

# The Nature of Underground Heating as Indicated by Numerical Modeling

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## ABSTRACT

A numerical model of the spontaneous combustion of coal has been developed and is being used to investigate the nature of self-heating in underground coal mines. Results to date confirm the complexity of the self-heating reaction in coal and illustrate the impact of the factors such as the coal reactivity, mass and airflow through the coal pile. Subtle differences in the chemical, physical and environmental conditions and make a significant difference in the development of a high temperature self-heating or a low temperature benign condition, the subtlety escaping normal underground observations. Additional work is planned to investigate the thresholds for such factors in the development of spontaneous combustion and its implications for detection by gaseous products.

## INTRODUCTION

Spontaneous combustion of coal in underground coal mines continues to represent one of the most significant hazards to the safety of workers in the mines in which they are employed. Many sources of ignition of methane gas have been removed from mines over the years, through their identification, and elimination by exclusion or changes in mining practices. These are generally associated with the mechanical aspects of mining coal or the ventilation of the underground workings. However, while ever coal mining takes place, crushed coal will be exposed to air and, under the right circumstances, spontaneous combustion can occur possibly leading to an open fire. If methane is present, a very dangerous situation can arise.

Inadequate detection methods and inappropriate control techniques can exacerbate the dangers of spontaneous combustion. Late detection means that a heating will be more advanced (hotter and /or larger) with the attendant greater risk of igniting methane. Inability to evaluate the state of a heating can easily lead to the use of inappropriate control techniques when the heating is too far advanced.

Explosions of methane, attributed to ignition by spontaneous combustion, have resulted in the deaths of 43 miners and the loss of three underground coal mines in Queensland over the last 25 years. Contributing factors in all three cases were inadequate detection and control techniques, much of which can be traced to a poor understanding of the nature of spontaneous combustion in underground coal mines. Very little is known regarding the nature of underground heatings and their controlling factors apart from rare anecdotal information on actual heatings, the results of gas analysis used in detection and the qualitative extrapolation from small scale laboratory tests. Some large scale self-heating tests have been carried out but with the emphasis on understanding of the stockpiling situation and are, due to their expense, limited in number and range of conditions studied.

A means of overcoming these difficulties is to develop a numerical model that may be used to examine a wide range of circumstances and conditions. Numerical modeling has been used in the past to examine the nature of spontaneous combustion in coal stockpiles but generally only over a limited range of coal types, particle size distributions, and configuration. The principles

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of modeling spontaneous combustion in stockpiles, however, can be adapted to understanding spontaneous combustion in underground coal mines to explain many aspects of this phenomenon.

To this end a number of numerical models that simulated self-heating of coal under conditions of forced ventilation, as occurs in underground heatings, have been developed and continue to be refined. Some of the factors that will be examined in the study will include the inherent reactivity and moisture content of coal, the geometry and mass of reactive coal as well as the rate of airflow through and permeability of the heating site. These will be related to in-situ conditions such as coal rank, the degree of fracturing and compaction of the heating site, and the pressure differentials required to cause heating. Modeling will also be used to predict the nature of the off-gas from a heating and used to evaluate current detection techniques such as Graham's ratio and carbon monoxide make.

This paper will discuss the basic understanding of spontaneous combustion, the basis of the models being developed and preliminary results obtained to date.

## THE BASICS OF SPONTANEOUS COMBUSTION

The phenomenon of spontaneous combustion is not limited to coal but is known to occur in a number of other materials such as charcoal, cattle feed, fertilizers, hay, cocoa beans, manure, oil-soaked rags (Haessler, 1989). No matter what material is involved, the basic principles that govern spontaneous combustion are the same in all cases. Spontaneous combustion is the process by which heat is generated spontaneously (without external initiation) within a substance by some reaction, under conditions that prevent the dissipation of the heat to the environment. Under these circumstances, the temperature of the reacting solid will rise leading in turn to an increase in the rate of reaction and greater heat generation. Left unabated the accumulation of heat can lead to the ignition of the solid reactant.

### The self-heating reaction

The nature of the reaction that produces the heat that may ultimately lead to ignition depends upon the nature of the substance under consideration. For example, spontaneous combustion in hay bales is initiated by bacterial activity until the temperature reaches about 75°C. Beyond this point the rate of aerial oxidation is greatly increased and continues to cause the temperature to increase, possibly to ignition.

In the case of coal, the source of heat is low temperature oxidation with oxygen from air. While the heat generated by this reaction is very little at ambient temperatures, under the right circumstances this heat may accumulate and cause the temperature of the coal to rise. The specific chemistry of the coal-oxygen reaction is very complex, not well understood, and need not concern us here. However, it is necessary to understand the factors that affect the rate of oxidation and the rate of heat generation that takes place in the coal.

The main factors involved are described below:

- (i) The oxidation reactivity of a coal pile,  $k$ , is determined by the inherent oxidation reactivity of the coal and its particle size. The inherent oxidation reactivity varies considerably from coal to coal, largely dependent upon the rank of the coal. In general low rank coals tend to be more reactive than high rank coals under the same set of conditions. The rate of oxidation is also a function of particle size being inversely proportional to particle size down to some threshold beyond which further size reduction has no effect. The combined contribution of inherent reactivity and particle size results in an overall oxidation reactivity for the coal in question, which might be regarded as the pile oxidation reactivity,  $k$ .
- (ii) The temperature of the reaction,  $T$ . Many studies have shown that the temperature dependence of the rate of oxidation can be described by the Arrhenius formula (Haessler, 1989) given by:

$$\frac{dq}{dt} \propto e^{\left(-\frac{E}{RT}\right)} \quad (1)$$

- $dq/dt$  = rate of oxidation (expressed in appropriate units such as gm O<sub>2</sub>/kg coal/min)  
 $E$  = the reaction activation energy,  
 $R$  = Boltzmann's gas constant, and,  
 $T$  = the absolute temperature.

The effect of temperature on the oxidation rate is to cause an approximate rate doubling for each 10°C rise.

- (iii) Accumulated oxidation,  $q$ . Coal, like many other substances, exhibits a reduction in oxidation rate as oxidation proceeds at a constant temperature and oxygen concentration (Carras and Young, 1994). This is described by the Elovich equation given by :

$$\frac{dq}{dt} \propto e^{(-aq)} \quad (2)$$

- $q$  = cumulative oxidation per unit mass of coal, and  
 $a$  = a constant.

- (iii) Oxygen concentration, O<sub>2</sub>%. As the oxygen concentration decreases the rate of oxidation also decreases for a constant temperature and degree of cumulative oxidation (Schmidt and Elder, 1940). This is best described by the equation:

(iv)

$$\frac{dq}{dt} \propto \left(\frac{O_2\%}{20.93}\right)^N \quad (3)$$

- $O_2\%$  = oxygen concentration by volume(%),  
 $20.93$  = oxygen concentration in normal air by volume(%), and,  
 $N$  = constant (approximately 0.6).

- (v) The heat of oxidation,  $\Delta H_{O_2}$ . The reaction that takes place between coal and oxygen is exothermic. The heat of oxidation is the amount of heat released per unit of oxygen adsorbed. In many of the previous studies it has been assumed that the heat of oxidation was the same for all coals and approximately equal to the heat of combustion or about 14250 J/gm oxygen adsorbed. Recent investigations by Taraba (1994) suggest that this is not the case. The heat of oxidation at temperatures of about 25°C appears to vary from about 3100 to 9300 J/gm O<sub>2</sub> depending upon the rank of the coal. Lower rank coals appear to have higher heats of oxidation. Further, the heat of oxidation is also a function of temperature and must, at high temperatures be equal to the heat of combustion. These effects must be considered in the modeling of spontaneous combustion.

The overall rate of heat generation due to oxidation can be expressed in the combined equation:

$$\frac{dH}{dt} = k \times \Delta H_{O_2} \times \left(\frac{O_2\%}{20.93}\right)^N \times e^{\left(-\frac{E}{RT} - aq\right)} \quad (4)$$

where  $k$  = the pile reactivity (for a given coal and particle size), and, other variables are as defined above.

This equation can be used to calculate the rate of heat generation by oxidation at any point in a coal pile at which the oxygen concentration, temperature, coal pile reactivity and accumulated oxidation are known. The rate of oxidation (consumption of oxygen) is given by:

$$\frac{dq}{dt} = k \times \left( \frac{O_2 \%}{20.93} \right)^N \times e^{\left( \frac{E}{RT} - aq \right)} \quad (5)$$

For the purposes of examining the production of off-gases, similar equations can be developed for the rate of production of gases such as carbon monoxide and carbon dioxide.

### Other sources of heat or heat transfer

While oxidation is the primary source of heat that drives the spontaneous combustion process, there are other sources of heat and heat transfer that play an important role in the development of a heating. Remembering the conditions for spontaneous combustion to occur, that some of the heat is retained in the solid causing its temperature to rise, it is clear that means of heat loss play an important part. Even though the rate of oxidation and heat produced may be very high, if it is all dissipated to the surroundings there will be no temperature rise and no self-heating.

Other possible forms of heat or heat transfer that can occur in a coal pile are those associated with the wetting and drying of coal, convective heat transfer between the coal and air, conductive heat transfer through the coal and convective heat transfer at the surface of the coal pile. All of these need to be considered in attempting to examine the self-heating behavior of coal.

The least well understood but most important of these is the wetting and drying of coal. Drying of coal is an endothermic process (requiring heat) which will affect the heat balance in an oxidizing pile of coal. The effect of drying will be to reduce the heat available to cause self-heating. The corollary is that wetting of coal is an exothermic process and will tend to accelerate self-heating. Whether or not wetting and drying can be regarded as a purely physical process is not clear as there some evidence that the presence of moisture can alter the inherent rate of oxidation. As a physical process wetting and drying can be determined from the moisture isotherm for a coal (Allardice, 1991) which relates the equilibrium vapour pressure of the surrounding air to the moisture content of the coal.

Convective heat transfer within the pile is controlled largely by the airflow through the coal and will be less significant at low flow rates than at high flow rates and convective heat losses at the pile surface are controlled by the pile surface temperature. Conductive heat losses are determined by the temperature distribution in the pile. All these heat transfer processes are dependent on the temperature distribution and geometry of the reacting coal pile. Stott et al (5) provide a succinct statement of the thermal equation applicable in one dimension being:

$$C_s \rho_s \frac{dT}{dt} A dx = \underbrace{KA \frac{d^2 T}{dx^2}}_{II} - \underbrace{C_g \rho_g V \frac{dT}{dx}}_{III} A dx + \underbrace{\Delta H_{O_2}}_{IV} \frac{dq}{dt} \rho_s A dx - \underbrace{\Delta H_{H_2O}}_{V} \frac{dM}{dt} V \frac{dT}{dx} A dx \quad (6)$$

- I = Rate of heat change in element dx causing the coal to self-heat,
- II = Rate of conduction heat transfer into element dx,
- III = Rate of convective heat transfer into element dx,
- IV = Rate of heat generation by oxidation in element dx, and,
- V = Rate of heat loss by evaporation in element dx,

and where:- subscript s = coal,  
subscript g = gas,  
A = cross-sectional area of element.

$C$  = specific heat,  
 $\theta$  = density,  
 $T$  = temperature,  
 $t$  = time,  
 $x$  = length of element,  
 $K$  = thermal conductivity,  
 $V$  = approach velocity of airflow,  
 $dq/dt$  = rate of oxidation (as per Equation 5 above),  
 $dM/dt$  = rate of evaporation of moisture,  
 $\Delta H_{O_2}$  = heat of oxidation, and,  
 $\Delta H_{H_2O}$  = heat of evaporation or condensation

The combined effects all of all these factors, the inherent reactivity of the coal, its particle size, oxygen concentration, accumulated oxidation, temperature, wetting and drying, convection and conduction, airflow and pile geometry, make the study of the nature of spontaneous combustion very difficult. Because of the vast range of conditions that can occur in a stockpile or underground, no single test can be used to assess the self-heating behavior with any degree of certainty or confidence. Even large scale self-heating tests involving many tonnes of coal can only provide a limited understanding of these complex interactions due to the limited number of tests that can be performed.

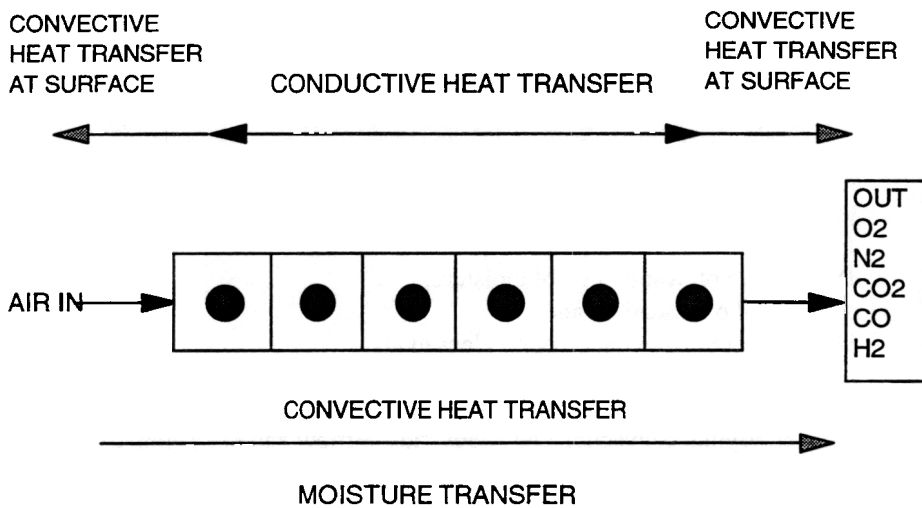
With a suitable numerical model it is possible to examine a very wide range of conditions, and the complex interactions involved in a heating. Further, it is possible to examine the production of other gasses such as carbon monoxide and carbon dioxide in the numerical simulation, so that the nature of the off-gas from a heating can be assessed against its development. This would provide an opportunity to examine the use of indicators such as CO make and Graham's ratio against the severity of a heating.

## BASIS OF NUMERICAL MODELING

Numerical modeling is the only way known to take into account the complex interplay between the factors discussed above. To this end a number of numerical models have been developed based on the same ideas. To simulate self-heating, a volume of coal is represented by a series of interconnected nodes. Each node is taken to represent a discrete volume and mass of coal through which air passes and in which oxidation, and therefore heat generation, take place. The mass is assumed to be concentrated at the nodes and all reactions, oxidation, wetting and drying, are assumed to take place at nodes. All heat transfer (convection and conduction) processes occur between nodes. The rate of oxidation at a node is described by Equation 4 and the heat transfer by Equation 5.

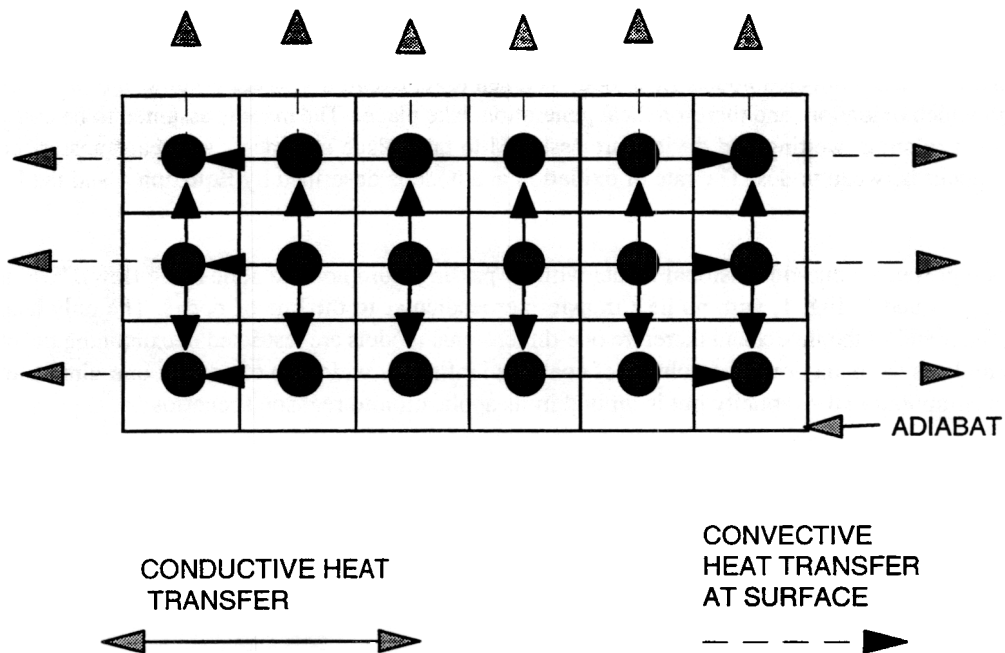
A single line of nodes represents a one-dimensional model with air passing from node to node (plug flow). Heat transfer is also from node to node as illustrated in Fig. 1, with no heat transfer perpendicular to the line of nodes. The only heat losses to the environment occur at either end of the model and therefore one-dimensional models are restricted in examining the effects of scale.

This type of model simulates the behaviour of a column of coal in an infinitely wide slab of coal. A one-dimensional model has the benefits of relative computational simplicity but is limited in its application to realistic scenarios.



**Fig. 1 – One dimensional heat transfer model.**

A two-dimensional model can be made to provide for more complex heat transfer processes as shown in Fig. 2. Airflow is still assumed to be homogeneous plug flow from one end of the node grid to the other, but conductive heat transfer can take place across a line of nodes. Convective heat losses can also occur at boundary surface other than the end surfaces. A two-dimensional model simulates a slice through a block of infinite width perpendicular to the plane of the nodal grid. Where an axis of symmetry exists across which there is no heat transfer (an adiabat), the nodal grid can be split to reduce the number of nodes in the simulation. The number of nodes required for a two-dimensional model is obviously far more than for a one-dimensional model, but the two-dimensional model is better suited to more complex geometries.



**Fig. 2 – Two dimensional heat transfer model**

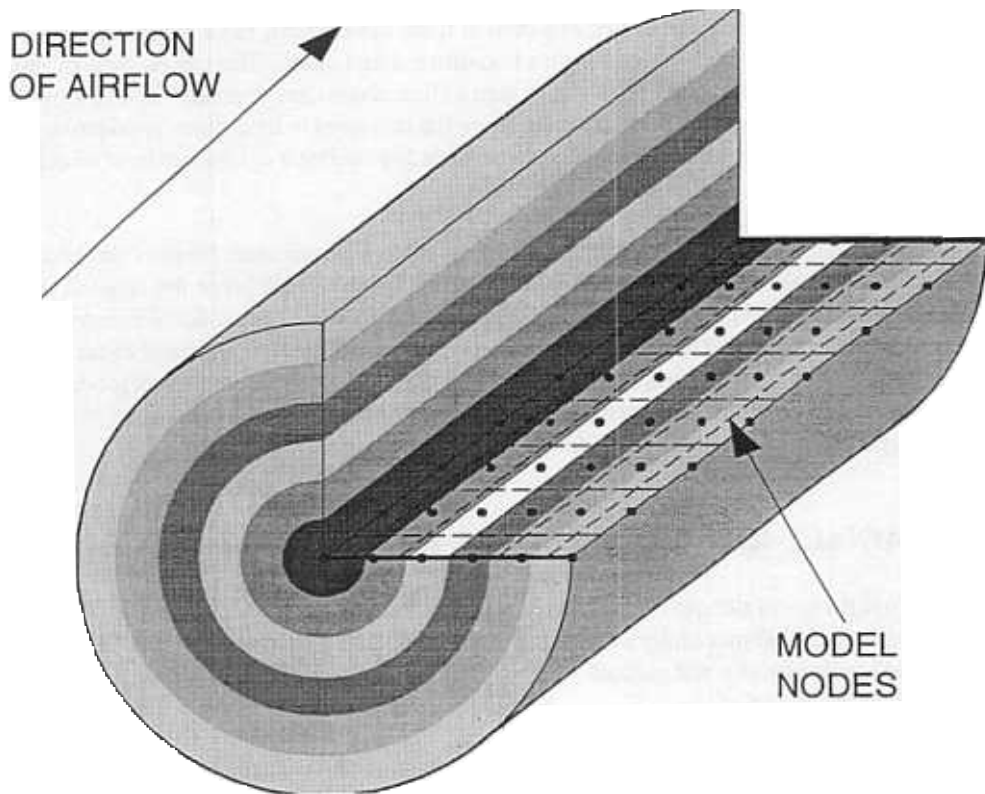
The complexity of modeling increases from one to two and then to three dimensions, but a method has been developed which allows a quasi-three-dimensional model to be developed from a two-dimensional model. This can be done by considering each node as representing a cylindrical shell as illustrated in Fig. 3, rather than a slice of constant thickness. In a homogeneous cylinder there is no heat flow tangentially, only axially and radially. By calculating the area used to determine conductive heat transfer between nodes based on this idea, the basic two-dimensional model can be made to simulate a cylinder of coal of definite dimensions and mass.

The original models developed were Quattro Pro spreadsheets utilizing macros to increment the time steps required to run a model. Each of the one, two and quasi-three dimensional models was a separate spreadsheet. Since the original paper describing these models was published (Humphreys, 1996), the models have been rewritten in Visual Basic for Windows. The separate one, two and quasi-three dimensional models have been combined into a single Visual Basic programme and as far as possible use common code. The main features of the Visual Basic models remain unchanged from the original spreadsheet models as described here, but their functionality and speed have been greatly enhanced. These numerical models are now being used to examine the self-heating of coal with a particular emphasis of understanding the nature of underground heatings.

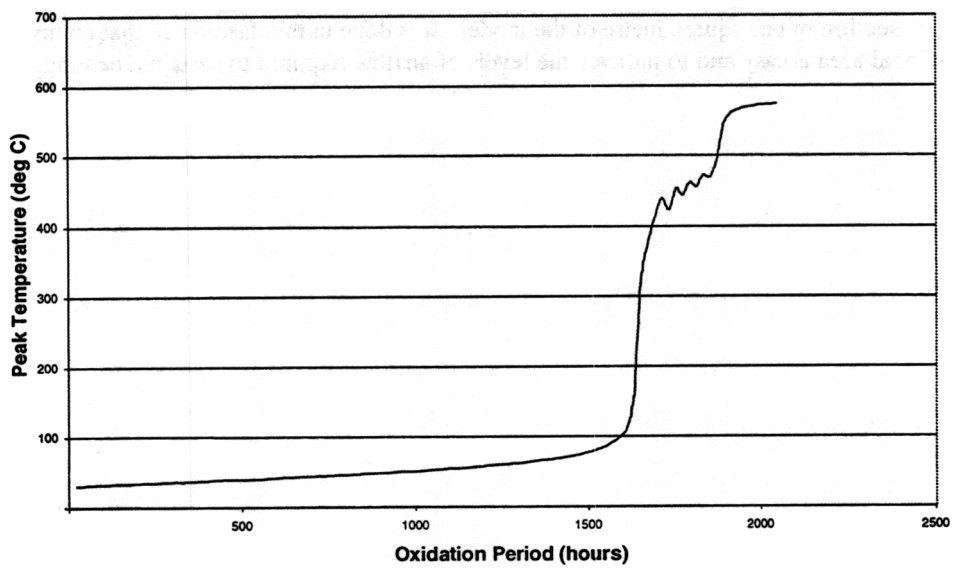
## **PRELIMINARY RESULTS OF THREE-DIMENSIONAL MODELLING**

Some preliminary results from the use of the quasi-three-dimensional model will help to illustrate the capability of the model and some of the areas that will be investigated more fully in time. It is hoped that this model will be able to be used to investigate a wide range of coal reactivities (inherent reactivity and particle size), airflow conditions (related to pressure differentials), mass of coal involved and moisture content of the coal.

The basic output from the model is a history of the temperature of the heating and the composition of the off-gas. An example is shown in Figs. 4 and 5 below. Fig. 4 shows the peak coal temperature as a model heating develops and Fig. 5 shows the basic composition of the off-gas from the same heating. The basic conditions modeled in this case were a cylinder of coal 6m long and 6m diameter, with an airflow flux of 25 lt/min/m<sup>2</sup>, and a oxidation reactivity approximately that of a Central Queensland sub-bituminous coal with a particle size of about 25mm. The airflow through the model is expressed as a flux representing the airflow passing through a cross-section of one square metre of the model. It is done in this fashion so that comparison between models of different cross-sectional area is easy and to indicate the levels of airflow required to sustain a heating.

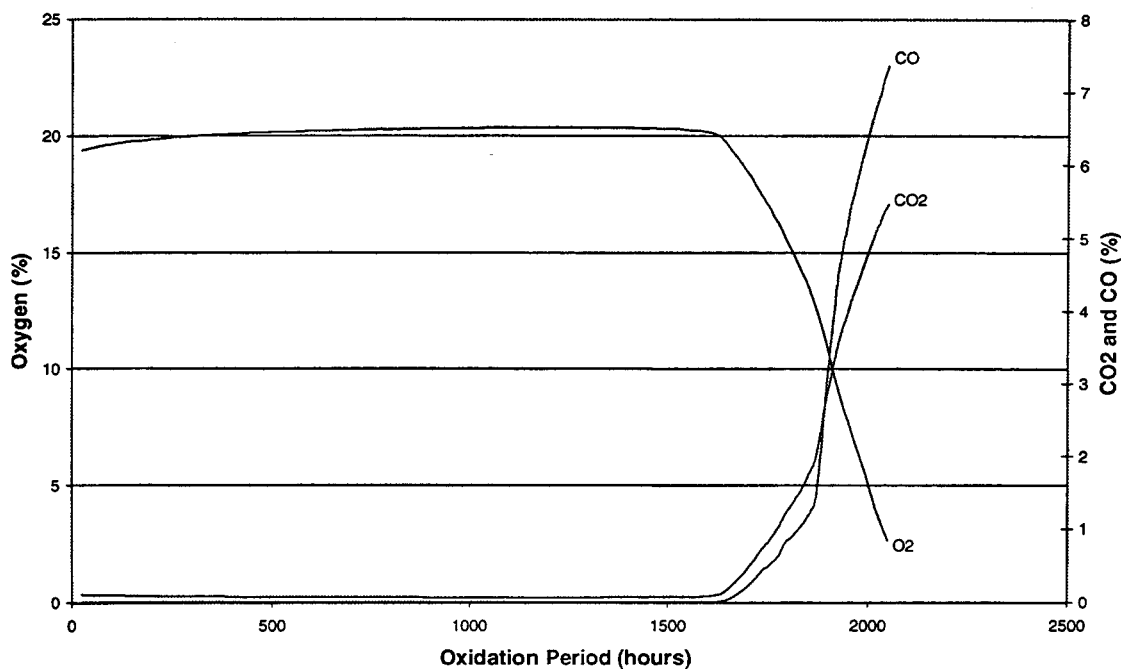


**Fig. 3 – Quasi-three dimensional heat transfer model.**



**Fig. 4 - Development of self-heating**





**Fig. 5 - Off-gas composition**

#### Variations in airflow

By adjusting the input parameters of the model it is possible to examine their impacts on the self-heating process. For example Fig. 6 shows the effects on the self-heating characteristics of varying airflow through a heating of approximately 200 tonnes of coal in a cylinder 6m long and 6m diameter. The coal pile reactivity is the same as that used for the results illustrated in Figs. 4 and 5, and it can be seen that variations in the airflow can have a significant effect on the development of a heating. At low flowrates (1.25 lt/min/m<sup>2</sup>) the rate at which the heating develops is considerably reduced and the maximum temperature reached by the heating is about 95°C after about 4500 hours. As the airflow is increased the maximum heating temperature increases, thermal run-away can occur and very high temperatures can be achieved.

The reasons for this behaviour can be seen from an examination of the way the heating develops in the numerical model. At low airflows, the amount of oxygen entering the pile is limited and is consumed near the upstream surface. This leads to the formation of a hot spot close to the air entry point. Its maximum temperature is limited by conductive heat losses to the upstream surface and by the limited oxygen supply. As the airflow increases, the hot-spot forms deeper into the pile due to increased convective heat transfer and greater penetration of oxygen. The peak temperature is less restricted by heat losses and oxygen supply and very high temperatures can be achieved.

#### Variations in pile reactivity and size

Clearly one of the most important controlling factors in the development of self-heating of coal is the reactivity of the coal in the pile whether due to its inherent reactivity or its small size. The impact of variations in coal pile reactivity can be gauged from the results shown in Fig. 7. Again the amount of coal is about 200 tonnes. As the reactivity decreases the initial rate of self-heating is also reduced and the time required to reach thermal run-away increases. However, beyond a certain reactivity the maximum temperature rise achieved is restricted and no thermal run-away occurs. The reactivities shown in Fig. 7 are expressed as a proportion of the inherent reactivity of a Central Queensland bituminous coal. These would be equivalent to coal with a particle size of approximately 6.25, 12.5, 25 and 50 mm for 32, 16, 8 and 4% reactivity, respectively.

Although the least reactive pile shown in Fig. 7 did not heat above about 50°C for the model size simulated, it may well do so if the pile was larger. This effect illustrated in Fig. 8, which shows the self-heating curves for coal with a relative reactivity of 8%, at different pile sizes. For a pile 7m long and 7m diameter, the heating reaches thermal run-away at about 1500 hours (63 days). This is slightly increased as the pile size is reduced to a 6m cylinder, but not significantly. When the pile size is further reduced to 5m, the heating does not exceed 75°C, and no thermal run-away occurs. It seems that there is a certain critical mass associated with the development of a spontaneous heating, which is related to the reactivity of the coal involved. In the example shown it is somewhere between and 5 & 6 m cylinder. The critical mass required for a heating will depend greatly upon the reactivity of the coal involved which is determine from the inherent reactivity and particle size.

### Off-gas composition and indicators of spontaneous combustion

The composition of the off-gas from self-heating is obtained as part of the results obtained by modeling. From this its possible to calculate various indicators of spontaneous combustion such as Graham's ratio, carbon monoxide make or carbon monoxide to carbon dioxide ratio. It is also possible to estimate the production of other indicator gasses such as hydrogen and ethane. The composition of the off gases obtained for the 6m cylinder with a reactive reactivity of 8% and airflow of 25 lt/min/m<sup>2</sup> are shown in Fig. 5. The primary indicators of Graham's ratio and CO make are shown in Fig. 9. Of most interest amongst these is the development of CO make during the modeled heating. Until the peak temperature exceeds 100°C, the CO make is very low and does not exceed 1 lt/min. This is followed by a period in which the peak temperature increases very rapidly to about 450°C and the CO make reaches about 10 lt/min. During this phase the heating hot spot becomes oxygen limited i.e. all the oxygen passing through the hot spot is consumed, and the hot spot begins to migrate upwind until it encounters the outer edge of the pile. At this stage the peak temperature increases again, and the CO make rises rapidly, in this case to exceed 50 lt/min. Eventually the heating reaches the surface of the pile and would certainly result in open fire. The development of Graham's ratio follows a similar pattern and results in values well above those normally encountered in an underground heating. However, it must be remembered that the modeling results take no account of the effect of dilution with other airflows, which are inevitable in an underground mine.

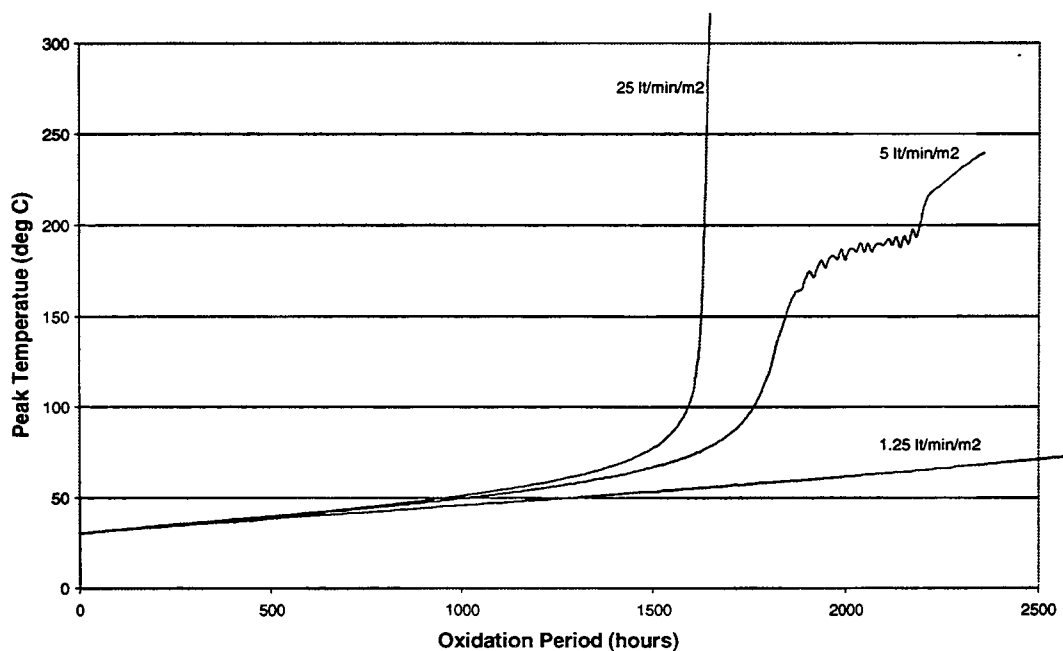


Fig. 6 - Impact of variations in airflow

The CO makes observed from the modeling undertaken so far, are similar to those used as trigger points in the industry, but appear

to occur at temperatures which would give cause for concern. From these early results it is not possible to draw any firm conclusions on the relationship between CO make levels and the state of a heating, but this is an obvious area for further investigation.

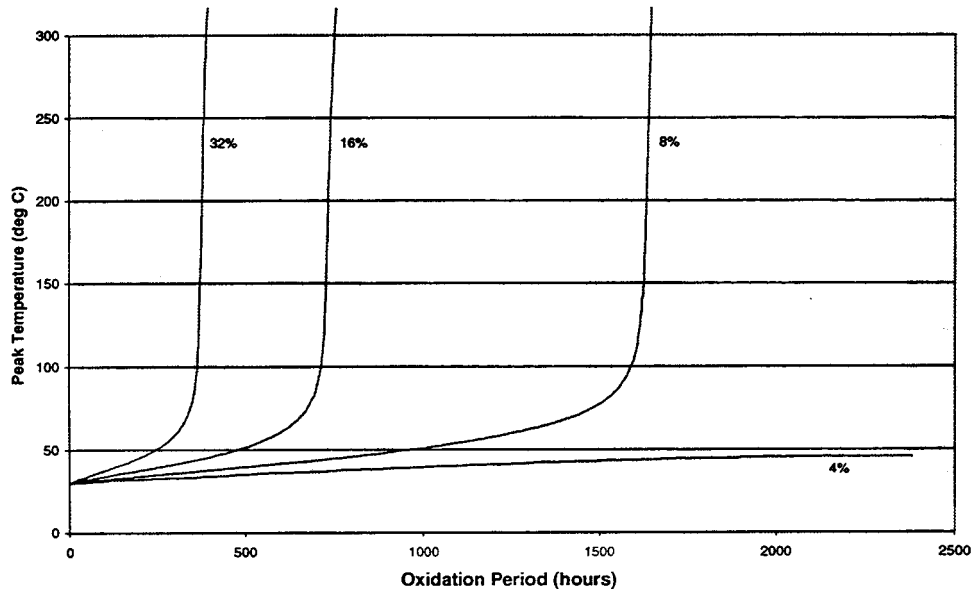


Fig. 7 - Impact of coal pile reactivity

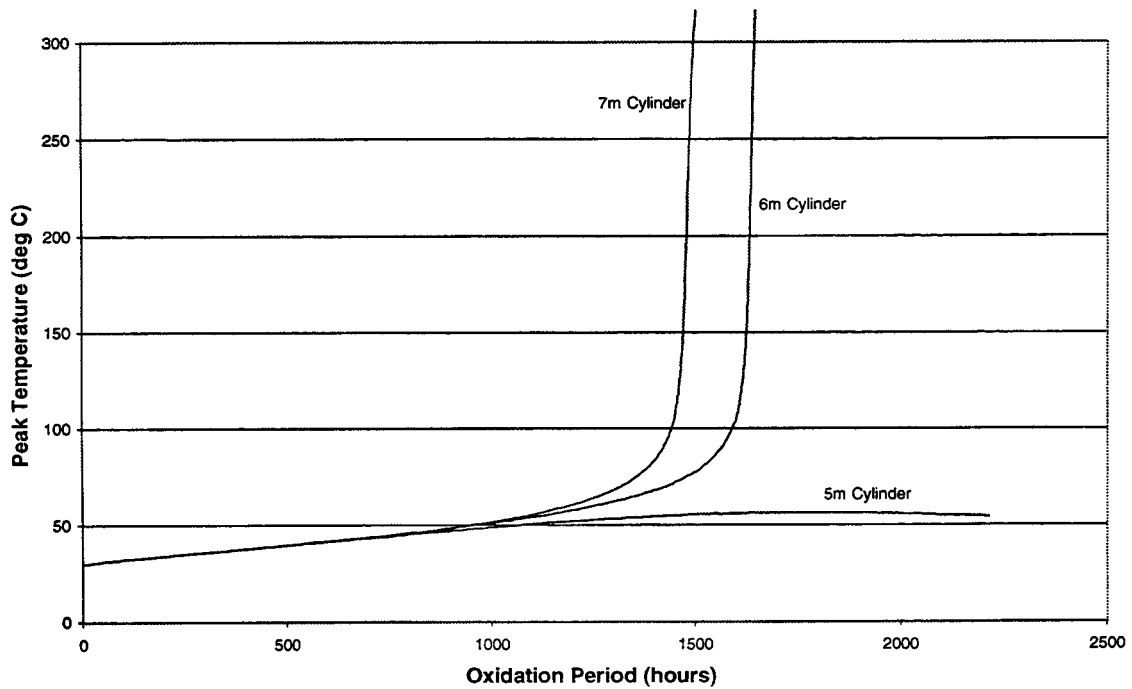
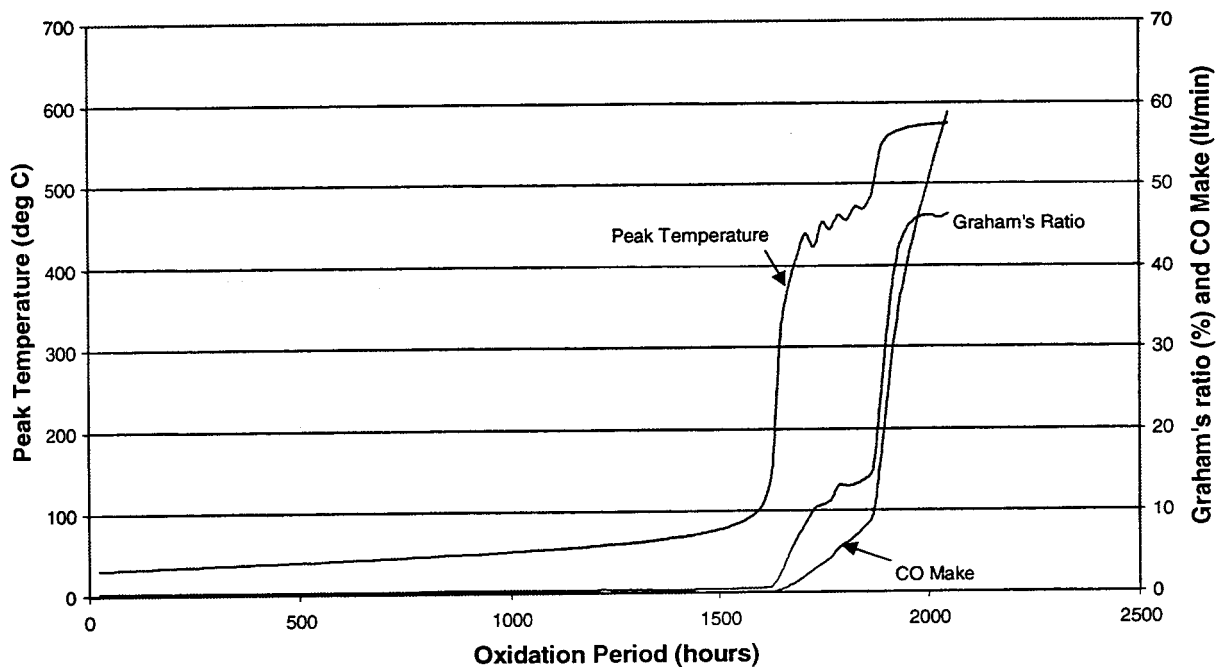


Fig. 8 - Impact of pile size



**Fig. 9 - Indicators of spontaneous combustion**

## CONCLUSIONS

The examples of modeling results given here illustrate the complexity of the self-heating reaction in coal and the main factors affecting self-heating. It can be seen that apparently slight changes in conditions of, say airflow (pressure differential) or mass of coal, can be the difference between the development of a significant self-heating with very high temperatures and a low level, low temperature event. These differences may not be noticeable in an underground mine yet still have a significant effect on the development of a heating.

The main factors considered to contribute to the occurrence of spontaneous combustion in underground coal mines are the reactivity, mass and moisture content of the coal involved and the airflow through the heating zone. It is intended to continue the study of spontaneous combustion using the techniques described here to more fully examine these factors. With additional modeling the occurrence of spontaneous combustion can be described in terms of coal reactivity, mass, airflow and moisture. Additional work will be undertaken to relate airflow to pressure differential which will identify potential heating sites underground.

Finally, an analysis of the gasses produced by the complex mass/temperature distribution will be carried out to relate the traditional indicators of spontaneous combustion to the state of a heating.

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