Modelling and parametric investigations on spontaneous heating in coal pile

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ABSTRACT

To predict the spontaneous heating of coal pile by computational fluid dynamics (CFD) is very meaningful for preventing the coal pile from self-ignition. A two-dimensional (2-D) numerical model, which could be simply implemented in FLUENT, was developed in this study. The chemical kinetic parameters of low-temperature oxidation of coal, which were expressed by the outer surface area of particles, were well measured in experiments. The coal piles under different conditions were calculated by using the developed model and measured kinetic parameters, in order to make clear the effects of some important factors. The simulation results indicated the evaporation of moisture from coal played a critical role. The pile height, coal type, wind velocity, and heat loss from bottom have significant effects on the process of spontaneous heating of coal pile. According to these effects, in order to increase the heat loss of pile and then effectively inhibit the self-ignition, the low pile height, good ventilation surrounding the pile, and ground material with high thermal conductivity below the pile should be used. The model developed in this model is expected to become a reliable tool to predict the spontaneous heating of coal pile.

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1. Introduction

Spontaneous heating of low-rank coal stockpile can lead to the waste of coal source and even life-threatening fires. In order to predict the behavior of the spontaneous heating, many mathematical models have been developed. These models can be generally classified as one-dimensional (1-D) [1–5] or two-dimensional (2-D) [6–7] models. Although the 1-D models have been developed and gradually improved for many years, they are still far from the real conditions. For example, a uniform gas velocity throughout the pile is usually assumed in the 1-D model, which is obviously different from reality condition. Furthermore, it is difficult to well simulate the effects of wind in surrounding air by using the 1-D models. However, the 2-D model is considered to be capable of catching the main features of real spontaneous heating process. Moghtaderi et al. [6] focused on the effect of wind flow on self-heating of coal stockpiles by a 2-D model. The calculations show that the wind flow can significantly alter the dynamics of flow field inside the pile and thereby affects the self-heating process. Akgun and Essenhigh [7] investigated the effects of pile height, pile angle, particle diameter and coal moisture with a 2-D model. Their work shows

that the spontaneous ignition can occur if the height exceeds some critical value with sufficient time. Nevertheless, it seems to be difficult to apply these models to the other cases. One of the reasons is that most of these models were developed by in-house code. Although some models can be implemented in commercial CFD software, they are still difficult to be used. For example, in these models, as an important chemical kinetic parameter describing the reaction rate of coal oxidation, the pre-exponential factor always has a unit of s^{-1}, which should be more reasonable to be a surface-basis unit for a gas–solid reaction.

In this study, a reliable 2-D model for the spontaneous heating of coal pile was built combined with the accurate measurement of coal oxidation rate. This model can be easily implemented in commercial CFD software. In addition, detailed parametric investigations were performed by applying this model to explore the effects of some important factors.

2. Experimental and modelling

2.1. Experimental

To obtain the accurate low-temperature oxidation rate of coal is very critical for the modelling of spontaneous heating. Fig. 1 shows the measuring system, which mainly consists of a heating reactor

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Nomenclature

a	oxygen reaction order (s)
A_0, A_1, A_2	pre-exponential factor (consistent unit)
C	inertial resistance factor (m^{-2})
C_p	thermal capacity ($J\,kg^{-1}\,K^{-1}$)
d	particle diameter, or diameter of main oxidation zone (m)
E	activation energy (kJ/mol)
h	height from ground (m)
H	heat (J/kg_{H_2O} for evaporation, or $J/kmol_{O_2}$ for oxidation)
Hu	Air humidity (%)
J	mass transfer rate ($mol\,m^{-2}\,s^{-1}$)
L	length of pile bottom (m)
m	mass in a cell (kg);
M	evaporation rate ($kg_{H_2O}\,m^{-3}\,s^{-1}$)
n	speed exponent (–)
Q	transfer rate of heat (W/m^2)
R	reaction rate ($kmol_{O_2}\,kg_{coal}\,s^{-1}$) or gas constant ($J\,mol^{-1}\,K^{-1}$)
S	specific surface area (kg/m^2), source term ($J\,m^{-3}\,s^{-1}$ for energy) or ($kg\,m^{-2}\,s^{-2}$ for momentum)
Δt	time step (s)
T	temperature (K)
ΔT	temperature difference (K)
U	wind velocity (m/s)
v	gas velocity (m/s)
$\vec{v}$	vector of gas velocity (m/s)

ΔV	cell volume (m^3)
x	characteristic length (m)
X	mole fraction (–)
ΔX	thickness for thermal conduction (m)
α	permeability (m^2)
β	thermal expansion coefficient (–)
ε	porosity (–)
λ	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
ρ	density (kg/m^3)
μ	viscosity ($kg\,m^{-1}\,s^{-1}$)

Subscripts and superscripts

0	atmosphere boundary layer, or ambient condition
c	coal
eff	effective
evap	evaporation of moisture
f	fluid
H_2O	moisture
i	coordinate x, y, or z
loss	heat loss
oxi	oxidation
O_2	oxygen
p	particle
rise	temperature rise
s	solid
sat	saturation status

for coal oxidation and a gas chromatograph (GC: GC3200, GL science) for measuring O_2 concentration. One sub-bituminous coal (coal A) and one bituminous coal (coal B) were used. The properties for the two coals are given in Table 1. Before the measurement, about 1.2 g of coal sample with particle size of 45–75 μm (mean diameter d_p = 53 μm) was put into a reacting tube (stainless steel, 3/8 in. in diameter), which was placed in the heating reactor. The mixture gas of O_2 (21 vol.%) and He with the flow rate of 0.015 l/min (STP) was passed through the reacting tube and reacted with the coal particles. The porosity of coal sample and residence time of mixture gas in the reacting tube were about 0.43 and 0.51 s, respectively. The heating reactor was heated electrically from 30 to 250 °C at a heating rate of 1 °C/min. Simultaneously, the O_2 concentration variations were measured by the GC and recorded by a computer. One measurement was repeated for six times. Finally, the changes of O_2 consumption rate or the oxidation rate of coal r_{oxi} ($mol_{O_2}\,kg_{coal}^{-1}\,s^{-1}$) with temperature were obtained. The relationship between the O_2 consumption rate and temperature can be expressed with an Arrhenius type of equation, as follows

$$r_{oxi} = A \exp\left(-\frac{E}{RT}\right) \tag{1}$$

Then

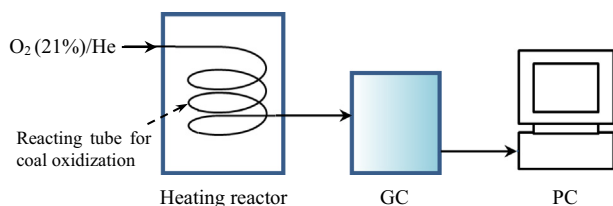$$\ln r_{oxi} = -\frac{E}{R} \cdot \frac{1}{T} + \ln A_0 \tag{2}$$

Fig. 1. Measuring system for oxidation rate of coal.

Then, the Arrhenius plot and the corresponding kinetic parameters (E and A) could be obtained. However, our previous study [8] showed that the particle size had a significant effect on the oxidation rate of coal, as shown in Fig. 2. It can be seen that the relationship between $\ln r_{O_2}$ and d_p at different temperatures for two bituminous coals can be described with a straight line with an inclination of about 1/3. In addition, the reaction order for oxygen concentration is around 0.5 [8]. Thus, the Eq. (1) can be rewritten as

$$r_{oxi} = A_1 d_p^{-1/3} X_{O_2}^{0.5} \exp\left(-\frac{E}{RT}\right) \tag{3}$$

or be expressed with outer surface area of coal particles,

$$r_{oxi} = A_2 S_p^{1/3} X_{O_2}^{0.5} \exp\left(-\frac{E}{RT}\right) \tag{4}$$

so that the pre-exponential factor (A_1 or A_2) can be unified for particles with various sizes. The obtained E and A_2 for coal A and B are also given in Table 1.

During the low-temperature oxidation of coal, physical adsorption and chemisorption occur together. However, physical adsorption is a reversible process which plays a major role only at very low temperature. In many studies, the physical adsorption was usually ignored. Furthermore, the heat of adsorption for physical adsorption is between 6.7 and 20.9 kJ/mol_{O_2}, while that of chemisorption is about 300 kJ/mol_{O_2} [9]. In this study, only the data in the temperature above 60 °C with a good linearity was used to calculate the kinetic parameters, which was considered to be the kinetics of only the chemisorption.

2.2. Modelling

ANSYS FLUENT 15.0 was employed to simulate the spontaneous heating of coal pile. The coal pile was modeled as a 2-D triangle, as shown in Fig. 3. One part of the surrounding space around the pile