# A mathematical model for stockpile management

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*Abstract*

The deterioration in the properties of coal during storage due to oxidation is a major problem in the coal export industry. The aim of the project was to develop a model to estimate the extent of deterioration in the quality of coal as a function of stockpile size, time and storage conditions and test its validity against results from experimental stockpiles. A one dimensional model for the oxidation of coal in stockpiles, which is based on the conservation of mass and energy has been developed for this purpose. The model was solved numerically and the results compared with experimental data for the three coals used in the study. The results obtained from the numerical solution of the model were found to be in satisfactory agreement with the data obtained from experimental stockpiles. Certain broad guidelines to minimise the extent of deterioration have emerged from the results of computer simulation for the engineering design, handling and management of coal storage facilities.

A model of the type developed should be applicable to simulating the deterioration of any stored product.

## Notation

| | | |
|---|---|---|
| Bi | Biot number | dimensionless |
| C | Oxygen concentration | $mol/m^3$ gas |
| $C_h$ | Oxygen concentration at boundary | $mol/m^3$ gas |
| $C_R$ | Specific heat of coal bed | J/kg/K |
| $C_c$ | Specific heat of coal | J/kg/K |
| $C_g$ | Specific heat of air | J/kg/K |
| $D_1$ | Diffusion coefficient (oxygen in air) | $m^2/s$ |
| $D_2$ | Thermal diffusivity of air | $m^2/s$ |
| $D_e$ | Diffusion coefficient for diffusion of oxygen in bed of coal | $m^2/s$ |
| $D_\eta$ | Particle size | mm |
| $\Delta H$ | Enthalpy of reaction | J/mol |
| 1 | Distance co-ordinate | m |
| L | Total length of bed | m |
| Le | Lewis number | dimensionless |
| n | Parameter in equation relating rate and time | dimensionless |
| p | Partial pressure of oxygen | atm |
| P | Pressure | Pa |
| Pe | Peclet number | dimensionless |
| q | Oxygen consumption | $gO_2$/(kg coal) |
| q* | Oxygen consumption | mol $O_2/m^3$gas |
| Q | Oxygen consumption | dimensionless |
| r | Rate of oxidation | mol $O_2$/mgas/sec |
| $r_1$ | Rate of oxidation at 1 hour | mol $O_2/m^3$gas/sec |
| $t_s$ | Time | second |
| T | Temperature | K |
| $T_b$ | Temperature at boundary | K |
| V | Wind velocity | m/second |
| X | Length of bed | dimensionless |
| y | Oxygen concentration | dimensionless |
| z | Temperature | dimensionless |
| $\lambda_B$ | Thermal conductivity of bed | W/m/K |
| $\rho_B$ | Bulk density of coal bed | $kg/m^3$ |
| $\rho c$ | Density of coal particles | $kg/m^3$ |
| $\rho g$ | Density of air | $kg/m^3$ |
| $\tau$ | Time | dimensionless |
| $\varepsilon$ | Porosity | dimensionless |
| $\mu$ | $Log_{10}$ (Gieseler maximum fluidity/dial divisions/ minute: ddpm) | dimensionless |
| $\mu 0$ | $Log_{10}$ (Gieseler maximum fluidity of unoxidised coal/dial divisions/minute) | dimensionless |
| $\alpha_e$ | Thermal diffusivity of bed | $m^2$/second |
| $\phi$ | Thiele modulus | dimensionless |

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## Introduction

Several properties of coal are adversely affected by atmospheric oxidation during storage (Nelson 1989). One of the properties which is most severely affected is the Gieseler fluidity (as measured by a Gieseler Plastometer) to such an extent that, because of deterioration, the stored coal can no longer be used for the purpose intended. The deterioration in the quality of coal in stockpiles is therefore a major economic problem in the coal export industry. To determine the extent of deterioration at a particular point in the stockpile, current practice involves expensive and time-consuming steps of taking a representative sample and testing it in laboratory. The aim of the project was to develop a model to estimate the extent of deterioration in the quality of coal (as measured by fluidity) as a function of stockpile size, time and storage conditions and test its validity against results from experimental stockpiles. Broad guidelines on the stockpile management techniques to minimise the extent of deterioration of any stored product should emerge from a sensitivity analysis of such a model.

## The Model

In this paper, the available correlations for the rate of oxygen consumption (Boyapati et al. 1991) as well as those between oxygen consumption and fluidity (Boyapati and Gupta 1992) have been incorporated into a one-dimensional model of a coal bed. The resulting equations have been solved numerically. Results from the model have then been compared with results obtained from the experimental stockpiles for three coal types (Liddell, Lilyvale and Wongawilli).

Nordon and Bainbridge (1983) have shown that the heat of wetting is unlikely to contribute significantly to the heating of coal in stockpiles under normal conditions. The effect of the relative humidity of the atmosphere was therefore not taken into account in the present model. The effect of solar radiation and fluctuations in the ambient temperature on the temperature rise in a coal stockpile were shown to be negligible (Davidson 1990) and were, therefore also ignored in the model. A one-dimensional model was used since two and three-dimensional models, though incorporating the same basic principles and therefore expected to yield similar results, become prohibitive in terms of the computing time required to solve them when balanced against the extra information that might be gained.

The major assumptions of the model are:

- Heat transfer occurs by conduction and convection.
- Mass transfer occurs by diffusion and convection.
- Air convection is due to the wind pressure gradients only and natural convection is negligible.
- The physicochemical properties of the bed (such as thermal conductivity, specific heat, diffusion coefficient, enthalpy of reaction) are constant with respect to temperature, moisture content and time.

With the assumptions using the conservation laws for mass and energy, the differential equations for oxygen and energy balance in a coal bed are:

$$\frac{\partial C}{\partial t_s} = D_e \frac{\partial^2 C}{\partial l^2} - u\frac{\partial C}{\partial l} - r \qquad \text{(oxygen balance)}$$

$$\rho B C b \frac{\partial T}{\partial t_s} = \lambda_B \frac{\partial^2 T}{\partial l^2} - \left( u\rho_g C_g \frac{\partial T}{\partial l} - \varepsilon r \Delta H \right) \qquad \text{(energy balance)}$$

The boundary conditions are:

At $l = 0$,

$$D_e \frac{\partial C}{\partial l} = uC - uC_b + \frac{D_1}{d_1}C - \frac{D_1}{d_1}C_b$$

$$\alpha e \rho_B C_B \frac{\partial T}{\partial l} = \rho_g C_g \left[ uT - uT_b + \frac{D_2}{d_2}T - \frac{D_2}{d_2}T_b \right]$$

and at $l = L$

$$D_e \frac{\partial C}{\partial l} = \frac{D_1}{d_1}C_b - \frac{D_1}{d_1}C$$

$$\alpha e \rho_B C_B \frac{\partial T}{\partial l} = \rho_g C_g \left[ \frac{D_2}{d_2}T_b - \frac{D_2}{d_2}T \right]$$

The above equations may be converted into dimensionless form by the following substitutions:

$$y = \frac{C}{C_b}; \tau = \frac{D_e t_s}{L^2}; X = \frac{1}{L}; r = \frac{\partial q^*}{\partial t_s}; Q = \frac{q^*}{C_b}$$

$$z = \frac{T}{T_b}; Pe_1 = \frac{uL}{D_e}; Le = \frac{\lambda_B}{D_e \rho_B C_B}; Pe_2 = \frac{u\rho_g C_g L}{\lambda_B}$$

$$Bi_1 = \frac{D_1 L}{d_1 D_e}; Bi_2 = \frac{D_2 L \rho_g C_g}{d_2 \lambda_B}; H = \frac{\varepsilon D_e C_b \Delta H}{\lambda_B T_b}; \phi^2 = \frac{L^2 r_1}{D_e C_B}$$

$$\text{Where } \frac{\partial Q}{\partial \tau} = \phi^2 \left( \frac{t_s}{3600} \right)^{-n}$$

$$t_s = \left[ \frac{Q C_b 3600^{-n}(1-n)}{r_1} \right]^{1/(1-n)}$$

Thus the dimensionless equations are:

$$\frac{\partial y}{\partial \tau} = \frac{\partial^2 y}{\partial X^2} - Pe_1 \frac{\partial y}{\partial X} - \frac{\partial Q}{\partial \tau}$$

$$\frac{1}{Le}\frac{\partial z}{\partial \tau} = \frac{\partial^2 z}{\partial X^2} - Pe_2 \frac{\partial z}{\partial X} - H\frac{\partial Q}{\partial \tau}$$

with the boundary conditions

At X = 0

$$\frac{\partial y}{\partial X} = [Pe_1 + Bi_1][y-1]; \frac{\partial z}{\partial X} = [Pe_2 + Bi_2][z-1]$$

and at X = 1.0,

$$\frac{\partial y}{\partial x} = Bi_1[y-1]; \frac{\partial z}{\partial X} = Bi_2[1-z]$$

The initial conditions are $y = z = 1.0$ (at all X).

In order to solve the above equations, data on the following input parameters are required: the diffusion coefficient of oxygen in a bed of coal, the enthalpy of reaction, the thermal conductivity of the bed, the heat capacity of the bed, the permeability of the coal bed to air, the bulk density and the particle density. For the present purposes, some of these have been determined experimentally and some have been obtained from the literature.

### Numerical solution of the model

The partial differential equations for the mathematical model were solved numerically using the NAG (Numerical Algorithms Group, U.K.) subroutine DO3PGF. This subroutine integrates a system of nonlinear parabolic partial differential equations in one space variable, using the method of lines and Gear's method. The results of calculations are discussed in some detail below.

### Comparison of model predictions with experimental results

The average particle sizes of the coals in the experimental stockpiles were calculated from the Rosin-Rammler size distribution graphs. The average particle sizes of the Liddell, Lilyvale and Wongawilli seam coals were 9.0 mm, 9.4 mm and 4.7 mm, respectively. The average particle sizes of four size fractions of Liddell seam coal were 0.23 mm (–0.4m fraction), 1.23 mm (–2+0.5 mm fraction), 4.89 mm (–8+2 mm fraction) and 19.65 mm (–50+8 mm fraction).

The experimental stockpiles (Boyapati et al. 1984) were 21 m long, 1.3 m wide at the top and 3.5 m at the base and 1 m high. For the calculations, a one-dimensional bed length of 2.4 m was used. Using L=2.4 m and an ambient temperature ($T_b$) of 289.5 K (calculated average temperature for the storage period of 11 months), the equations were solved for the head samples of the three coals and for the four size fractions of the Liddell seam coal.

Figure 1 shows the differences between the experimental and predicted values. The agreement is good except for the individual size fractions of the Liddell seam coal. This poor agreement results from assuming that the average particle sizes of Liddell seam coal in the stockpile are 0.23, 1.23, 4.89 and 19.65 mm, for the four size fractions, respectively. Therefore, the fact that these size fractions are mixed with the other sizes in the experimental stockpiles is not taken into account. Thus, the calculated fluidity values are higher (due to lower oxygen concentration) in the case of the smaller size fractions and lower in the case of the largest size fraction compared to the measured experimental data. A more accurate and rigorous calculation for the individual size fractions would use the population balance approach (Herbst 1979).

## Sensitivity analysis and model predictions

To obtain results for the extent of deterioration in the quality of a large hypothetical coal stockpile, a representative Lilyvale seam coal bed of 10 m length was considered. A sensitivity analysis was carried out to assess which of the factors have greater influence on the deterioration and to check whether a variation in the assumed values for some of the transport properties (taken from literature) would make a large effect on the results.

### *Effect of bulk density*

Changes in the bulk density (due to, for example, compaction of the stockpile) have two main effects: i.e., a decrease in the effective diffusion coefficient and a decrease in the permeability of the bed. The effect of bulk density on the extent of deterioration as a function of depth of bed (no convection) showed that the deterioration is greater when the bulk density is low, particularly near the boundaries. It has been found that, at low bulk densities, there is a deterioration even at the centre of the 10 m bed, because of the lower resistance to mass transfer.

To investigate the effect of the variation in bulk density for different heap sizes, beds of 1, 2, 5, 10 and 20 m were considered ($Pe_1 = Pe_2 = 0$). From the results of the calculations (shown in Fig. 2), it is clear that the greater the bulk density, the lesser is the deterioration, irrespective of heap size. For example after 6 months storage, Lilyvale seam coal stocked at 600 kg/m$^3$ bulk density as a 5 m bed would have a fluidity of 1400 dial divisions per minute (ddpm) whereas that stored at 1200 kg/m$^3$ would have a fluidity of about 4300 ddpm.

Figure 2 also shows that, for a given bulk density, storing coal in large stockpiles is advantageous in minimising the extent of deterioration. Further, the results clearly demonstrate the beneficial effects of compaction, particularly for small beds. In other words, for the same extent of deterioration, small coal heaps must be compacted to a greater bulk density than large heaps. For example, one year's storage in a 2 m heap at 1200 kg/m$^3$ produces about the same deterioration as in a 20 m heap at 600 kg/m$^3$ bulk density.

The effects of increasing bulk density, when convection is taken into account, are shown in Figure 3 for a 5 m bed. Whereas for the high bulk density bed, the deterioration is negligible except near the boundaries (about 0.5 m), at lower bulk densities, the effects can be devastating when the oxygen supply due to convection as well as diffusion creates a situation where the temperature rise can be significant.

Calculations show that when the bulk density is 600 kg/m$^3$, the maximum oxygen consumption occurs at about 0.4 m from the boundary, the maximum temperature being 320°C at about 1 m from the boundary. Such a situation, of course, is certain to lead to spontaneous combustion. An interesting result is that at low bulk densities, the fluidity near (0.1 m) the downstream boundary is higher than when the bulk density is high. This is because gases at this point are depleted of oxygen due to the high reaction rates (because of high temperature) earlier during its travel along the bed (due to the unidirectional nature of convection assumed).

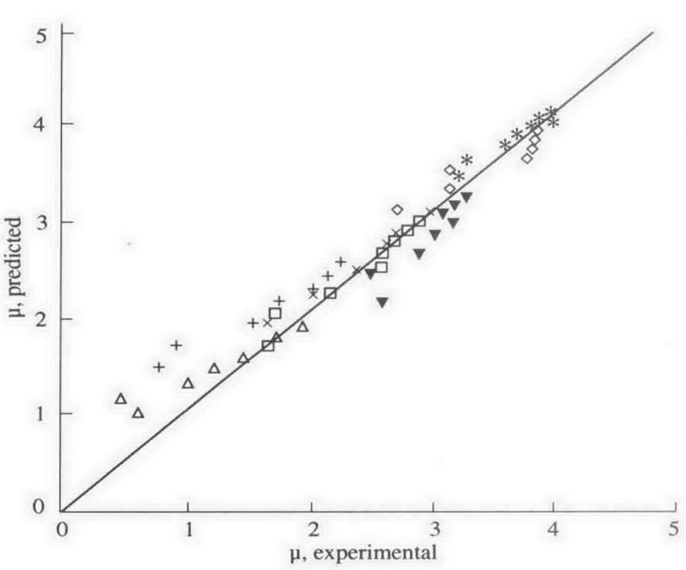


**Fig. 1.** Comparison of predicted versus experimental Gieseler Fluidity for: Liddell (□), Lilyvale (◇), and Wongawilli (*) seam coals; and four size fractions of Liddell seam coal: –0.5 mm (Δ), –2+ 0.5 mm (+), –8+2 mm (×) and –50+8 mm (▼). The values of the parameters, unless otherwise stated, were taken as Dp = 9.4 mm; L = 10 m; E = 30460 J/mol; $D_e = 1.75 \times 10^{-6}$ m$^2$/second; $T_b = 293$ K; $\Delta H = -3 \times 10^5$ J/mol; $\lambda_B = 0.18$ W/m/K; $\alpha = 1.0$; $\varepsilon = 0.28$; $\rho_B C_B = 11.3 \times 10^5$ J/m$^3$/K; $d_1 = d_2 = 0.01$ m (thickness of boundary layers); t = 8640 h; $u = 5.2 \times 10^{-6}$ m/second (superficial velocity of gas).

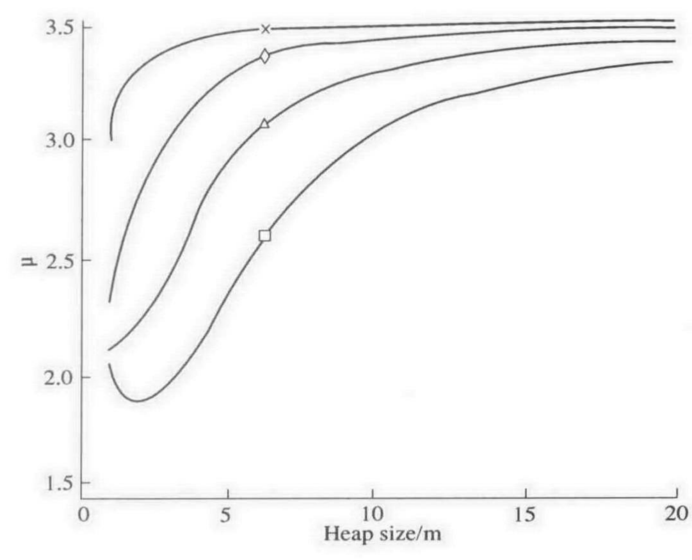


**Fig. 2.** Effect of bulk density of the bed on Gieseler Fluidity as a function of heap size of Lilyvale seam coal (no convection) (□) 600 kg/m$^3$; (Δ) 800; (◇) 1000; (×) 1200.

*Effect of ambient temperature*

The effect of the ambient temperature of storage was calculated between the range of 0°C and 40°C. Higher ambient temperatures result in greater deterioration at and near the boundaries. Significantly, the effects of large variations in ambient temperature are confined only to the surface of the heap.

*Effect of particle size*

The effect of particle size on the deterioration in quality was investigated for a 10 m bed after 1 year storage. The range of values used for the particle size was 0.1 to 60 mm. As is to be expected, the larger the particle size, the lower is the deterioration due to the lower rate of oxidation and hence the lower oxygen consumption. There appears to be an anomalous situation, however, for 0.5 and 1 mm particle sizes where the deterioration is greater than in the case of the 0.1 mm size. This is because, at very small particle size (0.1 mm), though the reaction rate is high initially, the rate falls rapidly so that the total oxygen consumption after 1 year of storage is lower than that in the case of 0.5 and 1 mm sizes.

*Effect of stockpile size*

To investigate the effect of the size of stockpile on the extent of deterioration, coal beds of varying maximum linear dimension of between 0.1 m and 40 m were considered with $Pe_1 = Pe_2 = 0$. Calculations showed that the size of the heap has an important bearing on the extent of deterioration. For example, after 1 year storage, the fluidity ($\mu$) of the coal falls from an initial value of 3.8 (6300 ddpm) to 2.2 (160 ddpm), in the case of a 1.0 m bed, whereas the fluidity is 3.45 (2800 ddpm) for a 20 m bed. When the smallest linear dimension of the heap exceeds 20 m, there is little change in the effect as the size of the bed increases. This is because the oxidation process at the centre of the bed is very slow due to the insufficient oxygen supply.

*Effect of time of storage*

The effect of time of storage was investigated both with and without convection. The results for no convection showed that, near the centre of the bed, the deterioration is marginal even after 4 years storage. Whereas the fluidity of the coal is completely destroyed at the boundaries, fluidity ($\mu$) is still 3.81 (initial value 3.825) at the centre. When convection is taken into account, with increasing time the zone of no (or negligible) deterioration shrinks and moves inward.

*Effect of velocity of air flow*

The effect of the velocity of airflow was investigated by using different values for Peclet numbers in the range of 0 to 90 for $Pe_1$ and 0 to 1.7 for $Pe_2$. This corresponds to a superficial velocity of between 0 (no convection) and $25 \times 10^{-6}$ m/second. As the velocity of air flow increases, the fluidity is lower and the point of maximum deterioration in fluidity moves away from the boundary (Fig. 4). Even at the highest velocity of airflow investigated, the deterioration at about 8 m from the upstream boundary is marginal since the coal at this point is still starved of oxygen. This underlines the importance of mass transfer control in minimising the deterioration of coal in stockpiles.

*Effect of coal rank*

The effect of coal rank was studied using only the three coals for which the data are available. The average particle size was assumed to be 10 mm for all the coals. The results show that the fluidity is substantially unchanged near the centre of the bed for all three coals after 1 year of storage. It can been seen that the deterioration is least for the higher rank Wongawilli seam coal.

A sensitivity analysis was also carried out to assess the effect of variation in values of the parameters such as boundary layer thickness, thermal conductivity of bed, specific heat of coal and enthalpy of reaction. The results showed that for a 10 m bed, uncertainty in the values assumed for these parameters (taken from the literature) would not have affected the results greatly. Further, the assumption that the values of physical properties are constant with respect to changes in moisture content, time and temperature is valid under these conditions.

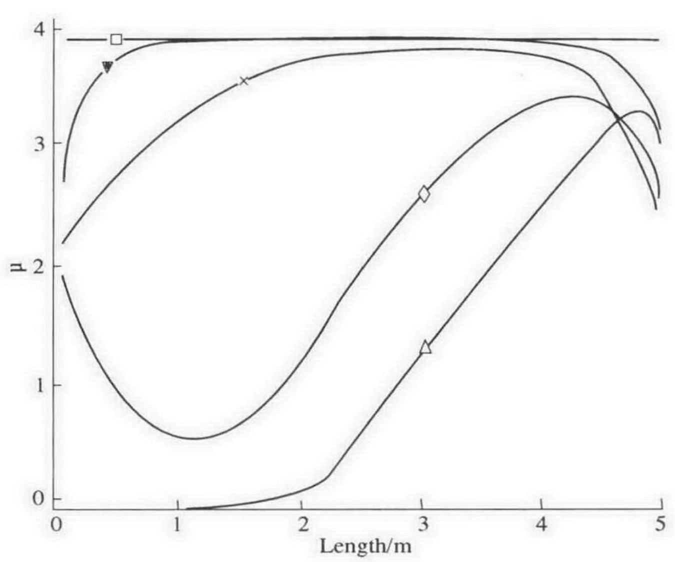


**Fig. 3.** Effect of bulk density of bed on Gieseler Fluidity as a function of depth of bed for a 5 m bed of Lilyvale seam coal (Δ) 600 $kg/m^3$; (◇) 800; (×) 1000; (▼) 1200; (□) Initial value.

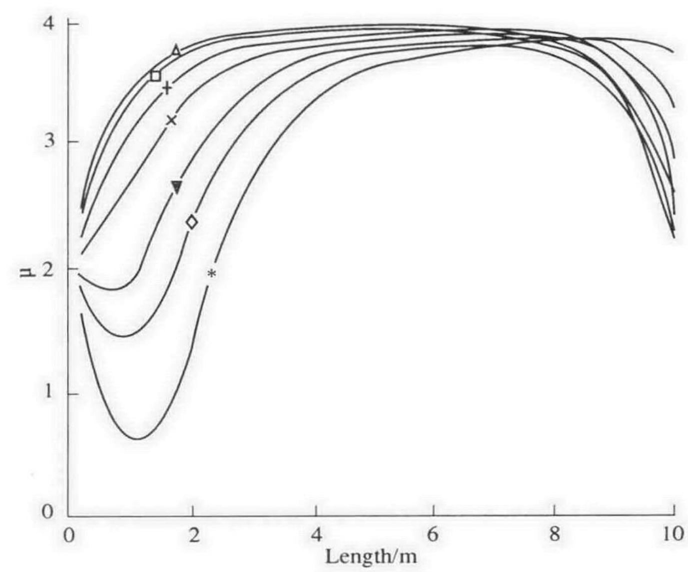


**Fig. 4.** Effect of velocity of air flow on Gieseler Fluidity as a function of depth of bed of Lilyvale seam coal (□) $Pe_1 = Pe_2 = 0$; (Δ) $Pe_1 = 1$ $Pe_2 = 0.02$; (+) $Pe_1 = 10$, $Pe_2 = 0.2$; (×) $Pe_1 = 20$, $Pe_2 = 0.4$; (▼) $Pe_1 = 40$, $Pe_2 = 0.7$; (◇) $Pe_1 = 55$, $Pe_2 = 1$; (*) $Pe_1 = 90$, $Pe_2 = 1.7$.

## Conclusions

1. The agreement between experimental and calculated values of the extent of deterioration in coal quality during storage was found to be satisfactory. The use of this approach could reduce the need for expensive and time-consuming tests on large experimental stockpiles to estimate the extent of the deterioration in the quality of stored products.
2. Other significant findings of the computer simulation include:

a) The results clearly demonstrate the important beneficial effects of increasing the bulk density of stockpiles by compaction. This need for compacting the stockpiles in minimising the extent of deterioration in the coal quality was shown to be particularly important for smaller heaps.

b) The maximum deterioration occurs near but not necessarily at, the surface of the heap, depending on the conditions of storage. In most cases, however, the deterioration in large heaps would be confined to a distance of about 1 m from the surface of the heap.

c) The smaller the heap, the greater is the deterioration. This implies that it is preferable to store coal in large heaps when practicable. When the smallest linear dimension of the heap exceeds about 20 m, however, no extra advantage will be gained by increasing the size.

d) The results show the important effects of deterioration due to oxygen supply resulting from forced convection (wind) and emphasises the need for a proper strategy in stockpile design and construction. The engineering design of storage facilities should take into account the prevailing wind direction, the strategic use of wind-breaks and topography of site.

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