

Modeling of Coal Spontaneous Fire in A Large-Scale Stockpile

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Abstract. The increasing need for energy consumption has resulted in the use of energy sources in coal continuing to increase. The transportation and distribution activities of coal also cause the pile to be exposed to heat when it is in a pile. Due to the kinetic characteristics of low-rank coal, the pile is very susceptible to spontaneous fire processes. Of course, this spontaneous fire phenomenon harms the safety and economic aspects of the coal pile. This study aims to model finite elements using Multiphysics simulation to determine the effect of the relative humidity of the pile on the temperature distribution of large-scale coal piles. Thus, handling methods and things that must be considered in storing and transporting coal piles can be formulated. Thermal phenomena modelling in coal piles is modeled using COMSOL Multiphysics software. The simulation is carried out by varying relative humidity of the environmental conditions (ambient). The simulation results show that this parameter can change the level of vulnerability of the pile to burn at an earlier time.

Keywords: Coal; COMSOL; Modeling; Relative humidity; Spontaneous combustion

1. Introduction

Coal spontaneous fires have received a lot of attention, especially in terms of safety. There have been catastrophic events in the coal industry due to the susceptibility of coal piles to burn themselves (Kong *et al.*, 2019). Although much of the spontaneous combustion of coal is related to laboratory scale, in reality, this problem often occurs in large-scale industries. Recently, studies on the tendency of coal piles to experience spontaneous fires continue to concern some researchers worldwide. Since 1924, testing methods have been introduced to determine the factors that play a role in the tendency of coal to burn on its own (Wang *et al.*, 2018; Davis and Byrne, 1924). However, the problems faced in industrial conditions are very different from what occurred on a laboratory scale; namely, coal piles have a vast dimension. Therefore, the approach or method of testing used in the laboratory must reflect physical and chemical phenomena at large scales. This statement has been discussed alongside overviews regarding typical industrial spontaneous combustion characteristics in ref (Shi *et al.*, 2022). Due to laboratory limitations in conducting large-scale testing, researchers continue to strive to study the phenomenon of spontaneous fires through numerical studies.

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The development of numerical studies related to spontaneous coal fires has entered the domain of CFDs (Taraba *et al.*, 2014) and multiphysics simulations (Thabari *et al.*, 2021; Saleh *et al.*, 2017). Large-scale simulations with stockpile conditions exposed to prolonged ambient thermal exposure have been done before (Zhang *et al.*, 2016; Taraba *et al.*, 2014). However, these studies ignore the influence of water content, both in the air in the form of relative humidity (RH) and the moisture concentration of coal in its simulation. In reality, RH is a vital parameter determining coal's susceptibility to spontaneous combustion phenomena. Another study (Wang *et al.*, 2018) provides that RH is vital in initiating spontaneous fires in coal piles.

This study seeks to improve previous studies by involving the influence of RH from the air in a simulated process. The simulation was conducted using COMSOL Multiphysics which proved capable of modeling spontaneous coal fire simulations on a large scale (Li *et al.*, 2021). The model is validated by comparing the simulation results with similar references, especially temperature and flow development.

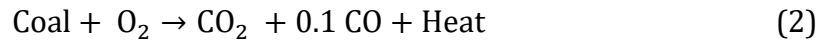
2. Modelling

2.1. Chemical Kinetics

The process of spontaneous combustion in coal is initiated by an oxidation reaction that is influenced by temperature and other factors. Despite its complexity, previous research conducted by Carras and Young (1994) and Yuan and Smith (2008) have determined that the rate of oxidation reactions in coal piles can be simplified to

$$r_{\text{ox}} = AC_{\text{O}_2} \exp\left(-\frac{E_a}{RT}\right) \quad (1)$$

Based on experimental studies that had been carried out (Yuan and Smith, 2008), the oxidation reaction of coal at low temperatures can be simplified to



The heat generated from the oxidation reaction in coal is described by the equation 3 as follow

$$Q = r_{\text{ox}} \Delta H_c \quad (3)$$

With ΔH_c is the amount of heat generated during the coal oxidation process. The value used in this study is 300 kJ/g-mol O_2 (Zhang *et al.*, 2016)

2.2. Momentum Conservation

In the section on porous media, the Brinkman equation models how fluid moves through the coal pile matrix. This is because coal piles are a coarse matrix with high permeability (Zhu *et al.*, 2013). The equation has been proved to be more accurate in simulating the fluid flow in a porous coal matrix where the high parameter of Reynold and Darcy are required (Wen *et al.*, 2017).

$$\rho \frac{\partial \mathbf{u}}{\partial t} = \nabla[-p\mathbf{I} + \mathbf{K}] - \left(\mu \kappa^{-1} + \beta \epsilon_p \rho |\mathbf{u}| + \frac{Q_m}{\epsilon_p^2} \right) \mathbf{u} + \mathbf{F}, \quad \beta = \frac{d\rho}{dp} \frac{1}{\rho} \quad (4)$$

$$\frac{\partial \epsilon_p \rho}{\partial t} + \nabla(\rho \mathbf{u}) = Q_m \quad (5)$$

$$\mathbf{K} = \mu \frac{1}{\epsilon_p} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu \frac{1}{\epsilon_p} (\nabla \mathbf{u}) \mathbf{I} \quad (6)$$

Assuming that the particle size is uniform, the Kozerny Carman permeability model is used

$$\kappa = \frac{d_p^2}{180} \frac{\epsilon_p^3}{(1 - \epsilon_p)^2} \quad (7)$$

2.3. Energy Conservation

The heat transfer phenomenon described in the model uses a heat transfer approach in porous media. The heat sources modelled in this simulation are convection and radiation phenomena from the ambient environment and heat generation due to oxidation reactions.

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \nabla T + \nabla \mathbf{q} = Q \quad (8)$$

$$\mathbf{q} = -k_{\text{eff}} \nabla T \quad (9)$$

$$(\rho C_p)_{\text{eff}} = \theta_p \rho_p C_{pp} + (1 - \theta_p) \rho C_p \quad (10)$$

$$k_{\text{eff}} = \theta_p k_p + (1 - \theta_p) k \quad (11)$$

The heat transfer that occurs from forced convection in an environment with ambient temperature occurs with the following equations 12 and 13 as follows:

$$-\mathbf{n} \mathbf{q} = d_z q_o \quad (12)$$

$$q_o = h(T_{\text{ext}} - T) \quad (13)$$

The heat generated from the oxidation reaction in a pile is modeled according to equation (1) and equation (3). However, equation (3) shall be modified by including porous fraction so that it becomes equation 14 as follows:

$$r_{\text{ox}} = A C_{\text{O}_2} \exp\left(-\frac{E_a}{RT}\right) (1 - \theta_p) \quad (14)$$

In the simulation with RH, the gas flow that enters the pile is considered air with certain humidity.

$$C_p = \frac{X_a M_a C_a + X_v M_v C_v}{M_a X_a + M_v X_v} \quad (15)$$

$$C_a = 1047.64 - 0.377T + 9.45 \times 10^{-4} T^2 - 6.02 \times 10^{-7} T^3 + 1.79 \times 10^{-10} T^4 \quad (16)$$

$$C_v = 4653.75 - 31.45T + 0.14T^2 - 3.31 \times 10^{-4} T^3 + 4.27 \times 10^{-7} T^4 - 2.88 \times 10^{-10} T^5 + 7.94 \times 10^{-4} T^6 \quad (17)$$

$$X_{\text{vap}} = \frac{\phi_i P_{\text{sat}}(T_\phi) M_v}{(P_\phi - P_{\text{sat}}(T_\phi) \phi_i) M_a} \quad (18)$$

$$X_v = \frac{c_v RT}{P_A} \quad (19)$$

$$c_v = \frac{X_{vap} P_A}{RT \left(\frac{M_v}{M_a} + X_{vap} \right)} \quad (20)$$

$$\phi = \frac{X_{vap} P_A}{P_{sat}(T_\phi) \left(\frac{M_v}{M_a} + X_{vap} \right)} \quad (21)$$

2.4. Species Conservation

The transport phenomena of chemical species in this model were assumed to be in convective manners. Fick's equation is used to model interactions between species in this model.

$$\rho \frac{\partial \omega_j}{\partial t} + \nabla \mathbf{j}_j + \rho (\mathbf{u} \nabla) \omega_j = R_j \quad (22)$$

$$\mathbf{j}_j = - \left(\rho D_j^f \nabla \omega_j + \rho \omega_j D_j^f \frac{\nabla M_n}{M_n} - \mathbf{j}_{c,j} + D_j^T \frac{\nabla T}{T} \right) \quad (23)$$

$$M_n = \left(\sum_j \frac{\omega_j}{M_j} \right)^{-1} \quad (24)$$

$$\mathbf{j}_{c,j} = \rho \omega_j \sum_k \frac{M_i}{M_n} D_k^f \nabla x_k \quad (25)$$

2.5. Boundary Condition

The model is assumed to be affected by the wind from one side of the pile. The pressure equation, which is affected by the wind flow speed, is chosen as the previous study (Krishnaswamy *et al.*, 1996)

$$P = P_a - \rho_{g,a} u_w^2 \left(\frac{\tan \theta}{2\pi} \right) \ln \left\{ \left(\frac{x}{2W - x} \right)^2 \right\} \quad (26)$$

On each side, there is heat transfer due to convection by external ambient conditions with a convective heat transfer coefficient of 7.5 W/m².K (Krishnaswamy *et al.*, 1996). The moving wind flow is assumed to be the air containing only O₂ in a 21% mass fraction. Table 1 contains all set parameters for the boundary conditions.

Table 1 Boundary Conditions

Parameter	Boundary			
	AB	BC	CD	DA
Pressure	Eq. 27	Eq. 27	$\frac{dP}{dy} = 0$	$\frac{dP}{dx} = 0$
γ_{O_2} (Mass fraction)	21%; inflow	outflow	-	-
γ_{CO_2} (Mass fraction)	-	outflow	-	-
γ_{CO} (Mass fraction)	-	outflow	-	-

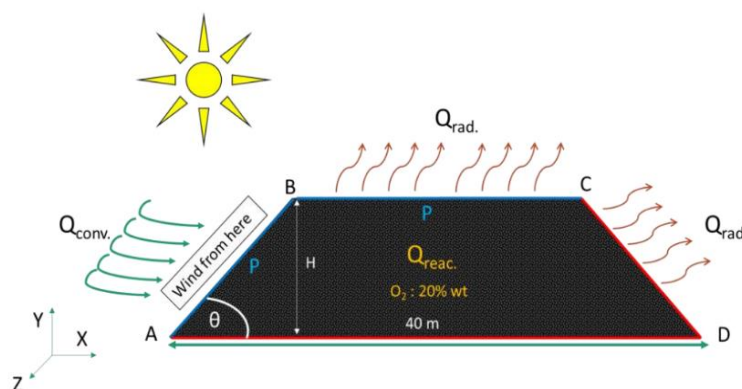
- : no flux

Table 2 Nomenclature

ρ	= coal density (kg/m ³)	C_v	= Vapor concentration in air (mol/m ³)
ϵ_p	= pile porosity	ϕ	= Relative humidity
β	= Thermal compressibility coefficient (1/Pa)	h	= Convective heat transfer coefficient (W/m ² .K)
μ	= dynamic viscosity (Pa.s)	d_z	= Geometry thickness (m)
C_p	= media specific heat capacity (J/kg.K)	d_p	= Particle size (cm)
T	= Temperature (K)	k	= Thermal conductivity (W/m.K)
t	= Time (s)	ω_i	= Species' 'i' mass fraction
k_{eff}	= Effective thermal conductivity (W/m.K)	j_i	= mass flux relative to mass average velocity (kg/m ² .s)
θ_p	= Porous medium volume fraction	D^f	= Coefficient of diffusivity (m ² /s)
X_a	= Air (dry) molar fraction	D^T	= Thermal diffusivity coefficient (kg/m.s)
X_v	= Air (vapor) molar fraction	u	= Velocity field (m/s)
X_{vap}	= Air moisture content	R_j	= Reaction rate (mol/m ³ .s)
A	= Pre-exponential factor (1/s)	E_a	= Activation energy (J/mol)
ΔH	= Heat of reaction (J/mol)		
C_{O_2}	= Oxygen concentration (mol/m ³)		
M	= Molar mass (g/mol)		

2.6. Model Geometry

Two coal pile geometries are depicted in two dimensions in this study. The geometry of the first pile refers to the following sources (Zhu *et al.*, 2013) to validate the species transport equation (can be seen in Figure 2). The coal pile is depicted as a trapezoid with a base length of 12 m and a height of 6 m. The angle of the inclined part of the pile is 56.3°. As seen from Figure 1, the second pile geometry is chosen to facilitate the change (variation) of some test parameters. The second pile also has a similar shape, namely a trapezoid with a height of 10 m, an angle value of 45°, and the length maintained at 40 m.

**Figure 1** Model Geometry

It is worth mentioning that the angle of pile correlates to the capacity of the coal-handling facility. Even though it is not discussed further in this study, this angle characteristic might be impactful because it correlates with the drag force of the wind. The model is assumed to have an infinite size in the z-axis direction. The simulation is carried out by taking a slice from the pile's center. With a very long geometry in the z-axis direction, the effect of the phenomenon in the z-direction is assumed to have no significant impact.

2.7. Model Assumption

The model in this study was developed by making assumptions in several parts. It is done to reduce the computational load but still provide representative results for the experiment. The assumptions are 1. The particle size of the pile is assumed to be uniform; 2. The porosity of the pile is assumed to be uniform for each point; 3. The spread of molecules in the stack occurs by diffusion; 4. The heat source involved in the heat transfer

process is the convection process from the environment and the heat from the oxidation process; 5. The phenomenon of movement of water particles (moisture) from coal is not modeled; 6. Coal is considered a dry pile; 7. The intrinsic effect of coal is neglected; 8. The characteristics of the simulated coal samples are taken from (Chen *et al.*, 2018) unless explicitly mentioned; 9. All simulations were transient simulations with the time step of 1 day; 10. All simulations were assigned with 303 K ambient temperature.

3. Results and Discussion

3.1. Model Validation

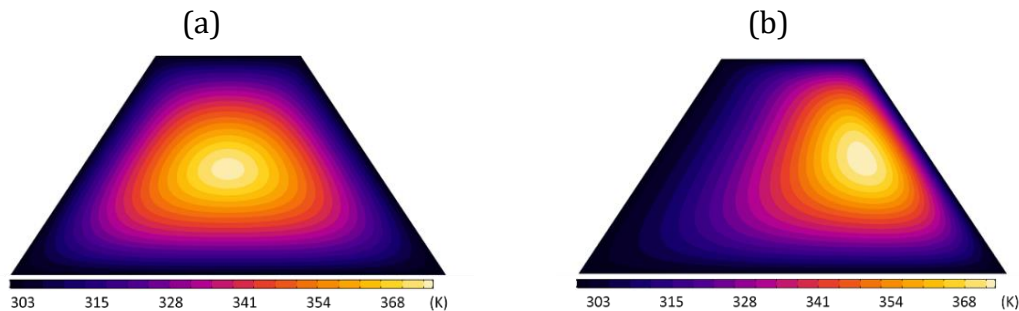


Figure 2 Simulation results for validation: (a) day 55; $v = 1$ m/s and (b) day 55; $v = 0.05$ m/s

The model is validated using the following reference (Zhu *et al.*, 2013), including the input physical and chemical parameters. This study selected a wind speed value of 0.05 m/s and 1 m/s to match the results with the reference. This study attempts to apply the transport of concentrated species interface to case studies. The Transport of Concentrated Species (TCS) interface is selected based on COMSOL usage guidelines that state that transport of diluted species is suitable for use when the number of solvents reaches 90% (COMSOL, 2019). In Zhu's study, the only species modelled was O_2 . In general, the composition of air is 21% O_2 and 79% N_2 by mass fractions (γ). Assuming that N_2 is solvent, the interface is less precise to use. N_2 is also considered inert and only used as a mass train (Wu *et al.*, 2016). It is known that the nitrogen content is still relatively stable to a temperature of 600°C (Pels *et al.*, 1995) and requires a temperature that can be reached up to 1200°C to be able to react to the process of pyrolysis coal (Jiao *et al.*, 2021) so the selection of N_2 as inert in this study is still entirely appropriate. In terms of validation, the isothermal contour distribution of the study results is comparable to the exact parameters of reference (Zhu *et al.*, 2013) through Figure 2.

It is seen that the models that apply the TCS interface can describe similar results with the reference. However, there is a slight difference from the maximum temperature value achieved. In the study with wind speeds of 0.05 m/s, the maximum temperature reached was 396 K. Meanwhile, the maximum temperature recorded by this study on the same day and conditions was 367 K. The same thing was also seen in the simulation results with wind speed conditions of 1 m / s. The maximum temperature value recorded from this study is 367 K. At the same time, the reference shows a value of 410 K. This difference is obtained due to the effort to use dynamic parameters in the simulation model. The dynamic parameters used are the air's thermal characteristics and the magnitude of the O_2 flux that goes into the pile. Thermal characteristics of air are obtained from the COMSOL Material Library, while flux O_2 is described through equation 27.

$$flux = \frac{0.21P}{RT} \quad (27)$$

Although discrepancies exist, it is worth noting that this study also reached a temperature (80 – 90°C) where coal pile spontaneous combustion has occurred, similarly like what was done in (Zhang *et al.*, 2016).

3.2. Flow Field Within the Pile

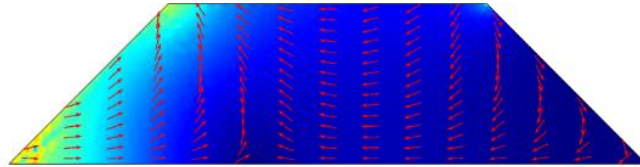


Figure 3 Flow field map within the pile of this study.

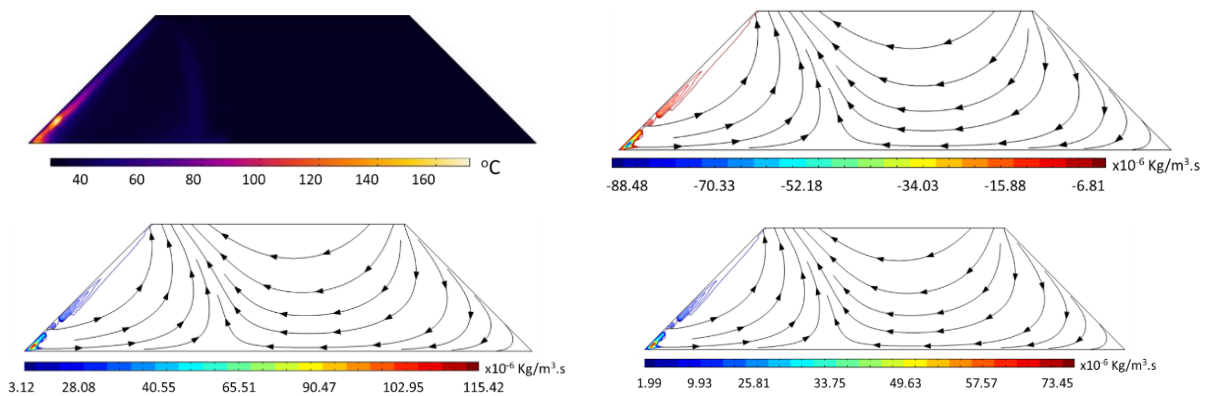


Figure 4 Temperature distribution (Top-Left); O₂ consumption rate (Top-Right); CO₂ production rate (Bottom-Left); CO-Production rate (Bottom-Right); on the 30th day with the following configurations (1 cm particle size, 0.3 porosity, 1 m/s velocity, 0.7 RH)

There are two studies described the flow patterns in large-scale coal piles when they are affected by wind (Taraba *et al.*, 2014, Zhang *et al.*, 2016). In both studies, the computing domain was determined as very large to minimize the outlet's influence of wind flow on coal piles. Based on Figure 3, the simulation results from this study showed a flow pattern in a good resemblance as reported in (Taraba *et al.*, 2014, Zhang *et al.*, 2016). Simulation results show that the flow is experiencing circulation where air enters from the side of the pile and goes towards the top end of the pile. In ref (Zhang *et al.*, 2016), this was described as the chimney effect. From the study, it can also be observed that although a stream of wind flows down the other side of the pile, the temperature development on that side is not very significant. It can happen because the flow does not provide the power to penetrate the cracks of the pile which allows oxygen to enter and initiate the dominant oxidation process.

The flow rate tends upwards because the pressure recorded at the top end of the pile is lower when compared to the pressure within the pile. Therefore, O₂ coming through the sides also experiences a tendency to move towards the flow. Nevertheless, the reactivity of coal makes oxygen consumed on its way to a low-pressure point. It is seen that the hot spot of the pile is centered around the area where the rate of O₂ consumption is very dominant. It gives the idea that the oxidation process continues to occur in the lower third of the pile where the pressure is more dominant, allowing O₂ to enter and penetrate the cracks of the

pile and react before the oxygen makes it to the top of the pile. The region where the highest temperatures are observed is also where the CO and CO₂ production rate is seen highest.

3.3. Relative Humidity

An earlier experimental study by the author (Nugroho *et al.*, 2008) showed that relative humidity played an essential role in self-heating, leading to spontaneous combustion. In order to study the effect of environmental humidity conditions toward the coal pile, simulations were carried out by varying relative humidity (RH) values. The selected humidity values estimate the expected value in tropical countries and Indonesia in particular. The effect of the difference in humidity can be seen in Figure 5.

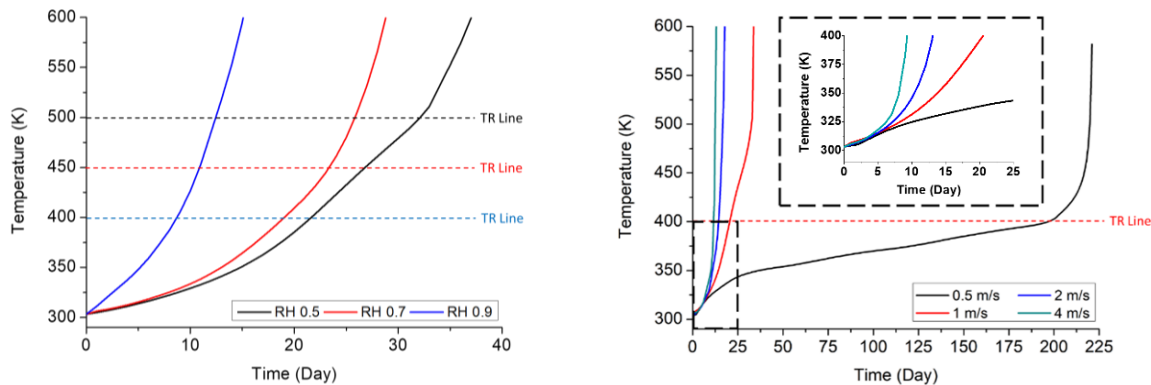


Figure 5 Left: T-t graph on RH variation. Right: T-t graph on velocity variation

The simulation results (Figure 5) show that with RH conditions of 0.5, the time required for the pile to reach the thermal runaway (TR) phenomenon is 33 days. Increasing the value to RH 0.7 shortens the time required for the pile to reach thermal runaway to 25 days. The pile becomes increasingly critical to experience thermal runaway when the RH value is at the highest value, which is 0.9. Temperature development results were similar (Wang *et al.*, 2018). The mentioned study observed that coal piles would experience an earlier temperature increase when irrigated with air with a higher RH value. It was also explained that the heat of rewetting occurs when extra heat is produced due to the condensation and wetting process of the bulk material. Similar to (Wang *et al.*, 2018), this model does not incorporate the competition between the evaporation of the pile's moisture content and heat from the condensation process because the pile is simulated as a dry pile. The heat (heat of rewetting) is caused by the condensation of the water content carried by air at the pile's bottom. Alongside the RH graph, the Temperature – time graph of the velocity effect shows that the coal pile's susceptibility toward spontaneous combustion increases as the velocity (wind) increases. Future developments can be made to simulate the competition process between moisture evaporation and heat of rewetting in order to better analyze phenomena that may occur in real-world conditions.

4. Conclusions

This study was done to observe how relative humidity could influence the susceptibility of coal piles to undergo spontaneous combustion. Two coal pile geometry were simulated, where one was done for model validation purposes only. This study's result strengthens the fact that a higher relative humidity value could make the coal pile more prone to spontaneous combustion. Given the result that ambient condition is influential toward spontaneous coal combustion, adjustments to the geographical conditions of the storage area or shipping lane to be traversed can provide knowledge for managers in preparing appropriate plans/scenarios in the storage or transportation process. Hence, it

can increase the safety factor of the pile for the mentioned scenarios. Nevertheless, this study was done in two-dimensional (2D) shape, where the assumption of very long geometry toward one direction (here, it is z-axis direction). This assumption might fall through for cases with intermediate sizes and might require three-dimensional (3D) simulations. Therefore, future study with 3D simulations might help to provide more understanding for coal spontaneous combustion in wider range of large pile in storage transportation.

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