

Modelling Spontaneous Combustion of Coal

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Abstract

Spontaneous combustion of coal is an important problem in mining and storage, in terms of both safety and economics. This is because coal reacts with oxygen in the air and an exothermic reaction occurs, even in ambient conditions. The heat of the reaction accumulates and the reaction becomes progressively faster and thermal runaway may take place to the point of ignition. A detailed computer model has been developed to simulate a bulk-scale, one-dimensional test column. Predictions from this model can then be used to simulate full-scale storage conditions. Model predictions are verified by using the experimental results from the test column at the University of Queensland. A 2-m column is being used in this laboratory to conduct a practical test capable of providing reliable data on coal self-heating.

Coal self-heating results produced with the 2-m column are consistent with theory. In particular, the hot spot development in test runs closely matches model predictions. Features of moisture transfer and hot spot migration are clearly visible, both in the model and in tests in the column.

Under the specific conditions considered in this study, it is shown that a subbituminous coal can reach thermal runaway in 4.5 days. This result is confirmed by observations made at the mine site, where hot spots have been found to occur within this timeframe.

The results obtained in this study indicate that there is a definite need to consider the influence of coal moisture on spontaneous combustion.

Key words: Spontaneous combustion, Callide coal, Hot spot development, Moisture transfer

Introduction

Spontaneous combustion of coal is an important problem in its mining, long distance transportation, and storage, in terms of both safety and economics. This is because coal reacts with oxygen in the air and an exothermic reaction occurs, even in ambient conditions. A problem arises when the rate of heat release produced by this process is more than is dissipated by heat transfer to the surroundings. The heat of reaction accumulates, the reaction becomes

progressively faster, and thermal runaway may take place to the point of ignition.

It is for these reasons that the phenomenon of spontaneous combustion of coal has been of fundamental and practical importance to scientists. Several theoretical and experimental studies have been performed on coal spontaneous combustion (Van Doornum, 1954; Nordon, 1979; Schmal et al., 1985; Brooks and Glasser, 1986; Arisoy and Akgun, 1994; Akgun and Arisoy, 1994; Krishnaswamy et al., 1996; Monazam et al., 1998; Arisoy and Akgun, 2000; Ak-

gun and Essenhigh, 2001). The main purposes of these studies were to develop methods for determining the conditions at which the coal pile could undergo spontaneous combustion, to predict the safe storage time under those conditions, and to determine the influences of factors contributing to the spontaneous heating.

Theoretical investigation of the spontaneous combustion of coal stockpiles is cost effective, and easier and faster than experimental investigations. However, the self-heating process depends on many factors, such as coal rank, temperature, airflow rate, the porosity of the coal pile, moisture content of coal and its changes, and particle size of coal. To provide a quantitative analysis of spontaneous combustion with a computer model requires knowledge of a large number of coal and gas properties. In addition, kinetic parameters appear in the model equations. These parameters must be obtained by methods that ensure realistic and representative data for full-scale storage conditions. For a dependable computer model, the predictions obtained with the model should be compared to bulk-scale test results and some parameters should be adjusted according to these results to provide an effective history match. A detailed computer model has been developed to simulate a bulk-scale, one-dimensional test column. Predictions from this model can then be used to simulate full-scale storage conditions.

A spontaneous combustion testing laboratory has been developed at the University of Queensland (UQ), School of Engineering. A 2-m column is being used in this laboratory to conduct a practical test capable of providing reliable data on coal self-heating. The results of experiments from the column are being used to verify the model predictions. This paper presents a history match of the hot spot development in subbituminous coal from the Callide Coalfield of Queensland.

Mathematical Model and Assumptions

The complete model involves considerable interaction among the physicochemical properties of coal, heat transfer, oxidant, water vapour, and moisture content of coal. This model is based on the following assumptions:

1. The model is one-dimensional.
2. A horizontal, cylindrical test column is considered.

3. There is heat loss at the outer surfaces of the column.
4. Only forced convection of air is considered. Thermal expansion of the heated gas in the bed and natural convection flows are neglected.
5. The coal pile is homogeneous and isotropic, with uniform spherical coal particles.
6. The coal density remains constant during the processes of oxidation, evaporation, and condensation.
7. The variation of gas flow rate along the coal bed due to oxygen consumption, CO, and CO₂ production, evaporation, and condensation is neglected.
8. The heat of wetting compared with that of condensation is negligible.
9. Oxygen consumption rate, which is described by the Arrhenius equation, is assumed to be first-order with respect to the oxygen concentration.

Governing Equations

The spontaneous combustion of a coal pile can be modelled by 6 one-dimensional time-dependent differential equations. These are conservation of oxygen, moisture, and energy for gas and solid phases. The equations to be solved are listed below:

Oxygen mass conservation in the gas phase:

$$(1 - \alpha) \frac{\partial \rho_{1o}}{\partial t} + V \frac{\partial \rho_{1o}}{\partial x} = D_{1o}^{(e)} (1 - \alpha) \frac{\partial^2 \rho_{1o}}{\partial x^2} - \alpha \varepsilon \rho_{1o} k \quad (1)$$

Oxygen mass balance in the coal particle:

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(D_{2o}^{(e)} \frac{\partial \rho_{2o}}{\partial r} r^2 \right) = \rho_{1o} k \quad (2)$$

Moisture conservation in the gas phase:

$$(1 - \alpha) \frac{\partial \rho_{1w}}{\partial t} + V \frac{\partial \rho_{1w}}{\partial x} = D_{1w}^{(e)} (1 - \alpha) \frac{\partial^2 \rho_{1w}}{\partial x^2} + \alpha r_w \quad (3)$$

Moisture conservation in the solid phase:

$$-\rho_s \frac{W'_0}{W_0} \frac{\partial w}{\partial t} = r_w = \rho_s K_w (w^* - w) \quad (4)$$

Energy conservation for the solid phase:

$$\begin{aligned} \alpha \rho_s c_p \frac{\partial T_s}{\partial t} &= \alpha \lambda_s^{(e)} \frac{\partial^2 T_s}{\partial x^2} + \frac{3}{R} \alpha h (T_g - T_s) - \\ \alpha \Delta H_w r_w + \alpha \varepsilon \Delta H_o \rho_{10} k - \frac{4}{\Phi} K_{sur} (T_s - T_a) \end{aligned} \quad (5)$$

Energy conservation for the gas phase:

$$\begin{aligned} (1-\alpha) \frac{\partial}{\partial t} (\rho_g c_g + \rho_w c_w) T_g + V \frac{\partial}{\partial x} (\rho_g c_g + \rho_w c_w) T_g = \\ (1-\alpha) \lambda_g^{(e)} \frac{\partial^2 T_g}{\partial x^2} - \frac{3}{R} \alpha h (T_g - T_s) \end{aligned} \quad (6)$$

The initial and boundary conditions used in the model can be written as:

$$\text{at } t = 0: T_s = T_a, T_g = T_a, \rho_{1o} = \rho_{ao}, \rho_{1w} = \rho_{aw}, W = W_0$$

$$\text{at } x = 0: \lambda^{(e)} \frac{\partial T_s}{\partial x} = h_0 (T_s - T_a), T_g = T_a, \rho_{1o} = \rho_{ao}, \rho_{1w} = \rho_{aw}, \frac{\partial W}{\partial x} = 0$$

$$\text{at } x = L: -\lambda^{(e)} \frac{\partial T_s}{\partial x} = h_0 (T_s - T_a), \frac{\partial T_g}{\partial x} = 0, \frac{\partial \rho_{1o}}{\partial x} = 0, \frac{\partial \rho_{1w}}{\partial x} = 0, \frac{\partial W}{\partial x} = 0$$

$$\text{at } r = 0: \frac{\partial \rho_{2o}}{\partial x} = 0$$

$$\text{at } r = R: \rho_{2o} = \rho_{1o}$$

The oxidation reaction of a coal particle at low temperatures can be considered to be controlled by both chemical rate and pore diffusion rate. In this regime, oxygen may reach the centre of the particle, but an oxygen concentration gradient within the particle occurs with an increase in temperature or particle size. The dependence of the overall oxidation rate on particle size and temperature is described by defining an effectiveness factor. Effectiveness factor ε is the ratio of the actual to the maximum volumetric oxidation rate. This factor is defined by analytical solution of the oxygen mass balance equation in a particle.

In this study, some of the physical constants and properties are evaluated using auxiliary empirical formulae and some known mathematical models.

Experimental Equipment

Beamish et al. (2002) describe the test equipment, the UQ 2-m column, which is 0.19 cm in diameter and has a 62-l capacity, equating to 40-70 kg of coal depending upon the packing density used. Coal self-heating is monitored using 8 evenly spaced thermocouples along the length of the column that are inserted into the centre of the coal at each location (Figure 1). Eight independent heaters correspond to each of these thermocouples and are set to switch off at 0.5 °C below the coal temperature at each location so that heat losses are minimised and, effectively, semi-adiabatic conditions are maintained radially. Temperature lag between heater and coal can be adjusted. Therefore, this column can experimentally simulate any type of radial heat loss from coal piles.

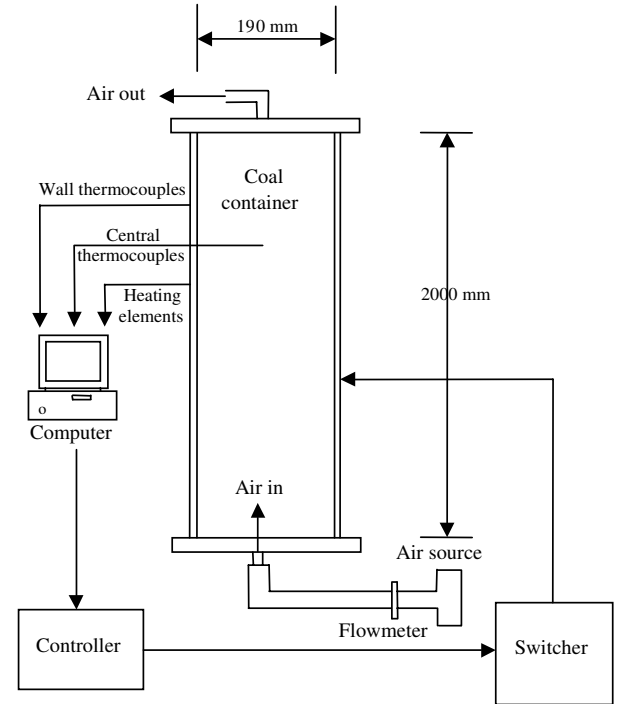


Figure 1. Schematic of the UQ 2-m column self-heating apparatus (modified from Arief, 1997).

Sample and Preparation

Samples of Callide subbituminous coal (UQ-COLQLD4) were obtained from a larger batch of fresh run-of-mine (ROM) coal for testing in the UQ 2-m column. Coal analytical data are given in Table 1. The coal particle size was kept below 75 mm,

representing normal product coal for the operation and the size distribution of the batch was determined prior to loading into the column (Table 2). The average particle size was 3.51 mm based on the procedure described by Kunii and Levenspiel (1991) for estimating the surface-volume average particle size from the size distribution of the coal. Three subsamples were taken at this stage to obtain data on the as-received moisture of the coal.

Test Procedure

A standard test procedure has been developed for the UQ 2-m column coal self-heating tests. The coal is loaded into the column with three 20-l plastic buckets. Once all the coal is in the column, it is sealed and the heaters are used to set the starting coal tem-

perature. This is achieved overnight. Air is then introduced to the coal. A computer records all data at 10-min increments. The column has several safety devices including computer-controlled trips on the external heaters and a temperature trip on the air inlet line. These are set to ensure maximum safety during operation of the column.

Results of Column Testing

Test results of UQCOLQLD4 coal are used in this study to compare to theoretical results from the mathematical model. This coal is subbituminous in rank, with an as-received moisture of 15.0% and an ash content of 15.0%, on a dry basis. Experimental conditions of the test are given in Table 3.

Table 1. Analytical data for Callide coal used in the bulk self-heating test of UQCOLQLD4.

| | Callide coal | Çan coal |
|---|--------------|----------|
| Moisture content (% , as-received) | 15.0 | 13.0 |
| Ash content (% , dry basis) | 15.0 | 17.7 |
| Volatile matter content (% , dry mineral matter free) | 35.4 | 32.3 |
| Calorific value (MJ/kg, dry ash free) | 31.30 | 44.3 |

Table 2. Particle size distribution of column sample.

| Size fraction (mm) | Average particle diameter, d_p (mm) | Coal mass (g) | Mass fraction | Mass fraction/ d_p |
|--------------------|---------------------------------------|---------------|---------------|----------------------|
| -75 + 45 | 60.00 | 7668.1 | 0.146 | 0.00244 |
| -45 + 26.5 | 35.75 | 7099.2 | 0.136 | 0.00379 |
| -26.5 + 13.2 | 19.85 | 8233.5 | 0.157 | 0.00792 |
| -13.2 + 6.7 | 9.95 | 74,88.2 | 0.143 | 0.01437 |
| -6.7 + 2.36 | 4.53 | 81,94.0 | 0.156 | 0.03454 |
| -2.36 | 1.18 | 13,684.2 | 0.261 | 0.22145 |
| Total | | 52,367.2 | | 0.28452 |
| Average d_p (mm) | | | | 3.51 |

Table 3. Experimental conditions used for 2-m column test.

| | |
|--------------------------|-----------------------------|
| Column length | 2 m |
| Column diameter | 0.19 m |
| Coal start temperature | 34 °C |
| Air inlet temperature | 23 °C |
| Air flow rate | 12.3 E-06 m ³ /s |
| Average particle size | 3.51 mm |
| Porosity | 0.4 |
| Initial moisture content | 15% |

Hot spot development in the column for sample UQCOLQLD4 is summarised in Figure 2, which shows the temperature profile changes that take place with time. In the initial stage of the heating, the airstream transfers moisture from coal nearest the air inlet to coal further downstream in the pile. Subsequently, a hot spot forms approximately 1.45 m from the air inlet (Figure 2) due to both coal oxidation and heat of condensation. After 2 days, the coal temperature plateaus at approximately 90 °C. The hot spot then progressively migrates towards the air inlet as the coal dries out and chases air to sustain the oxidation reaction.

On day 4.4, the hot spot reaches coal that is extremely dry, resulting in thermal runaway. This occurs approximately 0.6 m from the air inlet. The moisture distribution along the column at the end

of the test is shown in Figure 3. The minimum in moisture content at 0.6 m corresponds to the heat release of the hot spot at that location. The moisture transfer and the delay in thermal runaway until the coal dries out that was observed in this bulk coal experiment is consistent with the results of Bhat and Agarwal (1996), and Schmal et al. (1985).

Model Predictions

The computer program is run to predict the experimentally measured values. Predictions of the program are tested by comparing these values with the experimentally measured values. For this purpose, test conditions are given as input to the computer program. Input data are summarised in Table 4.

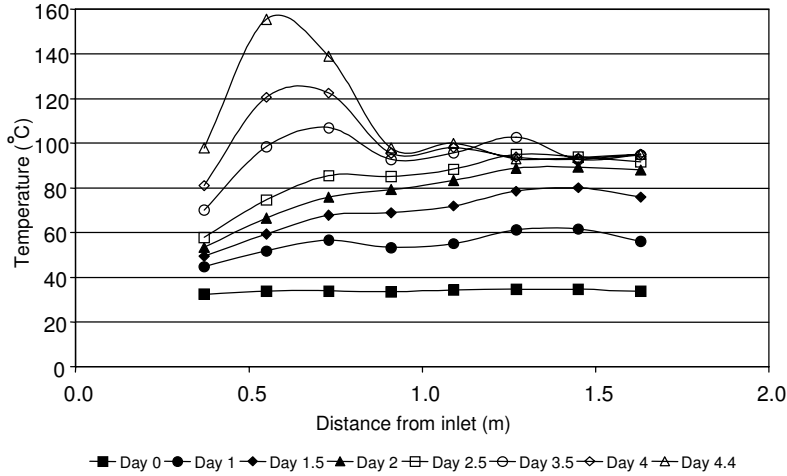


Figure 2. Temperature profile of coal self-heating in the UQ 2-m column.

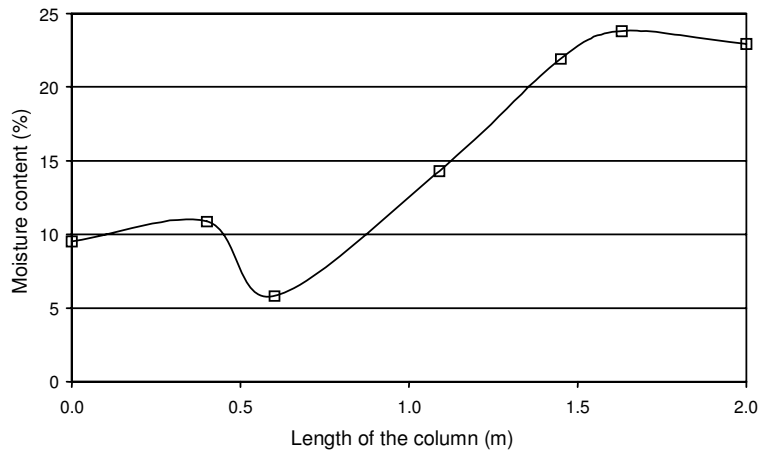


Figure 3. Moisture distribution along the column at the completion of the experiment.

Table 4. Input data for the model.

| | | |
|--|-----------------------------------|-----------|
| Compaction degree of coal bed | [m ³ /m ³] | 0.6 |
| Coal particle diameter | [m] | 0.00351 |
| Activation energy | [j/mol] | 41330 |
| Pre-exponential reaction factor | [1/s] | 1550 |
| Oxygen diffusion coefficient (in the gas) | [m ² /s] | 2.00 E-05 |
| Heat of reaction | [j/kg-O ₂] | 9.38 E+06 |
| Gas flow rate | [m ³ /s] | 12.3 E-06 |
| Density of coal | [kg/m ³] | 1125 |
| Density of air | [kg/m ³] | 1.16 |
| Coal initial temperature | [K] | 307 |
| Gas initial temperature | [K] | 296 |
| Initial relative moisture of air | [-] | 0.6 |
| Specific heat of water vapour | [j/kg-K] | 1870 |
| Convective heat transfer coefficient (coal-air entrance) | [W/m-K] | 4 |
| Convective heat transfer coefficient (coal-air exit) | [W/m-K] | 0.1 |
| Initial oxygen concentration | [kg/m ³] | 0.26752 |
| Initial moisture of coal (wet) | [kg/kg] | 0.15 |
| Initial moisture of coal (dry) | [kg/kg] | 0.176 |
| Evaporation rate coefficient | [1/s] | 2.00 E-04 |
| Diameter of reactor | m | 0.19 |
| Heat loss resistance of reactor | W/m ² K | 0.5 |

Reactivity of coal is determined by the pre-exponential reaction factor and activation energy. These 2 constants are obtained from the test results of UQCOLQLD4 coal. Specific reaction rate coefficients should be defined experimentally under spontaneous combustion conditions. Oxidation occurs throughout the body of the coal particle at low temperatures. Conventional coal combustion rate data at elevated temperatures is not useful for the spontaneous combustion case.

Other important data are evaporation/condensation rate coefficients. These coefficients should also be determined experimentally. Experimentally determined rate coefficients of Turkish ÇAN coal is used in this study. ÇAN coal properties are similar to those of UQCOLQLD4 coal and are given in Table 1.

Assumptions for heat loss coefficients are made considering physical conditions and other coefficients are taken from the relevant literature.

There are 5 dependent variables to be calculated by the program. These are coal temperature, gas temperature, coal moisture content, oxygen mass concentration in the gas phase, and moisture mass concentration in the gas phase. Predicted temporal and spatial distributions of these variables are given

in Figures 4-7.

In Figure 4, coal temperature distribution predictions are given. In the initial stage of the heating, the airstream transports moisture. Due to condensation downstream in the coal pile, the temperature increases. This situation continues until the end of the 3rd day. After that, thermal runaway starts developing in the relatively dry region closer to the inlet. At the end of the 4.5th day, considerable thermal runaway can be recognised 0.6 m from the inlet. These predictions coincide with the experimental results. The experimental maximum temperature plateau of 90 °C is established at 110 °C in the model predictions. The qualitative behaviour of theoretical predictions represents the test results very well. Quantitative differences are basically due to deficiency in rate data.

In Figure 5, predicted moisture content of coal is given. Initial moisture content is 0.176 kg/kg on a dry basis. Dry air causes a small amount of evaporation at the entrance for the test conditions. If the air were humid, condensation could occur instead at the entrance region. Downstream in the column, evaporation of the coal moisture is due primarily to the heat of reaction. This evaporated moisture is transported by the air flow and condenses over the coal

surface near the outlet of the column. Due to the degree of evaporation and temperature increase, part of the column is completely dried out in the thermal runaway region.

Moisture density in the gas phase is given in Figure 6. Moisture in the gas phase increases due to evaporation at the entrance region and decreases due to condensation towards the outlet of the column. Moisture level also increases with time and reaches a maximum value on the 3rd day. Then, the moisture level starts to decrease due to moisture carried by the gas flow.

In Figure 7, prediction of oxygen density in the

gas stream is given. The decrease in oxygen level indicates the exothermic oxidation reactions. Cumulative oxygen consumption along the coal pile results in a continuous decrease. At the end of the 2nd day, oxygen in the downstream gas flow is completely consumed. This region moves towards the entrance with time. The air feeding rate is very small, and after establishing a considerable amount of oxidation reaction, oxygen is consumed at the very beginning part of the coal pile and oxidation cannot progress further downstream of the pile. Again, due to lack of oxygen, thermal runaway moves towards the entrance of the pile where oxygen is still available.

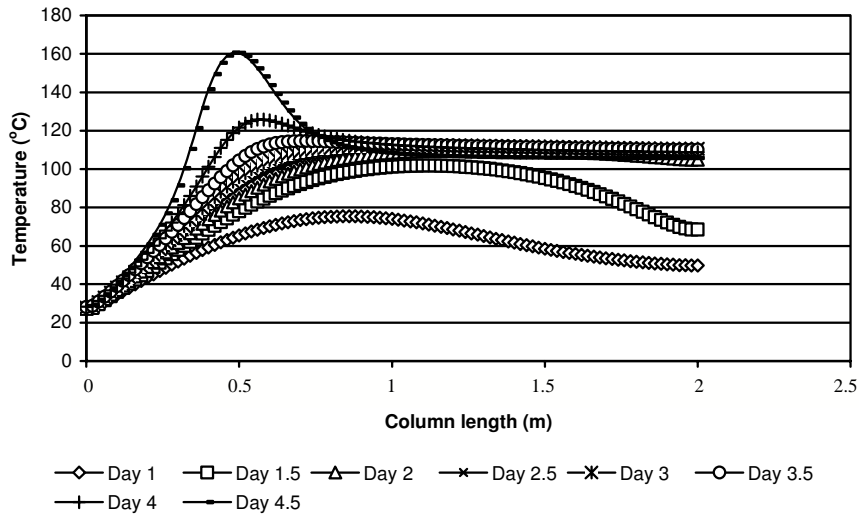


Figure 4. Theoretical predictions for temporal variation of coal temperature profiles.

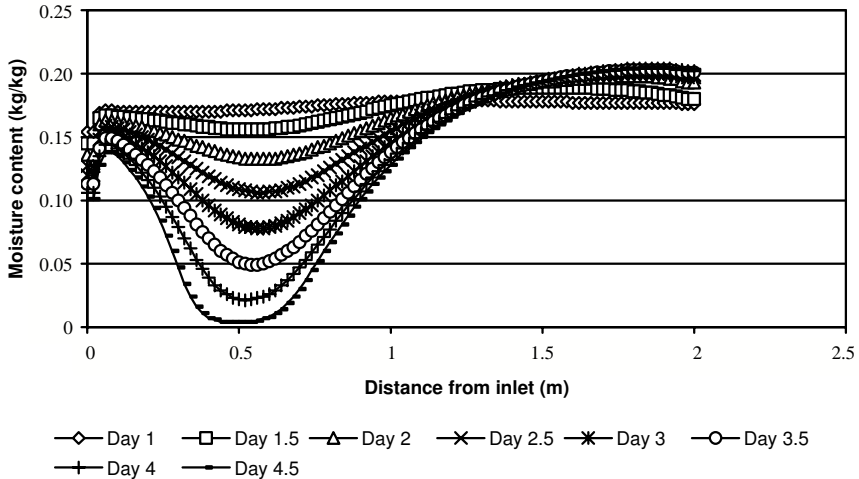


Figure 5. Theoretically predicted coal moisture distributions along the column.

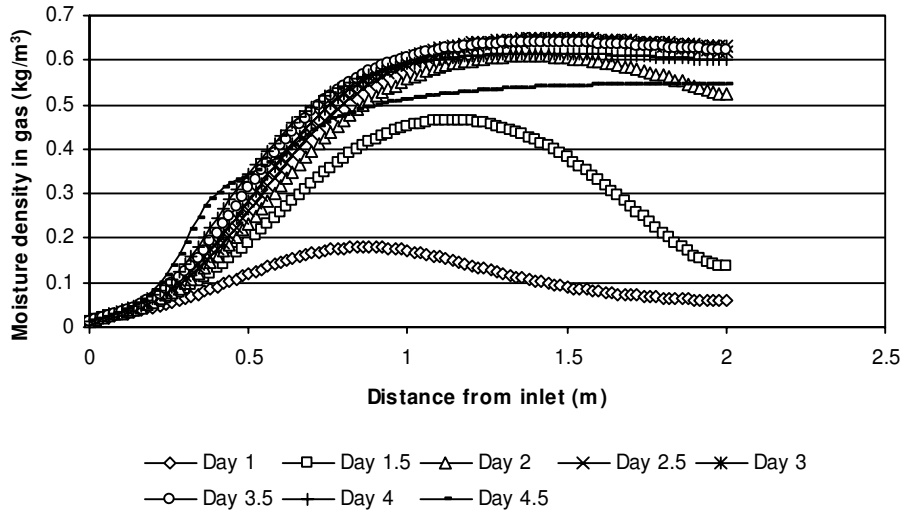


Figure 6. Theoretically predicted moisture densities in gas volume along the column.

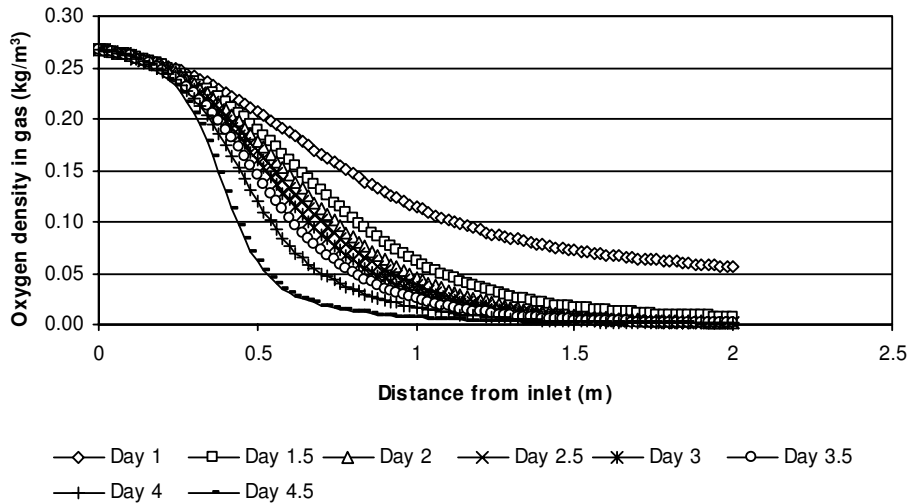


Figure 7. Theoretically predicted oxygen densities in gas volume along the column.

Conclusions

Spontaneous combustion of coal piles are investigated both theoretically and experimentally in this study. A computer program is developed for this purpose and tests are conducted in the UQ 2-m column.

Coal self-heating results are consistent between theory and experiments. In particular, the hot spot development in test runs closely matches the model predictions. Features of moisture transfer and hot spot migration in the column are clearly visible, both in the model and in tests.

Theoretical models can be successfully used to

investigate coal self-heating processes; however, to achieve dependable results, these theoretical models should be supported by experimental investigations.

Under the specific conditions considered in this study, it is shown that a subbituminous coal can reach thermal runaway in 4.5 days. This result is confirmed by observations made at the mine site, where hot spots have been found to occur within this timeframe.

The results reached in this study indicate that there is a definite need to consider the influence of moisture in the coal on spontaneous combustion, particularly with respect to the delay in reaching thermal runaway.

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Nomenclature

| | |
|--------------|---|
| C_p | specific heat capacity |
| D | diffusion coefficient |
| ΔH_0 | heat of reaction of oxygen with coal |
| ΔH_w | heat of evaporation of water |
| k | reaction rate |
| r_w | evaporation/condensation rate of water vapour |

| | |
|---------------|---|
| T | temperature |
| V | gas velocity |
| w | coal moisture content |
| w^* | balance moisture |
| W_0 | initial moisture rate of coal by wet base |
| W_0' | initial moisture rate of coal by dry base |
| α | compaction degree of coal bed |
| ε | effectiveness factor for oxidation |
| λ | thermal conductivity |
| ρ | density |
| Φ | column diameter |

Subscripts

| | |
|---|--------------------|
| g | gas |
| s | solid |
| w | water vapour |
| o | oxygen |
| a | ambient conditions |
| 1 | in gas phase |
| 2 | in solid phase |

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