

COMPUTATIONAL SELF-IGNITION OF COAL DUST ACCUMULATIONS IN OXY-FUEL COMBUSTION ATMOSPHERES

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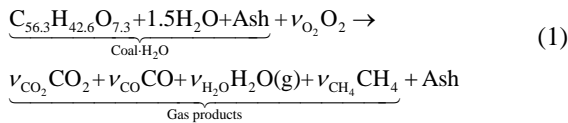
Introduction

Oxy-fuel combustion is one of the most promising technologies to reduce CO₂ and pollutant emissions. The concept replaces air with pure O₂ or a mixture of O₂ and recycled flue gas (mainly CO₂) and generates high-concentration CO₂ gas products for carbon storage. However, the risk of safety concerns for an oxygen-enriched combustion system, as one of the major technological challenges, has not been well studied. Dust may be processed or deposited in oxygen-enriched environments where little or nothing is known about the spontaneous ignition risk. In addition, the fire and explosion risks may vary in the CO₂-abundant ambient and further increase in the oxygen-enriched oxy-fuel combustion system.

A two-dimensional numerical model is developed to investigate the self-ignition behaviour in coal dust accumulations and predict the transient temperature and concentration fields during the self-ignition process. A modified one-step kinetic reaction considering mole fraction of oxygen in various mixture gases is adopted to describe the one-order thermal and oxidation rate. The numerical results are compared with the previous experiments [1].

Mathematical model

According to the elemental and proximate analyses [1,2], South African (SA) coal combustion can be simply specified as



where ν is the chemical stoichiometric coefficients and $C_{56.3}H_{42.6}O_{7.3}$ is the chemical formula of the active component on basis of 1000 g coal.

The reaction rate of self-ignition with one-order Arrhenius equation can be expressed by [1]

$$r_c = -(1 - \varepsilon_b) \rho_{c,0} A_{\text{cair}} g(X_{O_2}) \exp\left(-\frac{E_a}{RT}\right) \left(\frac{\rho_c}{\rho_{c,0}}\right)^a \left(\frac{X_{O_2}}{X_{O_2} + X_{GF}}\right)^b \quad (2)$$

where $g(X_{O_2}) = \left(X_{O_2} / 0.21\right)^{n_{O_2}}$ is the correction factor of the pre-exponential factor for O₂/CO₂ atmospheres.

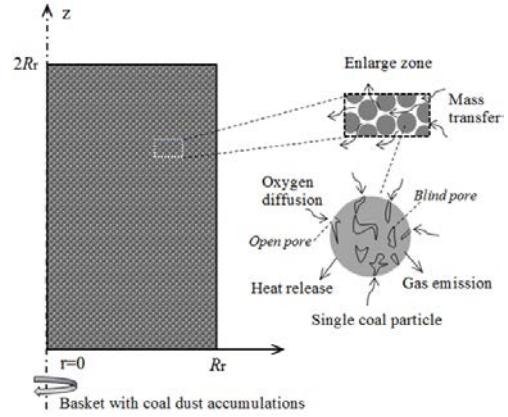


Fig. 1. 2D axisymmetric geometry of dust accumulation in an equidistant cylindrical basket

For the energy conservation:

$$((1 - \varepsilon_b) \rho_c c_c + \varepsilon_b \rho_g c_g) \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_c \nabla T) + r_c \Delta H_c \quad (3)$$

For the immobile solid coal, the mass conservation can be formulated:

$$(1 - \varepsilon_b) \frac{\partial \rho_c}{\partial t} = -r_c \quad (4)$$

For the gas species, the Maxwell-Stefan equations [3] accounting for all interactions of species in a solution are used in this paper

$$\frac{\partial(\rho_g Y_i)}{\partial t} + \nabla \cdot (\mathbf{j}_i) = -r_i \quad (5)$$

where Y_i is the mass fraction, $\sum_{i=1}^m Y_i = 1$, using the ideal gas law.

A Neumann condition was used for both the temperature field of bulk dusts and the concentration field of gas species (see Fig. 1). At $t=0$, the entire coal accumulation is unreacted, the temperatures of the coal and gas are constant, as well as the gas composition.

Simulation

COMSOL Multiphysics software is adopted to solve the partial differential equations in our study. Because the current work is only valid for self-heating period until ignition, all of the simulations were terminated once the temperature in the domain reaches a threshold which is defined as calculation termination temperature (210°C) in this paper.

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Results and discussion

A comparison of experimental and calculated SITs of SA coal at different dust volumes in various gas atmospheres is shown in Fig. 2. Clearly, SITs decrease from around 130 °C to even lower than 100 °C as the sample volume increases from 25 mL to 1600 mL, showing a strong size effect. In comparison with SITs in air, those for the ambient of 21% O₂/79% CO₂ are found to be only 0~1 °C higher for SA coal dust, agreeing with the experimental findings [1]. Such a small increment in SIT indicates a small inhibiting effect of CO₂.

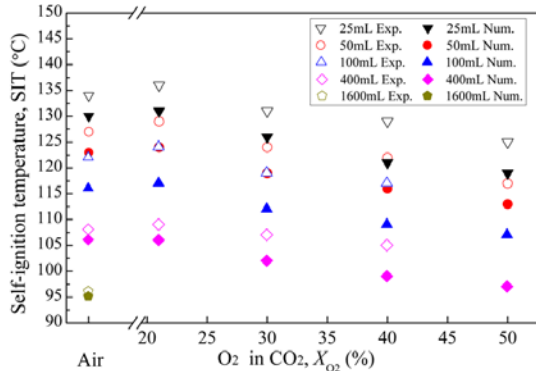


Fig. 2. Comparison of the numerical SIT and experimental SIT [1] of SA coal dust

Figure 3 shows t_i increases from 17.5 min (at 132 °C) to 618 min (at 96 °C) as the dust volume increases from 25 mL to 1600 mL for SA coal dust in air. This trend is converse with the effect of dust volume on the self-ignition temperature (SIT), which suggests that an increasing dust volume decreases SIT but increases t_i . Moreover, the ignition delay is found to decrease significantly as X_{O_2} increases for each dust volume.

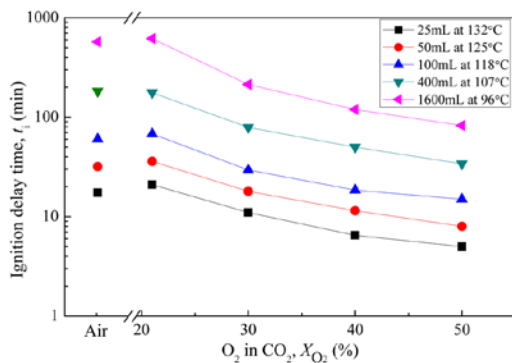


Fig. 3. Computed ignition delay time of SA coal vs. the oxygen mole fraction at the minimum supercritical temperature on the basis of 21% O₂/79% CO₂

Figure 4 demonstrates the temperature and gas components evolution at the central point (ignition location). Both the oxygen consumption rate and the gas products release rate are found to be comparatively small before ignition, which is consistent with the heat release rate. Fig. 5 compares the evolution of the central temperature and the Fick diffusivity of O₂ at the central point in air (21% O₂/79% N₂) and in 21% O₂/79% CO₂ atmosphere. It reveals that O₂ has a lower

diffusivity in CO₂ than in N₂, which may explain why SITs in 21% O₂/79% CO₂ were found to be slightly higher than in air.

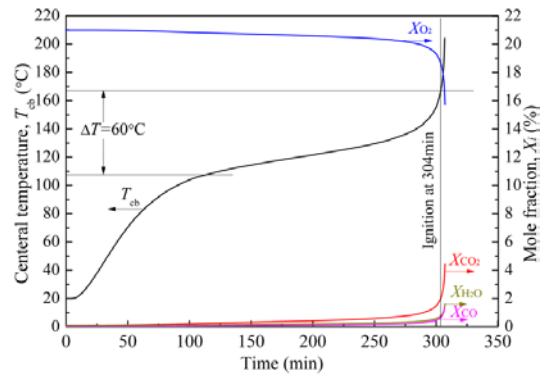


Fig. 4. The central point temperature and gas components evolution for 400 mL SA coal dust in air at oven temperature of 107 °C

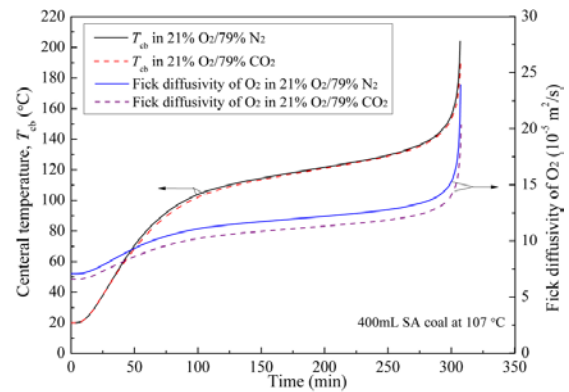


Fig. 5. The central point temperature and Fick diffusivity of O₂ evolution for 400 mL SA coal dust at oven temperature of 107 °C in air and in 21% O₂/79% CO₂.

Conclusions

The standardized hot-oven test under both air and O₂/CO₂ gas mixture conditions with O₂ mole fraction from 21% to 50% is simulated, and the transient temperature and concentration profiles are studied. Results show that the fire risk of self-ignition increases in the oxy-fuel combustion system: both self-ignition temperature and ignition delay time decrease with the increasing mole fraction of oxygen. The inhibiting effect of CO₂ is comparatively small for the self-ignition. These results indicate that the model provides a satisfactory explanation for self-ignition behaviour.

Acknowledgements

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