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A review on numerical solutions to self-heating of coal stockpile: Mechanism, theoretical basis, and variable study

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Abstract

Self-heating or even spontaneous combustion of stockpiled coal, which is likely to outbreak under favourable circumstances during its transport, process, and storage, is a long-standing thermal dynamic hazard. This hazard is harmful in diverse aspects: causing loss of coal resource and caking property, raising safety concerns upon occurrence of open fire, and giving off noxious/greenhouse effect gases. Due to the complexity of involved physical process (e.g. heat and mass transport) and chemical process (e.g. coal oxidation), formulating an analytical solution to the problem with or even without a transient approach would be a daunting task and the problem is thus more often addressed numerically. So far many numerical models to self-heating of coal have been developed and to summarise these erratic findings, this work critically reviewed these numerical solutions since the last four decades. Mechanism of self-heating on coal mass and low temperature coal oxidation especially kinetic modelling of coal oxidation is firstly investigated to clarify the involved physical and chemical processes. On basis of the mechanistic understanding, theoretical derivations and progressive advances on governing equations like energy, mass, and momentum conservation are reviewed and compiled in details. Through parametric studies or sensitivity check these models produced fruitful but slightly inconsistent findings. Therefore to provide industry more unbiased and comprehensive guides, the present work examined the influences of various contributors including wind flow, stockpile dimensions, coal particle size, moisture content, and packing porosity on the self-heating behaviour of stockpiled coal. Last not the least, major challenges and perspectives this subject may have are briefly discussed.

Keywords

theoretical, mechanism, stockpile, coal, study, review, variable, self, basis, heating, numerical, solutions

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A review on numerical solutions to self-heating of coal stockpile: mechanism, theoretical basis, and variable study

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Abstract

Self-heating or even spontaneous combustion of stockpiled coal, which is likely to outbreak under favourable circumstances during its transport, process, and storage, is a long-standing thermal dynamic hazard. This hazard is harmful in diverse aspects: causing loss of coal resource and caking property, raising safety concerns upon occurrence of open fire, and giving off noxious/greenhouse effect gases. Due to the complexity of involved physical process (e.g. heat and mass transport) and chemical process (e.g. coal oxidation), formulating an analytical solution to the problem with or even without a transient approach would be a daunting task and the problem is thus more often addressed numerically. So far many numerical models to self-heating of coal have been developed and to summarise these erratic findings, this work critically reviewed these numerical solutions since the last four decades. Mechanism of self-heating on coal mass and low temperature coal oxidation especially kinetic modelling of coal oxidation is firstly investigated to clarify the involved physical and chemical processes. On basis of the mechanistic understanding, theoretical derivations and progressive advances on essential terms like energy, mass, and momentum conservation are reviewed and compiled in details. Through parametric studies or sensitivity check these models produced fruitful but slightly inconsistent findings. Therefore to provide industry more unbiased and comprehensive guides, the present work examined the influences of various contributors including wind flow, stockpile dimensions, coal particle size, moisture content, and packing porosity on the self-heating behaviour of stockpiled coal. Last not the least, major challenges and perspectives this subject may have are briefly discussed.

Keywords

Self-heating, Coal stockpile, Numerical solution, Low-temperature oxidation

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A	Arrhenius pre-exponential factor	$(\text{kmol}/\text{m}^3)^{1-n}\text{s}^{-1}$
a	Empirical constant in Elovich equation	
C	Gas concentration	kmol m^{-3}
C_p	Specific heat capacity	$\text{J kg}^{-1} \text{K}^{-1}$
C_{Pr}	Pressure coefficient	
D	Diffusion coefficient of specie in the gas phase	$\text{m}^2 \text{s}^{-1}$
d	Diameter of coal particle	m
E	Apparent activation energy	kJ mol^{-1}
G	Specific porous media surface area	m^{-1}
g	Gravitational acceleration	m s^{-2}
h	Heat transfer coefficient	$\text{W m}^{-2} \text{K}^{-1}$
k	Permeability of the coal matrix	m^2
n	Apparent order of reaction	
P	Pressure	Pa
q	Amount of oxygen taken up per unit mass of coal	
R	Universe gas constant	$\text{kJ mol}^{-1} \text{K}$
Ra	Radius of coal particle	m
r	Consumption rate of oxygen	$\text{kmol m}^{-3} \text{s}^{-1}$
r_m	Rate of drying or wetting	$\text{kmol m}^{-3} \text{s}^{-1}$
$\check{r}$	Radial coordinate	m
S	Source term	
T	Temperature	K
t	Time	s
U	Gas superficial velocity	m s^{-1}
u	Velocity component in x direction	m s^{-1}
V	Free stream velocity	m s^{-1}
v	Velocity component in y direction	m s^{-1}
w	Velocity component in z direction	m s^{-1}
x	Longitudinal coordinate	m
y	Transverse coordinate	m
z	Axial coordinate	m
Greek letters		
α	Empirical constant in Elovich equation	
β	Thermal expansion coefficient	K^{-1}
ΔH	Heat of coal oxidation	$\text{kJ mol}^{-1} \text{O}_2$
ΔH_m	Heat of evaporation or condensation	kJ mol^{-1}
ε	Porosity	
λ	Thermal conductivity	$\text{W m}^{-1} \text{K}^{-1}$
μ	Gas viscosity	kg m s^{-2}
ρ	Density	kg m^{-3}
ψ	Stream function	$\text{kg m}^{-1} \text{s}^{-1}$
Subscripts		
am	Ambient	
b	Bulk coal	
c	Coal	
e	Effective	
g	Gas	
m	Moisture	
o	Oxygen	
r	Reference	

1 Introduction

Coal in all ranks, as a carbonaceous material, is able to be oxidised at low temperature with presence of oxygen rich air [1-19]. The interaction of coal with oxygen at low temperature is exothermic as a whole although some reaction sequences could be endothermic [15, 20]. It is widely recognised that low temperature oxidation is the main source of heat leading to spontaneous ignition of stockpiled coal. Other exothermic processes like microbial metabolism, interaction of coal with water, and oxidation of pyrite can also contribute to self-heating of coal mass [21]. Among them an important one is that heat evolves as moisture in both gas and liquid phase physically bonds with dry coal particles in which the process is termed as heat of “wetting” in some literatures [21-23]. Phenomenon of self-heating on a coal stockpile is likely to outbreak if the heat generated by coal oxidation and other mechanisms is not adequately dissipated to the surroundings via conduction, convection, and radiation. The excessive heat is, to a considerable extent, stored in the coal by virtue of its poor thermal conductivity and results in a net increment of temperature and meanwhile, very possibly, the reaction rate of coal oxidation. Once the temperature of a coal mass reaches a critical value at which thermal runaway occurs, a fire ensues if not averted with appropriate remedies [24-26]. The hazard of self-heating of coal stockpile is likely to take place in long term storage of thermal power station, in waste surface coal mining spoil piles, and transportation in cargo ship or train over large distances [26-30]. Spontaneous ignition and smouldering of coal stockpile burns the valuable fossil asset and poses a great threat to coal producers and users. In addition, serious and extensive oxidation of coal can also cause loss of its calorific value and coking property [31-33]. More recently, the liberation of large amounts of greenhouse-relevant gases and toxic gases, such as CO and NO_x, and hazardous substances, such as arsenic, selenium, mercury, and lead contributed from spontaneous combustion and low temperature oxidation of large-scale coal matrix has raised considerable concerns from global communities lately [34-38]. Figure 1 provides some of the photographic views of stockpiled coal fire collected from the worldwide.

Considering all of the raised concerns and the annoying fact that self-heating of coal stockpile is a long-standing problem, the hazard needs to be controlled. Although this imperative has long been acknowledged, it has also been accepted that the physical and chemical processes responsible for this problem is extremely complicated [28]. The problem was mitigated by practical means long before the scientific accounts emerged. However the theoretical research is in equal importance, on a quantitative basis, in assisting with the assessment and prediction of self-heating hazard and design of procedures and countermeasures to reduce this risk. Early efforts have been devoted to self-heating problem of bulky solids by thermal explosion theory, which laid firm foundation of the theoretical solution to the problem [39-42]. Afterwards a series of treatments of thermal explosion theory in solid material self-heating problem have been published

[43-53]. Although thermal explosion theory is able to determine criticality of a porous body with diffusion-controlled oxygen consumption [45, 49, 50, 53], it still has difficulties to directly apply this solution to self-heating problem of coal stockpile as more of the factors affecting self-heating are taken into account [28]. Additionally what raised much of the concern to coal operator is the induction period of a coal stockpile before catching a fire. The increasing demand of transient solutions poses significant challenges to the subject. Derivation of an analytical solution with less approximation to such a transient problem which might involves fluid dynamics, heat transfer, and chemical reaction kinetics would be a daunting or even impossible task so the problem is more often addressed numerically with increasing availability to high-performance computers. The main scope of this work is to review the numerical solutions to self-heating of stockpiled coal since four decades ago when the problem started to be embraced by numerical solutions.

To predict the self-heating behaviour of porous coal mass with progressively consumed gas species like oxygen and vapour, prior to the availability of high-performance commercial fluid dynamics simulation code, several rudimentary mathematical studies with many assumptions and simplifications though were conducted [23, 54-70]. Among these works, Sondreal and Ellman [23] calculated the material and energy balances for a stockpiled lignite in which heat is transferred only by conduction. Nordon [54] proposed a one-dimensional unsteady state model consisting of the differential equations for mass and energy conservation and for the reaction rate of coal oxidation. Schmal *et al.* [55] developed another one-dimensional model which included thermal impacts exhibited by evaporation/condensation of coal moisture. Both models analysed forced convection through the packed bed by varying the air flow velocity as a system parameter. Brooks and co-workers [56-59] differed from previous treatments in that natural convection was taken into account as an important mechanism for oxygen transport that is responsible for the occurrence of self-heating without the need to assume the existence of a pressure gradient over the coal bed. Young *et al.* [60] proposed a two-dimensional natural convection and conduction model in a packed bed containing a hot spot (i.e. coal stockpile, nuclear reactor) and this work reconfirmed natural convection is a feasible mechanism for oxygen transport into a coal pile where sufficient reaction may occur to sustain a hot spot. To predict the development of localized spontaneous heating within a porous coal matrix that is subjected to forced convection or in an otherwise quiescent environment in which buoyancy flow dominates, the Bureau of Mines developed three time-dependent mathematical models, which were used to calculate the temperature increase associated with chemisorption of oxygen by the coal [67]. Bradshaw *et al.* [61] studied the effect of natural convection on ignition in a laterally-unbounded coal pile and stable three-dimensional flow planforms for the model were predicted. Arisoy and Akgün [65] developed a one-dimensional non-equilibrium thermal model consisting of conservation equations for oxygen, water vapour, moisture of coal, and energy for both gaseous and

solid phases. Salinger and co-authors [69] critically reviewed the mathematical analysis of coupled reaction and transport in chemical reactors and analysed spontaneous heating of coal stockpiles by considering the nonlinear interactions of chemical reaction, heat transfer, and buoyancy-driven flows within and around the stockpile. Krishnaswamy and co-workers [8, 62] developed a reaction-diffusion model for low-temperature oxidation of coal and this model was incorporated in a two-dimensional model for spontaneous heating of open coal stockpiles where the influence of moisture migration can be negligible. Hull *et al.* [63, 68] developed a theoretical model for a confined space context where stockpile is sealed on all sides except the top which provides free surface and channels for oxygen diffusion. Monazam *et al.* [70] formulated a transient one-dimensional spontaneous heating model to describe the self-heating process at relatively low temperatures. Akgün and Essenhigh [64] proposed a two dimension transient model of self-heating of coal stockpile and found height and time are two primary factors in determining if a stockpile is unconditionally safe. Although the predictions of temperature ramping profile and incubation period are very likely beyond engineering accuracy due to substantial assumptions and restrictions having been made, these fundamental models are capable of providing subsequent researchers valuable insights to the problem and offering initial guidance to assist coal operators to stack stockpile more safely. No doubt the fundamental understanding of self-heating in coal stockpile has advanced but yet lacks clarification and summary especially for the period after the Carras and Young's review work [28]. Therefore the first intent of this work is to investigate more details of the mechanism of self-heating and heat & mass transfer process in coal matrix and on basis of this mechanistic understanding, core constituents and main features of these mathematical models are summarised and reviewed for future reference purpose.

More recently with the advance and development of more sophisticated numerical solutions, especially the availability of cutting-edge Computational Fluid Dynamics (CFD) modelling techniques and their increasing applications in coal and related industries [71], predictable interpretation of transient self-heating of coal mass with less restrictions and within tolerated engineering accuracy becomes possible [24, 26, 30, 31, 72-80]. Among these works, Moghtaderi *et al.* [30] studied the effects of wind driven flow field on self-heating behaviour of typical coal stockpiles and found wind flow plays a critical part in dynamics of flow field inside the pile and thereby affects the heating process. Krajčiová *et al.* [78] innovated a model including radiation energy balance of the coal stockpile surface and indicated solar radiation has a strong influence on the temperature ramping profile of stockpile. Yuan and Smith [75] studied effects of coal properties on self-heating problem in underground coal mine goaf areas by a CFD model. Yuan and Smith [24] further developed a three-dimensional equilibrium thermal CFD model to simulate spontaneous heating in a large-scale testing chamber with a forced ventilation system. Ejlali *et al.* [77] improved preceding models by employing a local thermal non-equilibrium

approach and stated the required time to vaporize the water content and the maximum temperature is a function of porosity of porous pile, moisture content and Darcy number. Taraba and Michalec [73] numerically investigated the effects of longwall advance rate on spontaneous heating in goaf areas by a CFD model. Kim and Sohn [72] numerically validated a novel method (air blowing from bottom of stockpile and/or instalment of dual barrier) to suppress spontaneous ignition of coal stockpiles in a coal storage yard. Zhu et al. [26] developed a theoretical model to predict the self-ignition time and locations of coal stockpiles with relatively large diameter of coal particle. Taraba et al. [74] developed a CFD model to study the influences of wind on the spontaneous heating process of a coal stockpile. Yang et al. [31] proposed a two-dimensional model to investigate the effects of coating the bottom of coal stockpile with fine particles to control self-heating hazard. Xia et al. [79] also used the CFD code to simulate the self-heating process of residual coal in longwall goaf. Zhang et al. [80] studied the low-temperature self-heating behaviour of multiple coal stockpiles under different prevailing wind conditions. Not only above works can eliminate more restrictions to enhance the applicability of numerical solutions to coal self-heating problems, considerable variable studies have also been conducted and many parametric findings have been reported. These key findings are however not strictly consistent so the applicability of these valuable suggestions to industry is somehow hindered. Hence to deliver more unbiased and objective guidance, these key findings must be clarified and examined in detail. A normal numerical solution is likely to undergo the following steps, refer Figure 2. Among them the important ones are mechanism analysis which determines the framework of the theoretical model, theoretical formulation which includes the most significant governing equations, and the parametric study which provides much more information and understanding of the problem. Therefore the present work mainly reviewed previous numerical models of self-heating of coal stockpile from above perspectives. Lastly some challenges the subject faces and possible improvements are discussed.

2 Mechanism of self-heating of coal stockpile and coal oxidation kinetics

2.1 Mechanistic understanding of the hazard

Analogous to many other biological and chemical porous reactors, a coal stockpile is essentially a coal mass consisting of heterogeneous distribution of porous coal particles and gases like oxygen, water vapour, and gaseous product liberated by oxidation reaction transporting in the inter-particle channels and the microstructures of coal particles [81, 82]. Figure 3 provides a schematic illustration of the process and main features of coal stockpile self-heating. Very briefly, phenomenon of self-heating could occur if the heat generated by coal oxidation and other exothermic processes exceed the heat dissipated to the surroundings by conduction, convection, and radiation. The air inside of stockpile can be constantly replaced and replenished through advective motion caused by forced or natural convection caused by presence of pressure gradient and diffusive motion caused by oxygen consumption of coal which results concentration of oxygen

in stockpile is lower than that of ambient atmosphere. The heat can be continuously produced if air supply is not eliminated. Interaction of coal with oxygen including coal oxidation and oxygen adsorption at low temperature is exothermic as a whole although it could be endothermic at some steps [15, 20]. The thermal effect of moisture might not be ignored at the initial stage of coal self-heating but heat generated by coal oxidation will dominate with progressive drying of coal. Therefore it is safe to argue that the major heat generation mechanism responsible for self-heating is still coal oxidation [28]. The heat of reaction during oxidation of lignite increased from approximately 313kJ per mole oxygen absorbed at 20°C to 376 kJ per mole oxygen at 90 °C [23]. Kaji et al. [7] measured the rates of heat liberation and oxygen consumption due to coal oxidation in the temperature range 20-170°C using coals ranging from subbituminous to anthracite and 75-90kcal (i.e. 300-379kJ) heat evolved per mole of oxygen at steady state was reported. The generated heat is transported out of the stockpile by conduction through coal mass, convection through wind, and radiation. If the rate of heat generation is greater than the rate at which heat can be dissipated to the external environment, the excessive heat will be stored in coal matrix and results in a temperature rise. The higher temperature would cause a more drastic reaction taking place, and if no controls are exercised, a fire is very likely to outbreak. Considering the factors that weathering coal particles at surface of coal stockpile are relatively inert in terms of oxidative reaction with long period of exposure to the ambient atmosphere and convective and conductive heat dissipation is stronger than heat production at surface area, the self-heating zone normally may reside at a few meters deep to stockpile surface, refer Figure 3. Besides the features described above, self-heating process of coal stockpile is also affected by local meteorological conditions through wind, rain/shower, varying ambient temperature and solar radiation. Water vapour is transported either into or away from the stockpile, depending on the relative ambient humidity and the equilibrium relative humidity within the coal for a given coal water content [28, 66, 83, 84]. Moisture has an impact on the process through both chemical and physical ways albeit the effects exhibited in chemical ways have not been fully grasped. More specific accounts of effects of moisture on coal oxidation and self-heating will be given at section 4.4.

To be more realistic to describe heat interaction inside a coal stockpile, heat transfer between coal particles should be treated in a non-equilibrium thermal approach because temperature differentials between air transported from ambient and coal particles could be substantially high. In other words, a stockpile should not be treated as a non-porous body and convective heat loss which takes place in the interior of stockpile ought to be featured. If the temperature differential between the solid coal particle and gas is important in the thermal behaviour, it is necessary to represent the energy stored in each individual phase as well as the exchange of thermal energy between them [85, 86]. Figure 4 is a close-up schematic illustration of intra-and inner-particle heat and mass transfer process. Heat conduction can occur between gas-

217 to-gas, gas-to-coal, and coal-to-coal where effective solid conductance is introduced because of narrow clearance existing
218 between coal particles which further reduce the thermal conductivity of coal. It is assumed that the porous coal stockpile
219 may be treated as homogeneous so that conduction can be modelled by a single effective thermal conductivity [60].
220 Effective thermal conductivity λ_e is often given by equation 1 [24, 26, 75, 82], other solutions for effective thermal
221 conductivity can be found in the literatures [67, 70, 72],

$$222 \quad \lambda_e = \varepsilon \lambda_g + (1 - \varepsilon) \lambda_c \quad (1)$$

223 The low thermal conductivity of coal is the main reason why thermal energy can be well contained in the deep stockpile.
224 Heat convection occurs between gas to coal and the efficiency of heat convection is mainly determined by velocity of gas
225 advection stream within narrow connected channels between coal particles. Whilst heat radiation could be a major
226 contributor in the surface of stockpile because of solar energy it absorbed but in deep stockpile heat radiation can be
227 negligible [78]. Another efficient heat transfer mechanism is interaction of coal with moisture in which the vaporisation
228 and diffusion of water from a hot region, followed by condensation in a cooler region, is accompanied by a considerably
229 higher effective rate of heat transfer than that which can occur by conduction alone [50]. The interaction of coal with
230 water proceeds much quicker than with oxygen molecule and that leads to the conclusion that interaction of coal with
231 moisture is an efficient heat transfer mechanism especially at temperature range 80~90°C. Air transported into coal
232 stockpile via convection and diffusion. Convective flow in both natural and forced ways is pressure-driven flow and
233 diffusive motion is caused by gas concentration gradients because neither oxygen is consumed nor gaseous products are
234 produced at an equal rate everywhere. Convective flow is the primary driver in micro-scale flow, even very small
235 pressure gradients will cause larger flux than flux generated by very steep concentration gradients [87]. Air convection
236 mainly occurs in inter-particle channels and diffusion mainly occurs in inner pores of coal particle and in deep region of
237 coal stockpile where convection is very weak. Irrespective of complex pore structure of coal, many numerical solutions
238 adopted a global surface reaction mechanism so detailed transport mechanism like gas diffusion into inner pores is
239 normally disregarded.

240 **2.2 A brief study of coal oxidation kinetics**

241 To define oxygen consumption rate of coal on a quantitative basis for numerical solution, the nature and chemical
242 kinetics of low temperature coal oxidation must be well studied. Mechanism of low-temperature coal oxidation has been
243 investigated by many studies but complete understanding has never been obtained because of very complex pore
244 structure and chemical composition of coal [4, 9, 15-18, 20, 28, 33, 88-103]. Despite of the incomplete understanding of
245 the mechanism and kinetics of coal oxidation, overall reaction paths have reached a general consensus. Very briefly two
246 parallel interaction sequences exist: direct burn-off and adsorption sequence. The burn-off reaction resembles direct

combustion of solid fuels which is strongly dependent on temperature and the reaction sequence is likely to occur at specific sites in a coal's aromatic or aliphatic structure, resulting in the direct formation of gaseous products including CO, CO₂, and H₂O [8, 9, 15, 95, 100, 104]. The adsorption sequence includes: (i) reversible physical adsorption; (ii) irreversible chemisorption of oxygen on the surfaces of pores and the formation of intermediate coal-oxygen complexes including peroxygen, hydroperoxide and hydroxyl species; (iii) the degradation of unstable solid coal-oxygen complexes to gaseous products and formation of stable solid compounds, e.g. carbonyl or carboxyl containing species; (iv) the decomposition of stable compounds and the exposure of new active sites for oxidation [15, 90], refer Figure 5 which is a very representative chart of interaction of coal with oxygen at low temperature. More kinetic models were summarized by Wang *et al.* [15], the compilation is further cited in this work to give a clearer picture of kinetic models, refer Table 1.

It is noticeable, at low temperature range, the number of the active sites for oxygen adsorption usually decays exponentially, which often correlates to exhibition of the Elovich effect. At present it is, however, unlikely to describe the burn-off reaction sequence in fundamental steps due to the lack of understanding and therefore, to a quantitative basis, many authors attempted to use the Elovich dependence (or partially) to describe the progressive decrease of the rate of sorption reaction regime with increasing uptake of active sites at a constant temperature [1, 15, 54, 90, 98, 105, 106]. The Elovich equation was often written as,

$$\frac{dq}{dt} = a \exp(-\alpha q) \quad (2)$$

Although the Elovich equation is often taken as a purely empirical term, it can be effectively applied to explain the rate of oxygen consumption with time, namely the “ageing” effect [1, 54, 107]. Whilst in reality temperature in stockpile is elevating as a result of heat accumulation and further due to the existence of burn-off reaction sequence which is highly dependent on temperature so consumption rate of oxygen is more frequently expressed in Arrhenius form with a given temperature and oxygen concentration [24, 26, 74, 75, 79], which was written,

$$r = A[C_O]^n \exp(-E/RT) \quad (3)$$

Authentic Arrhenius equation has its origin in gas phase reaction regime [108, 109]. An equation of the same form as Equation 3 has also found wide application to the oxidation of coal. However usually there is no mechanistic interpretation of A and E, simply an observed temperature dependence of rate that fits an equation of this form [110]. But some other studies indicated the activation energy, *E*, may be regarded as a measure of the energy barrier to reaction, while the pre-exponential factor, *A*, correlates to the available surface area for oxidation [111]. Thus, the pre-exponential factor depends heavily on the coal's pore structure and fine particles tend to have a larger pre-exponential factor [112]. Irrespective this dispute, it can be observed, from Equation 3, that coal oxidation rate is simply determined by the

277 reaction order and two Arrhenius constants at a given temperature and partial pressure of oxygen. It is assumed that
278 oxygen can penetrate throughout the coal without any diffusional resistance and the reaction rate between gaseous
279 oxygen and solid coal particle is expressed as if it is a homogenous gas phase reaction [1]. To consider the diffusional
280 restriction into the interior of coal particle, many studies introduced an effectiveness factor, which is conventionally
281 defined as the ratio of the reaction rate under diffusional limitations to the rate which would be observed in the chemical
282 control regime in the absence of transport or diffusional effect [96]. Detailed interpretation of the effectiveness factor can
283 be found in the literatures [8, 63, 65, 96]. The value of the reaction order in low temperature oxidation of coal and other
284 carbonaceous materials has been indicated to vary from 0.5 to 1 [28, 50]. More specific values of reaction order have
285 been published are: $n=1$ [23, 73, 113], $n=0.61$ [24, 114], $n=0.52$ [115], and $n=0.7$ [55, 116]. In the case of the
286 spontaneous combustion of coal, temperatures are extremely low and chemical kinetics play the main role on reaction
287 rate [1]. The kinetic constants are affected by unique coal properties such as pore structure, mineral matter, volatile
288 content, and coal rank so they varies from coal to coal. Even for a same coal the parameters can be affected by different
289 particle sizes [112] and heating stages [2]. The value of apparent activation energy, E , of different coals can vary between
290 12 and 95 kJ/mol and more values of activation energy for low temperature coal oxidation can be found in the review
291 work conducted by Wang et al. [15]. Taraba and Michalec [73] discussed the pre-exponential factor is of the greatest
292 uncertainty giving ordinarily values differing over several orders and another study also indicated the pre-exponential
293 factor has a typical value between 1 and $7 \times 10^5/\text{s}$ [24, 75]. As a result, the Arrhenius constants for a given coal oxidation
294 context must be determined experimentally. These experimental methods may include adiabatic testing method, heat
295 release measurement method, and differential thermal analysis [1, 117-120].

296

297 Self-heating of coal starts with low temperature oxidation stage at which adsorption reaction sequence might manifest so
298 the reaction rate of a coal could display a non-Arrhenius behaviour curve (more likely, a Elovich curve). In a study of the
299 oxidation rate of coal and coal char [107], it was shown that the oxidation rate of a coal char exhibits both an Arrhenius
300 and Elovich kinetics from 50~100°C. As can be seen in Figure 6(a), Jones and Newman [110] reported a non-Arrhenius
301 behaviour of a Chinese bituminous coal in a micro-calorimeter experiment at temperatures in the range 311~338K. More
302 recently an adiabatic testing figure of a high volatile bituminous coal from Hunter Valley coalfield of Australia indicated
303 that an Arrhenius dependence curve above 70 °C can be found and below this temperature a straight line is impossible to
304 be fitted at the $\ln(dT/dt)$ versus $(1/T)$ plot, refer Figure 6(b) [1]. A possible explanation is adsorption reaction sequence
305 proceeds at a high rate initially and manifests itself by driving reaction rate to a non-Arrhenius behaviour curve. With the
306 time elapsing and temperature increasing, the adsorption reaction tails off and the direct burn-off reaction step takes a

lead to the extent reaction rate starts to follow the Arrhenius-like dependence. Many numerical solutions adopted a simple Arrhenius approach with or without an effectiveness factor to mathematically deal with consumption rate of oxygen within a stockpile [24, 26, 31, 55, 58, 62, 64, 65, 72-75]. The conjunctive effects brought by the Elovich mechanism and Arrhenius equation at low temperature coal oxidation may introduce a new dimension for numerical simulation of self-heating behaviour on a coal mass although the need of numerical assessment of Elovich parameters was called long ago [54]. Another glance at the Equation 3 it can be known partial pressure of oxygen also plays a role in the rate of coal oxidation at a given temperature and Arrhenius constants. It is plausible to approximate that any solid coal-oxygen complex produced during low-temperature coal oxidation would not affect the rate of oxidation if Arrhenius reaction mechanism is presumed. Gaseous products (e.g. CO, CO₂, and H₂O) liberated by direct burn-off reaction and decomposition of solid complex would, however, disperse into the gas mixture and affect the concentration of oxygen although the amount of gaseous product is much less appreciable than that of consumed oxygen [95]. Early numerical works only considered the consumption of oxygen and some recent works started to incorporate effect of gaseous products with very simplified stoichiometric schemes though [24, 72-75], refer **Table 2** which summaries the main features such as transport mechanism and spatial dimension, and important parameters like physical properties and reaction kinetics of present numerical solutions to self-heating of coal mass.

3 Theoretical basis

On formulating a theoretical model for a numerical solution to self-heating of coal stockpile one is very likely to shed curiosity, to a mathematical sense, into how the heat is generated and transferred, how the oxygen is transported as being consuming by coal, how the gas flux flows inside stockpile, and how the moisture migrates from one site to another site. The mechanistic understanding of self-heating of coal matrix has been comprehensively discussed in the last section and having the fundamental knowledge in mind, core constituents of the mathematical model should include terms on heat and species (e.g. oxygen and/or water vapour) conservation, momentum balance and continuity equations for fluid flow in a porous matrix. This section will serve to discuss and record the progressive formulation and development of theoretical models. To keep the straightforwardness and simplicity of the discussion, energy term of heat radiation is not be included.

3.1 Energy conservation

3.1.1 Absence of moisture

The energy description starts with Sondreal and Ellman [23] who assumed heat is only dissipated by conduction of a coal mass, which yields,

$$\rho_b C_{pb} \frac{\partial T}{\partial t} = \lambda_e \nabla^2 T + S \quad (4)$$

337 The successive terms denote the storage of internal energy which manifest itself as a transient temperature rise of bulky
 338 coal, heat diffusion and energy source which denotes liberation of reaction heat. Later, Hull *et al.* and Young *et al.* [60,
 339 63] also used conduction as a sole heat transport mechanism when levelled stockpiles of coal are transported in a
 340 confined space like barges or rail cars, which gives,

$$341 \quad (1 - \varepsilon)\rho_c C_{pc} \frac{\partial T}{\partial t} = \lambda_e \frac{\partial^2 T}{\partial x^2} + (1 - \varepsilon)r\Delta H \quad (5)$$

342 In Schmal's one dimensional model [55], heat dissipated by convection (the second term in equation 5) was included in
 343 the heat balance equation, which results,

$$344 \quad (1 - \varepsilon)\rho_c C_{pc} \frac{\partial T}{\partial t} + \rho_g C_{pg} u \frac{\partial T}{\partial x} = \lambda_e \frac{\partial^2 T}{\partial x^2} + (1 - \varepsilon)r\Delta H \quad (6)$$

345 Brooks *et al.* [56-58] also incorporated convective heat term in heat balance but presuming a pseudo steady state, which
 346 produces,

$$347 \quad \lambda_e \frac{\partial^2 T}{\partial x^2} - \rho_g C_{pg} u \frac{\partial T}{\partial x} + r\Delta H = 0 \quad (7)$$

348 In the forced convection model of Edwards's work [67], a non-equilibrium thermal state between gas and coal was
 349 considered and the thermal transport equation was written in cylindrical coordinates, which yields,

$$350 \quad \varepsilon \rho_g C_{pg} \frac{\partial T_g}{\partial t} + (1 - \varepsilon)\rho_c C_{pc} \frac{\partial T_c}{\partial t} + \rho_g C_{pg} U_r \frac{\partial T_g}{\partial x} + \rho_g C_{pg} W \frac{\partial T_g}{\partial x} = \lambda_e \frac{\partial^2 T}{\partial z^2} + \lambda_e \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) + r\Delta H \quad (8)$$

351 And thermal transfer between the solid coal and the gas is governed by,

$$352 \quad \rho_c C_{pc} \frac{\partial T_c}{\partial t} = \frac{3h}{R} (T_g - T_c) \quad (9)$$

353 While in the wind-driven convection model, the gas and solid coal were, for a conservative estimate of induction period,
 354 assumed to be in thermal equilibrium. The energy transport equation was therefore written as,

$$355 \quad [\varepsilon \rho_g C_{pg} + (1 - \varepsilon)\rho_c C_{pc}] \frac{\partial T}{\partial t} + \rho_g C_{pg} u \frac{\partial T}{\partial x} = \lambda_e \frac{\partial^2 T}{\partial x^2} + r\Delta H \quad (10)$$

356 Krishnaswamy *et al.* [62] extended the heat conservation equation to two dimensions in Cartesian coordinate system,
 357 which yields,

$$358 \quad (1 - \varepsilon)\rho_c C_{pc} \frac{\partial T}{\partial t} + \rho_g C_{pg} \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \lambda_e \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + r\Delta H \quad (11)$$

359 To date commercial CFD code is capable of solving 3D problem in (non-)equilibrium thermal approach. Zhu and co-
 360 workers [26] used the code established a 2D energy conservation in thermal equilibrium, the equation is written as,

$$361 \quad [\varepsilon \rho_g C_{pg} + (1 - \varepsilon)\rho_c C_{pc}] \frac{\partial T}{\partial t} + \rho_g C_{pg} \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \lambda_e \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + (1 - \varepsilon)r\Delta H \quad (12)$$

362 Yuan and Smith [24, 75] used CFD code to develop a three-dimensional equilibrium thermal model for self-heating of
 363 coalbed in a testing chamber, which produces,

$$[\varepsilon \rho_g C_{pg} + (1 - \varepsilon) \rho_c C_{pc}] \frac{\partial T}{\partial t} + \rho_g C_{pg} \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} \right) = \lambda_e \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + r \Delta H \quad (13)$$

The most recently, Xia and co-workers [79] developed a non-equilibrium thermal model for self-heating of a longwall goaf, hence two separate energy equations are required,

For solid phase

$$(1 - \varepsilon) \rho_c C_{pc} \frac{\partial T_c}{\partial t} - (1 - \varepsilon) \nabla (\lambda_c \nabla T_c) = S + hG(T_g - T_c) \quad (14)$$

For gas phase

$$\varepsilon \rho_g C_{pg} \frac{\partial T_g}{\partial t} + \rho_g C_{pg} U_g \nabla T_g - \varepsilon \nabla (\lambda_g \nabla T_g) = -hG(T_g - T_c) \quad (15)$$

3.1.2 Presence of moisture

Although some fresh stockpiles are very dry due to low inherent water content of coal, they are likely to become moist with presence of rain, snow, and/or moist ambient air. In practice most coal stockpiles are moist especially some low rank coals with presence of high inherent water content and thereby heat exchanged via transition of water phase should be incorporated in the model. In Schmal's model, additional energy conservation was proposed for a moist coal pile [55]. To adjust the model, two extra terms were incorporated in Equation (6): one for evaporation (or, with the opposite sign for condensation, first term) and another one for convective heat transfer by water vapour (second term).

$$\Delta H_m \frac{\partial (U C_m)}{\partial x} + U_m \rho_m C_{pm} \frac{\partial T}{\partial t} + (1 - \varepsilon) \rho_c C_{pc} \frac{\partial T}{\partial t} + \rho_g C_{pg} u \frac{\partial T}{\partial x} = \lambda_e \frac{\partial^2 T}{\partial x^2} + (1 - \varepsilon) r \Delta H \quad (16)$$

By ignoring the convective heat transfer by water vapour, Monazam *et al.* [70] proposed another equation for energy balance of a damp coal mass,

$$(1 - \varepsilon) \rho_c C_{pc} \frac{\partial T}{\partial t} = \lambda_e \frac{\partial^2 T}{\partial x^2} - \rho_g C_{pg} u \frac{\partial T}{\partial x} + r \Delta H (1 - \varepsilon) + (1 - \varepsilon) \Delta H_m r_m \quad (17)$$

Arisoy and Akgun [65] improved Schmal's model by adopting a non-equilibrium thermal model to study the effect of moisture, which gives,

For solid phase:

$$(1 - \varepsilon) \rho_c C_{pc} \frac{\partial T_c}{\partial t} = \lambda_c \frac{\partial^2 T_c}{\partial x^2} + (1 - \varepsilon) \frac{3}{Ra} h (T_g - T_c) - (1 - \varepsilon) \Delta H_m r_m + (1 - \varepsilon) r \Delta H \quad (18)$$

For gas phase:

$$\varepsilon \frac{\partial}{\partial t} (\rho_g C_{pg} + \rho_m C_{pm}) T_g + u \frac{\partial}{\partial x} (\rho_g C_{pg} + \rho_m C_{pm}) T_g = \varepsilon \lambda_g \frac{\partial^2 T_g}{\partial x^2} - (1 - \varepsilon) \frac{3}{Ra} h (T_g - T_c) \quad (19)$$

Later Akgun and Essenhig [64] extended the one-dimensional non-equilibrium thermal model into two dimensions, which yields,

For solid phase:

$$(1 - \varepsilon) \rho_c C_{pc} \frac{\partial T_c}{\partial t} = \lambda_c \left(\frac{\partial^2 T_c}{\partial x^2} + \frac{\partial^2 T_c}{\partial y^2} \right) + (1 - \varepsilon) \frac{3}{Ra} h (T_g - T_c) + (1 - \varepsilon) r \Delta H - (1 - \varepsilon) r_m \Delta H_m \quad (20)$$

For gas phase:

$$\varepsilon \frac{\partial T_g}{\partial t} \rho_g C_{pg} + \rho_g C_{pg} \left[\frac{\partial}{\partial x} (u T_g) + \frac{\partial}{\partial y} (v T_g) \right] = \lambda_g \left(\frac{\partial^2 T_g}{\partial x^2} + \frac{\partial^2 T_g}{\partial y^2} \right) - (1 - \varepsilon) \frac{3}{Ra} h (T_g - T_c) \quad (21)$$

3.2 Mass conservation

Most models assumed mass of solid coal particle remains unchanged prior to ignition and therefore mass conservation study was focused on oxygen conservation and water vapour conservation (for a moist coal stockpile). Schmal *et al.* [55] proposed a one dimensional mass balance model for both oxygen and moisture, which yields,

For oxygen:

$$\varepsilon \frac{\partial C_o}{\partial t} + u \frac{\partial C_o}{\partial x} - \varepsilon D_o \frac{\partial^2 C_o}{\partial x^2} + (1 - \varepsilon) r = 0 \quad (22)$$

In which the successive terms represent the local accumulation of oxygen, the convective transport of oxygen, the diffusion of oxygen, and the consumption of oxygen due to coal oxidation.

For moisture:

$$\frac{\partial C_m}{\partial t} - \frac{\partial (u C_m)}{\partial x} = 0 \quad (23)$$

The successive terms represent the transient accumulation of moisture at the coal particle and the rate of evaporation (or condensation). Hull *et al.* [63] also used a one dimensional model to study the role of the diffusion of oxygen in a confined storage by eliminating volumetric convective component, which gives,

$$\varepsilon \frac{\partial C_o}{\partial t} = \varepsilon D_o \frac{\partial^2 C_o}{\partial x^2} - (1 - \varepsilon) r \quad (24)$$

Krishnaswamy *et al.* [62] developed the oxygen balance equation to two dimensions but molecular diffusion is ignored and a pseudo steady state is assumed, and these assumptions produce,

$$u \frac{\partial C_o}{\partial x} + v \frac{\partial C_o}{\partial y} = -r \quad (25)$$

Arisoy and Akgun [65] developed another one-dimensional conservation model for both oxygen and moisture, with similar form of Schmal's model,

For oxygen:

$$\varepsilon \frac{\partial \rho_o}{\partial t} + u \frac{\partial \rho_o}{\partial x} = \varepsilon D_o \frac{\partial^2 \rho_o}{\partial x^2} - (1 - \varepsilon) r \quad (26)$$

For moisture:

$$\varepsilon \frac{\partial \rho_m}{\partial t} + u \frac{\partial \rho_m}{\partial x} = \varepsilon D_m \frac{\partial^2 \rho_m}{\partial x^2} + (1 - \varepsilon) r_m \quad (27)$$

Akgun and Essenhigh [64] developed a more complete mass conservation model for both oxygen and moisture in two dimensions, which produces,

For oxygen:

$$\varepsilon \frac{\partial \rho_o}{\partial t} + \left(u \frac{\partial \rho_o}{\partial x} + v \frac{\partial \rho_o}{\partial y} \right) = \varepsilon D_o \left(\frac{\partial^2 \rho_o}{\partial x^2} + \frac{\partial^2 \rho_o}{\partial y^2} \right) - (1 - \varepsilon)r \quad (28)$$

For moisture:

$$\varepsilon \frac{\partial \rho_m}{\partial t} + \left(u \frac{\partial \rho_m}{\partial x} + v \frac{\partial \rho_m}{\partial y} \right) = \varepsilon D_m \left(\frac{\partial^2 \rho_m}{\partial x^2} + \frac{\partial^2 \rho_m}{\partial y^2} \right) - (1 - \varepsilon)r_m \quad (29)$$

Carras and Young [28] summarised a general form of mass balance which can be applied in both oxygen and water vapour, the general form was written as,

$$\varepsilon \frac{\partial C}{\partial t} + \varepsilon U \nabla C - D \nabla^2 C + S = 0 \quad (30)$$

Yuan and Smith [24, 75] developed a generic mass transfer equation in three dimensions by ignoring localized accumulation of gaseous species, which gives,

$$\rho u \frac{\partial C_o}{\partial x} + \rho v \frac{\partial C_o}{\partial y} + \rho w \frac{\partial C_o}{\partial z} = \rho D_o \frac{\partial^2 C_o}{\partial x^2} + \rho D_o \frac{\partial^2 C_o}{\partial y^2} + \rho D_o \frac{\partial^2 C_o}{\partial z^2} + S \quad (31)$$

More recently the oxygen conservation equation proposed by Zhu et al. [26] and Xia et al. [79] has the same form as the generalised description of Equation (30),

$$\text{Zhu's model} \rightarrow \varepsilon \frac{\partial C}{\partial t} + \left(u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} \right) = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - (1 - \varepsilon)r \quad (32)$$

$$\text{Xia's model} \rightarrow \varepsilon \frac{\partial C_o}{\partial t} + \nabla(-\varepsilon D \nabla C_o) + U \nabla C_o = r \quad (33)$$

3.3 Momentum balance

By making the Boussinesq approximation which essentially states that the temperature variation of the fluid properties can be ignored except for the density, and that the density dependence is only considered when it gives rise to buoyancy convection [121] and using Darcy's model to replace the shear stress tensor, Young et al. [60] proposed the motion equation in porous coal pile,

$$-\nabla P - \frac{\rho_{am} g}{k} U + \rho_g g = 0 \quad (34)$$

Later in buoyance-driven model of Edwards's work [67], a similar manner was used to develop the motion equation into two components, which shows,

$$\begin{cases} \frac{\partial P}{\partial x} = -\frac{\mu}{k} u \\ \frac{\partial P}{\partial y} = -\frac{\mu}{k} v + \rho_{am} g \left(1 - \frac{T_{am}}{T_g} \right) \end{cases} \quad (35)$$

The permeability k of coal matrix is approximated by the Blake–Kozeny equation for laminar flow in packed beds [24, 26, 62, 67, 72, 75, 77, 122], which gives,

$$k = \frac{\varepsilon^3 d^2}{150(1-\varepsilon)^2} \quad (36)$$

Many other works also used Darcy's law to describe flow in porous stockpile and additionally incorporates buoyancy convection as a possible mechanism of flow in porous medium as formulated by Edwards's work [30, 62, 64, 69]. The equation was generalised by Carras [28] and the universal form is written as,

$$U = \frac{k}{\varepsilon \mu} (-\nabla P + \rho g) \quad (37)$$

The first term in Equation (37) describes flow due to a pressure gradient while the second term describes the buoyancy due to gas density changes with temperature. For a very coarse coal stockpile (3~20cm), Zhu *et al.* [26] argued it is more appropriate to describe flow in Brinkman's law because of high Darcy number and Reynolds number [123], and motion of gas flow should be written as,

$$\begin{cases} \frac{\partial P}{\partial x} = \mu \frac{\partial^2 U}{\partial x^2} - \frac{\mu}{k} u \\ \frac{\partial P}{\partial y} = \mu \frac{\partial^2 U}{\partial y^2} - \frac{\mu}{k} v + \rho_g g \left(1 - \frac{T_{am}}{T_g}\right) \end{cases} \quad (38)$$

Nevertheless above models yields a steady flow field, to date, commercial CFD code is capable of handling a transient flow field which can be given by [82],

$$\rho_g \left(\frac{\partial U}{\partial t} + U \nabla U \right) = -\nabla P - \varepsilon U \frac{\mu}{k} + \mu \nabla^2 U - \rho_g g \beta (T_g - T_{am}) \quad (39)$$

In which the successive terms represent the transient momentum response, advection of momentum, pressure gradient, Darcy force, Brinkman effects and buoyant force.

3.4 Continuity

The continuity equation also assumes the validity of the Boussinesq approximation, which gives rise to the continuity equation [28, 60, 62, 69],

$$\nabla U = 0 \quad (40)$$

In a quasi steady-state approximation for the gas flow, the mass flux can be defined in terms of a stream function [60, 64, 67],

$$\begin{cases} \rho_g u = -\frac{\partial \psi}{\partial y} \\ \rho_g v = \frac{\partial \psi}{\partial x} \end{cases} \quad (41)$$

With CFD code, Kim and Sohn [72] proposed a three dimensional transient continuity equation with absence of the Boussinesq approximation, which yield,

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \quad (42)$$

If given appropriate initial and boundary conditions, quantitative information on self-heating phenomena can be produced. It should be noted, as a review study, any validation and analysis of mathematical model is not a task of present work. These theoretical terms are organised for general knowledge purpose so they might be modified or reworked when it comes to a numerical solution to a given context of self-heating of stockpiled coal.

4 Variable study

The last section compiles the theoretical basis of numerical solutions, one apparent point, as can be observed from these terms, is that self-heating behaviour of a coal stockpiles is governed by various variables, like coal reactivity which correlates to rate of coal oxidation and heat generation, moisture content which have an impact on heat transfer process, and geometry of stockpile which is likely to affect the distribution of wind induced pressure gradients around it. Considerable parametric studies based on these base models have been conducted to provide fruitful information to industry yet these valuable results are not strictly consistent. Therefore the aim of this section is to critically investigate and examine the impacts of different variables on the thermal behaviour of coal stockpile, and to clarify these findings and hopefully, shed light on practical industry operations. The main contributors to the self-heating of coal stockpile and the values they have been assigned are tabulated and attached in Appendix A. It can be seen some of the variables received intensive attentions and therefore the conduction of variable analysis is limited to those parameters, namely coal reactivity, particle diameter, compaction degree, moisture, wind, stockpile height and slope.

4.1 Coal reactivity

Two studies [124, 125] reviewed the factors affecting the susceptibility of coal to spontaneous combustion and the factors include: (1) Coal rank and petrographic composition, (2) Moisture content and volatile matter content; (3) Mineral matter type and pyrite content; (4) Particle size and physical properties; (5) Oxidation history and weathering. Among them one important intrinsic factor is rank of coal and coal rank is a measure of the extent of organic metamorphism of a coal, ranging from low-rank peat to high-rank anthracite [126]. It has reached a general consensus that low-rank coals are more liable to spontaneous heating than high-rank ones. Coal reactivity is a multi-factor driven parameter and it is difficult to determine their relative effects by varying one factor while retaining the others unchanged. As a result it appears impossible to develop a mathematical sense to consider all the factors in a numerical solution so the normal procedure is to manipulate the Arrhenius constants to denote different reactivity of different coals. This is plausible because the Arrhenius empirical constants are derived via real experimental data which might, to some extent, reflect the true nature of coal. Many studies have adopted this approach to investigate the influence of coal reactivity on self-heating behaviour of coal stockpile but what caused the variation of coal reactivity or Arrhenius parameters was not clearly stated. It is suspected the variation may attribute to some intrinsic factors of coal (e.g. coal rank, maceral or

physical composition) rather than some extrinsic ones (e.g. moisture content or coal particle size) because the external factors would have effects on both coal reactivity and other properties of coal and coal matrix. Schmal et al. [55] examined the effect of reactivity of coal by assigning different values of pre-exponential factor, refer Figure 7. The lower value of frequency factor stands for a less reactive coal, while the intermediate value represents a normal coal and the higher value signifies a more reactive coal. It is very noticeable the maximum temperature rise most rapidly for a more reactive coal due to faster coal oxidation which accompanies with more heat generation. A striking trend is that maximum temperature rise more slowly than that of a plain coal for a long run. A possible elucidation is that the hot spot of a more reactive coal stockpile move towards to the surface due to the depletion of oxygen. While the heat transferred by conduction is more efficient near surface, which results a pseudo steady state for a long run. However, the situation is very unlikely to occur because long before that the coal would become very inert. Brooks and Glasser [58] also studied coal reactivity by using different Arrhenius constants, refer Figure 8. In the model coal particle size was considered as an independent factor while maximum temperature was a dependent variable. It was found that pre-exponential factor is a more critical parameter than activation energy because safe particle size range varies more significantly with pre-exponential factor (Figure 8(a)) than with activation energy (Figure 8(b)).

Krishnaswamy *et al.* [62] investigated the effect of coal reactivity by using three values of pre-exponential factor for coal beds with various porosities, refer Figure 9. It was found from Figure 9(a) that decreasing the reactivity tenfold has little impact on the susceptibility of a coal stockpile to thermal runaway occurrence but the time required would be considerably extended. The reactivity of coal does not impact the self-ignitibility for a long run and it appeared to depend primarily on the amount of oxygen within the stockpile. Krajčiová et al. [78] studied the effects of coal reactivity by choosing four different coals among which Wyoming coal and Talcher coal are two extreme types with high pre-exponential factor ($8.83 \times 10^6/s$) and low activation energy (26 kJ/mol) respectively. It took approximately 10 days and 20 days to reach critical coal temperature for Wyoming coal and Talcher coal respectively. Therefore it might be summarised that more reactive coals (smaller value of activation energy and larger value of pre-exponential factor) could considerably decrease induction period for a coal stockpile to reach the critical temperature and for less reactive coals, thermal runaway is still possible to occur but would take longer.

The reactivity of coal also often correlates to the deterioration effect (also the Elovich effect) as more and more active sites attached to the surface area of coal are consumed with elapsing of time. Nordon and co-workers [54, 107] incorporated Elovich constants in the oxidation rate equation (Equation 43) to examine the deterioration effect of a

supercritical bed, as can be seen in Figure 10(a), the occurrence of thermal runaway totally changes with or without presence of Elovich constants. Schmal et al. [55] employed two rate reduction approaches (i.e. linear reduction and exponential reduction) to mimic the loss of reactivity, it was found that, unlike Nordon's result, it would not affect the occurrence of thermal runaway but the induction time is appreciably extended, refer Figure 10(b). Hence more numerical assessments are required to justify the influences of reactivity loss with time. The converged effects brought by the Elovich mechanism and Arrhenius mechanism at low temperature coal oxidation may introduce a new dimension for numerical simulation of self-heating behaviour on a coal mass although it may make the estimation of induction period less conservative.

$$\frac{dq}{dt} = r_r \exp[-(E + \alpha RTq)/RT] \quad (43)$$

4.2 Coal particle size

Increasing (or decreasing) coal particle diameter has two independent impacts on self-heating behaviour of a coal stockpile. One effect is to decrease (or increase) reaction rate of coal oxidation due to less (or more) exposure of inner surface of coal and another impact is to enhance (or reduce) permeability of coal mass. For coal particle sizes ranging from a few hundred microns to a few centimetres, it is widely reported that the rate of oxidation increases with a decrease in particle size because more internal surface area is exposed and most of the coal reaction surface is within the coal particle rather than on the exterior surface.[15, 23, 28, 65, 67, 95, 112, 113, 127]. The oxidation rate is widely reported to be inversely proportional to 0.1~0.7 power of particle size [15, 73, 95, 113, 127, 128]. However it has also been found the rate is independent of particle size if particle diameter is below a critical value. The values of critical diameter of coal particle were reported to be 2.31mm [116], 1mm [7], 5mm [23], and 0.05mm [127]. The difference of these values may attribute to coals with varying porosities and different testing configurations. To understand the physical and chemical connotation of the critical particle size, an illustration which divides the oxidation of a coal particle into three reaction regimes is given. As is well known, solid (coal)-gas (oxygen) reaction falls into three regimes, namely (a) kinetically dominated (b) kinetically and pore-diffusionally controlled (c) external mass transfer governed [16, 112, 116], refer Figure 11. Regime (a) often occurs in a very porous coal particle where overall oxidation rate is dominated by intrinsic chemistry of coal, oxygen molecule will diffuse deeply into the coal and the internal oxygen concentration (or concentration in pores) is equal to the bulk oxygen concentration. In the chemically-controlled regime, the gas transport restriction imposed by pore diffusion is eliminated and chemical composition and/or the number of reactive sites on the coal surfaces may be able to greatly influence reactivity. The reaction rate would be independent of coal particle size because the maximum diffusion capacity exceeds the amount of oxygen consumed by chemical reaction even within a

558 large diameter of coal particle. Reactions in regime (b) are characterized by less porous coal with higher effective
559 diffusivities for molecular oxygen. The chemical reaction is slower than diffusion, allowing gaseous oxygen to diffuse
560 into the coal particle before reacting. Oxygen concentration near the external surface approaches bulk concentration and a
561 concentration profile within the pore is expected. In this case the overall reaction rate is controlled by the combined
562 effects of chemical reaction and oxygen diffusion and is influenced by coal particle size. An extreme case may occur
563 (regime c) for a nonporous coal particle or a coal with strong internal diffusion limitations where the oxidation mostly
564 occurs on the superficial surface without any external diffusion resistance. Chemical reaction is fast relative to mass
565 transfer and therefore, oxygen concentrations on the external surface are close to zero. In this case reaction rate is
566 considered to be inversely proportional to the particle size. This regime occurs mainly in combustion at high
567 temperatures and is not the subject of low temperature oxidation [112]. The implication of critical value of coal particle
568 diameter is at which the oxygen diffused in internal and external surface equals to the maximum capacity of oxygen
569 consumption for low-temperature coal oxidation. Below the critical diameter the reaction of oxygen with coal falls into
570 fully chemical dominated regime (regime a) and any further reduction in coal particle size will not promote the reaction
571 rate. It is suspected the critical diameter of coal particle is relatively larger for a porous coal to a less porous coal.

572

573 To examine the effect of particle size on the rate of oxidation in a large coal stockpile, Akgun and Arisoy [112]
574 conducted a series of tests in a large testing cylinder by using four ranges of diameters (i.e. 2-5mm, 5-10mm, 15-20mm,
575 and 20-50mm) of a Turkish coal. The reported kinetic parameters of four coal samples are summarised in Figure 12. As
576 can be observed, a noticeable trend is both activation energy and pre-exponential factor drop with increasing diameters
577 and the variance of pre-exponential factor is more obvious than that of activation energy. The reduction of pre-
578 exponential factor correlates to less availability to surface reaction area and more restrictions for oxygen to diffuse into
579 interior of coal particle. The physical meaning of this reduction in activation energies is that the overall rate of oxidation
580 becomes less sensitive to temperature as particle size increases which may imply the transition of reaction regime from (b)
581 to (c). This is due to mass transfer regime might be dominated in large and intact particles and mass transfer is less
582 sensitive to temperature rise. Karnser and Perlmutter [116] and Kam et al. [100] also reported the reduction of activation
583 energy with larger diameter of coal particle. It was also indicated the apparent activation energy is approximately 20
584 kJ/mol if reaction rate is limited by external mass transfer and 63 kJ/mol for a very porous coal of which reaction rate is
585 governed by intrinsic chemical reaction [116]. While for coal reaction rated by combined effect of chemically and
586 diffusion control the value of activation energy is in the between [100]. It appears the reaction regime of four coal
587 particle size in Figure 12 falls into reaction regime (b) and further calculation reconfirmed this finding [112].

588

589 As the oxidation rate of most coals might be restricted by internal diffusion and therefore, for most cases reaction rate of
590 coal increases with decreasing diameter. It ought to note that a decrease in diameter can decrease the permeability of coal
591 mass (reduce particle size by twofold reduces the permeability by fourfold, Equation 36) and thus decrease the
592 availability of oxygen within coal stockpile as well. To examine the net effect, Edwards [67] scaled the value of pre-
593 exponential factor with direct ratio of particle diameter, which implies the reaction rate is governed by external mass
594 transfer. Three sizes of coal particles (0.05625mm, 0.1125mm, and 0.225mm) were studied in a wind-driven convection
595 model and the result is illustrated in Figure 13(a). The result shows a reduction in coal particle diameter, as a net effect,
596 leads to a greater increase in the maximum coalbed temperature and the hot spot moves towards surface of coalbed due to
597 starvation of and more difficulty to transport oxygen. As can be observed from Figure 13(b), Arisoy and Akgun reported
598 a similar finding that an increase in particle diameter cause less temperature rise but hot spot transports towards deeper
599 region of coalbed. In this study the reaction regime was considered to be chemically and pore-diffusion controlled
600 oxidation and the dependence of the reaction rate on particle diameter was described by defining an effectiveness factor
601 which is partly governed by particle size.

602

603 Krishnaswamy *et al.* [62] indicated the effect of particle size on bed permeability is more pronounced than its effect on
604 reaction rate in which an effectiveness factor was also introduced. In comparison of three sub-figures of Figure 14, it is
605 not hard to observe decreasing particle size is tending to catch an occurrence of thermal runaway more readily and
606 rapidly. It has also been noticed for low porosity (0.06) of coal stockpile with small particle, the thermal runaway would
607 not occur due to extreme transport restrictions of oxygen. However for a large particle, the fire incident is still likely to
608 outbreak for a long run, refer Figure 14(c). Thus the influence of particle size on pile permeability is deemed more
609 critical than that of global reaction rate. In consideration of the good limitation of oxygen ingress to a fine particle
610 stockpile, Yang *et al.* [31] demonstrated using fine particle coal coating coal stockpile could significantly decrease the
611 temperature rising rate. In practice, a possible strategy would be: (i) If a coal is very porous and the critical size of the
612 coal is quite large which implies coal reaction regime is chemically controlled, it is favourable to stack stockpile with
613 fine particle to restrict oxygen ingress because particle size has limited effect on reaction rate; (ii) whilst if a coal is less
614 porous and its critical size is very small which means the reaction is governed by oxygen diffusion and/or external mass
615 transfer, it is possibly safer to pack stockpile with large particles to slow down coal oxidation rate. However, it requires
616 more numerical assessment and field demonstration prior to any implementation with due consideration of alleviating the
617 self-heating hazard by changing particle size.

4.3 Porosity

Porosity represents the degree of compaction of a coal stockpile and its value has been generally categorised into three ranges to stand for three compaction scenarios [30, 55], refer Table 3. Porosity is a parameter which can be varied in practice by means of compaction and it has been a routine procedure for coal handlers to compact coal stockpile periodically due to more restriction of oxygen ingress for a more compacted pile [58, 64]. A detailed examination indicates an increase in porosity of a coal stockpile could affect self-heating behaviour in four aspects: (i) attract more airflow into stockpile and thus enhance availability of oxygen; (ii) provide more convective flow within pile and hence increase heat dissipation via convection in a non-equilibrium thermal model [64]; (iii) incur more difficulty to transfer heat via conduction due to more inter-particle clearance [55, 115]; (iv) has less reactive material per unit volume of pile. It has been showed that limitation of oxygen transport due to more compaction has an overwhelming effect on the self-heating process in many models [26, 55, 62, 67, 78, 115] and some of the representatives results are given in Figure 9, Figure 14, and Figure 15. It is obvious that at low porosities (0.06 for Krishnaswamy's model, 0.05 for Schmal's model, 0.165 for Edwards's model, and 0.1 for Fierro's model), the incident of thermal runaway is less likely to occur. While an exceptional result is given in Figure 15(d) which shows thermal runaway still outbreaks at low porosity of 0.1 for a stockpile composed of coarse particles (diameter >20mm). The similar finding has also been previously reported by Figure 14(c) with 9.6mm coal particle. This might attribute to only the large particle size has secured sufficient permeability as indicated by Equation 36 regardless the value of porosity.

There are two more studies presenting exceptional results [58, 64], refer Figure 16. As can be seen from Figure 16(a), thermal runaway will not occur in 80 days for porosity of 0.2 and for porosity of 0.3, maximum temperature rises steeply and thermal runaway takes place within 50 days. Interestingly, for porosity of 0.4, maximum temperature rises even more gently than that of porosity of 0.3. A possible explanation is that increasing the porosity results in more convective flow which enhances the heat dissipation and reduces the temperature rise. Despite of slightly slow temperature rise of porosity of 0.4 the thermal runaway still takes place which implies it is not an effective control measure to increase convection slow in this way. Additionally, as suggested in Figure 16(b), compacting coarse coal might be detrimental. A possible reason is the effect of having more reactive material per unit bed volume outweighs the effect of reducing oxygen ingress [58]. In consideration of all effects brought by porosity, it is concluded that periodic compaction of coal stockpile is able to prolong induction time but unable to make a stockpile unconditionally safe. The value of porosity is suggested to be below 0.2 for long time storage and extra pre-cautions needs to be taken upon compaction of a coarse stockpile.

648 4.4 Moisture

649 There have been many instances of combustible materials like linen stacks and grain-dust stockpiles being ignited by
650 moisture and this has been attributed to the latent heat of condensation, heat of adsorption (wetting) in the case of direct
651 addition of liquid, or indeed both [129, 130]. Coal, however, unlike other combustible material, exerts much more
652 complex processes interacted with moisture. It has been reported water is present in coal particles as many forms and a
653 generalised classification is bulk, capillary, multilayer, and monolayer water [131-133]. Bulk water dwells at the external
654 surface of coal particles or in the inter-particle voids and water condensed in a coal pore structure is usually denoted as
655 capillary water. Multilayer water, occurring in thin layers next to the walls of coal pores (a few molecular diameters in
656 depth), is weakly bonded to hydrogen atoms in coal aliphatic or aromatic structure, while monolayer water is strongly
657 hydrogen bonded to oxygen-containing functional groups at the pore surface [131]. More classifications of water in coal
658 can be derived in a review work conducted by Yu and co-workers [134]. The fact that water exists in many forms implies
659 the complex nature of coal-water interactions. Besides the mentioned physical interaction of coal with water, moisture
660 can also be a crucial part in chemical oxidation. The overall effect of moisture can be divided into two aspects, namely (i)
661 the effect of moisture transfer (evaporation, condensation, diffusion and convection) on the overall heat balance; (ii) the
662 effect of moisture (at equilibrium or during drying or wetting) on the rate of coal oxidation [135]. Moisture plays an
663 important part in determining the nature, rate and extent of self-heating in the stockpiled coal. It is widely reported water
664 in a coal may chemically and physically promote or inhibit coal oxidation and self-heating behaviour of coal. These
665 effects are briefly generalised and tabulated in Table 4 in which whether these effects were included in a numerical
666 solution is also discussed. The interactions between water vapour and coal can either exothermic or endothermic, mostly
667 depending on whether water condenses or evaporates. The equilibrium moisture content of coal is determined by the
668 difference between the humidity level of the surrounding air and the inherent moisture content [28]. It is thus necessary
669 to consider both of them simultaneously to study the effects of the moisture on the coal self-heating process. For example,
670 dry air flowing over moist coal stockpile will adsorb the moisture and leads in temperature decrease due to evaporation;
671 while moist air flowing over dry coal pile will condense the water vapour to coal surface and results in temperature rise
672 because of heat gain from condensation and wetting.

673 As inherent water plays a contradictory role in impacting consumption rate of oxygen, theoretically a critical moisture
674 range for a specific coal exists below or above which oxygen consumption rate is likely to be reduced. The implication of
675 the critical water content is that if water content is higher than this critical value, extra water forms multilayer at the
676 surface of coal pores increasing diffusion resistance for oxygen into interior of coal; whilst below this value, only a

677 portion of the active sites have access to the monolayer water molecules and this slows down the chemisorption reactions
678 [15, 131]. It has been suspected that the value of critical water content equals to the amount of water being adsorbed in
679 monolayer. Table 5 summaries some of the critical water contents for different coals. Due to existence of critical water
680 content and other complex interaction mechanisms of coal with water, extra precautions needs to be taken upon
681 preventing coal self-heating by spraying water.

682 The complex nature of the above effects hindered a comprehensive mathematical modelling as well as practical
683 applications. Consequently, many researchers only considered its physical effects by adding extra terms on energy
684 equations and mass equations in numerical solutions, refer Table 4. The heat of wetting is also not included because it
685 has been shown its value accounts for only 10% of the heat of evaporation [55] although it has been accepted
686 combustible material could be ignited by heat of “wetting”. As can be seen from Figure 17(a), moisture exhibits little
687 difference up to temperature 340K. However at higher temperature, the maximum temperature profile levels off at 350K
688 for a long period of time for a coal pile with 8% moisture content. This temperature rises again till the coal becomes
689 locally dry. At the pseudo steady state, it is postulated heat liberation due to oxidation approximately equals to heat
690 dissipation due to evaporation. This temperature level is maintained or slightly increased until the coal becomes totally
691 dry and then temperature may take off again. Not only the temperature rising rate is affected, the profile with distance
692 from surface of coal bed also has considerable difference, refer Figure 17(b). For a normal dry self-heating body,
693 generally the temperature profile across the body itself is roughly parabolic in shape with a peak at the hot spot [136],
694 like the result of dry coal. However the maximum temperature for moist coal becomes deeper and extended over a much
695 longer distance than for dry coal. Both phenomena are caused by the “heat pipe” effect, which is a very efficient heat
696 transfer mechanism and leads to a levelling of temperatures in a stockpile. The “heat pipe” effect appears even more
697 efficient at higher gas velocity as can be observed from Figure 17(c). The drying time is much shorter for a higher
698 velocity air stream. The calculations also implies the moisture can only serve to delay the onset spontaneous heating of
699 coal rather than a cure to this problem suggesting that safety of long-term storage of a coal stockpiles is independent of
700 moisture.

701

702 More calculations regarding effects of moisture for various airflow velocities were presented in Figure 18. Figure 18(a) is
703 the maximum temperature rising rate for both moist coal and dry coal with various airflow velocities. It can be seen
704 moisture has a great impact on self-heating behaviour and the levelling effect also manifest at high temperatures. There
705 are basically no differences between the heating rates of dry and damp coal initially because evaporation is very slow at
706 very low temperature. It can be also noticed the rate of temperature rise is greater at higher for dry coal for the entire

process and for moist coal only up to 330K. Upon the temperature the “heat pipe” effect governs the self-heating behaviour and the rate of temperature rise reduces owing to the more efficient water migration rate at higher velocities. The extended length of hot spot of wet coal was also reported, refer Figure 18(b). As the airflow velocity increases, the maximum temperature gradually drops and the length of the hot spot along the coalbed increases due to higher convective heat transport.

Figure 19 illustrates the influence of moisture on maximum temperature of a stockpile sourced from Akgun’s model [64]. In Figure 19(a) moisture levels of coal samples A, B, C are 16.8%, 1.8% and 35.4%, respectively. For coal B which is almost totally dry, the maximum temperature increases steadily with time as a normal case. For coal C which is very wet, temperature increases rapidly at the beginning and then evaporation becomes more effective and the temperature levels off. For coal A, the temperature rising profile resembles that of coal C but the steady state is much shorter than that of coal C probably because of quicker drying of coal A. However, Akgun’s calculation was running with a limitation that the chemical and physical compositions of the three coal samples are not identical and therefore it remains unclear whether moisture is the sole factor which causes the difference in the temperature ramping profiles of the three coal samples. One decade later Ejlali et al. claimed a similar finding in temperature rising profile for a wet stockpile [77]. Temperature rising profile of a wet coal underwent three stages: (i) slow rise due to self-heating, (ii) levelling effect due to energy exchange from alteration of water phase, and (iii) rapid rise due to drastic oxidation of dry coal at a relatively high temperature. Clearly numerical assessments on influences of moisture require to be substantially reinforced especially heat of “wetting” and how the moisture content affects coal oxidation kinetics need to be incorporated into the numerical model.

4.5 Wind

More recently intensive attentions have been drawn to study the complex effects of wind as more and more commercial CFD codes become available [26, 30, 72, 74]. Wind, as a kind of forced convection, plays a contradictory role in self-heating behaviour of a stockpiled coal. On one hand, the forced convection cools down the stockpile by taking more heat away; on the other hand, the wind is very likely to supply more oxygen into pile and generate more heat. Many studies used a constant velocity profile to mimic the wild wind [26, 62, 67, 115], to date a varying profile of incoming wind can be established either by power law [74] or log law [30] with the assistance of CFD code, refer Figure 20(a). Taraba et al. [74] further considered real changes in the velocity and direction of wind over time as deduced from meteorological data, refer Figure 20(b). It was also reported that the wind flow induces a wake region downstream from the pile and, consequently, creates an asymmetric pressure distribution, refer Figure 21.

737

738 To understand how air is transported into stockpile, the main requirement is a knowledge of the distribution of the
739 pressure around the pile. When wind confronts coal stockpile, locally higher velocity region is induced and higher
740 stockpile is more likely to result in even greater local velocity. Have another glance of momentum conservation equation
741 (Equations 37 and 39) it is not hard to notice that higher local velocity will contribute to more significant pressure drop.
742 Therefore lower pressure region where wind meets a higher obstacle, stockpile in this case, will be created and this lower
743 pressure region will draw air in. This quantity of pressure drop is conveniently presented in non-dimensional term using
744 the concept of a pressure coefficient [137]. The pressure coefficient, C_{Pr} , is defined via

745
$$C_{Pr} = \frac{2(P-P_0)}{\rho_{am}V^2} \quad (26)$$

746 Both Moghtaderi *et al.* [30] and Taraba *et al.* [74] reported the highest pressure is exerted at the front bottom of the pile
747 where the air flow is brought to rest (i.e. local velocity approaches zero) and pressure drops substantially at the top of the
748 pile before tailing off, refer Figure 22.

749

750 Moghtaderi *et al.* [30] and Akgun and Essenhigh [64] agreed that at initiation of oxidation, the resultant self-heating
751 rapidly becomes non-uniform throughout the pile and two local hot spot with maximum temperature will be created at
752 either side of the pile symmetrically when there is no wind. However it would be a totally different story with presence of
753 wind. Given that the equilibrium of symmetric mass transport and heat transfer is broken due to the wind, the distribution
754 of the hot spot is supposed to be asymmetric and indeed, almost all literatures agree this but the location of the hot spot
755 differs based on different models. Many models [30, 62, 74, 115] indicated that the hot spot always locates on the
756 windward side, while Zhu *et al.* [26] stated the location of the hot spot will move to the leeward for a coarse particle
757 stockpile with the increase of the velocity of wind. A possible reason is that more space and inter-particle channels can
758 be generated in a coarse coal stockpile and a stronger forced convection is induced at the windward side of the pile.
759 When wind becomes stronger, heat dissipated by the forced convection exceeds that generated by the oxidation and as a
760 result the hot spot moves to the deeper side or even the leeward side of the pile. Besides the lateral motion of hot spot,
761 Taraba *et al.* [74] further reported a vertical movement of the hot spot in the stockpile, refer Figure 23. At the initial stage
762 of self-heating (346K) the hot spot locates at top corner of windward side, it gradually moves to the bottom as self-
763 heating develops to an advanced stage (>397K). The buoyancy effects were deemed as a possible reason for the vertical
764 motion of the hot spot. Naturally convective airflow driven by buoyancy evidently promotes dissipation of the oxidation
765 heat in a hot spot located in the upper part of the pile and as a result, heat accumulation optimally commence to be
766 located at the bottom of the pile where the cooling effect of natural convection is weak. The ultimate location of hot spot

767 was demonstrated by field observation of another study [31], refer Figure 23. It can be seen the smoke and smouldering
768 fire locates at bottom of the stockpile and hence and coating stockpile bottom with fine particle coal can significantly
769 alleviate the hazard due to reduced ingress of oxygen into bottom zone.

770

771 Many studies also confirmed that the maximum temperature in the hot spot increases with the increased wind velocity
772 and some of the representative results are given in Figure 25. It appears the effects of more oxygen drawn into stockpile
773 promoting heat generation outweigh the effects of more heat dissipation via convection of higher wind velocity. It can be
774 also observed heat loss due to more wind convection has very limited effects especially at low temperature range, refer
775 Figure 25(d). Therefore installing artificial wind barriers confronting wind prevailing direction could be a possible
776 control to prevent self-heating and spontaneous combustion of the coal stocked [72, 138].

777 **4.6 Stockpile height**

778 For a specific spatial shape of stockpile decreasing pile height is widely reported to be capable of prolonging induction
779 period [26, 32, 64]. An apparent reason is heat for a lower stockpile can more readily be dissipated by conduction. Figure
780 26 shows influences of stockpile height on self-heating behaviour of stockpiled coals. A general trend is decreasing
781 stockpile height can make a safer stockpile. Thus the risk of spontaneous combustion on coal stockpile can be reduced by
782 stacking low pile. In addition, Akgun and Essenhigh [64], Zhu *et al.* [26], both agreed that a specific pile has a critical
783 value of pile height (1m in Akgun's model, 3m in Zhu's model) below which the stockpile becomes intrinsically safe or
784 can be safely stored for a very extended period of time. Each coal stockpile has a unique critical height and the critical
785 height is affected by many other factors like coal reactivity and moisture content. It is also found that the maximum
786 temperature rises of different coal piles have different sensitivities to pile height. If coal is very reactive and dry,
787 maximum temperature rise is very sensitive to the pile height. While if coal is very moist the occurrence of thermal
788 runaway exhibit independence of stockpile height, refer Figure 26(c). In practical coal storage and handling operation,
789 the pile height and storage capacity must be considered simultaneously because of the limitation of area of storage yard.
790 If a critical height of a reactive coal pile is less than 1m, it is obviously not suitable to stack that low pile in practical
791 operations. Figure 27 plots the loading capacity of a single stockpile in varied pile heights and slopes. Here a standard
792 truncated pyramid pile is assumed to be 100m long and 50m wide, and density of bulk coal is roughly 1.12t/m³
793 considering porosity of 0.2. It can be clearly seen from Figure 27(a), storage capacity of a single pile is becoming
794 increasingly insensitive to pile height and this insensitivity becomes more manifest at a gentle slope. For a very reactive
795 and gentle slope coal stockpile, decreasing pile height will considerably improve safe storage time and incur less loss of

the storage capacity. For a less reactive or very moist coal, increasing pile height will improve the storage capacity of pile and have less impact on self-heating behaviour.

4.7 Stockpile slope

Slope angel influences the self-heating process through wind-induced pressure gradient distribution. In the case of stockpiles with gentle slopes, the wind-induced pressure driving force for convective flow is smaller than for steep slopes. Two extreme situations are exemplified. If the wind attacks a very gentle or nearly flat pile, the variation on wind velocity will be negligible and therefore the effects on pressure variation can be ignored as well. If the airway is partial blocked by a nearly vertical porous pile, the local wind velocity will significantly rise and result in huge pressure coefficient drop. Therefore more air flows into the stockpile with a steeper slope and more oxygen can be supplied for coal oxidation. Figure 28 gives some of representative results of the effects of varying slopes on self-heating process of coal stockpile. Krishnaswamy *et al.* [62] indicated for a gentle slope, most porosities of stockpile is safe except for porosities above 0.3, while for a steeper slope, most porosities are not safe except for extremely low porosity of 0.06. Akgun and Essenhigh [64] also found that the self-heating behaviour is very sensitive to the side slope. As the slope decreases, the period of time when thermal runaway occurs considerably increases. However when it comes to a coarse particle stockpile (particle diameter>20mm), the pile slope has a very limited effect on self-heating behaviour [26]. A possible reason is big diameter of coal has secured enough permeability of oxygen ingress so slope has limited influence. It can be seen from Figure 27(b) the storage capacity of single pile is less dependent of side slope at lower heights. Thus for a low stockpile (<10m), a gentle slope can be employed to slow down self-heating process with less loss to the storage capacity.

5 Challenges and perspectives

As discussed self-heating of coal stockpile is a result of several complex processes and therefore most numerical models were developed with excessive assumptions and simplifications. The consequence of it is accuracy of the numerical outcome is questioned and even unable to meet engineering demand. Due to the lack of knowledge of coal oxidation mechanism, the mathematical description of oxygen consumption rate and heat generation rate would be a major dilemma. As indicated many investigators employed a simple Arrhenius dependence in defining coal oxidation rate and heat release rate in numerical models. This might be acceptable after coal thermal runaway occurs but the accuracy could be beyond engineering demand at low temperature as the time dependent term (i.e. the Elovich effect) is most effective at the beginning of the reaction [1]. The combination of Arrhenius and Elovich dependence could be a solution [1, 54] or utilization of two sets of Arrhenius parameters before and after thermal runaway could be an alternative [73, 74]. Although these treatments is very likely to make the result less conservative, the true nature of coal oxidation kinetics is

equally worthy of exploring. As previously discussed many studies introduced an effectiveness factor to describe the dependence of coal oxidation rate on particle size. The nature of this approach is to mathematically manipulate the oxygen transport limitation with the effectiveness factor upon changing particle size but the Arrhenius parameters remains constants. In fact Arrhenius parameters changes with particle size especially the pre-exponential factor varies considerably with particle size [112]. Therefore more tests are required to be undertaken to define the dependence of Arrhenius parameters on particle diameter. This approach may deal with effects of particle size on coal reaction rate more properly and the reaction rate is more conveniently to be described in a numerical model. Moisture affects self-heating behaviour of coal in many aspects but the previous models mainly considered heat transport arise from evaporation and recondensation. There are two effects of moisture should be worthy of more inspections: inclusion of heat of “wetting” and how oxidation rate varies with moisture contents owing to more/less exposure of oxidation surface. The inclusion of heat due to adsorption of moisture could be simulated by an increment of initial temperature. However the magnitude must be considered carefully because it is affected by the inherent moisture content of coal and humidity level of environment coal is stored [22] and more critically, the influence of initial temperature on self-heating behaviour of coal stockpile could be enormous [55]. How the moisture influences the coal oxidation rate is troublesome as dewatering or wetting of coal might be a highly dynamic process. The testing method in literature [139] might be a solution to define the reaction constants for different moisture contents of coal. How to enhance applicability of numerical models is also a major obstacle. To maintain simplicity and save computation load, most models were developed in one or two dimensions. Whilst a three dimensional model is in need as it is capable of providing a more clear picture of self-heating behaviour of a coal stockpile. To achieve that validation of the model would be paramount as many extrinsic factors would be functioning. A possible validation method would be the erection of wind, rain, solar radiation, and varying ambient temperature profiles accompanied with scattered temperature monitoring points inside stockpile. In addition more numerical assessments should be conducted to evaluate the control measures like wind shield, coating stockpile with inert and fine substances, and spraying coal particle with chemical inhibitor because research in this direction is scarce so far.

6 Summary remark

The phenomenon of self-heating of coal stockpile is a result of complex physical processes (e.g. airflow in porous coal stockpile, heat and mass transfer) and chemical processes (e.g. coal oxidation accompanied with heat liberation, interaction of coal with moisture). This hazard can be harmful in various aspects and be very persistent due to capability of coal oxidation at low-temperature. Equally important to practical mitigations, theoretical solutions draw immense attentions especially for prediction and management of the hazard. As an advanced tool numerical modelling has been

856 widely applied in investigating the transient self-heating behaviour of coal mass since last four decades. No doubt
857 substantial developments have been acquired but many findings needs to be critically reviewed and examined with
858 aiming to provide more comprehensive guidance to industry and to give inspiration of future works. This work firstly
859 investigated the mechanisms of self-heating of coal mass including interaction of coal with oxygen and characteristic
860 behaviour of heat and mass transfer at coal particle scale. The hazard is possible to take place if heat generated from coal
861 oxidation outweighs its dissipation via conduction and convection. On basis of the mechanistic understanding, derivation
862 and development of key theoretical terms of previous models were reviewed and compiled. It has also been recognised
863 the hazard is dependent on many factors like coal property, geometric feature of a stockpile, particle size and associated
864 compaction. To gain deep insights of the problem and deliver more objective guides to industry, variable analyses were
865 undertaken and several meaningful findings are listed:

- 866 a) Reactive coals are more readily to catch an occurrence of thermal runaway but less reactive coals are never
867 unconditionally safe. Pre-exponential factor appears to be a more critical parameter than activation energy if
868 Arrhenius reaction mechanism is employed;
- 869 b) Effect of coal particle size still remains a puzzle and requires further study. A possible strategy is: (i) If the
870 critical size of a specific coal is quite large, it is favourable to stack stockpile with smaller particle or coating it
871 with fine particles to restrict oxygen ingress; (ii) whilst if critical size is very small it is possibly safer to pack
872 stockpile with large particles to slow down coal oxidation rate;
- 873 c) Periodical compaction of stockpile can increase the induction period but need to keep porosity less than 0.2.
874 Extremely low porosity could make a stockpile intrinsically safe and extra precautions requires to be taken upon
875 compacting a coarse stockpile;
- 876 d) Temperature rise of a moist coal may undergo three stages: (i) slow rise due to self-heating, (ii) levelling effect
877 due to energy exchange from alteration of water phase, and (iii) rapid rise due to fast oxidation of dry coal. Extra
878 precautions are also required if control a heating hazard of stockpile by spraying water due to the existence of
879 critical water content;
- 880 e) Self-heating accelerates with increasing incoming wind velocity; both horizontal and vertical motion of hot spot
881 was observed with stronger wind;
- 882 f) Lower and gentle stockpile is safer in terms of prolonging incubation period but will compromise the loading
883 capacity of single stockpile. For a low stockpile (<10m), a gentle slope can be employed to slow down self-
884 heating process with less loss to the storage capacity.

885 Due to the complex nature of this problem, numerical models were often developed with too many assumptions and
886 simplifications. This subject faces two major challenges: one is the lack of a more reliable kinetic modelling of coal
887 oxidation especially at low temperature and another one is how to enhance its applicability. A new dimension is
888 introduced if more numerical assessments are conducted with due consideration of combined Arrhenius and Elovich
889 effect although this may make the result less conservative. More studies of effects of particle size are in need especially
890 how the Arrhenius parameters differ with different ranges of particle size. Heat of moisture adsorption and how coal

reactivity evolves with progressive drying of coal are two factors worthy of exploring upon considering effects of moisture on self-heating of coal stockpile. To enhance practical significance of this subject, a validated solution in three dimensions is in need. Erection of profiles of several internal temperature monitoring points with more considerations of local meteorological conditions like rainfall, varying ambient temperature, and gusty wind may facilitate the validation. More numerical assessment of control measures, like installing wind barrier, coating with fine particle substance, or spraying chemical inhibitor are also inspiring as studies in this directions are rare.

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(a) Alabama, U.S. [140]

(b) Jharia coalfield, India [141]

(c) Wuda coalfield, China [25]

(d) Hedland port stacker fire, Australia [142]

Figure 1 Photographic views of fire of stockpiled coal from the worldwide

Figure 2 Illustration of major steps for a numerical solution and work scope of this study

Figure 3 Schematic process and main feature of coal stockpile self-heating

Figure 4 A schematic view of heat and mass transfer between coal particles

Figure 5 Two processes of low-temperature interaction of coal with oxygen [92]

Figure 6 Two examples of non-Arrhenius behaviour of coal oxidation rate at low temperature (a) Plot of $\ln(\text{heat release})$ against $1/T$ for a China coal [110] (b) Plot of $\ln(dT/dt)$ against $1/T$ for an Australia coal [1]

Figure 7 Influence of pre-exponential factor on maximum temperature in a dry coal stockpile [55]

Figure 8 Influence of reactivity on maximum temperature of a coalbed [58]

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Figure 9 Influence of reactivity (pre-exponential factor) on maximum temperature [62]

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Figure 10 Influence of deterioration (reactivity reduction) on self-heating of coalbed [54, 55]

Figure 11 A schematic illustration of three coal oxidation regimes

Figure 12 Influence of coal particle size on kinetic constants and oxidation regimes

Figure 13 Influence of particle size on maximum temperature and location of hot spot [65, 67]

Figure 14 Influence of average particle diameter on temperature rise for various bed porosities [62]

Figure 15 Effect of pile porosity on self-heating behaviour [26, 55, 67, 115]

Figure 16 Exceptional findings of effect of pile porosity on self-heating behaviour [58, 64]

Figure 17 Influence of moisture on self-heating behaviour of a coalbed [55]

Figure 18 Influence of moisture on self-heating behaviour of a coalbed [65]

Figure 19 Influence of moisture on self-heating behaviour of three coal stockpiles [64]

(a) A log law governed vertical wind profile [30] (b) A representative fluctuation of wind velocity [74]

Figure 20 Profile of inlet wind velocity

Figure 21 Wake region induced by wind encountering a coal stockpile [30]

(a) Taraba's model [74]

(b) Moghtaderi's model [30]

Figure 22 Variation of the pressure coefficient around stockpile

Figure 23 Vertical shift of hot spot at various stages of self-heating: (a) 346 K; (b) 370 K; (c) 397 K; (d) 475 K [74]

Figure 24 Field observation of self-heating of coal stockpiles [31]

Figure 25 Influence of wind velocity on self-heating behaviour of coal stockpile: (a) Taraba's model [74] (b) Krishnaswamy's model [62] (c, d) Fierro's model [115]

Figure 26 Influence of stockpile height on self-heating behaviour of coal stockpile: (a, b, c) A moderate moist coal, a dry coal, a very damp coal [64] (d) a coarse coal stockpile [26]

(a) Varied pile height at different side slopes

(b) Varied side slope at different heights

Figure 27 Storage capacities of stockpiles with different pile heights and side slopes

Figure 28 Influence of bed slope on self-heating behaviour of coal stockpile: (a, b) sourced from [62] (c) Akgun's model [64] (d) Zhu's model [26]

1294 **Table 1 Comparisons of kinetic models developed by various investigators [15]**

Reference	Temperature range (°C)	Reaction mechanism	Model features
[99, 100]	200~225	➤ Direct burn-off reaction $\text{coal} + \text{O}_2 \rightarrow \text{CO}_2, \text{CO}, \text{H}_2\text{O}$ ➤ Sorption sequence $\text{coal} + \text{O}_2 \rightarrow \text{complex} \leftrightarrow \text{CO}_2, \text{CO}, \text{H}_2\text{O}$	❖ Prediction of oxygen consumption and gaseous products (CO_2, CO and H_2O), ❖ Analytical solutions for the reaction rates, as a sum of constant and exponential decay terms, ❖ Stoichiometric correlation between the reactants and the gaseous products
[95, 96]	150~160	➤ Direct burn-off reaction $\text{coal} + \text{O}_2 \rightarrow \text{CO}_2, \text{CO}$ ➤ Sorption sequence $\text{coal} + \text{O}_2 \leftrightarrow \text{physisorbed O}_2 \rightarrow \text{chemisorbed O}_2 \rightarrow \text{CO}_2, \text{CO}$ ➤ Separate water production $\text{coal} + \text{O}_2 \rightarrow \text{H}_2\text{O}$	❖ Prediction of oxygen consumption, gaseous products (CO_2, CO and H_2O) and solid intermediates, ❖ Site conservation among various active sites, ❖ Numerical solution of the model
[8, 9]	25~95	➤ Direct burn-off reaction $\text{coal} + \text{O}_2 \rightarrow \text{CO}_2$ ➤ Sorption sequence $\text{coal} + \text{O}_2 \rightarrow \text{oxycoal} \rightarrow \text{CO}_2$	❖ Prediction of oxygen consumed and carbon dioxide produced, ❖ Conserved active sites and exponential decay in the active sites for oxygen adsorption, ❖ Analytical solutions for the rates
[90]	60~90	➤ Direct burn-off reaction $\text{coal} + \text{O}_2 \rightarrow \text{CO}_2, \text{CO}, \text{others}$ ➤ Sorption sequence $\text{coal} + \text{O}_2 \rightarrow \text{carboxyl} + \text{carbonyl} + \text{CO}_2 + \text{unre active species}$, ➤ Carboxyl species $\rightarrow \text{CO}_2$ ➤ Carbonyl species $\rightarrow \text{CO}$	❖ Prediction of oxygen consumed and carbon oxides produced, ❖ Self-conserved active sites and reduction in active sites due to the formation of unreactive species, ❖ Analytical equations for the rates

Table 2 Main features and parameters of numerical solutions to self-heating of coal (char) mass

Reference		Main features					Chemical reaction parameters					Physical properties of coal (mass)						
		Coal type	Transien t(T)/Stea dy(S)	Spatial dimens ionalit y	Moisture(Y-yes/N- no)	Transport mechanism		Reac tion order	Arrhenius constants		Reaction mechanism	Heat of oxidation	Averag e particle diamet er	Poro sity	Dens ity	Specifi c heat capacit y	Thermal conductivit y	Oxygen diffusion coefficient in gas phase
						Heat	Oxygen		Activat ion energy	Pre- exponenti al factor								
[23]		A U.S. lignite	T	1D	N	Conduction	Forced convection	1	50	-	Oxygen consumptio n	376 kJ/mol O ₂	-	-	801	2263	0.2	-
[54]		Yallourn briquette char	T	1D	Y	Conduction & convection	Diffusion & forced convection	1	66	-	Oxygen consumptio n	300 kJ/mol O ₂	-	-	-	-	-	-
[55]	Dry coal	-	T	1D	Y	Conduction & convection	Diffusion & forced convection	1	7	4.2×10 ⁻¹⁰	Oxygen chemisorpti on	3 kJ/mol O ₂	-	0.05, 0.2, 0.3	1500	1000	0.12	2×10 ⁻⁵
	Moist coal							0.7	7.5	2.1×10 ⁻¹⁰		3.7 kJ/mol O ₂						
[58]		-	S	1D	N	Conduction	Natural convection	1	58.2	3600	Oxygen consumptio n	300 kJ/mol O ₂	0.01	0.3	-	-	0.2	2×10 ⁻⁵
[60]		-	S	2D	N	Conduction	Natural convection	-	-	-	-	400 kJ/mol O ₂	-	-	-	-	0.16	-
[56]		-	S	2D	N	Conduction	Natural convection	1	58.2	3600	Oxygen consumptio n	300 kJ/mol O ₂	0.01	0.3	-	-	0.2	2×10 ⁻⁵
[67]	Force d conve ction model	High- volatile C bitumino us coal	T	2D	N	Conduction & convection	Forced convection & diffusion	1	90	1.23×10 ⁹	Oxygen consumptio n	300 kJ/mol O ₂	0.076	0.33	1300	1004	0.114	1.5×10 ⁻⁵
	Buoya ncy- driven model			2D	N	Conduction & convection	Natural convection & diffusion	1	90	1.23×10 ⁹			0.076	0.33				
	Wind- driven model			1D	N	Conduction & convection	Forced convection & diffusion	1	90, 76.6	1.23×10 ⁹ , 5.96×10 ⁷			5.625× 10 ⁻⁵ , 1.125× 10 ⁻⁴ , 2.25×1 0 ⁻⁴	0.33, 0.16 5				
[61]		-	S	3D	N	Conduction & convection	-	0	-	-	-	-	-	-	-	-	-	-
[65]		Turkish moist coals	T	1D	Y	Conduction & convection	Forced convection & diffusion	1	70	2.933×10 ₆	Oxygen adsorption	9375kJ/kg O ₂	0.01, 0.02, 0.03	0.3	1100	1000	0.2	2×10 ⁻⁵
[69]		-	S	2D	N	Conduction & convection	Natural convection & diffusion	1	58.2	3600	Oxygen consumptio n	300 kJ/mol O ₂	0.01	0.4	-	-	0.2	2×10 ⁻⁵
[62]		Weather ed Wyomin g subbitu minous coal	T	2D	N	Conduction & convection	Forced & natural convection	1	57.5	8.83×10 ⁶	Burn-off	-	0.023	0.09 6	-	-	-	-
[63]		-	T	1D	N	Conduction	Diffusion	1	57.5	8.83×10 ⁶	Oxygen consumptio n	330 kJ/mol O ₂	-	-	-	-	0.2	2×10 ⁻⁵

[68]	-	T	1D	N	Conduction & radiation	Diffusion	1	57.5	8.83×10^6	Oxygen consumption	330 kJ/mol O ₂	-	-	-	-	0.2	2×10^{-5}
[70]	Wyoming subbituminous coal	T	1D	Y	Conduction & convection	Natural convection & diffusion	1	57.5	8.83×10^6	Oxygen consumption	330 kJ/mol O ₂	0.003~0.015	-	-	-	-	-
[30]	Australian bituminous coal	T	2D	Y	Conduction & convection	Forced convection & diffusion	0.7	7.5×10^{-7}	2.1×10^{-10}	Oxygen consumption	11560 kJ/kg coal	-	0.3	1260	1423	0.12	1.2×10^{-5}
[64]	Turkish brown coals	T	2D	Y	Conduction & convection	Forced convection & diffusion	1	46.81, 30.64, 21.89	1758, 1.485, 0.424	Oxygen consumption	-	-	0.3	-	-	-	-
[143]	A China coal	T	1D	N	Conduction & convection & radiation	Forced convection & diffusion	1	40	10	Oxygen consumption	-	-	0.5	-	1500	3.4	2×10^{-5}
[115]	A Spain coal	T	1D	N	Conduction & convection	Forced convection & diffusion	0.52	42	2.8×10^{-8}	Oxygen consumption	380 kJ/mol O ₂	-	0.1, 0.13, 0.15, 0.17, 0.2, 0.25, 0.3	1566	1132	0.113	-
[78]	Four coals	T	2D	N	Conduction & radiation	Diffusion	1	40, 26.88, 58, 30.64	10, 6, 8.83×10^6 , 1485	Oxygen consumption	-	-	-	-	1500	3.4	2×10^{-5}
[75]	Three U.S. coals	T	3D	N	Conduction & convection	Forced convection & diffusion	0.61	66.5, 73.6, 88.3	1.9×10^6 , 1.1×10^7 , 4.4×10^8	Coal+O ₂ →CO ₂ +0.1C O	300 kJ/mol O ₂	-	-	1300	1003.2	0.1998	1.5×10^{-5}
[24]	A U.S. High volatile bituminous coal	T	3D	N	Conduction & convection	Forced convection & diffusion	0.61	66.5	1.9×10^6	Coal+O ₂ →CO ₂ +0.1C O	300 kJ/mol O ₂	0.02	0.3	1240	1003.2	0.1998	-
[73]	A Czech bituminous coal	T	3D	N	Conduction & convection	Forced convection & diffusion	1	23.5 (subcritical), 51 (supercritical)	1.85 (subcritical), 13700 (supercritical)	Oxygen consumption	250 kJ/mol O ₂	-	-	-	-	-	-
[77]	A lignite	T	2D	Y	Conduction & convection	Forced convection & diffusion	1	55	1000	Oxygen consumption	22000 kJ/kg coal	-	-	-	1500	0.12	-
[72]	-	T	2D	N	Conduction & convection	Forced convection & diffusion	0	0.75	2.1×10^{-10}	Coal+O ₂ →CO ₂	-	-	-	1200	1050	0.12	-
[26]	A China coal	T	2D	N	Conduction & convection	Forced and natural convection & diffusion	1	50	180	Oxygen consumption	400 kJ/mol O ₂	-	0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4	-	1003.2	0.2	2×10^{-5}
[74]	A bituminous coal	T	2D	N	Conduction & convection	Forced & natural convection & diffusion	1	22 (subcritical), 50.5	1.85 (subcritical), 13500	Coal+O ₂ →0.1CO ₂ +0.4 H ₂ O+1.4O-COal	270 kJ/mol O ₂	0.01	-	-	-	-	-

								(supercritical)	(supercritical)	(subcritical) ; Coal+O ₂ → 0.2CO ₂ +0.8 H ₂ O+0.01C O+0.79O- Coal (supercritical)							
[79]	-	T	2D	N	Conduction & convection	Forced convection & diffusion	1	21.89	1	Oxygen consumption	300 kJ/mol O ₂	0.04	-	1300	1003.2	0.2	2×10 ⁻⁵

1312 Table 3 **Different compaction degree of coal stockpile and according value of porosity**

Porosity	~0.1	~0.2	~0.3
Compaction degree	Densely Compacted	Loosely compacted	Uncompacted

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1314 Table 4 **Generalised effects of moisture in coal oxidation and self-heating**

Literatures	Promotion of coal oxidation and self-heating	Numerical solution
[22, 144]	Heat gain in adsorption of water	N
-	Heat gain from vapour condensation	Y
[2, 15, 145, 146]	Drying can free more active surface	N
[145]	Water is a critical element in oxidation of pyritic sulphur	N
[15, 131]	Facilitate the formation of unstable intermediates at the early stage of coal oxidation	N
[147]	Tightly bound moisture generates radical sites	N
Literatures	Inhibition of coal oxidation and self-heating	Numerical solution
[15, 131, 145]	Water can occupy active sites in coal surface and block pores	N
[148]	Vapour pressure in pores blocks access for oxygen	N
-	Heat loss from evaporation	Y
[50]	Water can increase effective thermal conductivity of coal mass and thereby facilitate heat dissipation	Y
[149, 150]	Drying might cause collapse of some pore structures	N

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1316 Table 5 **Reported critical water contents for different coals**

Literatures	Coal type	Critical moisture content/%
[146]	A New Zealand subbituminous coal	8.1
[145]	Brown coals	5~10
	Two lignites	6~7
	A sub-bituminous coal	~6
[23]	A U.S. lignite	~20
[151]	Brown coals	5~8
	Subbituminous coals	1.5~2
	Bituminous coals to anthracites	0.5~0.7
[135]	A New Zealand sub-bituminous coal	8.3
[131]	A Australia bituminous coal	<0.8

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Reference	Examined variables and assigned values										
	Coal reactivity	Particle size (m)	Moisture content (% by mass)	Stockpile height (m)	Stockpile slope (o)	Packing porosity	Airflow velocity (m/s)	Bed length (m)	Thermal conductivity(W m-1 K-1)	Initial temperature (K)	Oxygen concentration (%)
[23]	-	-	-	-	-	0.1, 0.125, 0.15, 0.175	-	-	-	-	-
[54]	Various values of activation energy (8, 20, 40, 60) and rate constants, Elovich effect	-	-	-	-	-	0, 1×10^{-5} , 2×10^{-5} , 5×10^{-5} , 2×10^{-4}	3.4, 4.5, 4.6, 8	-	-	-
[55]	Various values of pre-exponential factor (1.2×10^{-10} , 4.2×10^{-10} , 1.2×10^{-9}), deterioration effect	-	0, 8	-	-	0.05, 0.2, 0.3	2×10^{-7} , 2×10^{-6} , 6×10^{-6} , 2×10^{-5} , 2×10^{-4}	-	0.12, 0.2	283, 293	-
[58]	Various values of activation energy (53, 62, 71) and pre-exponential factor (1, 10, 100)	-	-	-	-	0.2, 0.3, 0.4	-	1, 5, 10	-	-	-
[67]	-	5.625×10^{-5} , 1.125×10^{-4} , 2.25×10^{-4}	-	-	-	0.165, 0.33	2.2, 4.4	-	-	-	-
[65]	-	0.01, 0.02, 0.03	Dry, moist	-	-	-	0.5×10^{-5} , 1×10^{-5} , 2×10^{-5}	-	-	-	-
[62]	Two values of pre-exponential factors (8.83×10^7 , 8.83×10^5)	0.0023, 0.0096	-	-	11.3, 14, 18.4, 20, 21.8, 26.6, 39.8	0.06, 0.12, 0.18, 0.24, 0.3, 0.36	0.45, 2.23, 4.46, 6.69, 8.93	-	-	-	-
[70]	Varying values of pre-exponential factors	0.003~0.015	0~30	-	-	-	-	-	-	293~333	-
[32]	-	-	-	0.85, 1, 1.2, 1.8, 2.4, infinite	-	-	-	-	-	-	-
[64]	Three coals with different Arrhenius constants	-	16.81, 1.81, 35.4	1, 1.5, 2, 3, 4, 5	26, 34, 45, 63	0.2, 0.3, 0.4	-	-	-	-	-
[78]	Various values of activation energy (40, 26.88, 58, 30.64) and pre-exponential factor (10 , 6 , 8.83×10^6 , 1485)	-	-	-	-	0.2, 0.3, 0.35, 0.4	-	-	-	-	-
[115]	-	-	-	-	-	0.1, 0.13, 0.15, 0.17, 0.2, 0.25, 0.3	0, 5, 10	-	-	-	-
[26]	-	-	-	3, 4, 5, 6, 7.5, 9	45, 56.3, 71.6, 80.5	0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4	0.001, 0.05, 0.5, 1	-	-	-	5, 8, 10, 15, 18, 21
[74]	-	-	-	-	-	-	1, 2, 3, 4, 6, 10	-	-	-	-