



Full Length Article

Numerical investigation on the self-ignition behaviour of coal dust accumulations: The roles of oxygen, diluent gas and dust volume



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HIGHLIGHTS

- Both self-ignition temperature and ignition delay time of coal dusts clearly decrease with increasing oxygen mole fraction.
- The inhibiting effect of carbon dioxide is comparatively small on self-ignition and oxygen consumption increases dramatically after ignition.
- The model is valid to predict the transient temperature and concentration profiles of coal dusts until ignition.
- Heating value and kinetic parameters have a comparatively pronounced effect on self-ignition.

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ABSTRACT

Self-ignition of coal dust deposits poses a higher risk of fires in oxygen-enriched oxy-fuel combustion systems. In this work, we develop a numerical method, using the commercial software COMSOL Multiphysics, to investigate self-ignition behaviour of coal dust accumulations with a main emphasis on the roles of oxygen, diluent gas and dust volume. A one-step 2nd-order reaction kinetic model considering both coal density and oxygen density is used to estimate reaction rate using the kinetic parameters from previously conducted hot-oven tests. This model is validated to predict the transient temperature and concentration profiles of South African coal dusts until ignition. The computed self-ignition temperatures of dust volumes show a good agreement with experimental results. In addition, it is found that the inhibiting effect of carbon dioxide is comparatively small and oxygen consumption increases dramatically after ignition. Parameter analysis shows that the heating value and kinetic parameters have a comparatively pronounced effect on self-ignition temperature. The model provides a satisfactory explanation for the dependence of self-ignition behaviour on gas atmospheres, thus helping to further understand the fire risk of self-ignition in oxy-fuel combustion systems.

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1. Introduction

Oxy-fuel combustion is one of the most promising technologies to reduce carbon dioxide (CO₂) and pollutant emissions. The concept replaces air with pure oxygen (O₂) or a mixture of O₂ and recycled flue gas (mainly CO₂) and generates high-concentration CO₂ gas products for carbon storage [1,2]. However, the increasing fire risk in the solid-phase self-ignition [3] and the gas-phase explosion [4] for an O₂-enhanced combustion environment is still a technological challenge and has not been studied well yet. Dust accumulation often occurs in coal mills and power plants. Once exposed to

an oxidizing atmosphere and a mild heat source, this accumulated dust may self-heat to initiate smouldering combustion [5–7]. The fire and explosion risks may vary in the CO₂-abundant ambient and further increase in the oxygen-enriched oxy-fuel combustion system.

The self-ignition process refers to a physicochemical process of thermal runaway, which depends on the characteristics of combustible bulk materials and packing conditions (particle size, density, volume-to surface ratio, porosity, thermal conductivity, heat capacity etc.), as well as the ambient conditions (temperature, oxygen content, ventilation, etc.) [5,8–10]. Numerical simulations are promising approaches and have been developed to gain insight into the self-ignition behaviour of bench-scale coal dusts [11–13] and metal dusts [14], coal stockpiles [15–19], and underground

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Nomenclature

A	pre-exponential factor, $\text{m}^3/\text{kg s}$	<i>Greek symbols</i>	
c	specific heat, $\text{J}/\text{kg K}$	α	thermal diffusivity, m^2/s
d	diameter of a single dust, m	ε	bulk porosity
\mathbf{d}	diffusional driving force	ν	stoichiometric coefficient
\bar{D}_{ik}	Fick diffusivity, m^2/s	λ	heat conductivity, $\text{W}/\text{m K}$
D_{ik}	Maxwell-Stefan diffusivity, m^2/s	ρ	density, kg/m^3
E_a	apparent activation energy, kJ/mol	<i>Superscripts and Subscripts</i>	
h_m	mass transfer coefficient, m/s	0	initial
h_t	heat transfer coefficient, $\text{W}/\text{m}^2 \text{K}$	a	ambient of oven
ΔH_c	heat of reaction by per kg coal, kJ/kg	ac	active component of coal
\mathbf{j}	mass flux, $\text{kg}/\text{m}^2 \text{s}$	b	bulk of basket
K	constant	c	coal dust
Le	Lewis number	cb	centre of basket
M	molar mass, kg/mol	ct	calculation termination
m	number of the gas species	e	effective
n	order for Lewis number	g	gas
p	pressure, Pa	i	ignition
Q	volumetric heat release rate, W/m^3	i	gas species
r	rate of reaction, $\text{kg}/\text{m}^3 \text{s}$	j	gas species
R	ideal gas constant, $\text{J}/\text{mol K}$	k	gas species
R_r	radius of baskets, m	max	maximum
t	time, s	SI	self-ignition
T	temperature, K	wall	wall of basket
V	molar diffusion volume, m^3/mol		
X	mole fraction		
Y	mass fraction		
SIT	self-ignition temperature		

coal seams [20–24]. Several numerical models coupling heat and mass transfer equations have been developed to study the process of self-ignition of porous coal beds. However, all above models adopted 1st-order reaction kinetic models either on fuel-basis [11–14] or on oxygen-basis [15–18,21,22], might not well reflect the effect of oxygen and diluent gas on the ignition behaviour of dust layers in oxy-fuel combustion conditions. On the one hand, the corresponding fuel-basis kinetic parameters were typically estimated either by the Frank-Kamenetzki (F-K) model with basket heating methods [11,12,20] or by thermogravimetric analysis and differential scanning calorimetry (TGA-DSC) [25,26]. On the other hand, the oxygen-basis kinetic model might be more accurate to reflect the effect of oxygen mole fraction on the reaction rate. However, the technical challenge is that neither an effective method is available for kinetic parameters estimation, nor the accurate heating value of oxygen consumption ($\text{kJ}/\text{mol O}_2$) for a specific solid fuel.

Previous work in our laboratory experimentally investigated the fire risk posed by self-ignition of coal dust accumulations in various O_2/CO_2 atmospheres [3]. In this paper, we develop a two-dimensional numerical model to investigate the self-ignition behaviour of South African (SA) coal dust accumulations and predict the transient temperature and concentration fields during the self-ignition process. A one-step 2nd-order reaction kinetic model considering both coal and oxygen density is adopted to describe the thermal and oxidation rate. The numerical results are compared to previous experimental results [3]. The influences of the thermal and kinetic parameters are also analysed.

2. Mathematical model

As prescribed by the experimental investigation [3], the self-ignition temperature (SIT) and the ignition delay time (t_i) of the coal dust were determined using a 64-L oven and five equidistant cylindrical mesh wire baskets with volumes of 25, 50, 100, 400, and

1600 mL. Both the oven and coal dust sample were flushed by air or the premixed O_2/CO_2 gas prior to each experiment. When the test started, the rate of inlet ambient gas was set to 2 L/min which was monitored by a Rotameter. Once the oven was stabilized at the target temperature, the basket with a pre-flushed coal dust sample was placed in the oven for each test. More details can be found in the work of Wu et al. [3]. Considering the fact that the gas flow is comparatively low and the particle size is extremely fine, it is justified to ignore the effect of convection over diffusion in the coal dust accumulations domain. Furthermore, the cylindrical basket is axisymmetric, thus we solve the two-dimensional axis-symmetrical time-dependent conservation equations for the bulk material. The domain for the computation is shown in Fig. 1. The model geometry consists of three open boundaries (bottom, top and right sides) and the axisymmetric axis or vertical centreline $r = 0$ (left side). The radius of the dust accumulation domain is R_r and the height is $2R_r$. For simplicity, the following assumptions are made:

- Only the diffusional effect is considered in the domain as this is the dominant transport mechanism;
- The drying process in the simulations is not considered due to the small moisture content of the coal;
- Effects of gas conditions on the heat and mass transfer coefficients, as well as on the stoichiometric coefficients are neglected;
- Properties such as bulk porosity, thermal conductivity and specific heat capacity of both coal dusts and gas mixtures are independent of time and temperature;
- A one-step global oxidation reaction formulation is considered as shown in Eq. (1).

2.1. Chemical kinetics

Because coal has non-uniform a physical structure and a complex composition, the self-ignition process involves many

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