University of Wollongong
Research Online

Coal Operators' Conference

Faculty of Engineering and Information Sciences

2005

Anatomy of a Heating and Assessment of Critical Self-Heating Parameters

D. Humphreys

Publication Details

This conference paper was originally published as Humphreys, D, Anatomy of a Heating and Assessment of Critical Self-Heating Parameters, in Aziz, N (ed), Coal 2005: Coal Operators' Conference, University of Wollongong & the Australasian Institute of Mining and Metallurgy, 2005, 249-258.

Research Online is the open access institutional repository for the University of Wollongong. For further information contact the UOW Library: research-pubs@uow.edu.au

Anatomy of a Heating and Assessment of Critical Self-Heating Parameters

D Humphreys[1]

ABSTRACT

Numerical modelling is a valuable tool for simulating the fundamental processes that take place during a heating. The models presented in this paper have enabled a quantitative assessment of the effects of initial pile temperature, pile size and mass and coal particle size on the development of a heating. All of these parameters have a certain criticality in the coal self-heating process.

INTRODUCTION

Spontaneous combustion of coal has been a hazard to the mining industry from the very first attempts to mine coal.

The assessment of the propensity of coal for spontaneous combustion is largely based upon the results of any one of a large number of laboratory-based tests. Inevitably, there are compromises in the laboratory tests to increase the rate of oxidation and self-heating from that which would occur *in situ*. As a result, the assessment of the propensity of a coal for spontaneous combustion is reduced to a qualitative interpretation of the laboratory test results. Despite a plethora of different methods purporting to test the spontaneous combustion propensity of coal, too often the question arises 'What does this mean?' Quantitative assessment of the potential for spontaneous combustion in a coal mine is lacking. Numerical modelling offers distinct advantages to assess the anatomy of a heating and to quantify the effects of various intrinsic and extrinsic parameters.

BASIS OF NUMERICAL MODELLING

To better understand the complexities involved in the development of spontaneous combustion Humphreys (2004) developed a number of numerical models to simulate self-heating in one-, two- and quasi-three-dimensional models plus two commonly used laboratory tests. The multitude of factors that affect the oxidation of coal and therefore the development of spontaneous combustion have been extensively reviewed by many authors and will not be reviewed again here. However it is necessary to record that the numerical models took into account the impact of temperature, oxygen concentration, particle size, prior oxidation, the inherent reactivity, the heat of oxidation, and convective and conductive heat losses upon the gaseous interchanges taking and the temperature increases that occur during the development of spontaneous combustion in a coal pile.

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.

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 Figure 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 real scenarios.

A two-dimensional model can be made to provide for more complex heat transfer processes. 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 as well as 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 modelling 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, 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 resulting model is referred to as the Quasi-3D model.

1. MAusIMM, Managing Director, SkillPro Services Pty Ltd, PO Box 795, Booval Qld 4304. School of Engineering, The University of Queensland, Brisbane Qld 4072.

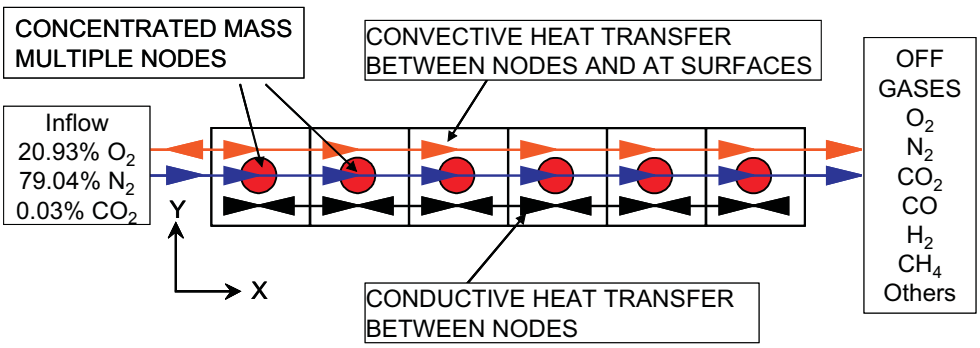

FIG 1 - One-dimensional heat transfer model.

Two additional models have also been developed to simulate the commonly used spontaneous combustion tests, the Adiabatic self-heating (R_{70}) test and the relative ignition temperature (RIT) test. These have been used extensively in Australia to characterise the spontaneous combustion of coals and a significant database of results exists. The numerical models for these tests simulate the conditions that apply to the tests by modelling the oxidation of coal in a single node with appropriate heat loss calculations for each test method (Humphreys, 2004).

MODELLING RESULTS AND DISCUSSION

The relationship between R_{70} and RIT test results and oxidation characteristics

Both the RIT and R_{70} tests purport to indicate the propensity of coal to spontaneous combustion. These two tests were developed independently many years apart and are often used by Australian operators to assess the potential for spontaneous combustion of coal. Australian Coal Industry Research Laboratories (ACIRL) has tested many Australian coals using both methods (Symmington, 1999). The assessment of the propensity to spontaneous combustion is based upon the qualitative assessments that coals with R_{70} greater than 1°C/h or RIT less than 130°C are highly prone or 'troublesome' coals. If the R_{70} is less than 0.5°C/h, or the RIT is greater than 120°C the coals are regarded as having low propensity to spontaneous combustion or are regarded as 'safe'.

The main properties of coals that vary from coal to coal and impact the greatest on likely self-heating characteristics of a coal are the inherent rate of oxidation (Ko) and the heat of oxidation (Ho(40°C)). The models developed to simulate the RIT and R_{70} tests were used to examine the effects of these coal properties on the RIT and R_{70} results. For a range of combinations of Ko (from 2000 to 22 000 g O_2/min/kg coal) and Ho (from 1000 to 15 000 J/g O_2), the R_{70} and RIT models were run to determine the corresponding R_{70} and RIT results. The relationships between these four parameters as indicated by modelling are shown in Figures 2 and 3.

From these results, it is clear that the two spontaneous combustion indices are affected in different ways. Consider the results obtained by modelling RIT as shown in Figure 2. The primary factor determining RIT is clearly the characteristic mineral-matter-free oxidation reactivity of the coal proportion, Ko. The heat of oxidation has only a minor effect on the RIT. Large variations in heat of oxidation (Ho(40°C)) from 1000 to 15 000 J/g oxygen adsorbed make very little difference to the RIT results obtained for a given rate of oxidation. On the other hand, it is clear from Figure 3 that R_{70} is dependent on both coal properties.

The explanation for this can be obtained by considering the nature of the two tests in relation to the coal properties that are involved. Taraba *et al* (1988) showed that the low temperature heat of oxidation was a function of temperature. Above about 80°C, the heat of oxidation for all coals was about the same (approximately 15 000 J/g O_2) but varied considerably from coal to coal at 40°C. Therefore in the RIT test, which begins at 70°C, there will be little variation in the heat of oxidation from coal to coal and it is reasonable to expect RIT to be independent of the low temperature heat of oxidation. This, however, is not the case in the R_{70} test, which starts at 40°C. Therefore R_{70} results will be influenced by the low temperature heat of oxidation and the oxidation reactivity. Clearly, this illustrates how important it is to understand any spontaneous combustion index in relation to the fundamental oxidation properties of coal to avoid the problems associated with purely qualitative assessments of spontaneous combustion.

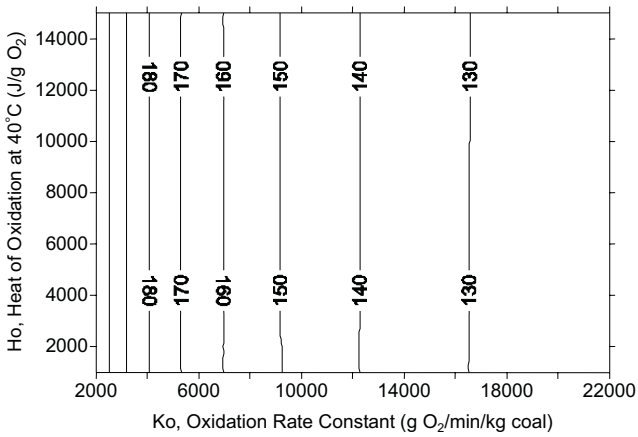

FIG 2 - RIT(°C) versus rate of oxidation and heat of oxidation as modelled.

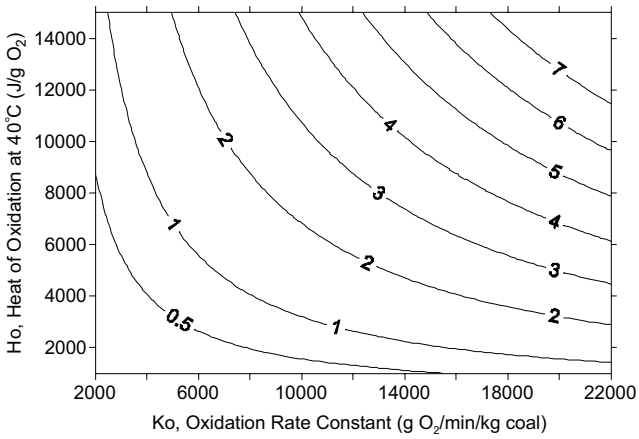

FIG 3 - R_{70}(°C) versus rate of oxidation and heat of oxidation as modelled.

It is reasonable to expect therefore that there is no direct correlation between RIT and R_{70} and this in fact is the case when one considers the distribution of RIT and R_{70} results obtained for a large number of Australian coals as shown in Figure 4. (Note however that the horizontal axis represents the self-heating period to 70°C from the R_{70} test (SHP(R_{70})) or 30/R_{70}. This places the apparently more prone (higher R_{70}, lower RIT) in the lower left corner of the diagram.)

How then are the test results related to each other and to the principal oxidation parameters Ko and Ho(40°C)? It is clear that there is not a simple correlation between RIT and R_{70}, but a more complex correlation involving the rate and heat of oxidation. The same data used to create Figures 2 and 3 has been plotted in Figure 4. This diagram shows lines of equal rate of oxidation and equal heat of oxidation. The actual test results fall within the range of reasonable values for the heat of oxidation, and there is an upper bound to the results when the low temperature heat of oxidation equals about 15 000 J/g of oxygen adsorbed. The results also provide a range for the rate of oxidation that will be useful in further modelling and a means of estimating the rate of oxidation and heat of oxidation based upon R_{70} and RIT testing.

This analysis explains the apparent conundrum that a coal may rate as prone to spontaneous combustion when tested in the Adiabatic (R_{70}) apparatus (say R_{70} = 1°C/h, SHP(R_{70}) = 30 hours) and less than 'troublesome' in the RIT apparatus (say RIT = 180°C).

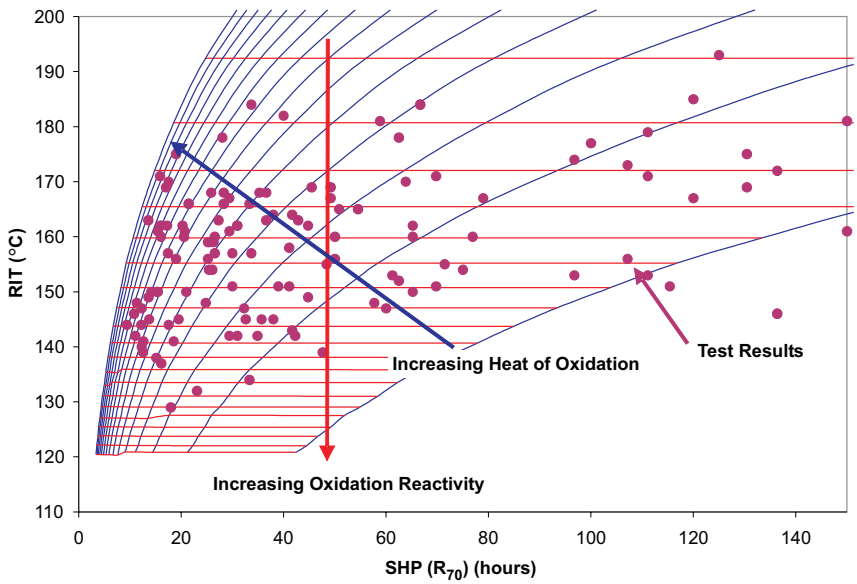

FIG 4 - RIT versus SHP(R_{70}) (ie 30/R_{70}) versus rate of oxidation versus heat of oxidation showing tested results for Australian coals.

Anatomy of a heating

The development of a spontaneous heating in coal is a complex phenomenon and is poorly understood, because it is so difficult to observe real heatings, particularly in underground coal mines, where they have the greatest potential to cause damage. Much of what is known about spontaneous heatings is derived from laboratory studies of very small-scale tests. These tests provide valuable data on the many parameters that affect the oxidation process and the production of off-gases that might be used for detection purposes. It is, however, virtually impossible to examine a real heating, to measure its temperature distribution, to measure the airflow involved, or to measure almost any aspect of its behaviour. It is impossible to conduct an 'autopsy' on a heating to see what has happened. Considerable insight can, however, be gained into the nature of real heatings by examining in detail the results obtained from a simulated heating.

Some understanding of the complexity involved can be obtained by examining the results of modelling the development of a heating in a pile of coal as simulated in the Quasi-3D model. The oxidation properties for the average test results shown in Figure 4 (R_{70} and RIT values of 0.90°C/hour and 162°C respectively) corresponding to values for Ko and Ho(40°C) oxidation reaction constants of 6500 g O_2/min/kg and 4500 J/g O_2 respectively. The relative oxidation rate was set to 25 per cent (equivalent to particle size of 91 to 400 mm) and the dimensions of the pile were set at 5 m diameter by 5 m long, simulating a heating in approximately 128 tonnes of coal. The airflow flux was set at 20 L/min/m^2 and the initial temperature was set to 35°C. This is referred to later as the 'base case'.

The main features of the development of the heating in the base case are illustrated Figure 5. The peak temperature in the pile, the position of the peak temperature (the hotspot) and the position of the minimum oxygen concentration in the pile are shown in Figure 5. At the very start of the heating, there is a moderately rapid increase in temperature, with the 'hotspot' located at the upwind surface of the pile and the minimum oxygen concentration at the back surface. The rate of temperature rise moderates (not visible on the figure but occurs nevertheless) and the position of the peak temperature moves gradually downwind. The position of the minimum oxygen remains at the back surface of the pile, although the minimum oxygen concentration is decreasing. After 275 hours, the peak temperature has moved to the furthest downwind position at about 1900 mm. The hotspot remains in this position until its temperature exceeds about 125°C.

This triggers a change in the behaviour of the heating and the hotspot begins to migrate forward. Shortly afterwards, the minimum oxygen concentration in the pile falls to zero as does the oxygen concentration at the hotspot. Despite this, the peak pile temperature is increasing rapidly, at approximately 8°C/hour.

Once the positions of the peak temperature and minimum oxygen concentration coincide, they begin to migrate together toward the upwind surface. This can only begin when the temperature profile in the coal ahead of the hotspot is sufficient to consume all the oxygen entering that part of the pile. The forward migration of the heating is limited by the upwind surface, which triggers another increase in the coal temperature. A short while after this, the temperature of the coal is sufficient to cause charring and a charline is formed in the pile. The final phase of the heating is the lateral expansion and downwind migration of the charline, as all the reactive elements in the coal are consumed by oxidation.

From this analysis, it is possible to divide the development of this heating into three distinct phases:

1. The incipient phase characterised by peak pile temperatures up to about 125°C. During this phase a hotspot develops from the upwind surface, migrates downwind to a maximum depth and remains static in that position.
2. The migration phase characterised by the forward migration of the hotspot. During this phase the minimum oxygen concentration in the pile falls to zero per cent and there is a very rapid increase in the peak coal temperature. Without remedial action, the heating continues to develop and could lead to the outbreak of fire at the upwind surface of the pile.
3. The charring phase, when the temperature in the pile is sufficient to cause the formation of unreactive char or the outbreak of open fire.

The most significant phase in any heating is the initial incipient phase up to about 125°C. Any spontaneous heating which is sufficiently large to pose a threat to safety will have to pass through the incipient phase. Most of the time required for a dangerous heating to develop will be in reaching 125°C. There may be circumstances in which a coal can be exposed to airflow and such a heating will not develop. For example, if the mass or thickness of the coal pile is insufficient, heat losses will

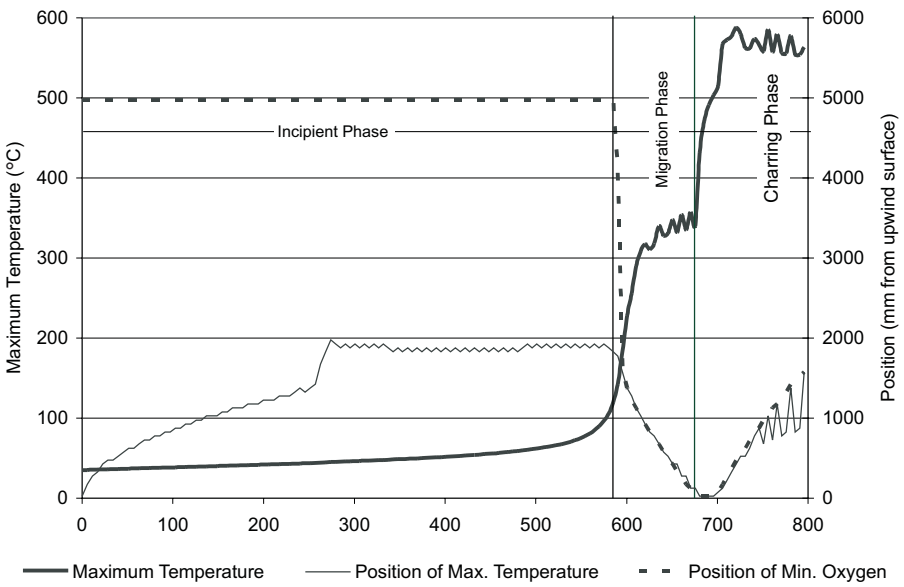

FIG 5 - Base case heating development – temperature and oxygen.

predominate at some temperature and a spontaneous heating will not occur. However, for heatings of significance, the incipient phase will be significant and there are a number of important factors in determining whether spontaneous combustion will occur in a particular coal.

Factors controlling the occurrence of spontaneous combustion

One of the main objectives of this study was to examine the nature of spontaneous heatings in coal and to relate the observed spontaneous combustion behaviour to measurable coal properties. Much of what is already known is based on an incomplete understanding of the phenomenon of spontaneous combustion.

What is poorly understood is the degree to which changes in many parameters affect the spontaneous combustion behaviour of coal. For example, consider the thickness of a coal seam. If it is assumed that the coal is broken up to a certain size and that there is airflow through the coal, how will the thickness of the seam affect spontaneous combustion behaviour? It could easily be accepted that if the seam is only 100 mm thick, there will be no spontaneous combustion, due to heat losses to the surrounding unreactive strata. But what will occur if the seam is 1 m thick, or 2 m or 3 m? As the coal seam thickness increases it could be expected that the heat losses relative to the heat generated by oxidation decrease and lead to higher and higher temperatures. At some critical thickness the temperature will be such that a heating will develop. There need be no changes in any of the other parameters for this to occur.

The same can be said of all the other parameters that have been listed. Any change which leads to greater heat generation, or lower heat losses, will cause the temperature in the coal pile to increase more rapidly and, at some critical value, will cause spontaneous combustion to occur.

The critical airflow flux to trigger spontaneous combustion

Airflow is essential for spontaneous combustion to take place. In any coal pile, without airflow through the pile, there is no oxygen available for oxidation and there can be no temperature rise. It has often also been said that high airflow is capable of carrying the heat generated by oxidation away from the pile and therefore can be used as a strategy to help control spontaneous combustion.

To examine the impact of airflow on the development of a spontaneous heating in a coal pile, a series of models using a one-dimensional model was run to simulate heating in a coal pile, such as a coal pillar in an underground mine. The airflow flux was altered over a wide range from 0.1 L/min/m^2 to 5000 L/min/m^2 with other model parameters the same as that used in the previous base case simulations.

It was found that at very low airflow flux levels, there is a temperature rise but the development of the heating restricted by the lack of oxygen entering the pile. Below about 3 L/min/m^2, the airflow flux has a significant effect on the development of spontaneous heating. Above 3 L/min/m^2, this effect becomes less significant and there is very little impact upon the development of the heating. For the purposes of additional modelling, it was decided therefore to use an airflow flux of 20 L/min/m^2 to ensure there was no effect due to inadequate flow of air through the model.

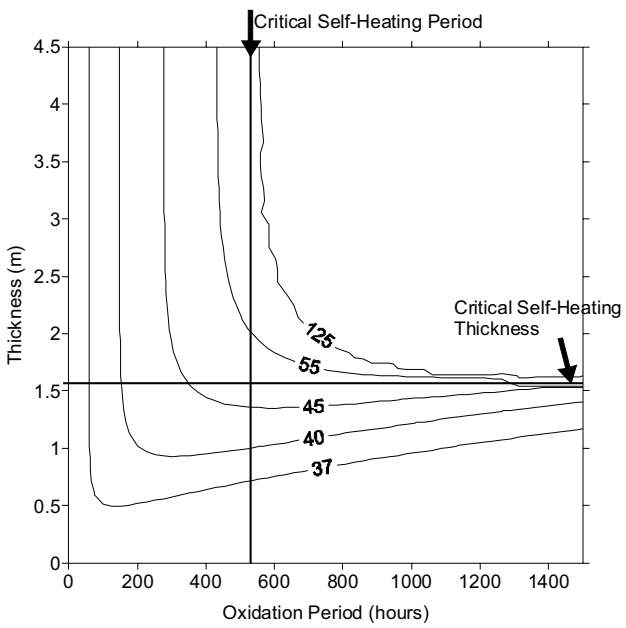

FIG 6 - The impact of pile thickness variations (peal pile temperature °C) on development of a heating.

It was also found that the impact of increasing airflow through the pile was to force the position of the hotspot formation further downwind in the pile. However, only if extreme values were simulated did the heating move significantly into the pile suggesting that it was not possible to rely on excess ventilation to control self-heating as has been suggested previously.

Critical spontaneous combustion characteristics

As discussed above one could expect that there is a critical thickness associated with a particular coal and size below which it would not be possible for spontaneous combustion to occur. The relatively high heat losses when the seam is thin prevent the necessary temperature rise required for transition from the incipient phase to the migration phase.

The impact of increasing seam or pile thickness was modelled using a variation on the 2D model to simulate the self-heating of coal in a deep pile of coal of varying thickness with the same coal properties as the base case. The initial thickness in the model was incremented until there was little change in the time-temperature profile. The results obtained are illustrated in Figure 6. As expected, for thin layers of coal, there is an initial temperature increase to some maximum value after which the coal begins to cool due to reduced rates of oxidation and heat transfer into the surrounds. As the coal thickness increases, the maximum temperature achieved before the coal begins to cool increases and the time at which this maximum is achieved increases. Up to some thickness, in this case about 1.5 m, the increase in oxidation rate due to increased temperature has been more than offset by the decrease caused by cumulative oxidation. Once the coal temperature exceeds about 70°C, however, a fine balance is achieved between these competing effects. Any further increase in temperature will see the domination of the effect from temperature. The result is that, above some critical thickness, the effect of temperature eventually dominates and there will be a very rapid temperature rise beyond 70°C. The critical self-heating thickness for the conditions modelled and illustrated in Figure 6 is 1.5 m. For the purposes of this study, the critical self-heating thickness is the maximum thickness for a given combination of coal properties (particle size, heat of oxidation, oxidation rate constant and initial coal temperature) at which self-heating to 125°C will not occur.

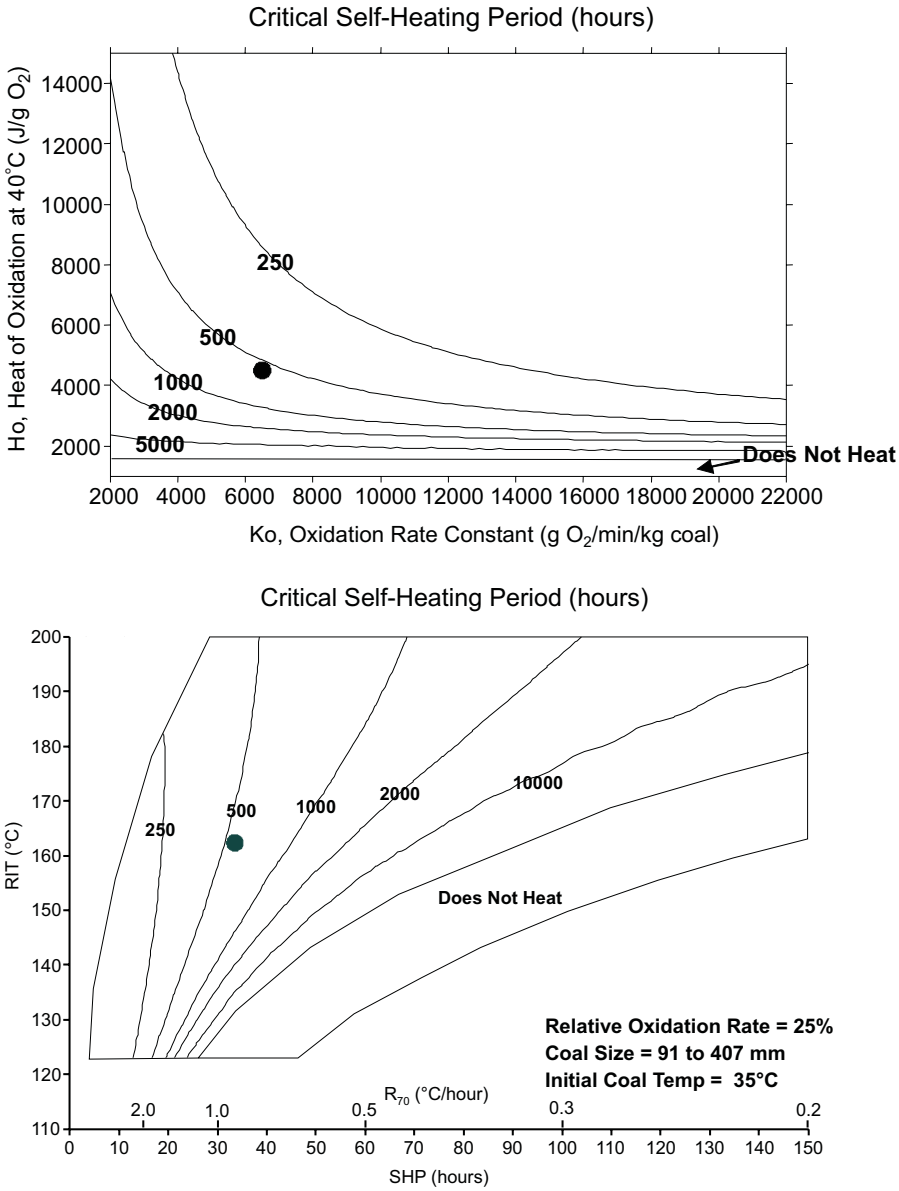

FIG 7 - Critical self-heating period for relative oxidation rate of 25 per cent (particle size of 91 to 407 mm) and initial temperature of 35°C.

If the coal thickness is greater than the critical self-heating thickness, spontaneous combustion will take place and very high temperatures will result. As the pile or seam thickness increases, the time required for the onset of rapid self-heating becomes less and less. As illustrated in Figure 6, this approaches some minimum value, shown as the critical self-heating period. In this case, the critical self-heating period is 550 hours. For the purposes of this study, the critical self-heating period is the minimum time taken for a given combination of coal properties (particle size, heat of oxidation, oxidation rate constant and initial coal temperature) to self-heat to 125°C.

Similarly, variations in the total coal mass can determine whether a heating will develop and affect the time required for the heating to develop. Clearly, the same logic applies when considering the impact of increasing the mass of coal in a pile. For very small piles, there will only be a small temperature rise, until heat losses balance heat generation. As oxidation proceeds, the rate of oxidation will decrease and the temperature of the small coal pile will begin to decrease. As the pile size increases, the maximum temperature achieved will increase until, eventually, the effect of increased oxidation is dominated by that of increased temperature and a fully developed heating with high temperatures will occur. For every combination of coal properties (particle size, heat of oxidation, oxidation rate constant and initial temperature) there will be a critical self-heating mass, which is the minimum mass of coal required to support self-heating to 125°C.

The critical spontaneous combustion characteristics of interest can therefore be defined as:

- the critical self-heating period (CSHP) – the minimum time in which spontaneous combustion will occur;
- the critical self-heating thickness (CSHThk) – the thickness of a coal pile or seam below which it is not possible for spontaneous combustion to occur; and
- the critical self-heating mass (CSHM) – the mass of a coal below which it is not possible for spontaneous combustion to occur.

The variation of critical self-heating period and thickness with oxidation properties can be assessed from Figures 7 and 8. In each of these figures the upper graph reflects the variation due to oxidation properties of the coal in the modelled critical self-heating period or thickness for coal with a relative oxidation

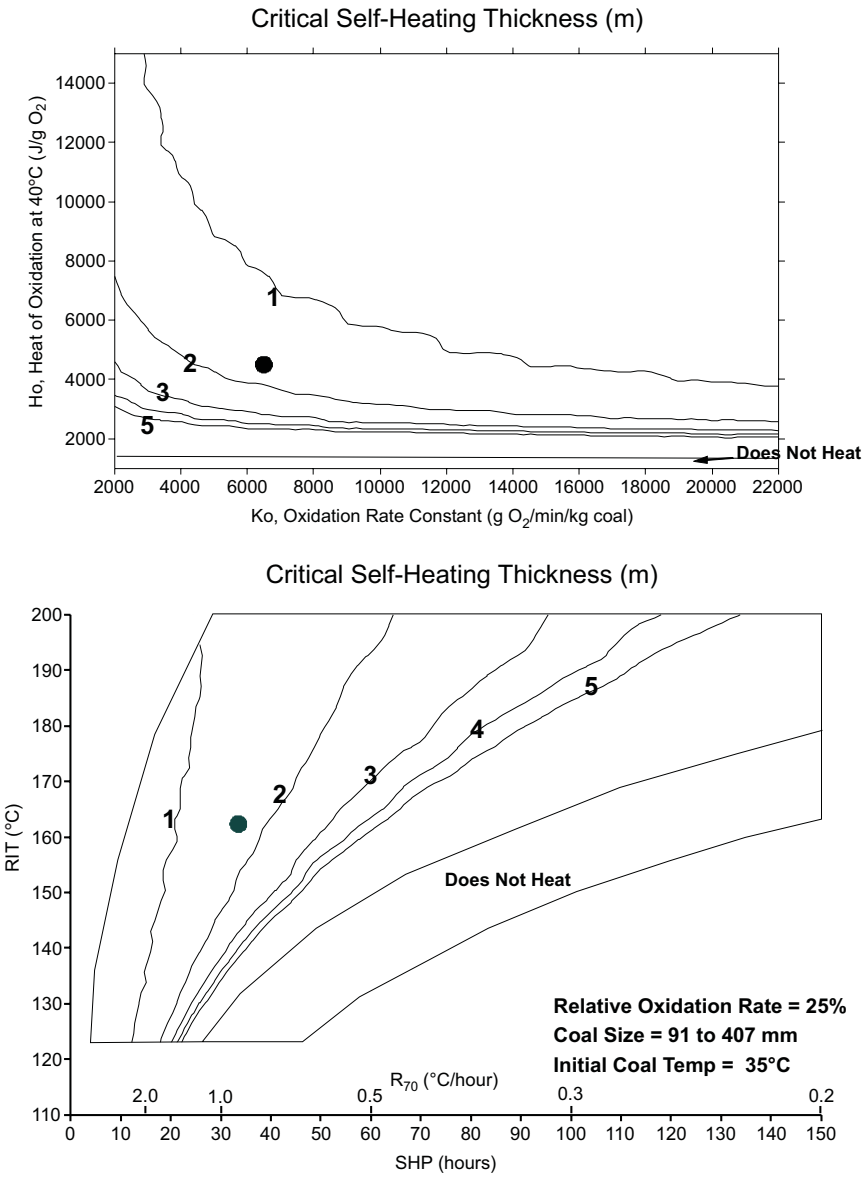

FIG 8 - Critical self-heating thickness for relative oxidation rate of 25 per cent (particle size of 91 to 407 mm) and initial temperature of 35°C.

reactivity of 25 per cent (95 per cent passing 91 to 407 mm) and an initial temperature of 35°C. The position of the average coal (Ko = 6500, Ho(40°C) = 4500) is also shown for reference. The lower graph shows the same critical self-heating parameter as a function of R_{70} and RIT.

It is clear from these results that the both critical self-heating characteristics decrease with increasing oxidation reactivity (Ko) and heat of oxidation at 40°C (Ho(40°C)) in a manner very similar to that of the critical self-heating period. It is also clear that neither R_{70} nor RIT results can claim to be a predictor of the critical self-heating period or thickness but that in combination these parameters can be used.

It should also be noted that it is predicted that some coals will not self-heat under the conditions modelled. The critical self-heating period and thickness are very high (infinite) and this is the case not matter how the particle size (relative reactivity) varies for these coals. This comes about because of the temperature dependence of the heat of oxidation suggested by the work Taraba (1988). Extrapolating his results to lower temperatures suggests that the heat of oxidation may become very low or zero. Therefore below some temperature, the critical self-heating temperature, it is likely that a particular coal is incapable of self-heating irrespective of the airflow, pile thickness, particle size, etc.

This behaviour is analogous to that seen in the USBM minimum self-heating temperature test described by Smith and Lazarra (1987) except that the critical self-heating temperatures are much lower than suggested by that test method. the relationship between the estimated critical self-heating temperature and the results of spontaneous combustion testing is shown in Figure 9. This adds one more parameter to the critical self-heating characteristics of coal being:

- the critical self-heating temperature (CSHT) – the initial coal temperature below which coal will not spontaneously combust irrespective of the thickness or mass of coal involved.

Use of the critical self-heating characteristics to assess the potential for spontaneous combustion

It is considered that the critical self-heating characteristics of temperature, thickness and period, as described above, can be used to provide a better means of assessing the spontaneous combustion potential in a mining, or stockpiling situation. It is quite apparent, based upon the modelling results obtained, that if the initial temperature of a coal seam in an underground mine is lower than the critical self-heating temperature of the seam, spontaneous combustion will not occur. Similarly, if the seam

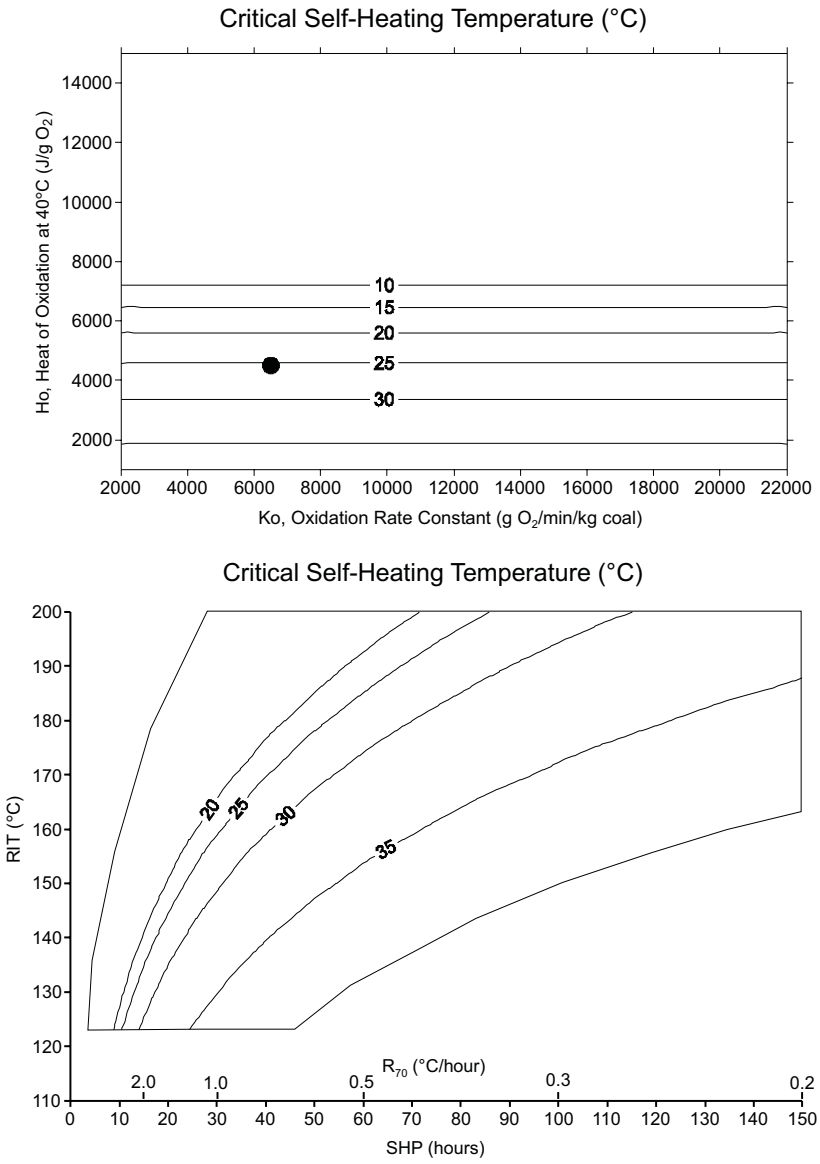

FIG 9 - Distribution of critical self-heating temperatures.

thickness is less than the critical self-heating thickness self-heating will not occur. This logic can be expressed in a simple flow chart as shown in Figure 10. This method of assessment represents a considerable improvement over the qualitative assessments of most spontaneous combustion test methods which leave the mine owner pondering the difference between high and low propensity to spontaneous combustion.

Obviously, caution must be used if it is predicted that there is no potential for spontaneous combustion and there is only a small difference between *in situ* properties and the critical self-heating characteristics of a coal. Small changes to *in situ* conditions could result in a different evaluation of the potential for spontaneous combustion. Caution must also be applied when the initial coal temperature is close to the critical self-heating temperature. Small variations in any of the coal properties especially determination of R_{70} or RIT and determination of the *in situ* initial coal temperature could have a significant impact on the outcome of the assessment of the spontaneous combustion potential. The method of assessment proposed here, however, is a considerable improvement over that which could be achieved if the only considerations were the results of the R_{70} and RIT results or any other qualitative interpretation of some laboratory test method.

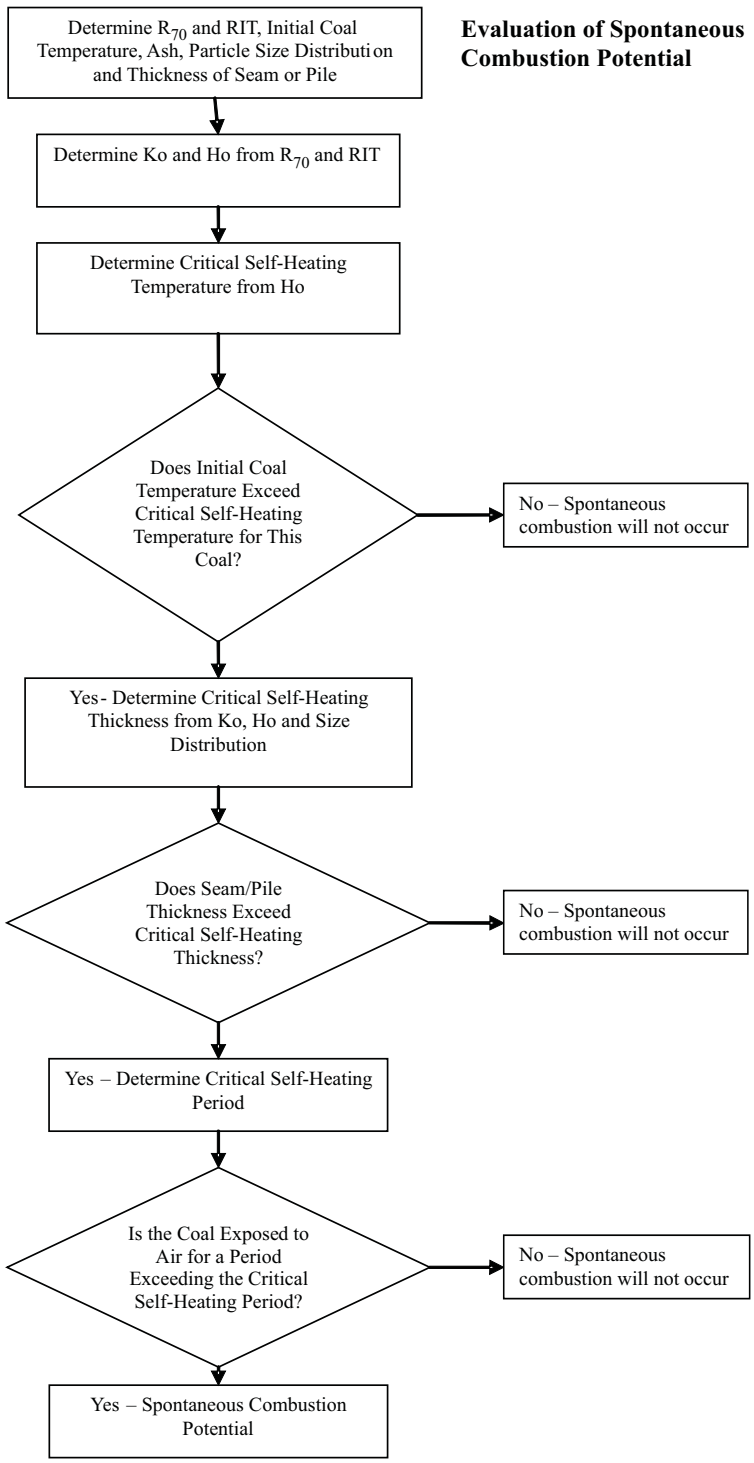

FIG 10 - A method of assessing the potential for spontaneous combustion in a mine or stockpile.

CONCLUSIONS

This study has attempted to combine a comprehensive knowledge of the many aspects of oxidation behaviour of coal and the heat loss mechanisms that play their part in spontaneous combustion to better assess the likely *in situ* or field behaviour of coals leading to the development of spontaneous heatings. This knowledge has been combined into a number of numerical modelling techniques that can simulate laboratory tests such as the R_{70} and RIT tests and to model the spontaneous combustion behaviour of coal in stockpiles, or in a mine. Fundamental oxidation parameters of reactivity and heat of oxidation are used as the basis for all models and therefore a direct link is established between results of the laboratory tests and predicted field behaviour.

The study has provided a fresh understanding of many aspects of the development of spontaneous combustion in coal leading in turn to the development a new more quantitative assessment of the potential for spontaneous combustion that better takes into account factors such as the initial pile temperature, pile size and mass, and coal particle size.

ACKNOWLEDGEMENTS

The author would like to acknowledge the valuable assistance of Stewart Gillies and Peter Golledge while studying as a PhD student at the University of Queensland and the support of Simtars and ACIRL in providing support for this study.

The views expressed in this paper are those of the author.

REFERENCES

Humphreys, D R, 2004. The application of numerical modelling to the assessment of the potential for, and detection of, spontaneous combustion in coal mines, PhD thesis, University of Queensland, Brisbane.

Smith, A C and Lazarra, C P, 1987. Spontaneous combustion studies of US coals, USBM Report of investigation 9079.

Symmington, A, 1999. Personal communication.

Taraba, B, Dobal, V, Cap, K and Harasta, M, 1988. Differential thermal effects during low temperature oxidation of coal, *Fuel*, 67:758-763.