

Mathematical modelling of the coal stockpile self-heating process. A case study

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Abstract

A simulation of the self-heating process occurring naturally in coal beds was carried out for a coal stockpile from Lupoaia (Romania). In order to obtain realistic results, meteorological data collected on site was used. Thermo-physical and chemical properties of coal used in the analysis were evaluated using samples from the actual stockpile. It was found that the self-heating process occurs at higher rate in the vicinity of the side slopes of the stockpile. Side slope exposure to wind is another factor that boosts the self-heating process.

Key Words: numerical modeling, coal, self-heating

1. Introduction

Self-heating in coal stockpiles occurs naturally especially in low grade coal with high content of volatile matter. The chemical process that results in self-heating is the low temperature oxidation, which is an irreversible exothermic reaction. The negative effect of self-heating is the decrease of coal quality (calorific value). If the self-heating is not controlled then a thermal avalanche type process occurs since increased temperature leads to a higher reaction rate.

Spontaneous self-heating is a major problem in transport and storage of coal since the process, if not controlled, results in fire and important production loss.

Coal storage in large stockpiles is essential in ensuring continuous supply for large capacity power units. Storage site must be properly prepared in order to minimize the risk of fire. Several rules of thumb in coal storage can be enumerated: the coal should be stored in several small piles instead of a large one in order to prevent temperature buildup and facilitate the inspection; stockpiles should not be higher than 4 m and should not contain more than 1500 t of coal; storage of coal with high content of moisture should be avoided.

The storage volume and the storage time are parameters depending on safety and continuity of coal supply to the power plant. Since the coal stockpile acts as a buffer between the coal extraction unit and power plant

the stockpile volume and storage time cannot be properly controlled.

Carras and Young [1] reviewed the methods used to predict the spontaneous heating tendencies in laboratory experiments. Some commonly used methods are crossing point measurements, isothermal and adiabatic calorimetry, oxygen sorption, and temperature differential. Although laboratory experiments provide some insight in the self-heating mechanism the results cannot be upscaled to a real stockpile since it is not possible to reproduce some scaling effects at small-scale experiments [2]. Two large scale spontaneous heating tests are available in the literature [3,4] designed to simulate the spontaneous heating under actual storage conditions.

2 Modeling of low-temperature coal oxidation

Low-temperature coal oxidation is a complex process not fully understood. Three types of processes are believed to occur (Carras and Young [1]): (1) physical adsorption; (2) chemical adsorption, which leads to the formation of coal-oxygen complexes and oxygenated carbon species; and (3) oxidation in which the coal and oxygen react with gaseous products released in previous phases, typically carbon monoxide (CO), carbon dioxide (CO₂), and water vapor (H₂O). Oxidation is by far the most exothermic reaction of all three. The temperature values for which the processes mentioned above occur can be found in [2].

The mathematical model used in this paper is described in detail in [5]. It is based on the classic equations of flow, heat and mass transfer and coal low-temperature oxidation.

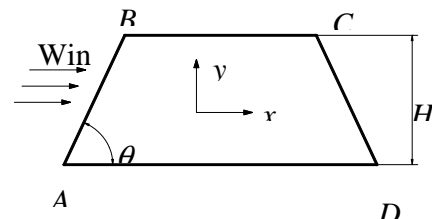


Figure 1

Continuity equation for the gaseous phase flow is given by:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0 \quad (1)$$

For the low values of flow velocity Darcy law can be applied. Momentum equation for the gaseous phase is:

$$\frac{\partial p}{\partial x} = \frac{\mu}{k} v_x \quad (2a)$$

$$\frac{\partial p}{\partial x} = \frac{\mu}{k} v_y + g\rho_{g,a} \frac{T - T_a}{T} \quad (2b)$$

Equation (2b) includes the natural convection modelled through Boussinesq approximation.

By combining (1), (2a) and (2b) the following equation is obtained:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = g\rho_{g,a} \frac{T_a}{T^2} \cdot \frac{\partial T}{\partial y} \quad (3)$$

Molecular diffusion of oxygen is not included in the analysis and the steady state is assumed. These assumptions yield the following equation:

$$v_x \frac{\partial y_{O_2}}{\partial x} + v_y \frac{\partial y_{O_2}}{\partial y} = -R_{O_2} \quad (4)$$

Internal temperature gradients in the coal particles are neglected. Coal particles and gas are considered at the same temperature at any specific location within the stockpile. The energy balance for the pseudo-homogenous medium consisting of the coal particles and gas can be written as:

$$(1-\epsilon_b)C_{p,c} \frac{\partial T}{\partial t} = -\rho_{g,a} C_{p,g} \left\{ v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} \right\} + k_{eff} \left\{ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right\} + R_{O_2} \Delta H_r \quad (5)$$

Heat conduction in the stockpile is governed by Fourier law with an effective thermal conductivity 0.2 W/(mK) (Brooks [6]).

Oxygen consumption rate is an essential parameter in the coal self-heating phenomenon. In this paper, a simplified expression was used [5]:

$$R_{O_2} = \eta_G (1-\epsilon_b) K_r y_{O_2} \\ R_{O_2} \approx \eta_G (1-\epsilon_b) k_1 y_{O_2} \quad (6a)$$

where:

$$K_r = K_{r0} \exp(-E_A / RT) \approx k_1 \quad (6b)$$

Equations (6a) and (6b) apply to both dry coal as well as to fresh wet coal introduced in the stockpile.

Equations (3-5) are coupled non-linear partial differential equations. With appropriate initial and boundary conditions these equations model the self-heating process of coal in the stockpile.

Initial conditions:

$$v_x = v_y = 0, \quad P = P_a, \quad T = T_a \\ x \geq 0, \quad 0 \leq y \leq H, \quad t = 0 \quad (7)$$

Boundary conditions:

Wind velocity and the angle of the side slope influence to an important extent the boundary conditions for the pressure variable. The boundary condition for pressure is obtained from theory developed for flow over steep slopes [7].

Along boundaries AB and CD:

$$P = P_a - \rho_{g,a} u_w^2 \frac{\tan \theta}{2\pi} \ln \left\{ \left(\frac{x}{2W-x} \right)^2 \right\} \quad (8a)$$

where $W = H / (2tg(\theta))$.

Along boundary BC:

$$P = P_a - \rho_{g,a} u_w^2 \frac{\tan \theta}{2\pi} \ln \left\{ \left(\frac{x}{2W-x} \right)^2 \right\} \quad (8b)$$

and:

$$k_{eff} \frac{\partial T}{\partial y} \Big|_s + \rho_g C_{p,g} v_y (T|_s - T_a) = h(T|_s - T_a) \quad (8c)$$

The convection heat transfer coefficient at the upper surface of the stockpile was considered $7.5 \text{ W/(m}^2\text{K)}$ according to [6].

On the boundary DA the following equations apply

$$\frac{\partial P}{\partial y} \rightarrow 0 \quad \frac{\partial T}{\partial y} \rightarrow 0 \quad T = T_a \quad (8d)$$

3 Numerical modeling.

Commercial software package ANSYS CFX was used to simulate the physical processes involved in the self-heating phenomenon. ANSYS CFX is a general purpose CFD solver with capabilities ranging from transport equations to chemical reactions modeling applications. The spontaneous heating of coal was modelled as a surface chemical reaction, coal oxidation, occurring on the coal surface in a porous medium. The heat generated from coal oxidation is dissipated by convection and conduction, while oxygen and oxidation products are transported by convection and diffusion.

The mass and heat transfer equations respectively are given by (in tensor notation):

$$\rho u_i \frac{\partial Y}{\partial x_i} = \rho D \frac{\partial^2 Y}{\partial x^2} + S \quad (9)$$

$$\begin{aligned} \left[\epsilon \rho_g c_{pg} + (1 - \epsilon) \rho_c c_{pc} \right] \frac{\partial T}{\partial \tau} + \rho_g c_{pg} u_i \frac{\partial T}{\partial x_i} = \\ = \lambda_{eff} \frac{\partial^2 T}{\partial x_i^2} + rQ \end{aligned} \quad (10)$$

The effective thermal conductivity is calculated as:

$$\lambda_{eff} = \epsilon \lambda_g + (1 - \epsilon) \lambda_c \quad (11)$$

In the equations above, index g refers to the gas phase and c to coal. ϵ is the porosity of the coal bed and is defined as the ratio between the bulk density and the coal particle density.

The physical model of the stockpile was developed on the following assumptions:

- truncated pyramid shape with the following dimensions: length 200 m, width 20 m, height 10 m, angle of the side slopes 60 °;
- initial temperature within the stockpile constant at any location and equal to 8 °C;
- coal particles have regulated shape (sphere);
- coal thermo-physical and chemical properties are presented in Table 1

Table 1. Thermo-physical and chemical properties of coal and coal bed

Coal particle density	1280 kg/m ³
Bulk density of the coal bed	840 kg/m ³
Specific heat capacity	1110 J/(kg K)
Thermal conductivity coefficient	0.175 W/(m K)
Heat of reaction	320 kJ/mol O ₂
Activation energy	70 kJ/mol
Pre-exponential factor	1.85E06 K/s
Coal particle diameter	0.01 mm

- temperature at the interface of the stockpile with the soil was 10 °C
- meteorological data (ambient temperature, wind velocity and direction, air humidity) was
- the stockpile is oriented in such a way that the one of the long slope side was exposed to the dominant wind direction

4. Results and discussion

A transient regime simulation was carried out using the data and assumptions presented in the previous paragraph. The simulation interval was considered 90 days. The two-dimensional temperature profile in the cross-section of the stockpile was recorded. Typical temperature profiles in the stockpiles are presented in Figure 2. A steady temperature increase caused by the heat generation due to low-oxidation reaction in the coal bed can be observed in the whole stockpile. More intense heat generation can be noticed in the vicinity of the side slopes, especially left slope, exposed to the dominant wind direction. The heat generation rate in the vicinity of the side slopes higher than in the rest of the stockpile can be explained by the favorable conditions for the low-temperature oxidation of coal. Access of oxygen and ventilation caused by the exposure to the dominant wind direction are considered the main factors that boost the low-temperature oxidation reaction. A very intense hot-spot appears in the vicinity of side slope exposed to the dominant wind direction appears at approximately one third of the height (measured from the base of the stockpile).

In the situation under analysis in this paper the high intensity hot spot mentioned above emerges approximately after 60 days from the beginning of storage. The presence of the hot spot is explained by the most favorable conditions for self-heating that appear in the hot spot area. The apparition of the hot spot at approximately one third of the stockpile height was also observed by Akgun and Essenhigh [8].

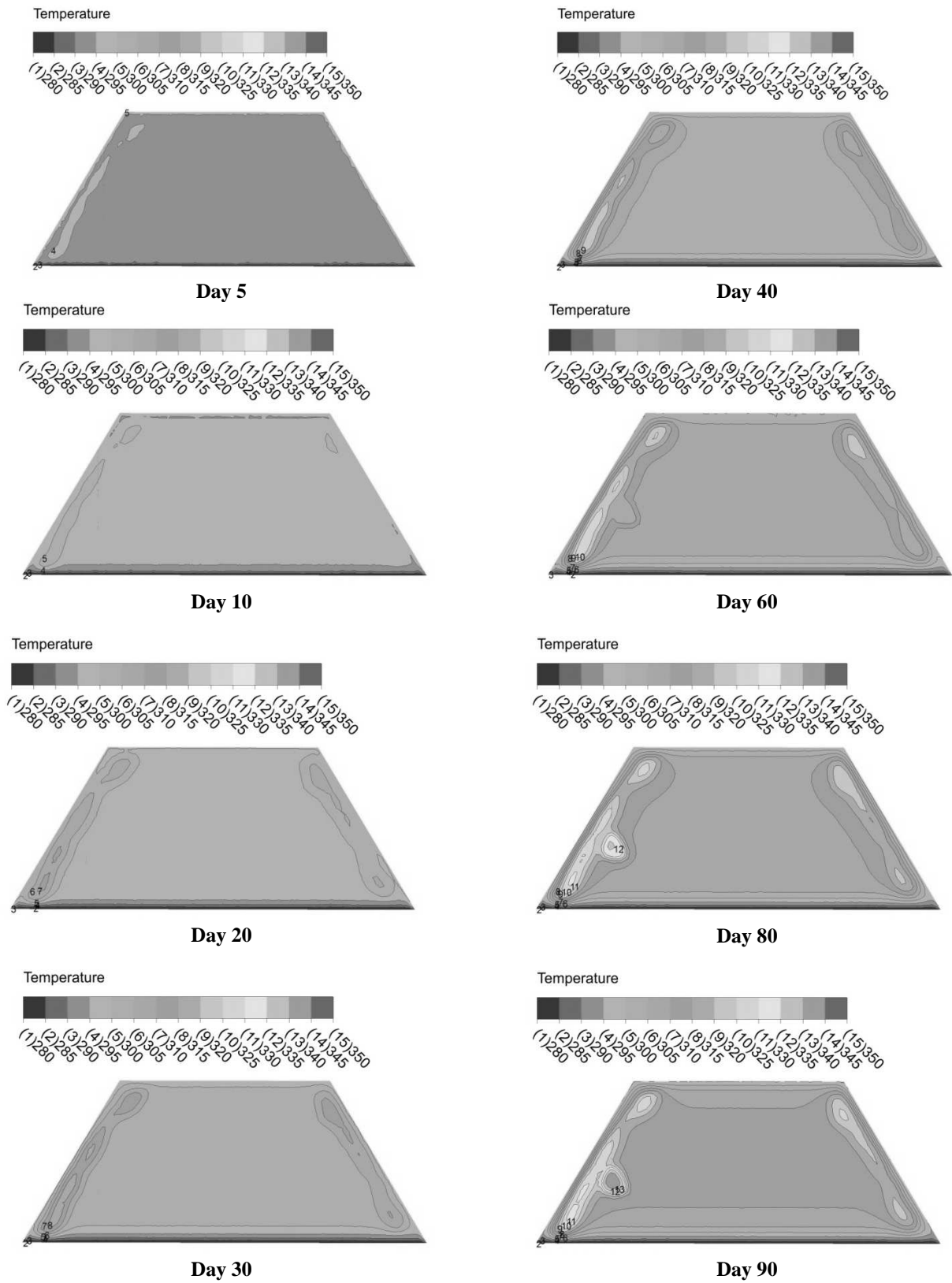


Figure 2. Two-dimensional temperature profile in the stockpile (cross section)

4 Conclusion

The self-heating process in coal beds occurs naturally due to the low-temperature oxidation reaction. The main factors that favour the self-heating are humidity and presence of oxygen. Continuous supply of oxygen as in the case of side slope coal stockpile exposed to wind increases the rate of the low-temperature oxidation reaction. Significantly higher temperature values and hot-spot were observed in the vicinity of the side slope exposed to the dominant wind. Oxygen penetration depth in the coal bed is influenced by the coal porosity and hence the hot-spots may occur at different depths in coal beds with different values of the porosity.

The humidity of the coal plays an important role in the dynamics of the self-heating process. Low-grade coal with high humidity content is more prone to self-heating. In such case, the temperature increases rapidly at the beginning of the storage process. As the temperature increases the evaporation will absorb heat and the temperature may approach a steady state [8].

Actions that could diminish the intensity of the self-heating process and prevent production loss through fires can be: preventing access of fresh air by covering the stockpile with asphalt, storage of coal with small particle size, storage of coal with low humidity, decreasing the storage interval to the minimum possible.

Nomenclature:

c_p	specific heat capacity
d_p	average particle diameter
E_A	activation energy for the oxidation reaction
g	gravity acceleration
G	molar flow rate of air
h	convection heat transfer coefficient
H	total vertical height of stockpile
ΔH_r	heat of oxidation reaction
k_1	rate constant for the burnoff reaction
k_{eff}	effective thermal conductivity of the coal bed
K_r	rate constant
K_{ro}	pre-exponential factor
L	length parameter
p_d	dimensionless pressure
p	pressure
Δp	pressure drop
R_{O_2}	oxygen consumption rate
R	molar gas constant
t	time

t_d	dimensionless time
T	temperature
T_d	dimensionless temperature
\bar{T}	average temperature within coal stockpile
u_w	wind velocity
$v_{x,y}$	velocity in the x and y respectively direction
x	length in x direction
x_d	dimensionless length parameter x direction
y	length in y direction
y_d	dimensionless length in y direction
y_{O_2}	oxygen mole fraction
W	width parameter ($W = H / (2 \tan \theta)$)
ϵ_b	bed porosity
η_G	global effectiveness factor
ρ	density
θ	angle of inclination
Subscripts	
a	ambient conditions
c	coal
g	gas
m	gas and coal mixture
s	surface

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