle population balance model was developed to predict the oxidation characteristics of an ensemble of char particles exposed to an environment in which their overall burning rates are controlled by the combined effects of oxygen diffusion through particle pores and chemical reactions (the zone II burning regime). The model allows for changes in particle size due to burning at the external surface, changes in particle apparent density due to internal burning at pore walls, and changes in the sizes and apparent densities of particles due to percolation type fragmentation. In percolation type fragmentation, fragments of all sizes less than that of the fragmenting particle are produced. The model follows the conversion of particles burning in a gaseous environment of specified temperature and oxygen content. The extent of conversion and particle size, apparent density, and temperature distributions are predicted in time.

Experiments were performed in an entrained flow reactor to obtain the size and apparent density data needed to adjust model parameters. Pulverized Wyodak coal particles were injected into the reactor and char samples were extracted at selected residence times. The particle size distributions and apparent densities were measured for each sample extracted. The intrinsic chemical reactivity of the char to oxygen was also measured in experiments performed in a thermogravimetric analyzer. Data were used to adjust rate coefficients in a six-step reaction mechanism used to describe the oxidation process.

Calculations made allowing for fragmentation with variations in the apparent densities of fragments yield the type of size, apparent density, and temperature distributions observed experimentally. These distributions broaden with increased char conversion in a manner that can only be predicted when fragmentation is accounted for with variations in fragment apparent density as well as size. The model also yields the type of ash size distributions observed experimentally.

Keywords: Fragmentation; Percolation; Coal; Solid; Particle

1. Motivation

The world's energy demands are projected to increase well into the 21st century and beyond. As much of this forecasted rise will occur in developing countries, use of cheap fossil fuels will continue to grow despite environmental concerns. Since fossil fuel combustion, in particular coal combustion, has a well-documented implication on climate change and air quality, burning the fuel cleanly and efficiently remains a paramount goal.

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Nomenclature

$b_{i,j}$	element i,j of the progeny matrix b, representing size distribution during fragmentation
$C_{i,k}$	fraction of particles in bin i,k that burn out of size-class i due to external burning
D	diameter of particle
$D_{i,k}$	fraction of particles in bin i,k that burn out of density-class k due to internal burning
D_O	oxygen bulk diffusion coefficient in particle boundary layer
k_d	mass transfer coefficient
k_{frag}	fragmentation rate coefficient
m	particle mass
$\widehat{M}$	molecular mass
N_{dens}	number of density classes implemented in model
$N_{i,k}$	number of particles which reside in size–density bin i,k
N_{size}	number of size classes implemented in model
Nu	Nusselt number
$P_{i,j,k,m}$	element i,j,k,m of the tensor P; represents the fraction of particles which [start in size class i, end in size class j, and start in density class k] that ends in density class m
P_g	oxygen partial pressure in ambient gas
P_s	oxygen partial pressure at the exterior particle surface
R	universal gas constant
R_{ex}	external reactivity of the particle (g/m^2/s)
R_{in}	internal reactivity of the particle (g/m^2/s)
q	overall burning rate of the particle (g/m^2/s)
S_g	specific internal surface area (m^2/g)
$S_{i,k}$	fraction of particles in size–density bin i,k which will fragment within time step dt
Sh	Sherwood number
T_p	particle temperature
T_g	ambient gas temperature
T_w	wall temperature to which particles radiate
x	conversion fraction
x_i	diameter of size-class i

Greek symbols

ΔH	heat of reaction
$\Delta\rho_k$	apparent density difference between density class k and $k+1$
Δx_i	diameter difference between size class i and $i+1$
α	size sensitivity parameter for fragmentation
ε	particle emissivity
λ	thermal conductivity of gas
γ	constant factor by which size interval varies for each size bin, $\gamma = x_i/x_{i+1}$
γ_o	change in volume upon reaction per unit oxygen consumed
η	effectiveness factor which relates internal reactivity to maximum possible internal reactivity
ρ_c	apparent density of the carbonaceous material
ρ_k	density of density-class k
ψ	structural parameter used to fit internal surface area throughout the course of conversion
σ	piecewise standard deviation of the Gaussian distribution used to predict fragment densities
σ_{sb}	Stephan–Boltzmann constant
ω	density sensitivity parameter for fragmentation
υ_O	moles O_2 reacted per mole carbon reacted

The efficient burning of any particular fossil fuel relies on accurate characterization of the fuel conversion process so that optimal reaction conditions can be identified. This requires the development of models that accurately predict fuel conversion rates for specified temperature, pressure, and gas composition. With porous solid fuels, the models must not only have parameters that accurately describe the rates of chemical reactions that consume the carbonaceous material but they must also have parameters that accurately describe the transport of reactive gases through particle pores as well as parameters that accurately describe the mode of burning, i.e., how the size and apparent density of the particle vary with mass loss during the conversion process. Even with accurate chemistry, transport, and mode of conversion models, accurate prediction of mass loss during the combustion of solid fuels will depend upon the extent of fragmentation during the conversion process. All coal particles fragment to some extent during coal combustion. Fragmentation reduces the particle size, and small particles are converted to gaseous species at faster rates than large particles. Fragmentation occurs during coal devolatilization and during char