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A Parametric Study of Spontaneous Ignition in Large Coal Stockpiles

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Abstract. Self-heating of coal during its storage and transportation has been a serious problem for decades. Coal stored in large piles for long duration is subjected to weathering by atmospheric air that prevails with different temperatures and moisture content. Chemisorption of atmospheric oxygen results in low-temperature oxidation of pile, which generates heat due to exothermic reactions. If the local heat release rate is higher as compared to the heat dissipated, a significant increase in temperature is possible and this results in spontaneous ignition of the pile. The presence of moisture in coal delays the occurrence of self-heating. This motivates to analyze a scenario of using moist coal to delay or even prevent the self-ignition in dry coal until a given time period of its storage. The main objective of this work is to investigate the critical conditions, which may lead to spontaneous ignition in large coal stockpiles containing dry and moist coal layers. A one-dimensional numerical model is used for this purpose. A parametric study is carried out considering different porosity, superficial air velocity and reactivity values. The time period of coal pile storage is fixed as 360 days. The location and time taken for self-ignition in the pile within this period is reported for each case. In summary, considering several cases, the simulations systematically reveal that highly reactive coal with high pile porosity and higher superficial gas velocity takes the least time to reach the self-ignition temperature.

Keywords: Coal pile, Self heating, Spontaneous ignition, Moisture, Porosity, Numerical model

1. Introduction

Spontaneous ignition in coal piles causes serious damage to life and property. It also reduces the calorific value of coal that is left unburned. A large number of accidents are reported in the past. Depending on the conditions prevailing, it can take few months to several years to reach the self-ignition temperature in the pile. Self-heating of piles is caused due to imbalance between the heat generated by processes such as adsorption, oxidation, condensation and heat dissipated by conduction, convection and evaporation. Large amount of experimental data is available in literature, but are strictly dependent on the environmental conditions and

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the properties of coal. These experiments may take several months or even years before any valuable data can be obtained from them. The classical hot-plate experiment and oven-basket experiments are conducted on small scale piles and the results are extrapolated to large scale piles. However, there may be significant differences in the temperature distribution in the large pile. In order to reduce the experimental cost and time, the focus has shifted towards theoretical and numerical modelling. However, due to complexity in modeling the actual scenario, several assumptions are made in formulating the model. Most of the models are one-dimensional, although two-dimensional models have started to appear in literature more recently.

Several mathematical models [1–10] have been developed and used in the earlier studies. Nordon [2] developed a numerical model to explain the importance of transport processes of reactants and energy in affecting the self-ignition temperature. Handa et al. [3] carried out numerical simulation using a 2-dimensional mathematical model. They concluded that the mechanism of self-heating was complicated and strongly depends on kinetics parameters and environmental conditions. Schmal et al. [4] formulated a one-dimensional numerical model and validated it with the experimental data obtained from large stockpiles. They did a comprehensive study of various parameters and successfully predicted the location and the time taken to reach self-ignition temperature in the pile. Brooks and Glasser [5] studied the pressure variations over the pile in addition to the transport processes. The model included natural convection as a mechanism of oxygen transport. However, the effect of moisture was neglected. Based on the parametric study, the piles were classified as safe, unsafe or conditionally safe, depending upon whether the pile was oxygen limited or heat transfer limited. Arisoy and Akgun [6] developed a one-dimensional model to examine the influence of gas velocity, particle size and moisture content on self-ignition characteristics. They showed that the evaporation of moisture decreased the rate of temperature rise. Increasing the gas velocity further increased the evaporation rate and this resulted in a further decrease in pile temperature. Moreover, the high temperature region moved downstream due to convective transport of heat at higher velocities. Boyapati and Oates [7] developed a one-dimensional model to study the effect of pile height, storage time and storage conditions on the extent of deterioration in coal quality. The results revealed that small piles and piles subjected to high wind velocity are susceptible to greater deterioration. Further, compacting the pile minimized the extent of deterioration. Akgun and Essenhigh [8] studied the influence of pile height, particle size, porosity and coal moisture content on self-ignition characteristics using a two-dimensional unsteady model. They found that ignition temperature and time depends on pile porosity and self-heating occurred on piles greater than 2 m height for the coal considered in their study. Yuan and Smith [9] numerically investigated the self-heating potential of coal in long wall gob area with ventilation. They observed that the temperature rise was highly depended on coal surface area than coal reactivity. However, the effect of moisture and weathering of coal were not accounted in their model. Later, Yuan and Smith [10] used the model to analyze the effect of air velocity and order of reaction on self-heating of coal in underground mines. Their model accurately predicted the induction time for self-heating although a higher oxygen concentration and lower temperature were reported. Further, the order of reaction had a major effect in predicting the induction time. The effect of moisture on self-heating of cellulose materials stored in large layers was reported by Mehaffey et al. [11]. The exothermic heat released during moisture condensation resulted in spontaneous ignition near the middle layer. Arisoy and Akgun [12] analyzed the effect of pile height on spontaneous ignition of coal with different moisture content and reactivity. It was observed that in high moisture content coal, the temperature increases rapidly until the evaporation rate dominated and then the temperature remained almost constant till the coal becomes locally dry. After this, the temperature again increased rapidly with time. The results also revealed a critical storage height to prevent spontaneous ignition that was dependent on the safe storage time of the coal. Green et al. [13] studied the effect of initial temperature and compacting process (pile porosity) on the formation of hotspots in large stockpiles. They found that uncompacted pile (low porosity) resulted in an enhancement of oxygen transport by diffusion and was the major cause for the emergence of hotspot. Moghtaderi et al. [14] showed that external wind flow altered the flow dynamics within the pile, which enhanced the oxygen transport and affected spontaneous heating. Taraba et al. [15], from his simulations, reported that self-ignition process was always dominant on the windward side of the pile. It was also noted that, at low velocities, the hot spot moved to the surface of the pile as a result of oxygen starvation and accumulation of heat of oxidation near the top surface. However, at higher velocities, the hot spot moved downwards due to buoyancy assisted heat dissipation. Fierro et al. [16] outlined several methods to control the spontaneous ignition of large coal piles and finally concluded that covering the pile with fly-ash slurry was the best method to prevent spontaneous ignition. Later, more advanced methods to increase the incubation period for prevention of spontaneous heating was reported by Tripathi [17]. Zhang et al. [18] used a 2-D numerical model to study the effect of various parameters such as pile height, particle size, reactivity and wind velocity. They identified that the presence of localized hot spots can significantly enhance the spontaneous heating. Joshi et al. [19] investigated the effect of weathering on spontaneous combustion of coal through their experiments. They observed that weathering changed the reactivity (pre-exponential factor and activation energy) of coal. Wang et al. [20] conducted a series of experiments on lab and industrial scales using low-rank coal-piles by varying the ambient temperature and pile height. They observed that piles with large volume had greater possibility of inducing self-ignition when coal was stored at temperatures close to the critical self-ignition temperature. However, the induction period for reaching self-ignition temperature is longer as compared to smaller volume piles. Fernandez and Garcia [21] experimentally determined the minimum ignition temperature of coal and other solid fuels such as wood and biomass. They observed that the ignition temperature varied depending on particle size and compaction. Krishnaswamy et al. [22] formulated a mathematical model and performed a parametric study on large open piles, where migration of moisture was negligible. A general correlation was obtained for estimating the time taken for spontaneous ignition in pile. Bhat and Agarwal [23] extended the earlier model to include the condensation and evaporation of moisture from coal particles. They also conducted parametric studies by varying the ambient temperature, humidity, reactivity and particle size. It was observed that partial wetting of coal reduced the possibility of spontaneous ignition in the moist region; however, it enhanced the self-ignition in the dry region of coal particle due to the release of heat of condensation. Further, it was noted that low rank coals have a greater tendency to self-ignite. Hooman and Maas [24] theoretically studied the self-heating phenomena of moist coal stockpile subjected to natural convection. An expression for temperature rise was obtained from scaling analysis. The theoretical model predicted the experimental and numerical data available in the literature. Arisoy et al. [25] showed that moisture moderation prevented ignition in coal above a critical moisture content and below that value, the temperature rise due to reactivity was dominant than the heat loss due to vaporization. They also accurately predicted the evaporation rate of moisture during different stages of self-heating. More recently, Yuan et al. [26] developed a computational model to investigate the susceptibility of self-heating in piles with different coal origins. Their model accurately predicted the self-ignition temperature for all experimental configurations (hot-plate and oven-basket experiments) of different scales. However, their model did not include absorption or desorption of moisture from coal.

It is clear that several numerical models have evolved over decades to study the self-heating phenomena in coal piles with or without moisture content. However, the combined effect of packing dry and moist coals over each other has not been analyzed in detail yet. The present work focuses on a parametric study on ignition behavior when moist and dry coal layers are in different configurations in large-scale stockpiles. Following the simple model reported by Schmal et al. [4], since self-heating is a low temperature oxidation process, the model does not solve for combustion reactions for CO oxidation and water gas shift.

2. Numerical Model

The formulation reported in the one-dimensional numerical model of Schmal et al. [4] is used in the present study. The model solves transient governing equations for energy, oxygen and water vapor in gas phase and in coal. The low temperature oxidation of coal is modeled using a single-step Arrhenius type reaction based on oxygen concentration. It is assumed that the air surrounding the coal particles, in the porous region, and that in the ambient, is assumed to be saturated with moisture, except in the dry layers [4]. Further, air flowing from top to bottom (in this one-dimensional case or in any direction from ambient to the coal pile in a generic case) transports moisture evaporating from the top layer to the bottom layer. The convective air flow rate is the dominant transport mechanism for water vapor than diffusion. Hence diffusion is neglected in the transport equation. Second order central difference scheme is used for the spatial discretization and first order forward difference scheme is used for time discretization.

The governing equations (presented in "Appendix") are solved using a program written in FORTRAN language. The numerical model is quantitatively validated with the results reported in Schmal et al. [4] and Arisoy and Akgun [6], and qualitatively validated against the experimental data of KEMA [27]. Further, validation against smaller scale experimental results, carried out in a wire mesh of 100 cm × 100 cm have also been carried out. Figure 1 presents the profiles of pile temperature, oxygen concentration in the gas phase and oxygen adsorbed in dry coal at three different time instances. The results obtained using the present code matches the numerical data with good accuracy.

Figure 2 presents a parametric study showing the influence of superficial gas velocity, porosity and reactivity in a dry coal pile. The values of the parameters used (changed) in each case is shown in the respective figures. All other parameters and property values are kept the same. The present code closely predicts the

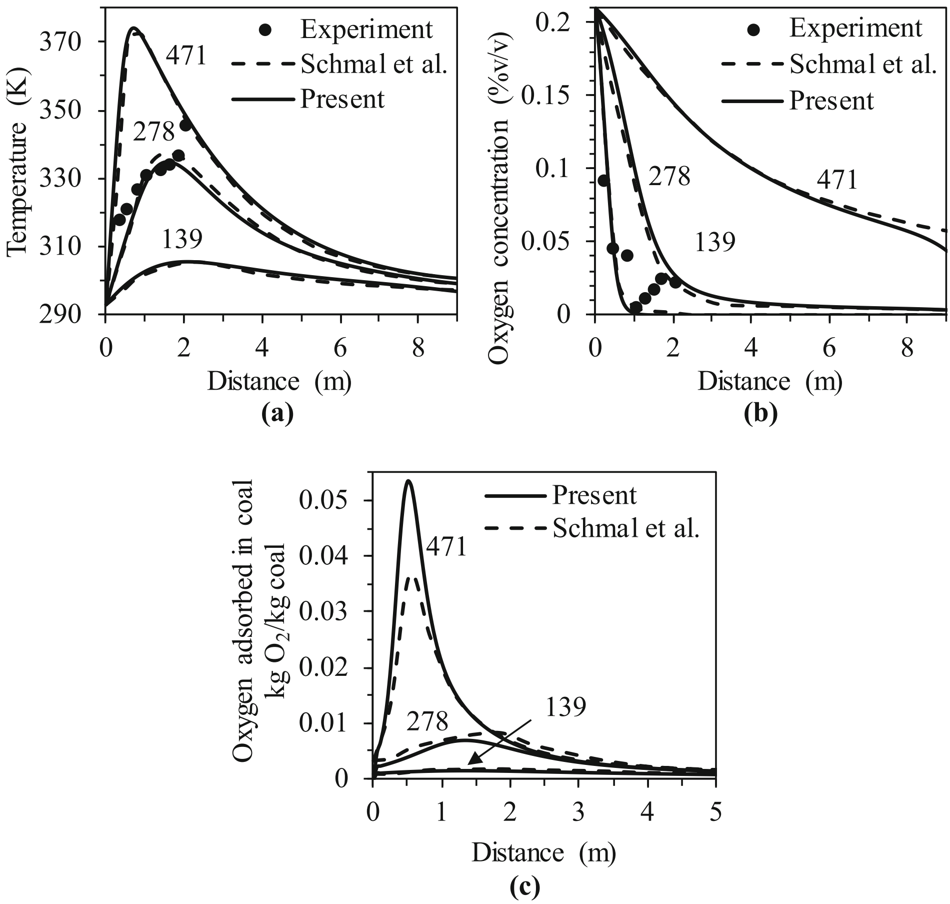

Figure 1. Comparison of predicted profiles of (solid lines) a temperature b oxygen concentration and c oxygen adsorption in a dry coal pile after 139, 278 and 471 days, compared against the numerical model of Schmal et al. [4] and measurements by KEMA report [27].

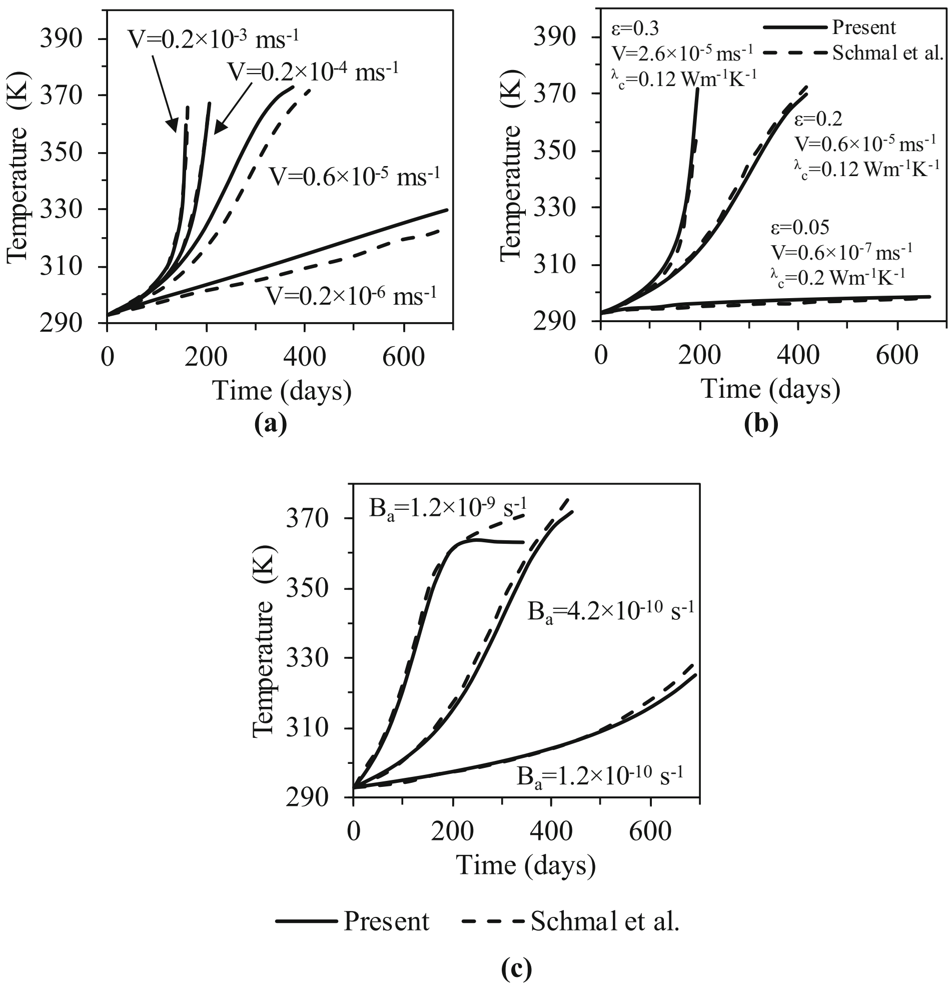

Figure 2. Influence of a superficial gas velocity b pile porosity and c coal reactivity on the maximum temperature in the dry coal pile.

numerical data of Schmal et al. [4] at low gas velocities (Fig. 2a). At higher velocities, the numerical trend is captured quite accurately. However, as the time progress a small temperature difference is observed between the two codes. The present code also accurately predicts the peak temperature reached in piles with different porosity and different coal reactivity (Figs. 2b, c).

The temperature profiles in the moist coal pile is shown in Fig. 3 at different time instances. It should be noted that the moisture content in this coal is only 8% (Schmal et al. [4]). The temperature profile near the top surface and the peak temperature in the pile are predicted well by the present code. But it underpredicts the temperature profile away from the top surface. The code also captures the

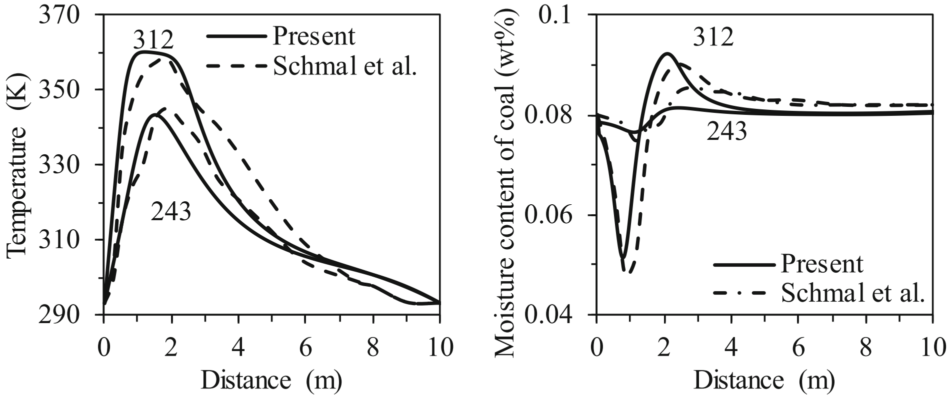

Figure 3. Comparison of temperature (left) and moisture content of coal pile (right) in a moist coal pile after 243 and 312 days, with the present numerical model.

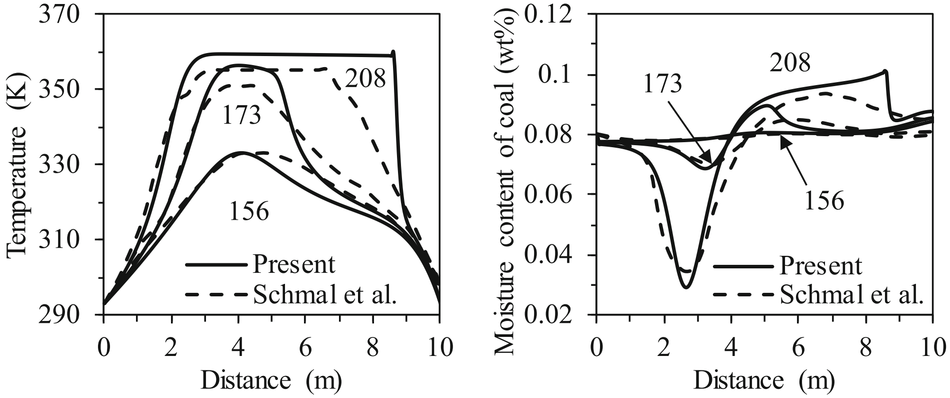

Figure 4. Comparison of predicted temperature (left) and moisture content of coal pile (right) at V = 3 × 10^{-5} m/s in a moist coal pile after 156, 173 and 208 days.

variation in moisture content of coal very closely besides predicting the location where the coal runs locally dry.

Figure 4 presents a comparison of temperature profiles in the moist coal at high gas velocity. The present code overpredicts the peak temperature by a small amount (~ 5°C). The constant temperature region extends for meters into the pile as predicted by the present code. The moisture content profiles reveal that the code is able to predict the exact location where coal runs locally dry.

The present code is compared with the model formulated by Arisoy and Akgun [6] for predicting spontaneous combustion in moist coal. All the model parameters are kept the same as reported in Schmal et al. [4], except for the moisture content

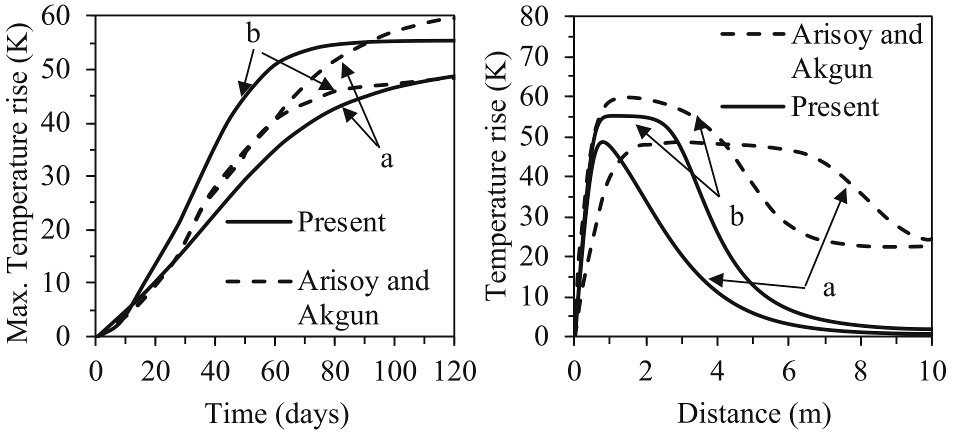

Figure 5. Predicted maximum temperature rise (left) and temperature profiles in moist coal after 120 days (right) for gas velocities of a: 0.5 m/s and b: 1.0 m/s, compared with Arisoy and Akgun [6].

in the coal, which is taken as 10%. However, the model reported by Arisoy and Akgun [6] differs from the present model in the following aspects.

1. The size of coal particle is considered by Arisoy and Akgun [6]. The oxidation rate is dependent on the size of the coal particles, which is defined by an effectiveness factor.
2. The rate of evaporation in their model depends on the particle size, energy of water-coal bonding, which is the additional energy required to remove moisture from coal surface, the moisture content in gas and solid phases, and temperature of coal particles [6].

Figure 5 shows the comparison of maximum temperature rise profiles in moist coal at two different gas velocities. The present code predicts the trends quite accurately for both the cases. However, the present code over-predicts the temperature for a gas velocity 0.5×10^{-5} m/s while it under-predicts for 1×10^{-5} m/s.

The maximum temperature rise in the pile increases with an increase in the gas velocity as compared to the results of Arisoy and Akgun [6]. They predict a decrease in pile temperature with air velocity. This is due to the combined effect of reduction in the oxidation rate with decreasing particle diameter and the evaporation of inherent water in coal which in turn reduces the pile temperature. These effects are not considered in the present model, which causes discrepancy in the result obtained with the present model. Further, weathering of coal is not considered in the simulations which also leads to higher temperatures predicted by the model. It should be noted here that the numerical results of Arisoy and Akgun [6] have not been compared with experimental data.

To have additional validation of the predictions from the present model, experimental case reported in Wang et al. [20] has been compared against the numerical predictions. The experiment reported in Wang et al. [20] focuses on determining the Critical Self Ignition Temperature (CSIT) of low rank coals. Coal particles were packed in a wire mesh basket of different sizes and kept in a constant temperature chamber where ambient air temperature was controlled to be a constant. Temperature probes (thermocouples) were used to detect internal temperatures at different positions including the center of the coal pile. The dimensions of the wire-mesh basket and thermocouple positions are shown in Fig. 6. The properties of coal used in the simulations is given in Table 1.

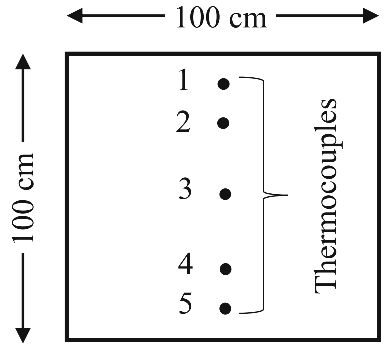

Figure 6. Schematic of the wire mesh basket with thermocouples (Label: 1–10 cm, 2–20 cm, 3–50 cm, 4–80 cm, 5–90 cm).

Table 1
Properties of Coal Used for Simulation of the Case from Wang et al. [20]

Property (units)	Symbol	Value	References
Density of coal (kg/m^3)	ρ_c	1300	Wang et al.
Density of air (kg/m^3)	ρ_a	1.16	Wang et al.
Specific heat of coal (J/kg-K)	C_{pc}	1990	Wang et al.
Specific heat of air (J/kg-K)	C_{pa}	1000	Wang et al.
Diffusion coefficient of O_2 (m^2/s)	D_a	2×10^{-5}	Schmal et al.
Porosity of pile	ε	0.46	Wang et al.
Activation energy (J/kmol)	E_a	1.39×10^{8}	Wang et al.
Frequency factor (1/s)	B_a	1.2×10^{-11}	Schmal et al.
Superficial air velocity (m/s)	V	0.5×10^{-7}	Schmal et al.
Thermal conductivity of pile (W/m–K)	λ_c	0.12	Schmal et al.
Heat of reaction (J/kmol-O_2)	ΔH	3×10^{8}	Schmal et al.
Heat of vaporization (J/kmol-H_2O)	ΔH_w	4.2×10^{7}	Schmal et al.
Moisture content in coal (%wt)	c_4	27.2%	Wang et al.

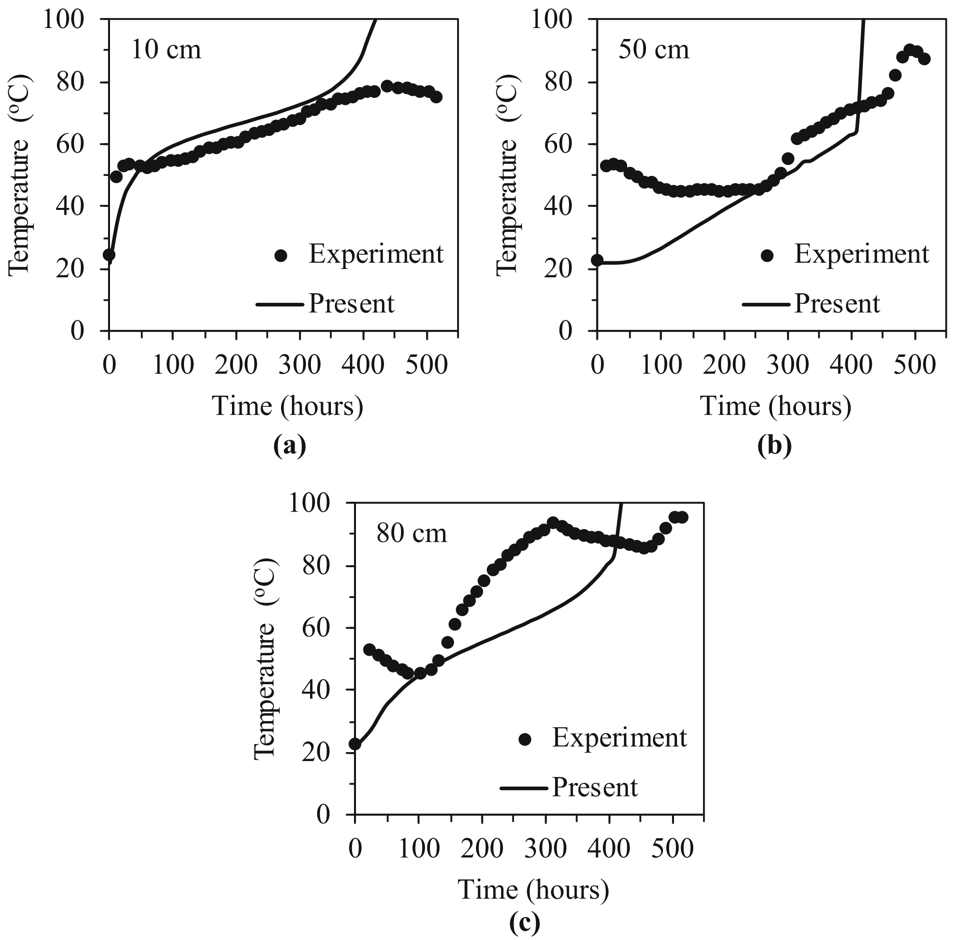

Figure 7. Temperature profiles at different positions in coal sample packed within a wire mesh of 100 cm × 100 cm at an ambient temperature of 75°C, at locations of a 10 cm b 50 cm and c 80 cm; solid line shows present numerical predictions and symbols shows experimental results of Wang et al. [20].

The ambient temperature of 75°C has been considered. Figure 7 presents the comparison of experimental temperature profiles with the present model at three different depths measured from the top surface. The model predicts the experimental data with good accuracy at 10 cm from the top surface. However, at other locations (50 cm and 80 cm) there are notable deviations from the experimental data. At higher depths, natural convection causes an increase in the superficial gas velocity due to high temperature in the pile [20]. Further, the particle size of coal also influences the self-heating temperature which is not considered in the present model. A constant superficial gas velocity, assumed in the present model that is applicable for large piles, and the effect of particle size forms the possible reason for the discrepancy between the experimental and model results. From this exercise, it is quite clear that the present numerical model is able to capture the trends for self-heating in several scenarios and can be used for first-hand predictions of the self-ignitions in several cases.

3. Computational Domain

The coal pile of 30 m height is considered in this study. Figure 8 shows the schematic of layered dry and moist coals in the pile. The distance X is measured from the bottom of the pile. A uniform grid with spatial resolution of 0.05 m is used to spatially discretize the 30 m high coal pile. A time step of 50 s is used for time marching. These values have been arrived at by working out a suitable combination of grid size and time step, where the solution smoothly converges rather than producing oscillations. Table 2 reports the property values of different parameters used in the model, as taken from Schmal [29].

4. Boundary Conditions

Temperature Both isothermal and adiabatic conditions are imposed depending on the physical conditions that prevail in the pile according to the parametric values considered in this study. For isothermal case, the temperature at the top and bottom surface of the pile is assumed to be equal to the ambient temperature (293 K). Further, the initial temperature of coal is also assumed to be equal to the ambient temperature for all the cases, which is a very restrictive assumption. Adiabatic condition is imposed on the bottom surface for certain cases.

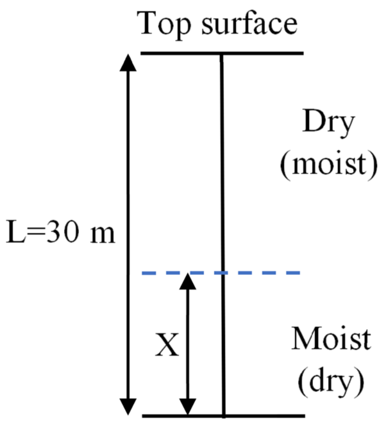

Figure 8. Schematic of domain with dry and moist coal layers; systematic parametric variations are considered, where moist (or dry) coal will be present for a given depth from top surface and remaining will be dry (or moist) coal.

Table 2
Properties of Dry and Moist Coal [29] Used (Standard Conditions)

Property (units)	Symbol	Dry coal	Moist coal
Density of coal (kg/m^3)	ρ_c	1500	1500
Density of air (kg/m^3)	ρ_a	1.1	1.1
Specific heat of coal (J/kg-K)	C_{pc}	1000	1000
Specific heat of air (J/kg-K)	C_{pa}	1000	1000
Diffusion coefficient of O_2 (m^2/s)	D_a	2×10^{-5}	2×10^{-5}
Porosity of pile	E	0.2	0.2
Activation energy (J/kmol)	E_a	7×10^7	7.5×10^7
Frequency factor (1/s)	B_a	4.2×10^{-10}	2.1×10^{-10}
Universal gas constant (J/kmol-K)	R	8314	8314
Superficial air velocity (m/s)	V	0.6×10^{-5}	0.6×10^{-5}
Thermal conductivity of pile (W/m–K)	λ_c	0.12	0.12
Order of reaction of O_2 with coal	n	1	0.7
Heat of reaction (J/kmol-O_2)	ΔH	3×10^8	3.7×10^8
Heat of vaporization (J/kmol-H_2O)	ΔH_w	–	4.2×10^7
Moisture content in coal (%wt)	c_4	–	12%
Weathering function	$f(c_2)$	1	1

Oxygen concentration The initial oxygen concentration in air and the oxygen content near the top surface is taken as a constant equal to 0.21. The initial concentration of oxygen in the coal is taken as zero.

Moisture content Bituminous coals normally contain 5%–15% water on weight basis, depending on the type of coal and the season [13]. Keeping this in mind the initial moisture content is taken as 12% in moist coal layer.

Table 3 reports the cases considering dry coal and moist coal layers. Case A is that of dry coal being present for the entire length. In this study, constant initial moisture content of 12% has been considered. Cases B, C and D configure moist coal layer of different height in the bottom of the dry coal layer, and cases E, F, G and H considers initially dry coal layer at the bottom of a moist coal layer at the top. These conditions replicate the moisture absorption from the top (cases B, C and D) of the pile or that from the bottom of the pile (cases E, F, G and H).

5. Results and Discussion

The influence of various parameters on self-heating of pile is studied by systematically varying the pile porosity, superficial gas velocity and coal reactivity. All the simulations are executed considering an ambient temperature of 293 K. The initial temperature of coal is assumed to be equal to the ambient temperature following literature [4]. In all these cases, the storage time of the pile is taken as 360 days (around 1 year). Due to slow nature of the oxidation process it is assumed that the temperature of coal is always equal to the temperature of air inside the pile. It should be noted that the seasonal and daily variation in ambient temperature is neglected and a constant value is kept throughout the simulations. Further, the

Table 3
List of Cases with Layers of Moist and Dry Coal Layers

Case	X	Moisture content in the bottom, X (%)	Moisture content in the top, (L–X) (%)
A	L	0	0
B	0.25L	12	0
C	0.5L	12	0
D	0.75L	12	0
E	0.1L	0	12
F	0.25L	0	12
G	0.5L	0	12
H	0.75L	0	12

weathering of coal due to oxidation is not considered in these simulations. Furthermore, the self-ignition of the pile is expected to occur when the temperature has reached 100°C [4, 8]. That is for a worst case scenario, the coal pile is assumed to be self ignited when the maximum temperature in the pile reaches a value of 373 K (100°C).

The temperature and oxygen concentration profiles are plotted from top to bottom of the coal pile. They are extracted either at the end of 360 days for the cases those have not self-ignited or at the time instant when the self-heating temperature of 373 K is attained inside the coal pile.

5.1. Standard Conditions

In these simulations, all the parameters are kept at standard conditions shown in Table 2 ($V = 0.6 \times 10^{-5}$ m/s, $\varepsilon = 0.2$ and $B_a = 4.2 \times 10^{-10}\ s^{-1}$). The temperature at the top and bottom boundary is assumed to be equal to the ambient temperature of 293 K. Figure 9a presents the variation of maximum temperature in the pile plotted as a function of number of days for case A. Monotonic increase in temperature with time is seen. Maximum temperature in the pile increases to 360 K at the end of 360 days. The same trends are observed for cases B, C and D, and hence these are not reported in Fig. 9a. Considering the trend in Fig. 9a, it is likely that the cases would self heat to ignition temperature, however, at a time interval greater than 1 year. Figure 9b shows the temperature variation within the pile for cases A, B, C and D. It is clear that the peak temperature is attained within 2 m from the top surface in all cases. The pile temperature decreases rapidly after the peak and a sharp decrease occurs up to a distance of around 5 m from the top surface in the dry coal region. After this, the reduction in temperature is quite gradual. Other cases with larger quantities of moist coal at the bottom (cases B, C and D) present similar trends, however, with a small variations in temperature in the moist coal layer. It is observed from the temperature profiles that the moist coal layer present below the dry coal layer has no effect on the temperature rise in the dry region of the pile.

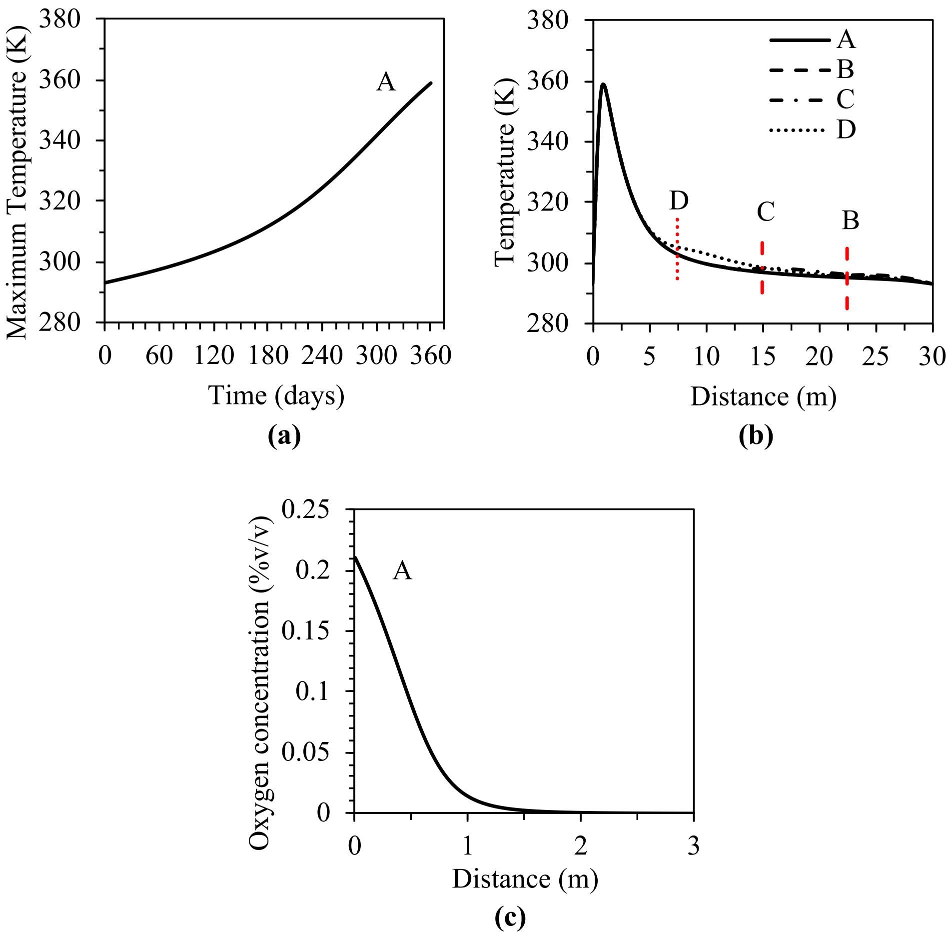

Figure 9. a Maximum temperature versus time in days and profiles of b temperature and c oxygen concentration from top to bottom of the pile.

Figure 9c presents the oxygen concentration profile for case A from top to bottom of the pile. The oxygen concentration decreases steeply and aymptotically reaches the zero value. This high rate of consumption of oxygen within the dry coal layer is the reason for rapid increase in temperature in this region. Due to low porosity and low gas velocity (as per the standard conditions, Table 2) the moist coal region at the bottom is starved of oxygen. Hence, the temperature in the moist coal region is well below the ignition temperature. The influence of changing the porosity will be discussed later.

Figure 10a presents the maximum temperature in the pile as a function of time in days for case A (with complete dry coal layer) and case E (with moist coal layer on top and dry coal occuping 10% of the height at the bottom). It is clear

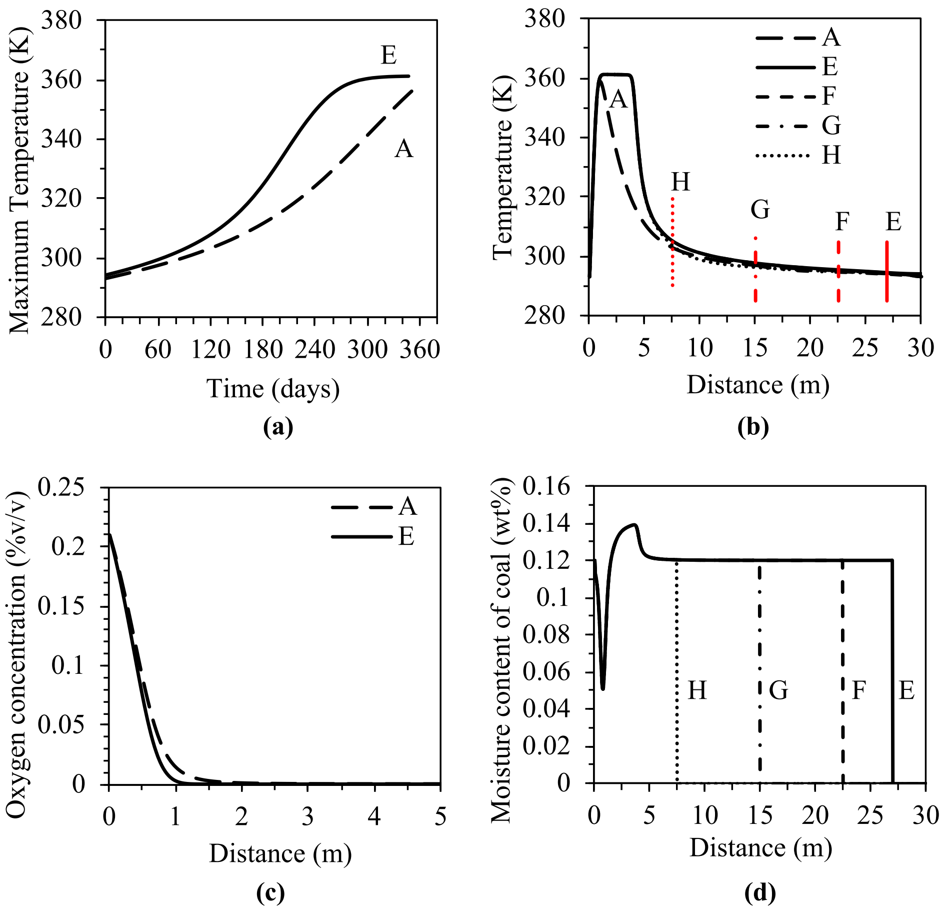

Figure 10. a Variation of maximum temperature versus time, profiles (from top to bottom of the pile) of b temperature, c oxygen concentration and d moisture content in coal at ambient temperature of 293 K.

that for case E the maximum temperarature increases and reaches a value of 360 K (quite close to ignition temperature of 373 K) and then it remains constant at 360 K for further days. Cases F, G and H also follow the trend of case E. It is reported in Schmal et al. [4] that ignition can occur at any time after the attainment of 360 K, this process is quite rapid and the numerical simulation becomes unstable. Thus, they used to denote the ignition using dashed line [4]. Therefore, it can be concluded that cases A, E, F, G and H are expected to self-ignite since all cases have reached the constant maximum temperature of 360 K, even though they have not produced any spikes. It is observed that irrespective of the amount of moist coal present at the top of the pile, the time taken to reach the maximum temperature of 360 K is 307 days. Figure 10b presents the temperature profiles in the pile at the end of 360 days. After an initial rise in temperature, an almost constant temperature plateau of around 360 K is maintained in the moist coal region. The peak temperature remains constant up to a certain depth into the coal layer (Fig. 10b) and then decreases sharply at a distance of 5 m to 6 m from the top surface of the pile. Figure 10c presents the oxygen concentration profiles for cases A and E. Faster consumption of oxygen is seen for case E. This happens within 1 m from the top surface. Figure 10d shows the variation of coal moisture content in the pile for cases E to H. The moisture content in coal is 0.05 percent at around 1.5 m from the top surface for all the cases. High temperature due to oxidation of coal near the top surface helps in the evaporation process of the moisture in the coal pile. Some of the water vapor diffuses downstream. In all cases, the moisture content locally increases to a value of around 14%, at a location of around 4 m from the top of the pile. The evaporation or condensation of moisture and its variation within the pile are determined by the pile temperature as given by Eqs. (4) and (5) in "Appendix". Based on the pile temperature, moisture in the coal pile evaporates and its variation within the pile becomes dependent on the gradient of temperature, the value of which is dependent on the ambient (or the initial) temperature. The rate of evaporation of the moisture, the local minima and maxima of moisture concentration and their locations are clearly dependent on the variation of pile temperature. It is also observed that the evaporation and condensation of moisture occurs completely in the moist coal region irrespective of differences in the level of moist coal layers in the pile.

5.2. *Influence of Pile Porosity*

The porosity of a coal pile is a dimensionless quantity defined as the ratio of the volume of the voids (pores) to the total volume of the coal stockpile. The value of porosity can vary between 0.05 and 0.4, [4, 8]. The general guidance for storing large stockpiles of coal is to pack it to a density of 1100 kg/m^3 to 1200 kg/m^3 corresponding to porosity in the range of 0.12 to 0.13 [28]. The experiments in Schmal et al. [4] also show that porosity plays a significant role in the self-heating of large stockpiles of coal. The current study analyses the influence of the layering of moist-dry coal in combination with different porosity values on self-heating hazard.

Initially, simulations are carried out with a low porosity value of 0.1. For this, the superficial gas velocity and thermal conductivity are taken as 2.6×10^{-7} m/s and 0.2 W/m–K, respectively. Similar values are reported in Schmal et al. [4] for a porosity value of 0.05. Values of all other parameters are kept the same. Figure 11 shows the temperature profiles in pile for cases A to H, at the 360th day. It is clear that the pile temperature, even though increases beyond its initial value, is well below the self-heating temperature for all the cases, irrespective of the order of layering the coal. This is because of the limited availability of oxygen due to low porosity of the pile. Small changes in the temperature profile are observed between the cases in the moist coal layer. This may be due to the accumulation of heat of condensation in the moist coal layers as a result of low porosity of the pile. The cases E to H (Fig. 11b), with moist coal layer on top, attains a higher

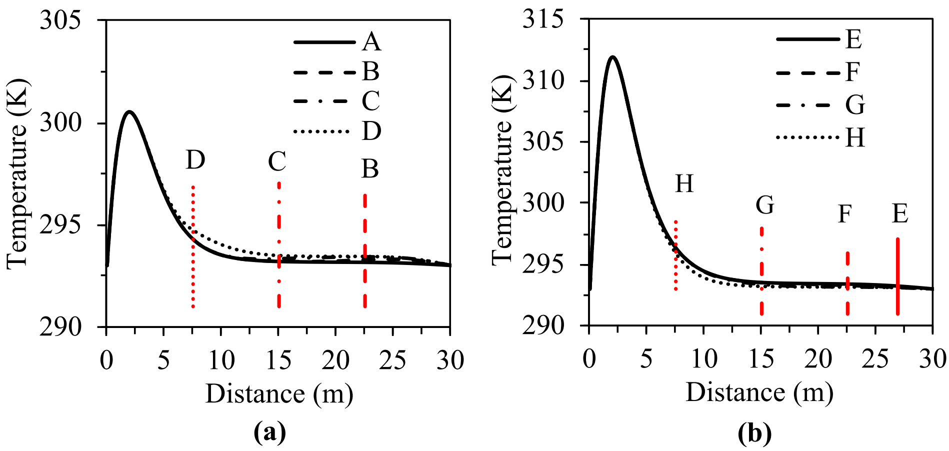

Figure 11. Profiles of temperature for a cases A, B, C, D and b cases E, F, G, H, with porosity, ε = 0.1, superficial air velocity, V = 2.6 × 10^{-7} m/s and thermal conductivity 0.2 W/m-K, at ambient temperature of 293 K.

maximum temperature due to the moisture content in the top layer, indicating that coal pile should be packed with lower porosity when moist coal layer is available at the top.

At a higher porosity of 0.3, the corresponding superficial velocity value has been increased to 2.6 × 10^{-5} m/s (around four times the standard value), following Schmal et al. [4]. Such conditions pose favorable scenario for self-ignition. All other parameters are kept the same as in the previous cases. Figure 12a presents the oxygen concentration profiles in the pile for case A. It is observed that the oxygen is consumed within 3 m from the top surface. Similar trends are observed for cases B, C and D. It is also noted that the oxygen transport is enhanced as compared to pile subjected to standard conditions (shown in Fig. 9c). This is due to increased pile porosity assisted by a higher superficial air velocity. For all these cases ignition takes place after 197 days at a location of 1.8 m from the top surface. Figure 12b shows the oxygen concentration profiles in the pile for cases E to H. The oxygen concentration decreases rapidly to zero at around 2.5 m from the top layer. The high porosity has clearly influenced the oxygen distribution to the coal present at the top of the pile.

Figure 13a presents the variation of maximum temperature with time in days for case A. Similar trends are observed for cases B, C and D. The temperature increases non-linearly to 380 K at the end of 200 days, indicating self-ignition of the pile. For cases E to H, temperature increases in a non-uniform manner and reaches a value of around 360 K. Then, it remains the same for a few days. Self-ignition in these cases are observed by a spike in temperature profile. This spike is observed after 240 days for all the cases. It should be kept in mind that, for these cases, the pile can self-heat to ignition temperature at any location where the constant temperature zone (∼ 360 K) prevails and hence the pile temperature must be

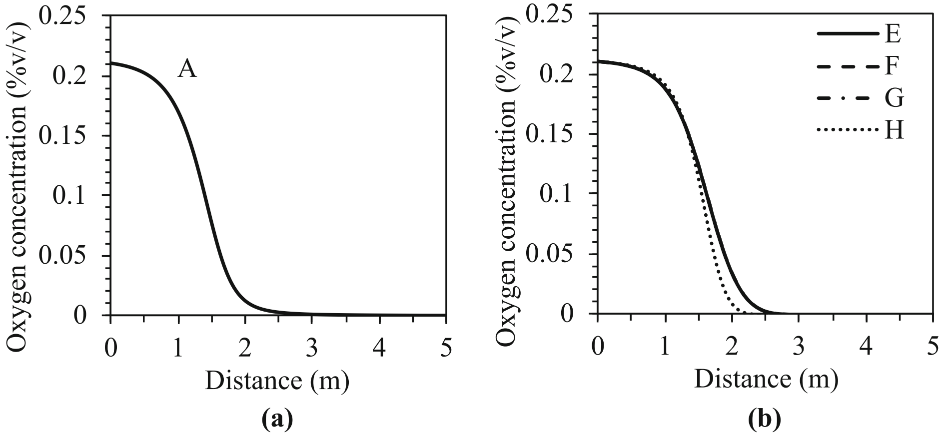

Figure 12. Profiles of oxygen concentration for a case A and b cases E, F, G, H with porosity, ε = 0.3 and superficial air velocity, V = 2.6 × 10^{-5} m/s at ambient temperature of 293 K.

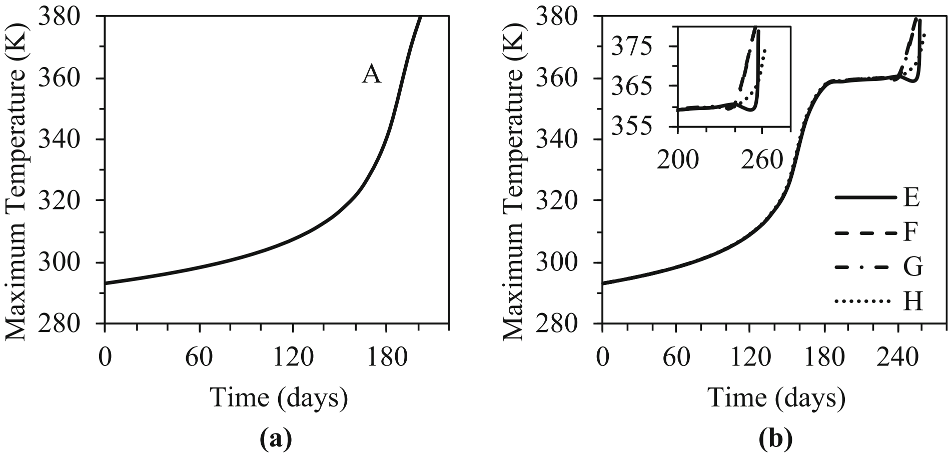

Figure 13. Variation of maximum temperature with time in days for a case A and b cases E, F, G and H with porosity, ε = 0.3 and superficial air velocity, V = 2.6 × 10^{-5} m/s at ambient temperature of 293 K.

kept below the constant temperature value for safety. Two factors dictate the non-linear variation in temperature in these cases. First factor is the oxidation rate that depends directly upon the pile temperature (which is initially at the ambient temperature) and inversely depends upon the ambient temperature (as per Eq. (1) in "Appendix"). The second factor is the rate of vaporization that depends upon the temperature gradient within the pile. Oxidation is an exothermic reaction and phase change is an endothermic process. These two factors, in combination, determines the variation in the temperature profiles.

The vaporization and condensation dynamics are illustrated by plotting the maximum and minimum moisture content in the coal pile and their locations as a function of time. Figures 14a, b present the variations in maximum and minimum moisture content of coal with time in days for cases E to H. It is observed that the moisture condensation increases gradually with time and the increase becomes notable after around 160 days for all the cases, especially for case H. Around the same time, a constant temperature region develops in the pile as shown in Fig. 13b. Figure 14c reports the locations of maximum moisture content in the pile for case E. It is visible that the maximum moisture content is present at the interface of the moist coal-dry coal layers (at 22.5 m) for about 140 days. With further increase in time, the location of maximum moisture moves up then gradually moves down into the pile. All other cases (F, G and H) show similar trends. Figure 14d shows the location of minimum moisture content in the pile for case E. The location of minimum moisture content is present near the top surface for around 150 days. The pile temperature controls the phase change process and both pile temperature and ambient temperature control the oxidation rate. As a result of these, moisture content in the coal varies and it contributes back to the resultant temperature profiles. Other cases (F, G and H) show similar trends.

5.3. Influence of Superficial Air Velocity

The air velocity is chosen as 0.2×10^{-3} m/s (around two orders of magnitude higher than the standard conditions). Such velocities are observed in coal piles stored in highly windy regions. As seen earlier, the effect of superficial air velocity is connected to the porosity of the pile. The pile must have large porosity to allow for higher air velocity to have an influence on the oxygen transport and heat convection processes. Therefore, the porosity of the pile is chosen as 0.3 instead of 0.2. The large superficial velocity causes rapid transport of oxygen and heat into the pile. The temperature at the bottom of the pile increases quickly and an abnormal decrease occurs towards the bottom of the pile with a sudden drop in temperature to the ambient value (due to boundary condition). Since the moisture content in coal is determined by the pile temperature (Eqs. (4) and (5) in "Appendix"), imposing an isothermal condition causes excessive condensation of moisture at the bottom of the pile, which does not occur physically. This causes numerical instability while calculating the moisture content in coal. Therefore, these simulations are executed with adiabatic boundary condition at the bottom of the pile.

Figure 15 presents a comparison of the temperature profiles in the pile simulated with adiabatic and isothermal conditions at the bottom boundary. It is much clear that the temperature profiles are identical except that at the boundary, for both boundary conditions. Further, it should be noted that altering the boundary conditions (temperature only) does not have any effect on the location or time or the value of peak temperature reached in the pile.

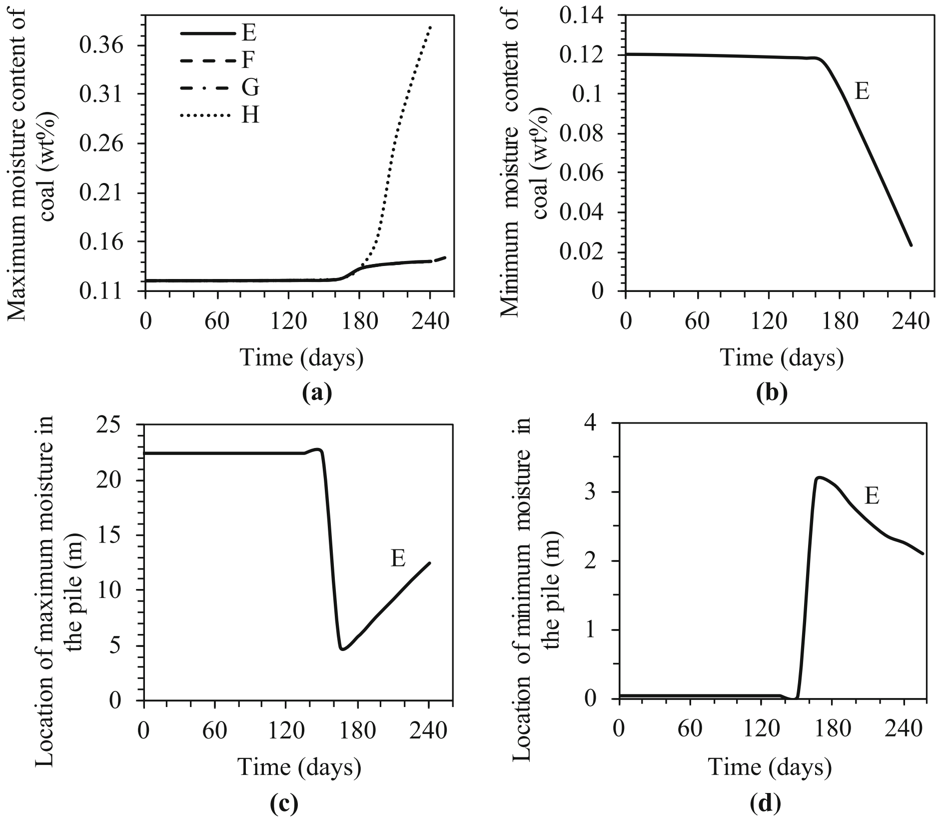

Figure 14. Variation of a maximum moisture content b minimum moisture content c location of maximum moisture and d location of minimum moisture with time in days for pile with porosity, ε = 0.3 and superficial air velocity, V = 2.6 × 10^{-5} m/s at ambient temperature of 293 K.

Figure 16 presents the temperature profiles in a dry coal pile for cases A to D. For case A, the temperature rises steeply, reaches a maximum and then decreases gradually towards the bottom of the pile. The temperature rises to a peak value in the dry coal region for all the cases. With higher porosity ($\varepsilon = 0.3$), and air velocity ($V = 0.2 \times 10^{-3}$ m/s) self-heating occurs within 7 m from the top surface of the pile for all the cases. A second peak in the temperature profile is observed in the moist coal region for cases B, C and D. This is due to high availability of oxygen in the moist coal layers. The value of the second peak is lower than the first because of the presence of moisture in coal at that location. However, for case D, a constant temperature region is observed indicating the evaporation and condensation of moisture in this region. For all the cases considered, the pile ignites after 160 days at a location of 5.5 m from the top surface.

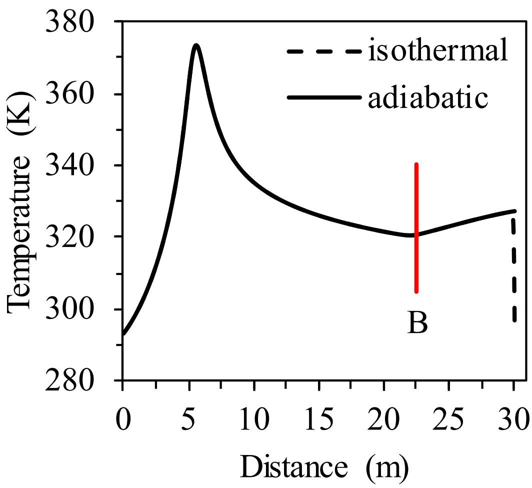

Figure 15. Profiles of temperature for isothermal condition and adiabatic condition prescribed at the bottom of the pile for case B ($V = 0.2 \times 10^{-3}$ m/s, $\varepsilon = 0.3$).

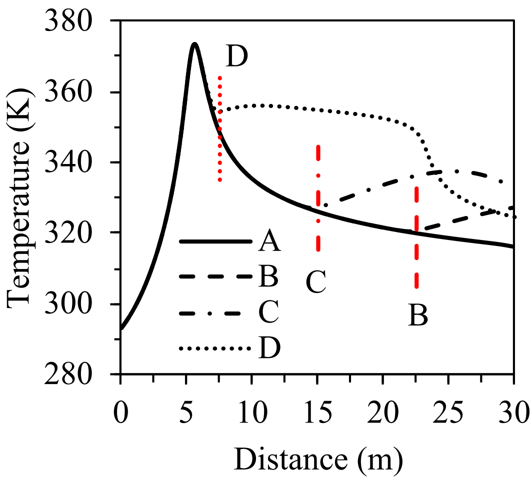

Figure 16. Temperature profiles for cases A, B, C and D ($V = 0.2 \times 10^{-3}$ m/s, $\varepsilon = 0.3$) at ambient temperature of 293 K.

Figure 17 shows variation of the maximum temperature as a function of time for the pile packed with moist coal on top and dry coal at the bottom (cases E, F, G and H). It is clear that pile temperature increases steeply after around 140 days and self-ignition occurs for all these cases within 160 days. The variation trends observed here are quite different from those observed in Figs. 10a and 13b, where the maximum temperature remained constant at 360 K for a few days and sudden

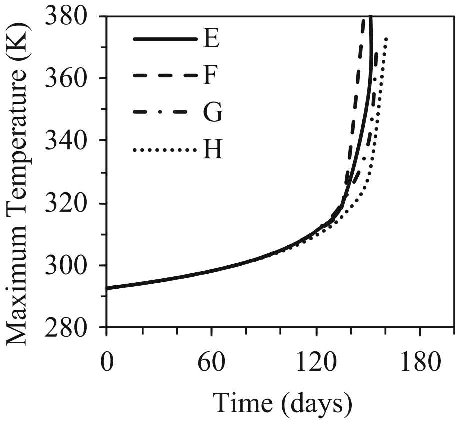

Figure 17. Maximum temperature as a function of time in days for cases E, F, G and H at ambient temperature of 293 K (V = 0.2 × 10^{-3} m/s, ε = 0.3).

Table 4
Time Taken for Ignition and Ignition Location for Cases E to H (V = 0.2 × 10^{-3} m/s and ε = 0.3) at Ambient Temperature of 293 K

Case	X	Time (days) [Location (m)] 293 K
E	0.1L	151 [22]
F	0.25L	151 [22]
G	0.5L	157 [15.3]
H	0.75L	160 [9.65]

self-ignition occurred as indicated by a spike in the maximum temperature variation. Here, the temperature increases in a non-uniform (exponential) manner and reaches the self-ignition temperature of 373 K.

The ignition location and time taken to attain ignition temperature (373 K) is given in Table 4. As discussed earlier, the dependency of the phase change process with ambient temperature form the reason for these variation trends.

5.4. *Influence of Coal Reactivity*

The coal reactivity is studied by varying the value of the frequency factor, B_a, from 4.2×10^{-10} s^{-1} to 1.2×10^{-9} s^{-1}. The values of ε and V are taken as 0.3 and 0.2×10^{-3} m/s, respectively, to evaluate the favorable conditions for the occurrence of self-ignition. The values are chosen such that the pile takes the least amount of time to reach self-ignition temperature. It should be kept in mind that the reactivity of dry coal is only changed and the reactivity of moist coal is taken

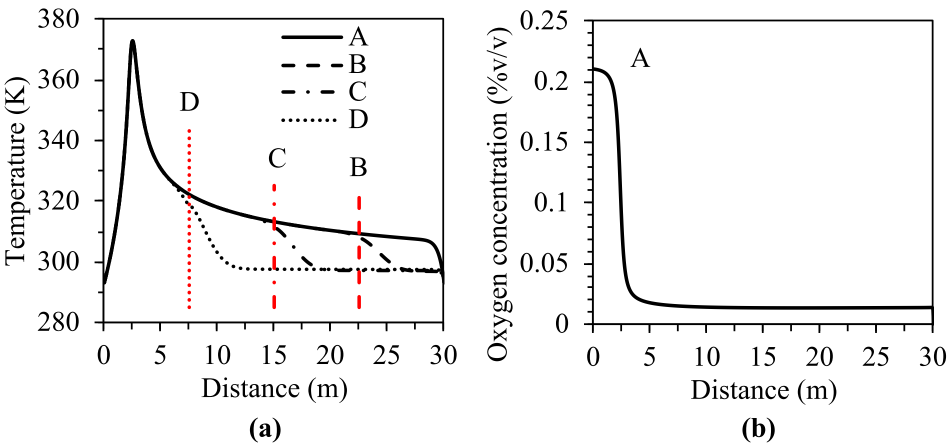

Figure 18. a Temperature and b oxygen concentration profiles at ambient temperature of 293 K ($V = 0.2 \times 10^{-3}$ m/s, $\varepsilon = 0.3$ and $B_a = 1.2 \times 10^{-9}\ s^{-1}$).

as $2.1 \times 10^{-10}\ s^{-1}$ (standard value in moist coal studies). The coal reactivity also depends on activation energy. However, the activation energy is kept constant in the present simulations.

Figure 18a presents the temperature profiles in the pile having dry coal on top and moist coal at the bottom (Cases A to D). It is observed that there is a steep temperature rise near the top layer of the pile due to higher reactivity. The temperature profile drops at the interface, where the moist coal layer is present. This is due to low reactivity of the moist coal. The low reactivity of coal coupled with high porosity of the pile is the reason for almost uniform temperature distribution in the moist coal region at the bottom.

Figure 18b shows the oxygen concentration profiles in the pile when self-ignition occurs. The oxygen near the top layer is consumed rapidly as expected. Further, the oxygen profiles in the moist coal region remains almost constant. This is quite different from the dry coal region, where the temperature continues to increase due to abundant availability of oxygen and high reactivity of coal.

For all the cases considered, the time taken for self-ignition is about 57 days and ignition takes place within 3 m from the top layer. As discussed earlier, the presence of moist coal at the bottom does not affect the location or the time taken to reach the maximum temperature in the pile.

6. Conclusions

A parametric study is carried out to analyze the effects of dry and moist coal layers present in different configurations on self-heating of coal piles, considering different porosity, superficial air velocity and reactivity values. The time period of coal pile storage is fixed as 360 days. The location and time taken for self-ignition in the pile within this period is reported for each case. The results indicate that pile with higher porosity takes lesser time to reach self-ignition temperature. A higher superficial air velocity aids in transporting the heat and reactant to the vicinity of a hot spot. This improves the heat transfer rate in the pile and further reduces the time taken to reach self-ignition temperature. In piles simulated with standard conditions, the temperature rises to 360 K at the end of 360 days in piles with dry coal layer at the top. Self-ignition also occurs for all the cases with moist coal at the top. Increasing the superficial air velocity, reduces the time taken to reach the self-ignition temperature. For highly reactive dry coal, the pile is ignited within 57 days.

Appendix: Mathematical Model

The governing equations for the one-dimensional mathematical model as reported by Schmal et al. [4] are given below.

Equation for low-temperature oxidation of coal

$$\frac{\partial c_2}{\partial t} = B_a c_1^n f(c_2) \exp\left[-\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \tag{1}$$

Equation for mass conservation of oxygen

$$\varepsilon \rho_a \frac{\partial c_1}{\partial t} + \rho_a \frac{\partial (V c_1)}{\partial x} - \varepsilon D_a \rho_a \frac{\partial^2 c_1}{\partial x^2} + (1-\varepsilon)\rho_c \frac{\partial c_2}{\partial t} = 0 \tag{2}$$

Equation for conservation of heat

$$\rho_c c_{pc}(1-\varepsilon)\frac{\partial T}{\partial t} + \rho_a c_{pa}\frac{\partial (VT)}{\partial x} - \lambda_c \frac{\partial^2 T}{\partial x^2} = \frac{\Delta H}{MW_{O_2}}(1-\varepsilon)\rho_c \frac{\partial c_2}{\partial t} + \frac{\Delta H_w}{MW_{H_2O}}(1-\varepsilon)\rho_c \frac{\partial c_4}{\partial t} \tag{3}$$

Equation for evaporation or condensation of water

$$\frac{\partial (V c_3)}{\partial x} = 1.4 \times 10^7 \frac{V_a \exp(-r_v/RT) \times (r_v/RT - 1)}{T^2[1 - 1.15 \times 10^6 \exp(-r_v/RT)]^2} \frac{\partial T}{\partial x} \tag{4}$$

Equation for mass conservation of moisture in coal

$$\frac{\partial (V c_3)}{\partial x} + (1-\varepsilon)\frac{\rho_c}{MW_{H_2O}}\frac{\partial c_4}{\partial t} = 0, \tag{5}$$

where ε is the pile porosity, c_1 is the mole fraction of oxygen in the gas phase, c_2 is the amount of oxygen adsorbed in coal (kg-O_2/kg-coal), V is the superficial air velocity including the water vapor (m/s), V_a is the superficial velocity of the inflowing dry air (m/s), D_a is the diffusion coefficient of oxygen (m^2/s), c_3 is the concentration of water in gas phase ($kmol/m^3$), c_4 is the amount of water adsorbed in coal (kg-H_2O/kg-coal), ρ_c is the density of coal (kg/m^3), ρ_a is the density of air (kg/m^3), c_{pa} is the specific heat of air (J/kg-K), c_{pc} is the specific heat of coal (J/kg-K), λ_c is the thermal conductivity of coal bed (W/m–K), T is the absolute temperature (K), ΔH is the heat of adsorption of oxygen (J/kmol) and ΔH_w is the heat of adsorption of water (J/kmol). Since the moisture content in atmospheric air is much less, V_a is assumed to be equal to V. These governing equations are solved in a coupled manner using finite difference method.

References

1. Sondreal EA, Ellman RC (1974) US Bureau of mines. Report of Investigations, 7887
2. Nordon P (1978) A model for the self-heating reaction of coal and char. Fuel 58:456–464
3. Handa T, Morita M, Sugawa O, Ishii T, Hayashi K (1983) Computer simulation of the spontaneous combustion of coal storage. Fire Sci Technol 3(1):13–23
4. Schmal D, Duyzer JH, van Heuven JW (1985) A model for the spontaneous heating of coal. Fuel 64:963–972
5. Brooks K, Glasser D (1986) A simplified model of spontaneous combustion in coal stockpiles. Fuel 65:1035–1041
6. Arisoy A, Akgun F (1994) Modelling of spontaneous combustion of coal with moisture content included. Fuel 73:281–286
7. Boyapati IE, Oates A (1994) A mathematical model for stockpile management. In: Proceedings of the 6th international working conference on stored-produce protection, vol 2
8. Akgun F, Essenhigh RH (2001) Self-ignition characteristics of coal stockpiles: theoretical prediction from a two-dimensional unsteady-state model. Fuel 80:409–415
9. Yuan L, Smith AC (2008) Numerical study on effects of coal properties on spontaneous heating in longwall gob areas. Fuel 87(15–16):3409–3419
10. Yuan L, Smith AC (2009) CFD modeling of spontaneous heating in a large-scale coal chamber. J Loss Prev Process Ind 22(4):426–433
11. Mehaffey JR, Richardson LR, Batista M (2000) Self-heating and spontaneous ignition of fibre-board insulation panels. Fire Technol 36(4):226–235
12. Arisoy A, Akgun F (2000) Effect of pile height on spontaneous heating of coal stockpiles. Combust Sci Technol 153:157–168
13. Green U, Aizenshtat Z, Metzger L, Cohen H (2012) Field and laboratory simulation study of hot spots in stockpiled bituminous coal. Energy Fuels 26:7230–7235
14. Moghtaderi B, Dlugogorski BZ, Kennedy EM (2000) Effect of windflow on self-heating characteristics of coal stockpiles. Trans IChme 78:445–453
15. Taraba B, Michalec Z, Michalcova V, Blejchar T, Bojko M, Kozubkova M (2014) CFD simulations of the effect of wind on spontaneous heating of coal stockpiles. Fuel 118:107–112
16. Fierro V, Miranda JL, Romero C, Andres JM, Arriaga A, Schmal D, Visser G (1999) Prevention of spontaneous combustion in coal stockpiles experimental results in coal storage yard. Fuel Process Technol 59:23–34
17. Tripathi DD (2008) New approaches for increasing the incubation period of spontaneous combustion of coal in an underground mine panel. Fire Technol 44:185–198

18. Zhang J, Ren T, Liang Y, Wang Z (2016) A review on numerical solutions to self-heating of coal stockpile: mechanism, theoretical basis, and variable study. Fuel 182:80–109
19. Joshi K, Raghavan V, Rangwala AS (2013) Effect of weathering of coal and organic dusts on their spontaneous ignition. Fire Technol 49:843–856
20. Wang Y, Zhang X, Sugai Y, Sasaki K (2017) Determination of critical self-ignition temperature of low-rank coal using a 1 m wire-mesh basket and extrapolation to industrial coal piles. Energy Fuels 31:6700–6710
21. Fernandez-Anez N, Garcia-Torrent J (2019) Influence of particle size and density on the hot surface ignition of solid fuel layers. Fire Technol 55:175–191
22. Krishnaswamy S, Agarwal PK, Gunn RD (1995) Low-temperature oxidation of coal 3. Modelling spontaneous combustion in coal stockpiles. Fuel 75:353–362
23. Bhat S, Agarwal PK (1996) The effect of moisture condensation on the spontaneous combustibility of coal. Fuel 75:1523–1532
24. Hooman K, Maas U (2014) Theoretical analysis of coal stockpile self-heating. Fire Saf J 67:107–112
25. Arisoy A, Beamish B, Yoruk B (2017) Moisture moderation during coal self-heating. Fuel 210:352–358
26. Yuan H, Restuccia F, Richter F, Rein G (2018) A computational model to simulate self-heating ignition across scales, configurations, and coal origins. Fuel 236:1100–1109
27. Kok A (1981) KEMA Report, WSK/2780-55
28. Dungan KW (2003) Storage and handling of solid fuels. In: Cote AE (ed) Fire protection handbook, 1st edn. National Fire Protection Assoc, Quincy
29. Schmal D (1987) A model for the spontaneous heating of stored coal. Ph.D. Thesis. https://repository.tudelft.nl/islandora/object/uuid%3A680f83d3-be29-45d1-9e27-a33644f2d9c3