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Mathematical modeling of reactants' transport and chemistry during oxidation of a millimeter-sized coal-char particle in a hot air stream

An Marcel Beckmann[a], Jakub Bibrzycki[a,b], Marco Mancini[a], Andrzej Szlęk[b], Roman Weber[a,*]

[a] Clausthal University of Technology, Institute for Energy Process Engineering and Fuel Technology, Agricolastr. 4, Clausthal-Zellerfeld 38678, Germany
[b] Silesian University of Technology, Institute of Thermal Technology, Konarskiego 22, Gliwice 44-100, Poland

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ABSTRACT

A two-dimensional time-dependent model for mathematical description of the oxidation process of a coal-char particle placed in an oxidizer stream has been developed. The model is used to simulate the oxidation process of a 5.2 mm char-particle for which the kinetic parameters for heterogeneous reactions have been measured. The initial morphology has been determined using mercury porosimetry. The calculated char-particle mass-loss agrees well with the measured data and the model predicts slower oxidation rates at the end of the process due to alterations to the particle morphology. The importance of both the Boudouard reaction and CO_2 diffusion inside the particle has been underlined.

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1. Introduction and objectives

Predicting combustion rates of char particles has been an important issue since such information is required for designing pulverized coal boilers, fluidized bed combustors, fixed bed combustors and gasifiers. Recent works attempt to clarify the oxidation mechanisms by examining limitations of power-law kinetics as opposed to Langmuir kinetics [1] and to examine correctness of expressions for calculating CO/CO_2 ratio as a function of particle temperature, diameter [2] and oxygen partial pressure [3]. The reaction order and activation energies are subjects of numerous experimental and theoretical investigations [1,4] so is particle morphology development during oxidation [5,6]. Existing combustion models have been fit [7] to experimentally determined overall oxidation rates for a number of coal chars. Despite all these works, accurate predictions of oxidation rates, or more generally, accurate predictions of burnout, in the last 20% range, are still impossible without (often ad hoc) corrections to current char oxidation models [6,8,9]. One of the issues is the ash behaviour and its either catalytic or inhibiting effect on the oxidation rates. Not surprisingly, the most recent work concerning combustion of micron size (100 μm) char particles, has attempted to clarify the effect of ash film and ash dilution on the oxidation rates [10].

This work is concerned with combustion of a 5.2 mm coal-char particle in a stream of hot air (see Experiments). During the particle combustion, an ash layer has been formed which inhibits the oxidation rate. In this paper, a mathematical model is formulated for computer simulations of the experiment. The model calculates the development of the oxidation front within the particle and predicts the ash layer development. It will be shown later that the model replicates well the experiment and the slow-down of the oxidation process, occurring during the last 20% burnout, is also well reproduced.

2. Experiments

Recently, Bibrzycki et al. [11,12] have reported a series of measurements concerning oxidation rates of 5.2–6.3 mm char particles. In this paper, experimental run No. 1 is considered only (see Table 2 in [11]) where a char particle of 5.2 mm diameter is oxidized in a stream of hot air (1069 K, 101325 Pa) approaching the particle with 3.3 m/s velocity. Simplistically, the experiments can be described as recording mass loss and surface temperature of a particle placed in a hot air stream, as shown in Fig. 1. The particle mass has been recorded every second using an analytical balance while the particle surface temperature, on the downwind side, has been recorded every three seconds using an infrared camera. The composition of the char (char generation method is described in [11]) has been determined, using another ten char particles, to be: ash content 0.128, moisture 0.015, volatiles 0.077, fixed carbon

* Corresponding author.
E-mail addresses: roman.weber@ievb.tu-clausthal.de, weber.rom@gmail.com (R. Weber).

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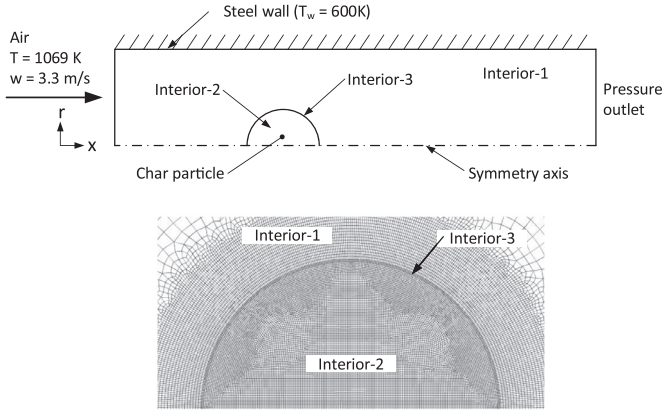

Fig. 1. (Top) Simplified representation of the experiment [11,12]; also computational domain and boundary conditions, (Bottom) numerical mesh in and near to the particle.

0.78 so that the average ash content of the char particles is 0.14 on moisture and volatiles free basis. 169 s are needed to achieve 85% char conversion while the process is completed after 300 s. At the end of the oxidation process, the remains constitute 100% of the initial ash mass. The infrared images show that in experimental run No. 1 [11] the particle diameter stays approximately constant due to the fact that the ash remains on the particle.

Mercury porosimetry has been used to determine the particle true density ($\rho_{\text{true}} = 1628\,\text{kg/m}^3$), volumetric pore length ($L_V = 2.47 \times 10^{14}\,\text{m/m}^3$), porosity ($\varepsilon = 0.286$), pore structural parameter ($\psi = 2.28$), initial internal volumetric surface area ($S_{V_0} = 3.11 \times 10^7\,\text{m}^2/\text{m}^3$) and pore tortuosity ($\tau_{\text{pore}} = 1.20$) (see Tables 3 and 4 in [11]). The intrinsic kinetics for the char considered have been determined using TGA operated in isothermal mode to eliminate both the complexity and ambiguity in deriving the kinetic parameters at non-isothermal operation [13]. Assuming that the char consists of ash and carbon only, the char oxidation is described by the following stoichiometric equation:

$$C + \gamma O_2 \Rightarrow (2\gamma - 1)CO_2 + (2 - -2\gamma)CO \tag{1}$$

where the CO/CO_2 ratio is taken to be temperature dependent [14]

$$\frac{CO}{CO_2} = 2512 \cdot \exp\left(-\frac{6244}{T_p}\right) \tag{2}$$

and the stoichiometric coefficient (γ) is calculated as

$$\gamma = \frac{1 + 0.5(CO/CO_2)}{1 + (CO/CO_2)} \tag{3}$$

The pre-exponential factor and the activation temperature of the Arrhenius expression

$$k_{\text{int}} = A_{\text{int}} \cdot \exp\left(-\frac{E_{a,\text{int}}}{R \cdot T}\right) \tag{4}$$

for Reaction (1) have been determined to be $A_{\text{int}} = 4.04 \times 10^3\,\text{m/s}$ and $E_{a,\text{int}}/R = 15,450\ K$ [11]. The latter corresponds to a 128 kJ/mol activation energy which is lower than typically quoted values of around 140 kJ/mol [4] or 160 kJ/mol [15]. The pre-exponential factor and the activation temperature for oxidation of the same char in carbon dioxide (Boudouard reaction)

$$C + CO_2 \Rightarrow 2CO \tag{5}$$

have been determined to be $A_{\text{int}} = 2\,775\,\text{m/s}$ and $E_{a\ \text{int}}/R = 26,177$ K [11]. Thus, a 218 kJ/mol activation energy [16,17] has been measured. The ratio of CO_2 gasification to oxidation rate at 1073 K is then 3.13×10^{-5} which aligns well with typical values (see Table 2 in [16]). In the experimental determination of the above kinetic constants, reactions (1) and (5) are taken to be first order.

3. Two-dimensional char combustion model

The above described experiments are measurements of the overall oxidation rate of char particles placed in a stream of hot air (Fig. 1). The oxidizer flow is laminar (flow Reynolds number = 465) and the particle Reynolds number is 140 so that the boundary layer around the particle is also laminar and a time dependent wake is formed on the downwind side. The intention is to formulate a mathematical model describing the time dependent char oxidation process. The model is to account for the reactive laminar flow around the particle as well as for the reactants' transport and their reactions inside the particle so that the propagation of the reaction front inside the particle could be calculated. It is expected that the mathematical model reproduces the alterations to the particle structure and shows the build up of the ash layer with time. It is assumed that heterogeneous reactions (1) and (5) take place inside the particle (on the walls of the particle pores) and on the particle external surface. The reactions produce both CO and CO_2 and, if oxygen is available, CO can be further oxidized to CO_2 in the particle voids and in the air flow. In formulating the model we draw upon the work of Yang et al. [18] and Buczynski et al. [19]. Yang et al. [18] have considered time dependent combustion of a biomass particle suspended in a methane flame using a modeling approach somewhat similar to our approach (see below). The work of Buczynski et al. [19] has been used in the development of the porous particle model described in Section 3.3.

3.1. Computational domain, initial and boundary conditions

The computational domain contains three interiors, as shown in Fig. 1. Interior-1 represents the gas-flow, while Interiors-2 and -3 represent the porous particle. Interior-3 is a 0.05 mm thick zone placed on the particle outskirts which is used to account for the radiation exchange between the particle and the surroundings, see below. In each of the three interiors a numerical mesh is created (see Fig. 1); 26 326 cells are used in total. Throughout the simulations, air at 3.3 m/s velocity and 1069 K temperature enters the computational domain and the steel pipe temperature (T_{wall}) remains at 600 K, as shown in Fig. 1. The initial conditions for the particle are: 5.2 mm diameter, 300 K temperature, 14% ash and 86% carbon mass fractions, morphology as specified previously.

3.2. Conservation equations for gas-phase (Interior-1)

In Interior-1 (see Fig. 1), where gas-phase is present only, the conservation equations include continuity

$$\frac{\partial(\rho_g)}{\partial\tau} + \nabla \cdot (\vec{w} \cdot \rho_g) = 0 \tag{6}$$

momentum conservation

$$\frac{\partial(\rho_g \cdot \vec{w})}{\partial\tau} + \nabla \cdot (\vec{w} \cdot \vec{w} \cdot \rho_g) = -\nabla \cdot p + \nabla \cdot \bar{\bar{\tau}} \tag{7}$$

species mass balance

$$\frac{\partial(\rho_g \cdot g_i)}{\partial\tau} + \nabla \cdot (\vec{w} \cdot \rho_g \cdot g_i) = \nabla \cdot (\rho_g \cdot D_{g\,i-\text{mix}} \cdot \nabla g_i) + R_i \tag{8}$$

and energy balance

$$\frac{\partial}{\partial\tau}(\rho_g \cdot h_g) + \nabla \cdot (\vec{w} \cdot (\rho_g \cdot h_g)) = S_{\text{he}} + \nabla \cdot (\lambda_{\text{eff}} \cdot \nabla T) \tag{9}$$

In the above equations w and ρ_g stand for gas velocity and density, respectively while τ represents time, $\bar{\bar{\tau}}$ is the stress tensor of the laminar flow; g_i is the i^{th} species mass fraction, $D_{g\,\text{i-mix}}$ is the diffusion coefficient in the gas mixture (for computing the diffusion coefficients see Eqs. (21, 22)). The terms R_i are mass sources/sinks due to CO oxidation to CO_2 while S_{he} is the energy

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