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NUMERICAL MODELLING OF LOW RANK COAL FOR SPONTANEOUS COMBUSTION

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ABSTRACT: Transportating and stockpiling low-rank coals are puts them under risk of spontaneous combustion, because they are very easy to get self heating ignition after drying or removing moisture due to high moisture and oxygen contents. In this study, the modified concept of Equivalent Oxidation Exposure-time (EOE-Moisture time) has been presented for row-rank coals. The equations for the EOE-Moisture time have been formulated by considering moisture content and oxidation capacity in low temperature range to predict the heat generating rate as functions of coal moisture saturation and oxygen concentration in the pile. Numerical simulations were carried out by applying the EOE-Moisture time on self-heating of low rank coal by changing the coal stockpile size. It has been shown based on the numerical simulations that the temperature rising rate of the pile is increased with lower initial moisture saturation of low rank coal. It has been shown that coal including a large percent of moisture is easy to increase temperature and has a smaller critical diameter of coal stockpile size compared with coals with low moisture.

INTRODUCTION

Demand for low rank coals, such as brown coal and lignite, has been increasing, because they have better characteristics for coal gasification and Coal Water Mixture (COM). However, they include high contents of water and oxygen and during transporte are under risk of spontaneous combustion, because they are prone to self-ignition after drying or removing moisture that ranges around 30 to 50 % of their weight. Thus, some schemes to transport the low rank coals have been required.

As shown in Figure 1, the schematic process of spontaneous combustion was presented by Sasaki and Sugai (2011). Oxidation heat generated in the coal starts from the outside surface of the stockpile, because oxygen is supplied from the atmosphere. Some heat is lost to the atmosphere, but some also diffuses to inward to the centree of the stockpile. The outer part of the stockpile returns to the atmospheric temperature, θ^0, after enough time. However, the oxygen concentration in the pile is kept at a relatively low concentration, because oxygen does diffuse to the inner zone via the oxidation zone. When coal at the centre of the pile is preheated slowly without oxygen, a high temperature spot at the centre is generated. The oxidation and heat generation zone gradually moves from the pile surface to the centre while shrinking and rising in temperature. Finally a hot spot is formed at the centre.

In this study, the modified model on high moisture and reactive coal (hereinafter EOE-Moisture) has been presented based on the Equivalent Oxidation-Exposure time (EOE-time) that was presented by Sasaki and Sugai (2011) for bituminous coal piles in a low temperature range. The models of heat generation rate or O_2 consumption rate and the EOE-Moisture time have been derived by multiplying a function of moisture saturation in micro pores characterizing low-rank coal matrix to the EOE-time model for a bituminous coal-pile. The model of EOE-Moisture time has been applied to simulate changes of temperature, oxygen concentration and moisture saturation in the coal pile.

EOE-MOISTURE TIME AND HEAT GENERATION RATE OF LOW RANK COAL

Heat generation rate from coal

In the present model, coal oxidation reaction includes physical adsorption and chemical adsorption via oxygen reaction at low temperatures. Measurement of the heat generation rate at the early stages of the process show that an exponential decrease has been reported by many experiments, such as that by Kaji *et al*., (1987), as shown in Figure 2. Based on their measurement results, the heat generation rate

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per unit mass of coal at temperature *θ*(ºC), *q* (W/g), can be expressed with a function of elapsed time after being first exposed to air, *τ*(s):

$$q = C \cdot A\exp(-\gamma\tau) \tag{1}$$

where, *A* (kW/kg) is heat generating constant, *C* is molar fraction of oxygen, and γ(s^{-1}) is the decay power constant. The initial order of heat generating rate of coal for exposing air is $q(0)$≈0.01 to 0.001 kW/kg.

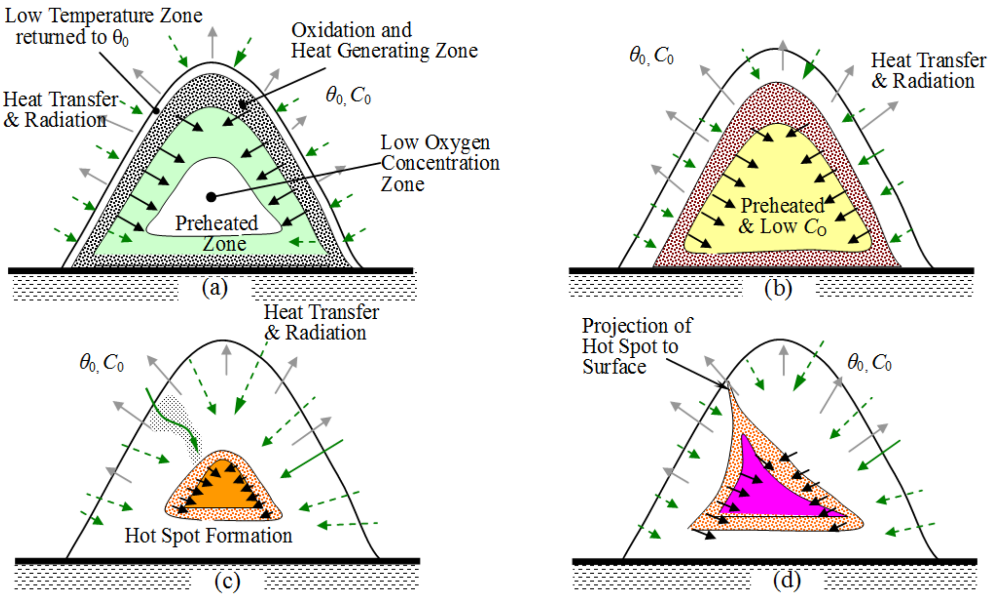

Figure 1 - Schematic figure showing self-ignition process of coal stockpile (Sasaki and Sugai, 2011)

Arrhenius equation by oxidation

Kaji *et al*. (1987) measured rates of oxygen consumption due to coal oxidation in the temperature range 20 to 170 ºC using coals ranging from sub-bituminous to anthracite. They reported that heat generated per unit mole of oxygen at steady state is *h* = 314 to 377 (kJ/mole), and their results of the Arrhenius plots, the oxygen consumption rate versus inverse of absolute temperature T^{-1} (K^{-1}), shows the model of Arrhenius equation. Thus, the higher the coal temperature; the faster the oxidation or adsorption rate. When the heat generation rate is proportional to oxygen consumption rate, the heat generated, *A*, can be estimated using the following equation,

$$A = A_0 \cdot \exp\left(-\frac{E}{RT}\right) \tag{2}$$

where, A_0 (kW/kg) is the pre-exponential factor, *E* (J/mole) is the activation energy, *R* is the gas constant (J/mol/K), and *T* (=273+*θ*) (K) is the absolute temperature. Kaji *et al.* (1987) has reported that the coals have almost the same activation energy of around *E*=50 kJ/mole for the temperature range of 20 to 170 ºC. On the other hand, the activation energy of fresh coal is expected to be much lower than that of exposed coal in air, because fresh coal adsorbs oxygen physically at an initial stage of self-heating. Average activation energy and decay power constant. For Japanese bituminous coals (see Tables 1 and 2), were used for the present numerical simulations.

Equivalent oxidation exposure time (EOE-time)

The heat generating rate, *q*, is expressed as a function of *θ*, *C*, and *τ*. Equations (1) and (2) can be used to calculate *q* for a constant temperature. However, they are not applicable for the calculation of the normal coal temperature change versus elapsed time. Its concept is partly similar to Elovich equation (see Nordon, 1979), but it provides a scheme to estimate *q* follows change of temperature of coal and

EOE-time (see Figure 3). For an example, assume a coal lump is placed in an environment in which C = 0.1 and θ =45 ºC, for elapsed time; τ =1 h, and then it is stored in one of C =0.2 and θ = 70 ºC for another 1 h period. It is not possible to reconstruct this situation by adding the former and later times with different oxidation rates. In the numerical simulations, suppose the coal pile surface is exposed to air of oxygen concentration, C_0, air temperature, θ_0, thermal diffusion and O_2 gas diffusions are numerically calculated (see Figure 1).

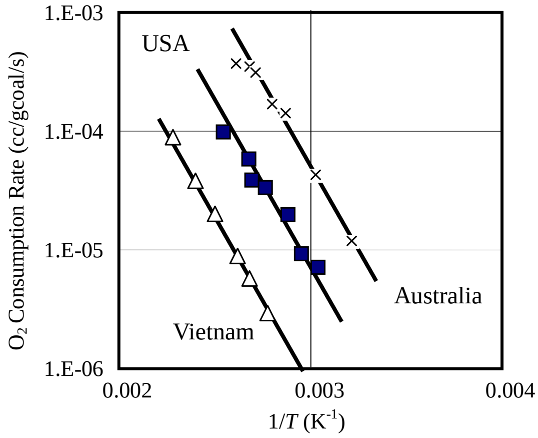

Figure 2 - O_2 consumption rate of coals vs. inverse of absolute temperature measured by Kaji *et al.* (1987) (Coal samples were mined in USA, Australia and Vietnam)

Table 1 - Physical properties of coal used for numerical simulations (Sasaki and Sugai, 2011)

Coal Density	Moisture Content	Specific Heat of Coal	Thermal Diffusivity of Coal	Diffusion Coefficient
ρ_{coal}	w_0	C_p	A	D
1291 kg/m^3	Bituminous c. : 5g/g Low rank c.: 30g/g	1.21 kJ/kg/°C	6.8×10^{-8} m^2/s	7.1×10^{-6} m^2/s

Table 2 - Heat generating properties of coal used for numerical simulations (Sasaki and Sugai, 2011)

Decay Power Constant	Pre-exponential Factor	Activation Energy
Γ	A_0	E
3.0×10^{-4} s^{-1}	Bituminous coal: 29 kW/kg Low rank coal: 88 kW/kg	20 kJ/mol

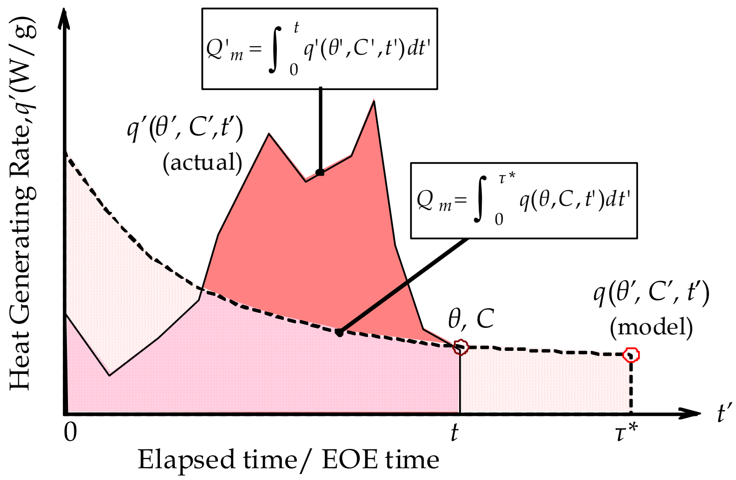

Figure 3 - Schematic definition of EOE-time of bituminous dry-coal to estimate heat generating rate by matching total heat generations (Sasaki and Sugai, 2011)

A new model of the elapsed time that considers the aging degree of the coal is required to overcome this difficulty. The cumulative generated heat of the coal, Q_m' (J/g) from elapsed time 0 to t, is defined as,

$$Q'_m = \int_0^t q'(\theta', C', t')dt' \quad (3)$$

where, the actual heat generation rate, $q'(\theta', C', t')$, θ' and C' are changing with the elapsed time, t'. However, the cumulative heat, Q_m, for constant θ and C, can be derived using Equations (1) and (2) from time 0 to τ^*:

$$Q'_m = \int_0^{\tau^*} q(\theta, C, t')dt' = Q_m \quad (4)$$

If the amounts of accumulated heat, Q'_m and Q_m, defined in Equations (3) and (4), are equal, τ^* in Eq. (4) expresses the aging time of the coal for constant temperature; $\theta = \theta'(t)$ and constant concentration; $C = C'(t)$, for the actual elapsed time ($t' = t$). In this paper, τ^* is defined as the EOE-time (see Figure 3). It is calculated based on a summation of generated heat $q'(\theta', C', t')\cdot\Delta t'$ over a numerical calculated interval time, $\Delta t'$.

Characterisation of low-rank content of low-rank coals

Low-rank coals are characterised by high porosity and internal surface area with low-rank content. As shown in Figures 4 and 5, internal surface area porosity were characterised against saturated moisture value based on measurement results of Illinois coals (Thomas and Damberger, 1976) in order to build up a modified numerical-model on oxidation and self-heat generation for low-rank coal.

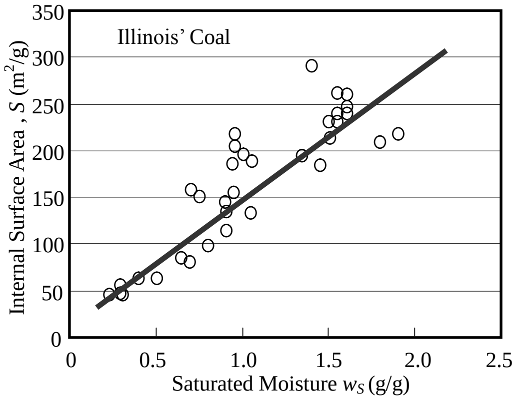

Figure 4 - Model of the relationship between saturated moisture and internal surface area of low rank coal (see Thomas and Damberger, 1976)

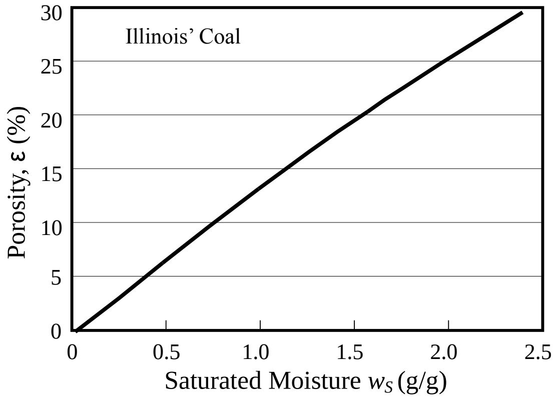

Figure 5 - Model of the relationship between saturated moisture and porosity of low rank coal (see Thomas and Damberger, 1976)

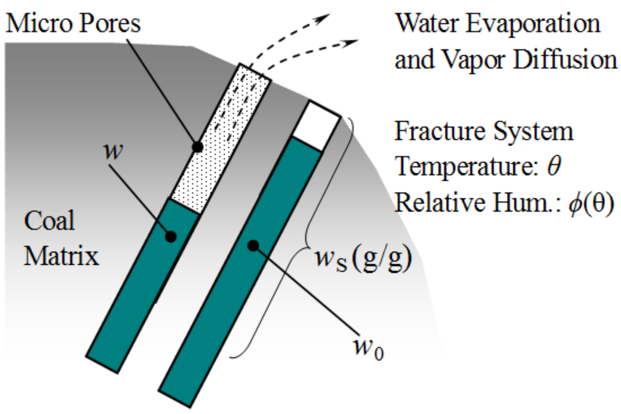

Figure 6 - Model of moisture saturation in micro-pores oflow-rank coal matrix

Formulation of EOE- Moisture model

Figure 6 shows a physical model of moisture saturation in micro-pores of coal matrix. The water evaporation rate (g/s), $\partial w/\partial t$, from micro pores to fracture channels in coal matrix is assumed to be proportional to the difference between moisture saturation and relative humidity as given by

$$\frac{\partial w}{\partial t} = \beta\left(\frac{w}{w_S} - \varphi(\theta)\right) \tag{5}$$

where β (g/s) is mass transfer rate, $\phi(\theta)$ is relative humidity at coal temperature θ, and w_s(g/g) and w(g/g) are saturated moisture and moisture at a elapsed time in the micro pores of unit mass of coal matrix, respectively. The numerical modified models of frequency factor, A(kW/kg), and EOE-Moisture time, τ^*, for low-rank coal are given by following equations (6) and (7) using moisture saturation as the analytical variable, because the internal surface area in the coal matrix can be assumed to be proportional to (1-w/w_s).

$$A(\theta, w) = A_0 \cdot \exp\left(-\frac{E/R}{273+\theta}\right)\cdot\left(1-\frac{w}{w_S}\right) \tag{6}$$

$$Q_m(\theta, w, \tau^*) = \int_0^{\tau^*} q(\theta, w, C, t)dt \tag{7}$$

For examples, when moisture is saturated (w=w_s), the frequency factor becomes A= 0, while A=A_0 for bituminous dry coal (w = 0). Thus, the presented model has a function to promote self-heating after drying of coal matrix often observed in low-rank coals.

In the present numerical simulations, molecular diffusions of O_2 and water vapor (moisture) in the coal pile as a porous media are considered by solving both partial differential equations for their concentrations with O_2 consumption and water vapor evaporation rates. The block temperatures in the coal pile are also calculated numerically at each time step based on heat generation, EOE-Moisture time defined by Equation (7) and latent heat for water evaporation from micro pores. The drying process of coal matrix in the pile starts from initial moisture saturation, w_0(g/g), and relative humidity, $\phi(\theta_0)$, in atmospheric air.

NUMERICAL SIMULATION RESULTS AND DISSCUSSION

Case of bituminous coal pile

Figure 7 shows the numerical simulation results of centre temperature, θc(°C), of a bituminous dry-coal pile with sphere shape (diameter range: d_0= 0.3 to 10 m) versus elapsed time. The temperature at the centre of the pile is increased with elapsed time, but the cases of $d_0 \le 2$ m show the temperature returns to atmospheric and initial temperature θ_0 =25 ºC. This is because that the EOE-time increased by heat transfer to surrounding air makes reducing heat generation rate of coal lump even if its location is at the centre. However, the case of $d_0 \ge 4$ m, coal at the sphere centre receiving enough heat in low oxygen concentration before oxygen diffuses into the centre, and lower EOE-time induces higher heat generation than that of $d_0 \le$ 2m before ignition and combustion of coal. The critical diameter getting self-ignition is roughly evaluated as d_0= 3m for the initial temperature of θ_0 =25 ºC. The critical diameter depends on the activation energy, E and the decay power constant, γ, of the heating of coal pile.

Case of low-rank coal pile

Numerical simulations on self-heating were carried out by applying the EOE-Moisture model for low-rank coal by setting various initial moisture saturation and relative humidity levels for atmospheric air. Figure 8 shows comparisons of temperature-time curves at the centre of a pile 10m in diameter to compare bituminous and low-rank coals. The results show that temperature rising of low-rank coal with w_0=0.3 and ϕ=0.7 is higher than that with w_0=0.8 and ϕ=0.7 after 400 days. The reason that low-rank coal of w_0=0.8 showed low temperature rise is due to large latent heat of the drying process.

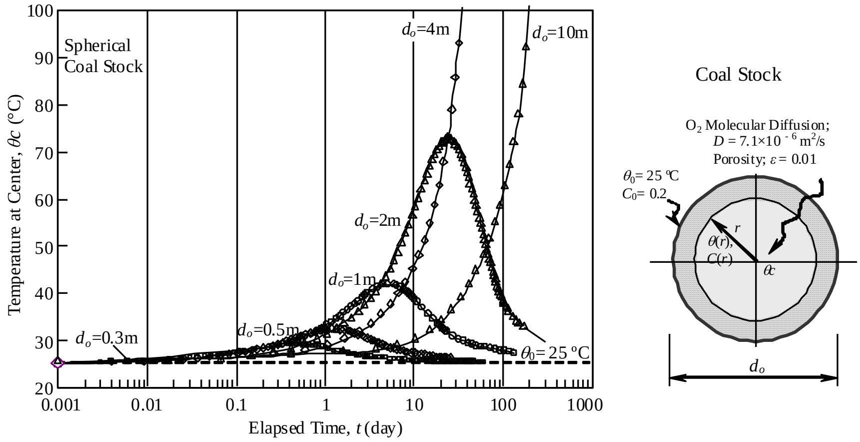

Figure 7 - Numerical simulation results on centre temperature of spherical coal stockpile of bituminous dry-coal with different diameter, d_0 (m) (Tables 1 and 2)

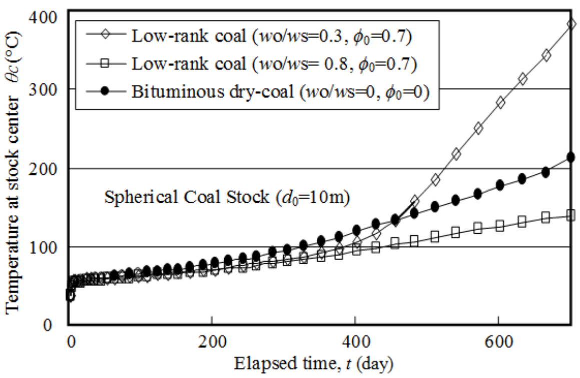

Figure 8 - Temperature-time curves at the centre in pile of bituminous and low-rank coals

CONCLUSIONS

In this study, the modified concept of EOE-Moisture time has been presented for row-rank coals. The equations for the EOE-Moisture time have been formulated by considering moisture content and oxidation capacity in a low temperature range to predict heat generating rate as functions of coal moisture saturation and oxygen concentration in the pile. Numerical simulations were carried out successfully by applying the EOE-Moisture time on self-heating of low rank coal by changing the coal pile size. It has been simulated that temperature rising rate of the pile is increased with lower initial moisture saturation of low rank coal.

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