

THE NATURE OF UNDERGROUND HEATINGS AS INDICATED BY NUMERICAL MODELING

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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 which 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 conditions of coal type, particle size, configuration etc. The principles 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 air flow 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 (1). 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 which 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 and need not concern us here. However, it is necessary to understand the factors that affect the rate of oxidation, and hence the rate of heat generation, that takes place in the coal.

These are:

(i) The reactivity of the coal in the reaction zone which is determined by the inherent reactivity of the coal and its particle size. The inherent reactivity varies considerably from coal to coal, largely dependant 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 effect of decreasing particle size is to increase the rate of oxidation. In general the rate of oxidation is inversely proportional to particle size up to some threshold particle size beyond which further size reduction has no effect. The combined contribution of inherent reactivity and particle size results in an overall reactivity for the coal in question, which might be regarded as the pile reactivity.

(ii) The temperature of the reaction. Many studies have shown that the temperature dependence of the rate of oxidation can be described by the Arrhenius formula given by :

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

where dq/dt = rate of oxidation (appropriate units may be, for example, gm O₂/kg coal/min)

E= the reaction activation energy

R= Boltzmann's gas constant

T= the absolute temperature.

Figure 1 shows this effect for typical values applicable to coal. As can be seen there is an approximate doubling of the rate of oxidation for each 10°C rise in temperature.

(iii) Accumulated oxidation. Coal, like many other substances, exhibits a reduction in oxidation rate as oxidation proceeds at a constant temperature and oxygen concentration (2). This is described by the Elovich equation given by :

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

where q = cumulative oxidation per unit mass of coal.

Figure (2) illustrates this effect.

(iv) Oxygen concentration. As the oxygen concentration decreases the rate of oxidation also decreases for a constant temperature and degree of cumulative oxidation (3). This is best described by the equation:

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

where k_3 = constant
 O_2 = oxygen concentration (%)
 20.93 = oxygen concentration in normal air (%)
 N = constant (approximately 0.6).

The overall rate of oxidation taking into account all of these effects can be expressed in the combined equation:

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

where k = the coal pile reactivity.

This equation can be used to calculate the rate of oxidation at any point in a coal pile at which the oxygen concentration, temperature, coal pile reactivity and accumulated oxidation are known. Given the heat of oxidation, the rate at which heat is produced by oxidation can be determined. 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, i.e. 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 is 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 (4) 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 dependant 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:

$$C_s \rho_s \frac{dT}{dt} A dx = KA \frac{d^2T}{dx^2} - C_g \rho_g V \frac{dT}{dx} A dx + \Delta H_{O_2} \frac{dq}{dt} \rho_s A dx - \Delta H_{H_2O} \frac{dM}{dt} V \frac{dT}{dx} A dx \quad (5)$$

- | | | | | |
|---|---|--|---|--|
| I | II | III | IV | V |
| 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 | V = Rate of heat loss by evaporation in element dx |

where:-

- subscript s = coal
- subscript g = gas
- A = cross-sectional area of element
- C = specific heat
- ρ = density
- T = temperature
- t = time
- x = length of element
- K = thermal conductivity
- V = approach velocity of air flow
- dq/dt = rate of oxidation (as per equation 4 above)
- dM/dt = rate of evaporation of moisture
- ΔH_{O_2} = heat of oxidation
- ΔH_{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 DEVELOPED.

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 one-dimensional model is represented by a single line of nodes with air passing from node to node (plug flow). Heat transfer is also from node to node as illustrated in Figure 3, 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.

A two-dimensional model can be made to provide for more complex heat transfer processes as shown in Figure 4. 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.

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 Figure 5, 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.

Numerical models for one, two and quasi-three dimensions have been developed, the main features of which are described above, and are being used to, examine the self-heating of coal under varying conditions.

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 Figures 6 and 7 below. Figure 6 shows the peak coal temperature as a model heating develops and Figure 7 shows the basic composition of the off-gas from the same heating. The data beneath the caption give the coal pile reactivity (k in equation 4 above), the mass of coal modelled (m), and the airflow flux (q) through the model. (For the results shown here the coal mass is as a cylinder with the length equal to the diameter, and the coal moisture content is zero unless otherwise stated). The results of modeling for a particular coal pile reactivity (k) are applicable to a range of inherent coal reactivities and particle sizes in combination. As an indication, the reactivity shown in Figures 6 & 7 is approximately that of a Central Queensland high volatile bituminous coal with a particle size of 25mm. The airflow flux (q) shown is the airflow passing through a cross-section of one square metre of the model. The airflow in the model is expressed as airflow flux so that comparison between models of different cross-sectional area is easy and to indicate the levels of airflow required to sustain a heating.

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 Figure 8 shows the effects on the self-heating characteristics of varying airflow through a heating of approximately 15 tonnes of coal while all other parameters remain unchanged. The coal pile reactivity is the same as used for the results illustrated in Figures 6 & 7, and it can be seen that variations in the airflow can have a significant effect on the development of a heating. At low flowrates (3.125 lt/min/m²) the maximum temperature reached by the heating is about 125°C, after which the temperature begins to fall. As the airflow is increased the maximum heating temperature increases, thermal run-away can occur and very high temperatures are achieved. However, beyond a certain airflow the trend is reversed and again the maximum heating temperature falls.

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. However, at some point the hot-spot is pushed back towards the downstream surface and its maximum temperature is again limited by conductive and convective heat losses. It is literally blown out of the back of the pile. The range of airflows that will produce thermal run-away is determined by the depth of coal and the pile reactivity and can be very wide.

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 Figure 9. Again the amount of coal is about 15 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 Figure 9 would be representative of 6.25, 12.5, 25 & 50 mm diameter particle size for a Central Queensland bituminous coal.

Although the least reactive pile shown in Figure 9 did not heat above about 50°C for the model size simulated, it may well do so if the pile was larger. This is illustrated in Figure 10 which shows the self-heating curves for the least reactive coal of Figure 9, but for progressively larger masses. At 15t (2.5m diameter), there is no self-heating above about 50°C. As the mass of coal increases, the peak heating temperature also increases, so that at 28t (3.125m diameter) the peak temperature increases to about 80°C. Further increases in coal mass lead to even higher peak temperatures until, beyond a certain critical mass, thermal run-away is achieved. For the example shown this is somewhere between 28 (3.125m diameter) and 48 tonnes (3.75m diameter). (All the self-heating curves shown in Figures 9 & 10 are for the most rapid self-heating obtained under varying airflow conditions.)

VARIATIONS IN MOISTURE CONTENT.

All of the examples given above are for dry coal, so that the effects of wetting and drying have been ignored. However, moisture can play an important part in self-heating. In general, low rank coals which have the greatest inherent oxidation reactivity also have the highest moisture content. On the basis that the role of moisture in the self-heating reaction is limited to wetting and drying i.e. there is no catalytic effect or reduction in oxidation rate due to the presence of moisture, Figure 11 shows the impact of moisture on self-heating. The coal reactivity used is quite high, about equivalent to a sub-bituminous coal of about 100mm particle size. As can be seen, until the coal temperature reaches about 85°C the presence of moisture has no impact on self-heating. However, beyond about 85°C for moist coals, the rate of self-heating is reduced and the heating may "stall" for a period as the coal dries. The degree to which the rate of self-heating is reduced and the length of the "stall" period is dependant on the initial moisture content. The reason for this behaviour is that the equilibrium vapour pressure of the coal increases very rapidly near 100°C, resulting in very high drying rates and large heat losses from the coal. These heat losses balance the heat of oxidation and the rate of self-heating is reduced until the coal dries sufficiently and there is again an excess of heat from oxidation.

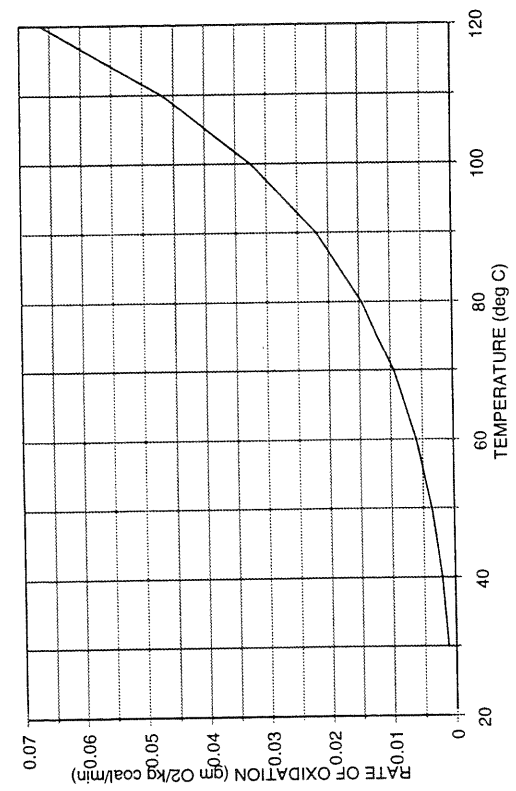


Figure 1 - Effect of Temperature on Rate of Oxidation.

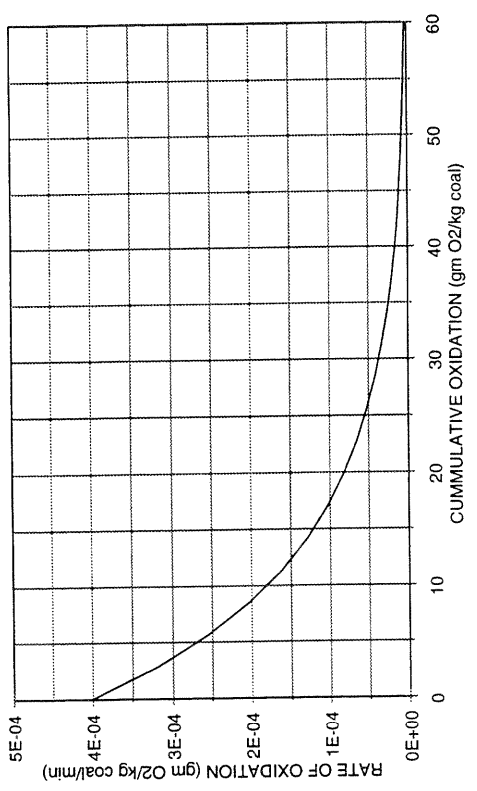


Figure 2 - Effect of Cumulative Oxidation on Rate of Oxidation.

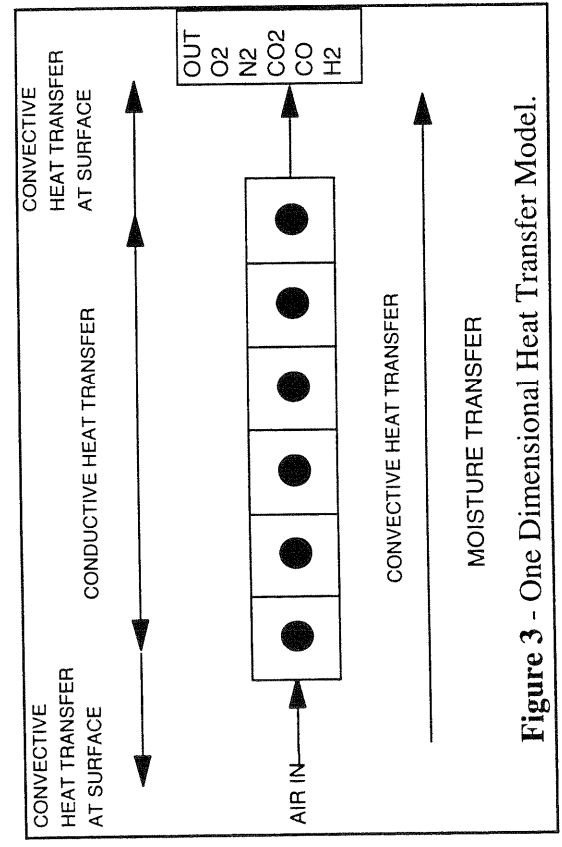


Figure 3 - One Dimensional Heat Transfer Model.

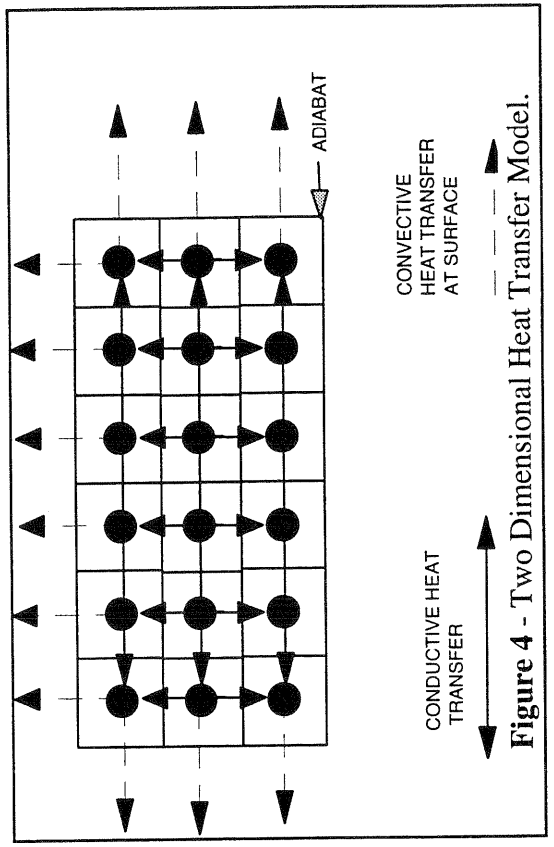


Figure 4 - Two Dimensional Heat Transfer Model.

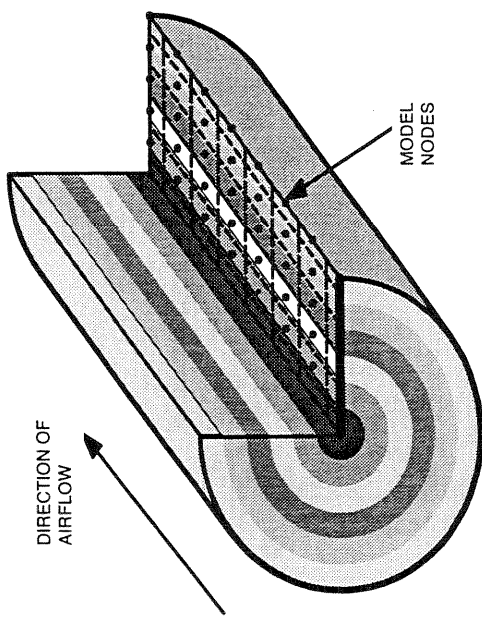


Figure 5 - Quasi-three Dimensional Heat Transfer Model.

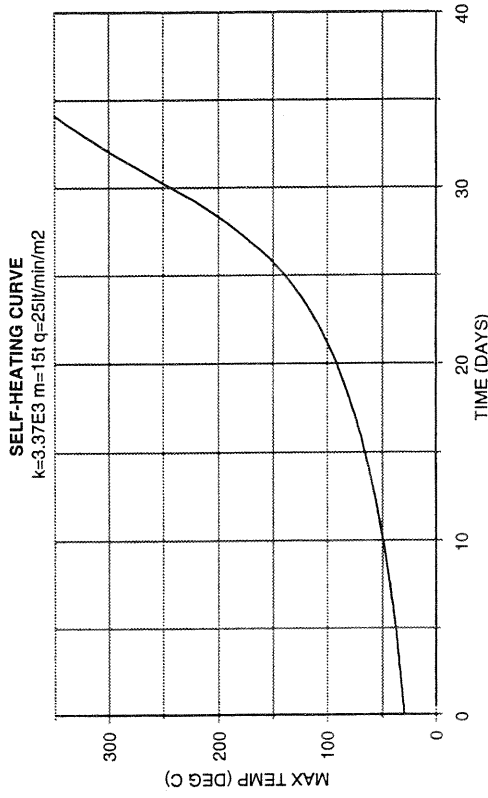


Figure 6 - Typical Self-Heating Curve from 3D Modelling.

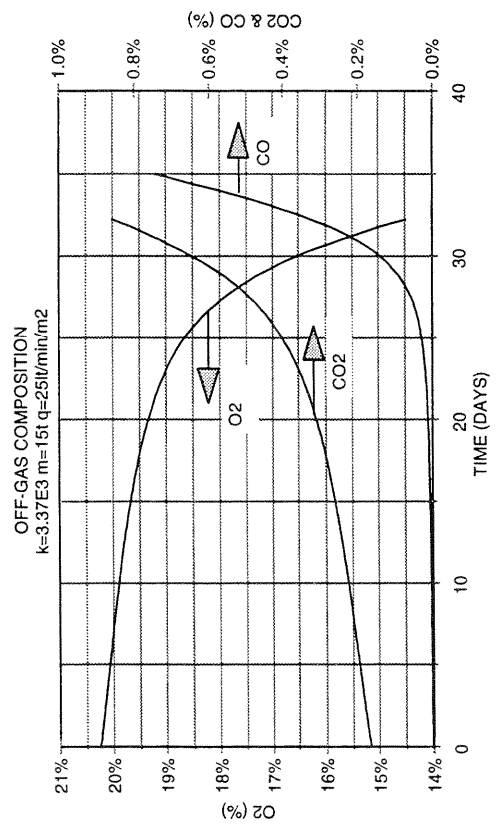


Figure 7 - Typical Off-gas Composition from 3D Modelling.

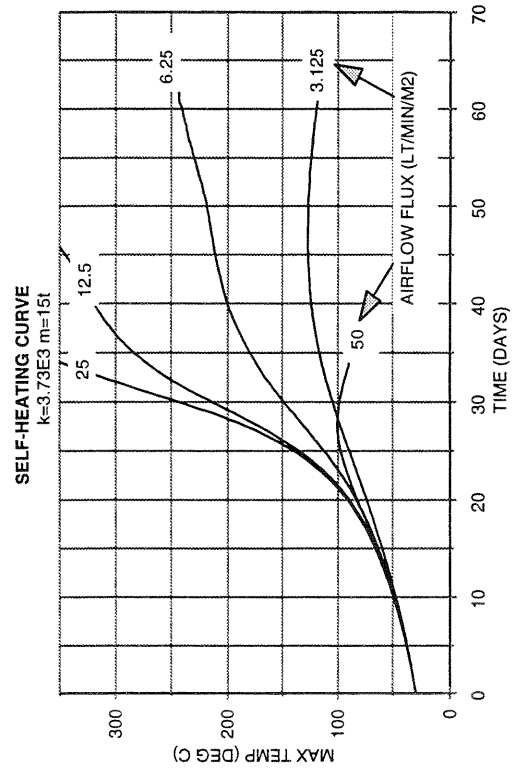


Figure 8 - Impact of Variations in Airflow on Self-Heating.

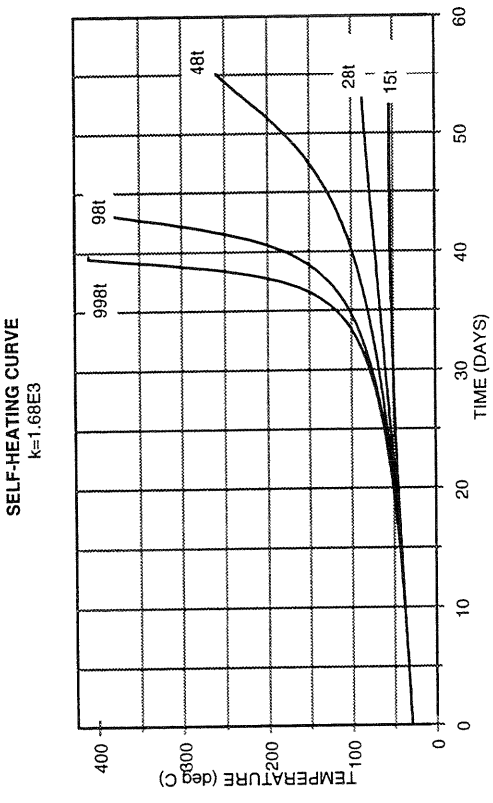


Figure 9 - Impact of Coal Pile Reactivity on Self-Heating.

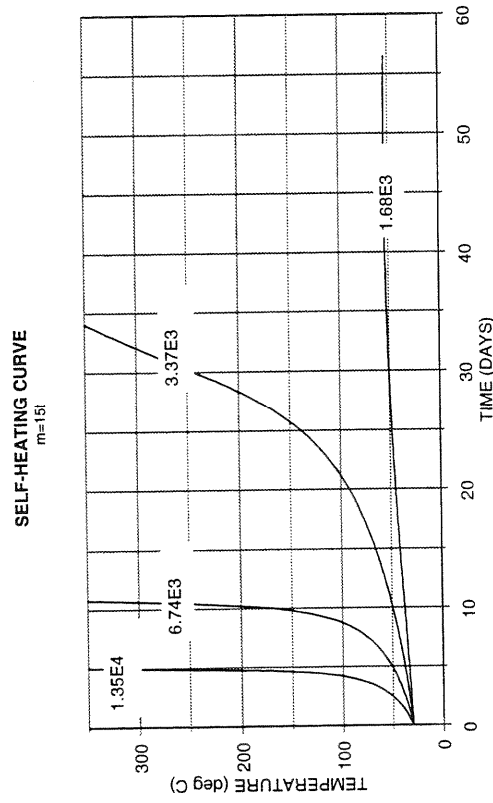


Figure 10 - Impact of Variations in Coal Mass on Self-Heating.

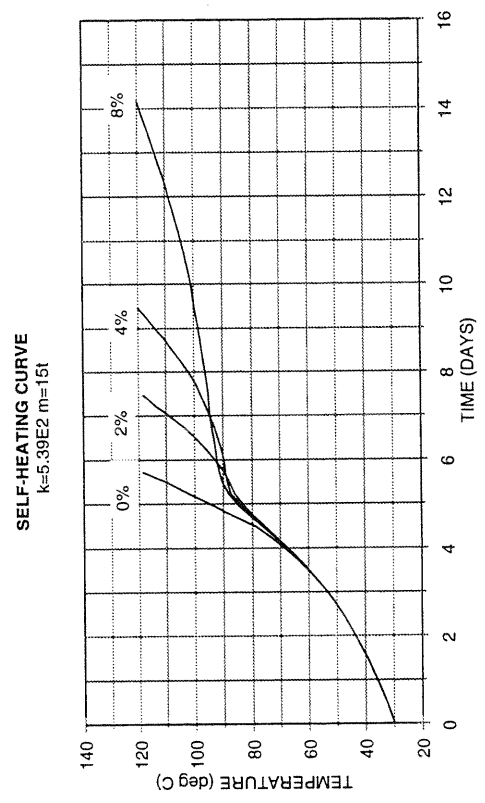


Figure 11 - Impact of Coal Moisture on Self-Heating