Computational study on self-heating ignition and smouldering spread of coal layers in flat and wedge hot plate configurations

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Abstract

Porous fuels have the propensity to self-heat. Self-heating ignition has been a hazard and safety concern in fuel production, transportation, and storage for decades. During the process of self-heating ignition, a hot spot forms at a specific location in the fuel layer and then spreads as a smouldering fire. The understanding of hot spot and smouldering spread is of importance for prevention, detection, and mitigation of fires. In this paper, we build a computational model that unifies the simulation of ignition and smouldering spread by adopting a two-step kinetic scheme. The model is validated against hot plate experiments of coal in both flat and wedge configurations. The comparison between predictions and experiments shows that the model predicts the minimum ignition temperature (T_{ig}) and transient temperature profiles reasonably well. The simulation results demonstrate that the hot spot originates at the hot plate and then spreads towards the free surface due to oxygen consumption. In the wedge configuration, the simulations show that the height of maximum temperature point decreases with increasing wedge angle and that the influence of wedge angle can be explained by the heat transfer. This model brings together the two combustion phenomena (self-heating ignition and smouldering) that were traditionally studied separately and analyses the transient behaviour of hot spot and smouldering spread in detail. It deepens our understanding of self-heating fire events and can help mitigate the hazard in the future.

Key words: Self-heating, ignition, smouldering, coal, and hot plate

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Nomenclature

A	pre-exponential factor,1/s
c	solid specific heat capacity, J/kg-K
C	gas specific heat capacity, J/kg-K
D	mass diffusivity, m^2/s
E	activation energy, kJ/mol
$\bar{h}$	specific enthalpy, J/kg
h_c	convective coefficient, W/m^2-k
h_m	diffusive mass-transfer coefficient, kg/m^2-s
h_{vl}	heat loss coefficient, W/m^3-k
ΔH	change in enthalpy, MJ/kg
k	thermal conductivity, W/m-k
L	the height of sample, mm
$\dot{m}''$	mass flux, kg/m^2-s
M	molar mass constant, g/mol
n	heterogeneous reaction order
P	pressure, Pa
t	time, s
T	temperature, ^oC
x	horizontal length, mm
Y	mass fraction
z	vertical length, mm

Greeks

ε	emissivity
κ	permeability, m^2
$\bar{\rho}$	bulk density, kg/m^3
v	viscosity/stoichiometry
ϕ	porosity
$\dot{\omega}$	reaction rate, 1/s
$\dot{\omega}'''$	volumetric destruction/formation rate, kg/m^3-s
σ	a weighted collision diameter, Å

Subscript

0	initial
a	ash
ad	adsorption
c	coal
cr	critical
f	formation
d	destruction
g	gas
hc	heterogeneous combustion
hp	hot plate
ig	ignition
j	gaseous species number
k	reaction number
N	nitrogen
O	oxygen
M	The oxy-complexes
∞	free surface

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1 Introduction

Self-heating is the temperature rise of a material due to exothermic processes taking place within the material bulk [1-3]. Self-heating can lead to ignition when the rate of heat generation is greater than the rate at which the heat is dissipated to the surroundings. Self-heating ignition of fuel has been a hazard and safety concern in production, transportation, and storage for decades.

Various experimental methods [4] (such as DSC-TGA, R_{70}, hot plate, and oven-basket) have been used to study self-heating and ignition of fuels. As one of the two most used methods (along with oven-basket experiment), the hot plate experiment is proposed for the situation where material accumulates on a hot surface, which is a common hazard in industry. The hot plate experiment can be carried out in different configurations. The most typical configuration is flat configuration [5, 6], where a uniform thin layer of dust is placed on top of a flat hot plate. The temperature of the hot plate is maintained at a constant value and the top face of the layer is exposed to the ambient air and the side face is framed by a metal ring [7, 8]. The plate temperature is increased between different experimental runs until ignition is observed. The aim of the experiment is to measure the critical temperature of the hot plate that triggers the ignition of a dust layer. This critical temperature is referred to as the minimum ignition temperature (T_{ig}) [6].

Flat configuration is the most commonly used configuration in industry. However, this configuration does not represent the geometry of realistic hazards. In most industrial accidents, fuel layer ignition initiates in wedged-shape corners where the fuel is trapped [9]. In order to better understand the self-heating hazard in realistic geometrical conditions, Joshi, et al. [9] designed a hot plate experiment in the wedge configuration. In this configuration, two plates are joined together to form a wedge-shape geometry to hold the fuel sample. Despite the difference in geometrical setup, the wedge configuration has the same experimental procedure

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and aims as flat configuration.

To gain theoretical insights on the self-heating ignition of fuel layers in hot plate configurations, a number of numerical studies have been conducted to simulate self-heating ignition in both flat configuration [10, 11] and wedge configuration [12, 13]. Yuan, et al. [10] found a compensation effect between two kinetic parameters across different coals and well predicted the T_{ig} for coal of various sources under flat configuration. Sahu, et al. [12] built a multi-dimensional computational model to simulate the wedge configuration experiment and the influence of geometry on the ignition location was studied. [12] is the first computational study to simulate the wedge configuration experiment and the simulation results demonstrate that the ignition location rises as the wedge angle becomes smaller.

However, these studies focus on the onset of ignition alone. The investigation on transient behaviour during the whole self-heating process (i.e from ambient to ignition) is limited. Experimental studies show that during self-heating of a fuel layer hot spot forms at a lower part inside the sample and spreads upward after ignition [1, 14], at which stage the solid fuel smoulders [1, 15-17]. Therefore, the formation and upward spread of hot spot are relevant to smouldering. The understanding of the relationship between hot spot and smouldering spread is of great importance for prevention, detection, and mitigation of self-heating fires. However, the literature lacks a computational study that investigates and analyses the transient characteristics of hot spot and smouldering spread in detail.

In order to fill this gap, in this paper we build a two dimensional computational model to simulate self-heating ignition and smouldering spread of fuel layers in different hot plate configurations by adopting a two-step kinetic scheme. Among all solid fuels, only coal has been experimentally studied in both flat [7] and wedge configuration [9]. Due to the availability of experimental data, coal is therefore chosen as the material to validate the model. Using the validated model, we simulate the self-heating ignition and smouldering spread in different hot

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plate configurations and explain the influence of wedge angle.

2 Computational model

2.1 Governing equations

Self-heating of coal is driven by the exothermic heterogeneous reactions occurring between solid phase reactant (coal) and gas phase reactant (oxygen) inside the pores of the porous layer. Our model is built based on Gpyro [18]. Gpyro is an open-source code which integrates mechanisms of mass transfer, heat transfer, and chemistry for reactive porous media and has a robust inbuilt stiff solver capable of solving complex smouldering problems [19-21].

The governing equations are Eqs.(1)-(6), which impose conservations of (1) mass, (2) species and (3) energy in the solid phase as well as (4) mass, species, and (6) momentum (Darcy's law) in the gas phase. Subscripts *z* and *x* refer to the vertical and horizontal directions respectively. Subscripts i and j refer to the solid species and gas species respectively. All the other symbols are explained in the nomenclature table. Further details on the formulation of Gpyro and solution method can be found in [22].

The thermo-physical properties of solid species and gas species are assumed to be constant. The gas-phase temperature is assumed to be the same as the condensed-phase temperature (thermal equilibrium). The coal is assumed to be dry and therefore the effects of water drying are not considered in the simulation. All the gas species are assumed to have the same specific heat capacity c_g=1100 J/kg-K [18].

$$\frac{\partial \bar{\rho}}{\partial t} = -\dot{\omega}'''_{fg} \tag{1}$$

$$\frac{\partial \left(\bar{\rho} Y_i\right)}{\partial t} = \dot{\omega}'''_{fi} - \dot{\omega}'''_{di} \tag{2}$$

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$$\frac{\partial\left(\bar{\rho}\bar{h}\right)}{\partial t}=k\frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}\right)+k\frac{\partial}{\partial z}\left(\frac{\partial T}{\partial z}\right)+\dot{\omega}_{di}'''(-\Delta H_i)-h_{vl}(T-T_\infty) \tag{3}$$

$$\frac{\partial}{\partial t}(\rho_g\bar{\phi})+\frac{\partial \dot{m}_x''}{\partial x}+\frac{\partial \dot{m}_z''}{\partial z}=\dot{\omega}_{fg}''' \tag{4}$$

$$\frac{\partial}{\partial t}(\rho_g\bar{\phi}\bar{Y}_j)+\frac{\partial}{\partial x}(\dot{m}_x''Y_j)+\frac{\partial}{\partial z}(\dot{m}_z''Y_j)=-\frac{\partial}{\partial x}\left(\bar{\phi}\rho_g D\frac{\partial Y_j}{\partial x}\right)-\frac{\partial}{\partial z}\left(\bar{\phi}\rho_g D\frac{\partial Y_j}{\partial z}\right)+\dot{\omega}_{fj}'''-\dot{\omega}_{dj}''' \tag{5}$$

$$\dot{m}''=-\frac{\bar{\kappa}}{\nu}\frac{\partial p}{\partial z}-\frac{\bar{\kappa}}{\nu}\frac{\partial p}{\partial x}\qquad\left(\rho_g=\frac{P\overline{M}}{RT}\right) \tag{6}$$

2.2 Two-step reaction scheme

The kinetics scheme used to simulate self-heating in previous studies was simplified to a lumped one-step reaction [10-13]. However, a one-step scheme is not able to capture the transient behavior encompassing both self-heating ignition and smouldering spread. The literature [23-25] has shown that there are two main reaction sequences occurring in parallel: oxygen adsorption and smouldering combustion (burn-off reaction), which can be described by a two-step reaction scheme as shown in Eq. (7) and (8).

$$\nu_c\text{coal}+\nu_{a,o}\,\mathrm{O_2}\rightarrow\nu_{a,M}\,\text{coal}\cdot\mathrm{O_2} \tag{7}$$

$$\nu_c\text{coal}+\nu_{c,o}\,\mathrm{O_2}\rightarrow\nu_{c,a}\,\text{ash}+\nu_{c,g}\,\text{gases} \tag{8}$$

During oxygen adsorption (Eq.(7)), oxygen is absorbed by coal to form a chemical complex. The adsorption process is exothermic [25-27]. When the temperature of coal increases to a certain degree, the coal starts to burn (Eq. (8)). Referred to as burn-off reaction in the literature [23-25, 28-30], this reaction is the heterogeneous combustion (smouldering) occurring between oxygen and coal to produce ash and gases.

The two-step reaction scheme has also been identified in microscale (TGA) experiments. Li, et al. [24] investigated the kinetics of coal self-heating ignition using thermogravimetric analysis-differential scanning calorimetry (TGA-DSC). They found that there are two stages

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during self-heating and determined the corresponding kinetics parameters for three different coals. In the first stage, the dominant reaction is oxygen adsorption. In the second stage, the dominant reaction is heterogeneous combustion [24].

Both adsorption and heterogeneous combustion depend on temperature [24] as well as the mass fractions of coal (Y_c) and oxygen (Y_O) [25, 28, 30]. Their reaction rates follow the Arrhenius law. The rate for reaction k is expressed by Eq. (9) . $n_{c,k}$ and $n_{O,k}$ represent the reaction order of coal and oxygen respectively. The two reactions happen in parallel in the simulations as shown in the literature [25, 28, 30].

In Gpyro, solving the conservation equation of species (Eq.(2)) requires calculating the volumetric destruction and formation rates ($\dot{\omega}_d'''$ and $\dot{\omega}_f'''$) for different species [18]. For example, the destruction rate for coal in reaction k is calculated by (10) based on the calculation of reaction rate. The formation and destruction rates for other species are calculated accordingly [18].

$$\dot{\omega}_k = A_k e^{-E/RT} Y_c^{n_{c,k}} Y_O^{n_{O,k}} \tag{9}$$

$$\dot{\omega}_{dc,k}''' = \overline{\rho} Y_c A e^{-E/RT} Y_c^{n_{c,k}} Y_O^{n_{O,k}} \tag{10}$$

2.3 Mass transport of gas species

The consumption and transport of oxygen inside a porous fuel layer is an important phenomenon during self-heating ignition and smouldering. In Gpyro, the overall mass transport in gas phase is solved by Eqs.(4)-(6) simultaneously. The parameters (i.e diffusivity, kinematic viscosity, and permeability) used in these equations are set as follows:

Gaseous diffusion coefficients are calculated by Chapman–Enskog theory [18, 31]. The binary diffusion coefficient (units of m^2/s) for species A diffusing into species B is:

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$$D_{AB} = 0.018829 \frac{\sqrt{T^3 \left(\frac{1}{M_A} + \frac{1}{M_B} \right)}}{P \sigma_{AB}^2 f(\frac{T}{\varepsilon_{AB} / k_b})} \tag{11}$$

In Eq.(11), M_A and M_B are the molar mass constants of species A and B; σ_{AB} is a weighted collision diameter of species A and B; k_b is the Boltzmann constant; ε_{AB} is the maximum energy of attraction between molecules A and B. σ_{AB} and (ε_{AB} /k_b) are Lennard Jones parameters that describe the binary diffusion coefficient of species A into species B using a function of $T/(\varepsilon_{AB} / k_b)$. σ_{AB} and ε_{AB} are weighted averages between molecules A and B for Eqs.(12) and (13).

$$\sigma_{AB} = \frac{1}{2}(\sigma_A + \sigma_B) \tag{12}$$

$$\varepsilon_{AB} = \sqrt{\varepsilon_A \varepsilon_B} \tag{13}$$

Table 1 The values of Lennard-Jones parameters used for calculating the diffusivity of gases in the simulations [31]

	Gas species	M (g/mol)	σ (Å)	ε/k (K)
A	oxygen	32	3.434	113
B	nitrogen	28	3.667	99.8

Several approximations are made for the calculation of mass transport in gas phase. It is assumed that the background gas (Species B) that the O_2 (Species A) diffuses into has the same Lennard Jones parameters as N_2, because N_2 accounts for the largest mass fraction in air and smoke. The Lennard Jones parameters for O_2 and N_2 are obtained from [31] as listed in Table 1; All gaseous species have unity Schmidt number and therefore the kinetic viscosity of gas species has the same value of diffusivity as shown in Eq. (14).

$$\nu \approx D_{AB} \tag{14}$$

The permeability for different solid species is given in Table 3. The weighted permeability of solid mixture in Eq.(6) is calculated on a volume basis [18]:

$$\overline{\kappa} \approx \sum X_i \kappa_i \tag{15}$$

3 Parameterization

3.1 Chemical parameters

The parameterization for the chemical parameters used in the simulations is shown in Table 2. A and E are obtained from TGA experiments in [24], where several coals have been analysed. Since the Pittsburgh seam coal used in the experiments [7, 9] that the model is validated against is not studied in [24], here we choose activation energies of 67 kJ/mol and 68.8 kJ/mol (for the coal Type B in [24]) for adsorption reaction and smouldering combustion. The reason for choosing these two values is because they are in the middle of the range (49.4 to 104.6 kJ/mol) reported in literature [32-34] for Pittsburgh seam coal. The kinetic difference between coal type B in [24] and Pittsburgh seam coal is considered by varying the pre-exponential factors. The simulations show that when 2.5×10^3 (1/s) and 1.28×10^3 (1/s) are used for the pre-exponential factors of adsorption reaction and smouldering combustion respectively, the model shows a good prediction for T_{ig} and hot spot spread compared to the experiments. These two values of pre-exponential factors are within the range (7.06×10^2 to 6.0×10^4 1/s) reported for Pittsburgh seam coal in [32-34]. The reaction orders for oxygen (n_o) and coal (n_c) in adsorption reaction are reported to be 1 [25, 28, 30], while those for heterogeneous combustion are 0.68 and 1 respectively [35].

The values for stoichiometry and heat of reaction are also obtained from literature. For adsorption, it is reported that 1 kg of coal adsorbs 0.1kg O_2 [28], releasing 2MJ of heat [27]. For heterogeneous combustion, 1.1 kg of coal reacts with 2.1 kg of oxygen to generate 3.1 kg of gases and 0.1kg of ash [11, 36]. The heat of combustion for Pittsburgh seam coal is -29.8 MJ/kg [7].

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Table 2 The values of chemical parameters used in the simulations

Parameters	Adsorption reaction	Source	Heterogeneous combustion	Source
A (1/s)	$2.5\times10^{3*}$	[24, 32-34]	$1.28\times10^{3*}$	[24, 32-34]
E (kJ/mol)	67	[24]	68.8	[24]
n_c	1	[25, 28, 30]	1	[35]
n_O	1	[25, 28, 30]	0.68	[35]
v_c (kg/kg)	1	[28]	1.1	[11]
v_o (kg/kg)	0.1	[28]	2.1	[11]
v_a (kg/kg)	-	-	0.1	[11]
v_M (kg/kg)	1.1	[28]	-	-
v_g (kg/kg)	-	-	3.1	[11]
ΔH (MJ/kg)	-2.0	[27]	-29.8	[7]

*Calibrated

3.2 Thermal-physical parameters of solid species

The parameterization for the thermal-physical parameters of solid species is shown in Table 3. Most of the properties for Pittsburgh seam coal were measured in the flat configuration experiment [7], except for heat capacity c and permeability κ. c is obtained from [37]. Pan and Connell [38] reported that the range of values for the permeability of coal is 10^{-15} to$\cdot10^{-13}$ m^2, therefore a middle-range value $5\cdot10^{-14}$ is used in the simulations. $\mathrm{Coal}\cdot\mathrm{O}_2$, the oxy-complex produced during the adsorption reaction (Eq. (7)), is assumed to have the same properties as coal, except for density, which increases by 10% due to the oxygen adsorption. (The coal has a larger density than the one in flat configuration as reported in [9]. The densities for the coal and oxy-complex in the wedge configuration are shown in the round brackets in Table 3). For ash, the density is obtained from [39] and the permeability of ash is set according to [40]. The other properties of ash are from [20].

Table 3. The values of thermal-physical parameters for solid species used in the simulations

Parameter	Unit	Coal	Complex	Source	Ash	Source
ρ	kg m^{-3}	532(580)	585.5(632)	[7, 9]	800	[39]
k	W $m^{-1}K^{-1}$	0.1	0.1	[7]	0.06	[20]
c_p	J kg^{-1} K^{-1}	1080	1080	[37]	880	[20]
ϕ	-	0.59	0.65	[7]	0.03	[20]

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κ	m^2	$5 \cdot 10^{-14}$	$5 \cdot 10^{-14}$	[38]	10^{-16}	[40]

4 One-dimensional flat configuration

4.1 Computational domain and boundary conditions

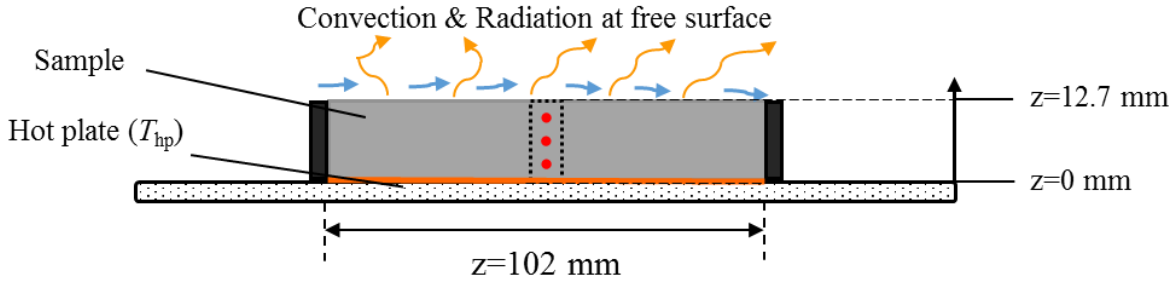

Figure 1 Schematic of flat configuration[7] for layer thickness L = 12.7 mm; The position of the three thermocouples are z=4 mm , 7 mm, and 10 mm as marked by the red dots.

The model is first validated against the flat configuration to obtain a fundamental understanding of the mechanisms and transient characteristics. We simulate the hot plate experiment conducted in [7], where most of the thermophysical parameters required in the simulation were measured with accuracy and high quality. The experiment aimed to measure the critical temperature of the hot plate that triggers the ignition of a dust layer (the schematic is shown in Figure 1). Three thermocouples were mounted evenly at the centreline of the sample to monitor the temperature change. The ignition is considered to occur when the temperature measurement at any of the three thermocouples is 50 ºC over the hot plate temperature according to ATSM standard [5]. The critical hot plate temperature is the minimum ignition temperature (T_{ig}) [6].

The computational domain of the flat configuration experiment follows Figure 1. In the flat configuration, the sample is a circular-shaped thin layer. Since the thickness of the layer is significantly smaller than its diameter, the radial heat and mass transfer in the horizontal direction can be neglected [10, 11]. The limiting transport phenomena occurs only along the vertical direction and therefore a 1D model is used to simulate the flat configuration [10].

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The boundary conditions for the flat configuration are defined by Eq. (16)~(19). Eq. (16) and (17) are for heat transfer at the bottom (z=0) and top (z=L) boundary. For the bottom boundary, the temperature of the hot plate T_{hp} is fixed. For the top boundary, both convective and radiative heat losses are considered. An empirical value for convective heat transfer coefficient, h_{c} = 10W/m^2 -K [41], is used and the emissivity (ε) of coal is set at 0.8 [42]. Eq. (18)-(19) are the boundary conditions for gas diffusion. The top free surface is open to the atmosphere; the bottom surface is impermeable to mass flow. h_{m} is the diffusive mass transfer coefficient calculated through h_m= h_c/C_{g} based on the mass-heat transport analogy. This coefficient is used to calculate the diffusive mass flux of gaseous species at top surface [18]. C_{g}, the specific heat capacity for gas species, is assumed to be 1100 J/kg-K[18]. Eq. (20)-(21) are the pressure boundary conditions. At the bottom, there is no pressure gradient as it is impermeable. The pressure on the top surface is atmospheric.

$$T\big|_{z=0} = T_{\mathrm{hp}} \tag{16}$$

$$-k\frac{\partial T}{\partial z}\bigg|_{z=L} = -h_{\mathrm{c}}\left(T\big|_{z=L} - T_{\infty}\right) - \varepsilon\sigma\left[\left(T\big|_{z=L}\right)^4 - T_{\infty}^4\right] \tag{17}$$

$$\frac{\partial Y_j}{\partial z}\bigg|_{z=0} = 0 \tag{18}$$

$$\bar{\psi}\rho_g D\frac{\partial Y_j}{\partial z}\bigg|_{z=L} \approx -h_m\left(Y_j^{\infty} - Y_j\big|_{z=L}\right) \tag{19}$$

$$\frac{\partial P}{\partial z}\bigg|_{z=0} = 0 \tag{20}$$

$$P\big|_{z=L} = P_{\infty} \tag{21}$$

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4.2 Validation

A grid and time step independence study was first conducted to ensure the simulation results converge with time and spatial discretization. The solution converges for grid sizes finer than 0.1 mm and time steps smaller than 0.01 s. Thus, the simulations in this study are conducted at Δz=0.1 mm and Δt= 0.01 s.

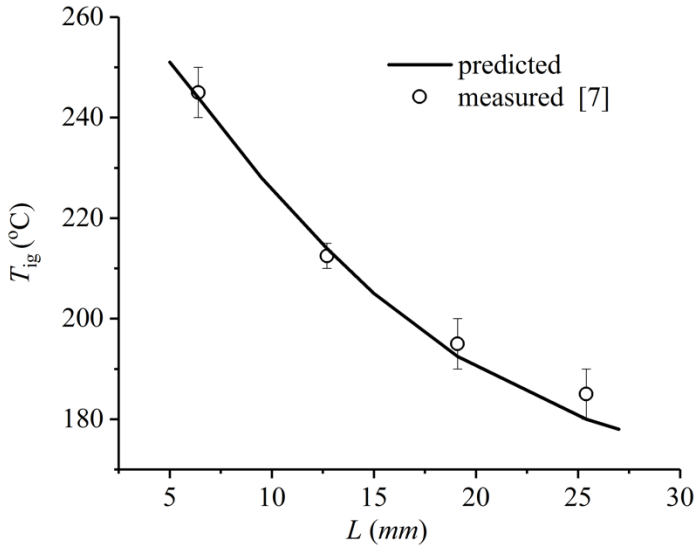

Figure 2 Comparison between predicted and measured [7] minimun ignition temperature for samples of different heights;The error bar is ±5°C for the cases of L= 6.4, 19.1, and 25.4 mm and ±2.5°C for the case of L= 12.7 mm.

Minimum ignition temperature (T_{ig}) is the essential measurement in the self-heating experiments and correctly predicting it is the starting point of this research. Thus the model is first compared with measured T_{ig} as shown in Figure 2. In the simulations, the hot plate temperature is increased by 2°C between two consecutive runs until ignition is predicted. The simulation gives a satisfactory prediction of T_{ig} for all 4 experiments with a margin of error smaller than 5 °C.

As the focus of the study is the transient behaviour, the model is further validated by comparing the predicted and measured temperature profiles at different times for the case L = 12.7 mm as shown in Figure 3. The case of L =12.7 mm is chosen here for validation because it has the lowest experimental uncertainty (the T_{ig} uncertainty for L = 12.7 mm is 5 °C, whereas

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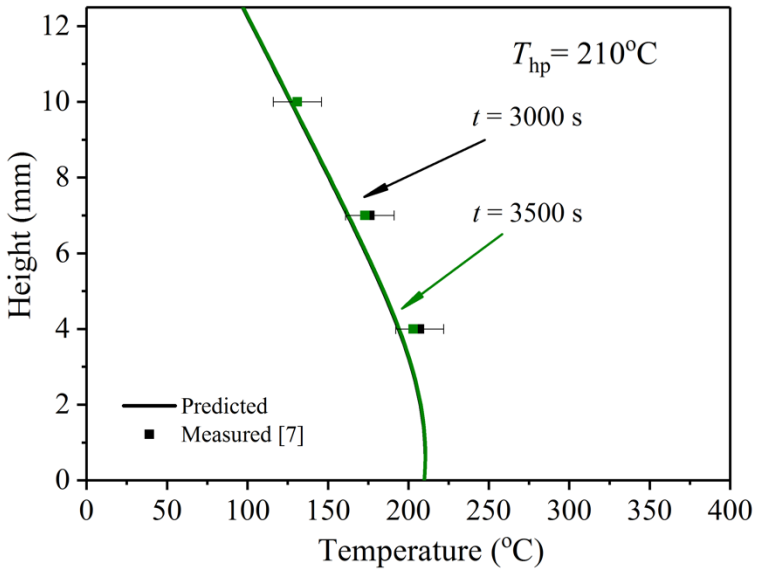
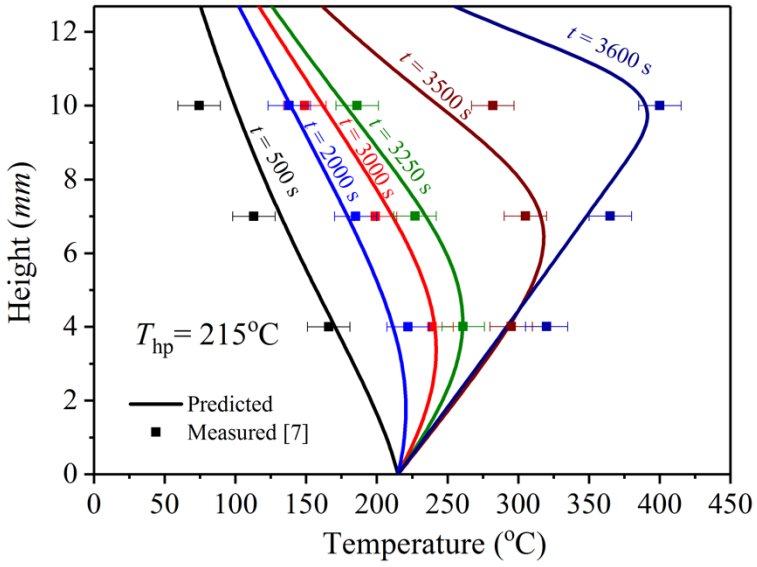
for the other cases the uncertainty is 10 ºC).



(a)



(b)

Figure 3 Comparison between predicted temperature profiles and experimental measurements [7] for the case L =12.7mm at two hot plate temperatures; (a) is the subcritical condition, where T_{hp} = 210 ºC; (b) is the supercritical condition, where T_{hp} = 215 ºC. The measurement uncertainty for transient temperature is ±15 ºC according to [9].

As shown in Figure 3(a), at subcritical condition (T_{hp} = 210 ºC), when the hot plate temperature is below the threshold for ignition, the temperature profile is parabolic, where the highest temperature point in the sample is close to the bottom. After 3000 s, steady state is reached (the temperature profiles of t =3000 s and 3500 s overlap) due to the balance between

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heat dissipation and heat generation.

At the supercritical condition (T_{hp} = 215 ^{o}C), the sample self-ignites. Figure 3(b) clearly shows the formation, growth and upward spread of the hot spot. At t =500 s, the highest temperature in the sample is still the hot plate temperature and the location of highest temperature is at the contact with the hot plate. At t =2000 s, the highest temperature exceeds the hot plate temperature and a hot spot forms. From 2000 s to 3250 s, the temperature increases all over the sample and the hot spot slowly moves upward. At t = 3250s, the highest temperature in the sample is 260 ^{o}C, 45 ^{o}C higher than the hot plate temperature. At this instant, ignition is about to occur according to the ASTM standard [5], which defines the ignition as when sample temperature is 50 ^{o}C above the hot plate temperature. After this point, the hot spot moves up quickly. At t = 3600s, the location of hot spot has move to 10 mm with the highest temperature increasing to 380 ^{o}C. In general, there is reasonable agreement between the predictions and the experimental measurements. This is the first time the upward spread of hot spot after self-heating ignition is accurately predicted.

4.3 Upward spread of smouldering

To better understand the transient characteristics during the process of self-heating ignition and smouldering spread, the transient profiles of temperature and oxygen from 500 s to 3500 s are predicted in Figure 4. Each curve refers to the profile at a single time step. The time difference between two adjacent black curves is 500 s. From 500 s to 3000 s, an upward movement of the hot spot is observed. During the same period, oxygen starts to be consumed and by t = 3000 s the oxygen concentration of bottom part reduces down to 10 % .

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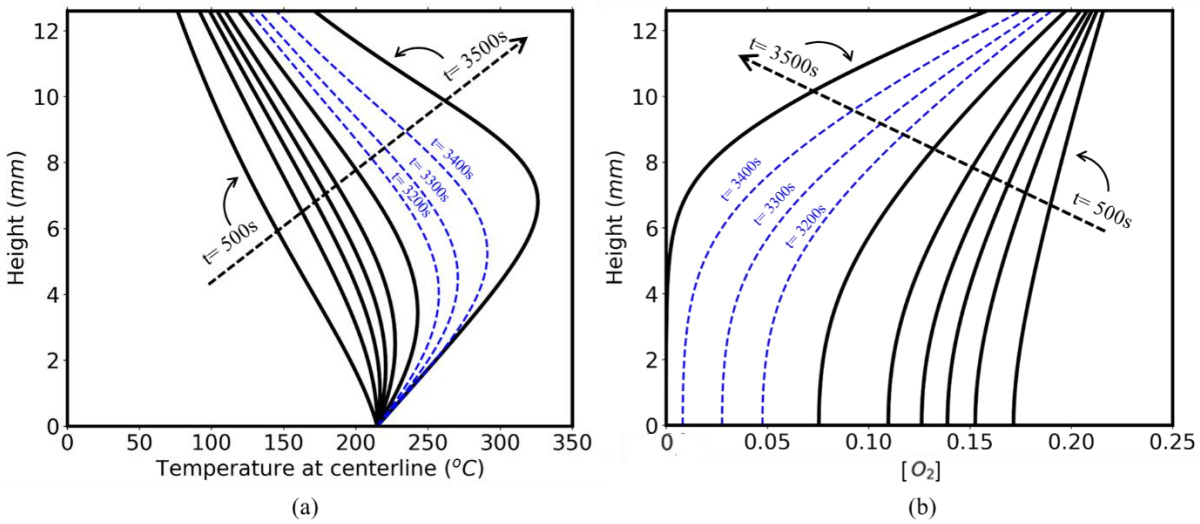

Figure 4 The predicted profiles of temperature (a) and oxygen concentration (b) at different times (from 500 s to 3500 s) for supercritical condition (T_{hp}= 215 °C); The time difference between two ajacent **black solid** curves is 500 s; the blue dashed are profiles at higher time resolution between 3000 s and 3500 s

From 3000 s to 3500 s, the temperature profile changes rapidly and there is a significant upward movement of the hot spot (the transient behaviours during this period is displayed in detail with blue dashed curves in Figure 4). At the same time the smouldering reaction accelerates and the oxygen at bottom layer is depleted. In 1984, Bowes [1] put forward the hypothesis that a temperature wave would form and move upward when ignition occurs. This hypothesis of temperature wave is tested and confirmed to be true here using a validated computational model.

We further analyse the chemical process for adsorption and smouldering in Figure 5 and Figure 6. Figure 5 shows the reaction rates for two reactions before 3000 s, when ignition has not occurred yet. Before ignition, the maximum temperature of the sample is below 250 °C and the reaction rates of adsorption and smouldering are of the same order of magnitude. The reaction peak moves upward slowly from the bottom (500 s) to 4 mm (3000 s) with an average spread rate of 0.1 mm/min.

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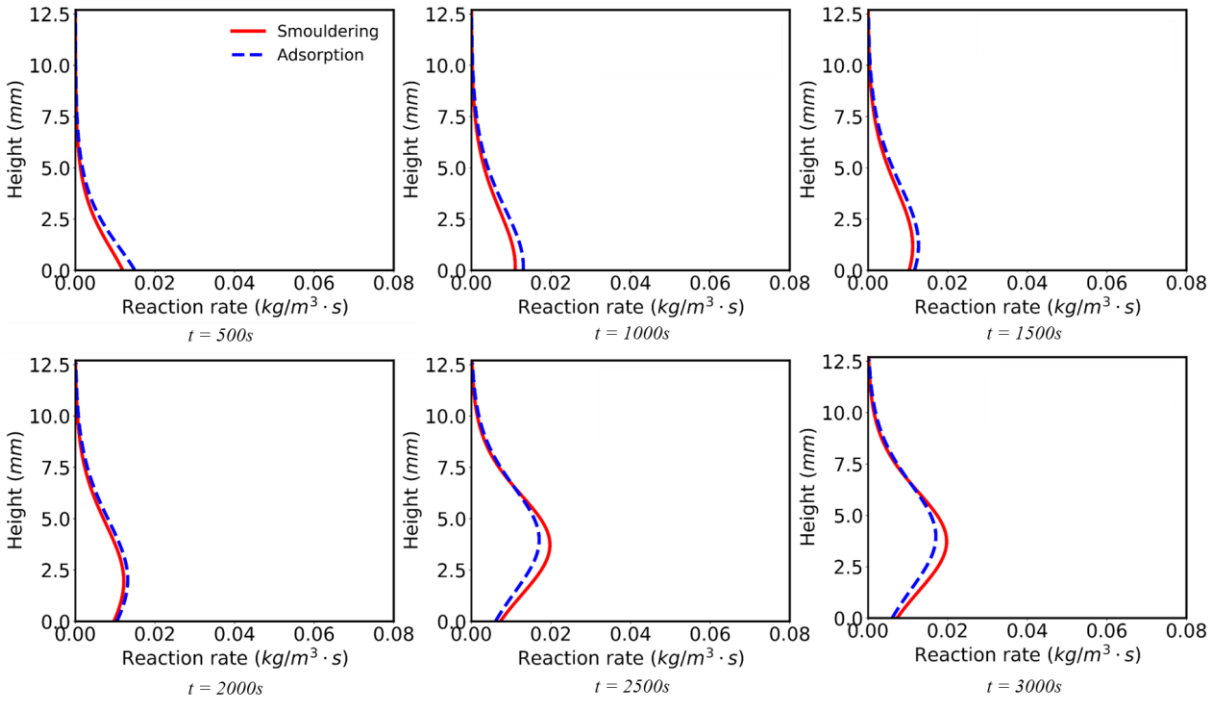

Figure 5 The predicted reaction rate profiles of adsorption and smouldering (heterogeneous combustion) at different times (from 500 s to 3000 s) for the case L=12.7 mm & T_{hp}= 215 ºC;

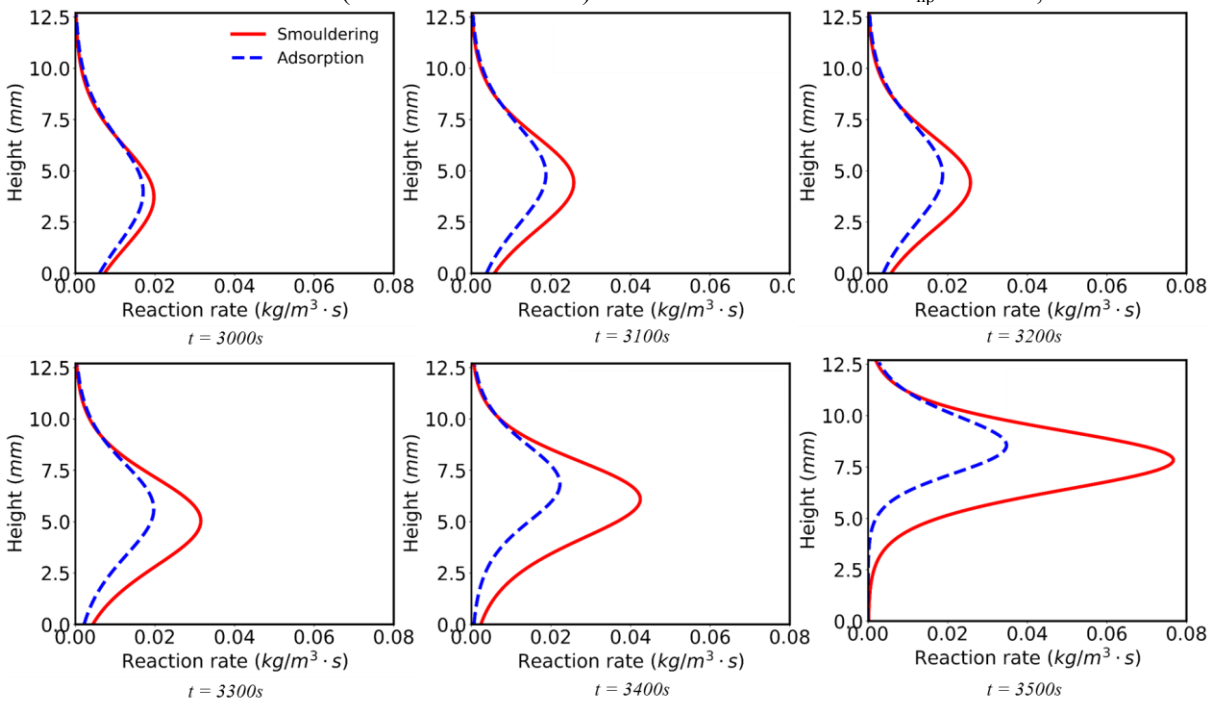

Figure 6 The predicted reaction rate profiles of adsorption and smouldering (heterogeneous combustion) at different times (from 3000 s to 3500 s) for the case L=12.7 mm & T_{hp}= 215 ºC;

Figure 6 shows the situation after ignition. Smouldering reaction accelerates and the peak smouldering rate increases by a factor of 4 (from 0.02 to 0.08 kg/m^3-s). During the same period, the peak adsorption rate increases from 0.015 to 0.035 kg/m^3-s. Smouldering becomes the main reaction once ignition has been triggered. This is in agreement with experimental findings [24]

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that at a higher temperature range there is a change of dominant chemical pathway and smouldering becomes the main reaction [1, 15]. In addition, the location of reaction peak moves upward much faster after ignition and the average spread rate of smouldering is 0.5 mm/min, five times higher than before ignition. This is because the oxygen at the lower part of the layer is rapidly consumed due to the acceleration of smouldering and the reaction zone starts to move towards the free surface to seek more oxygen supply. By comparing hot spot (in Figure 4) and smouldering reaction peak, we find that they spread upward at a similar rate. In other words, the upward movement of the hot spot reflects the smouldering spread after ignition.

5 Two-dimensional wedge configuration

5.1 Computational domain and boundary conditions

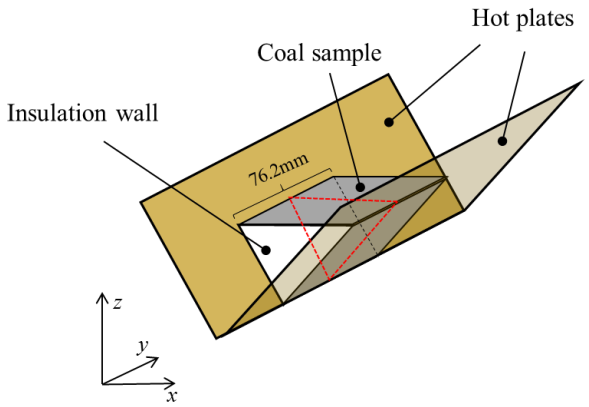

Figure 7 Schematic of hot plate experimental setup in wedge configuration [9]; The red triangle indicates the section used in the simulations; Two insulation walls are put at both ends in y direction.

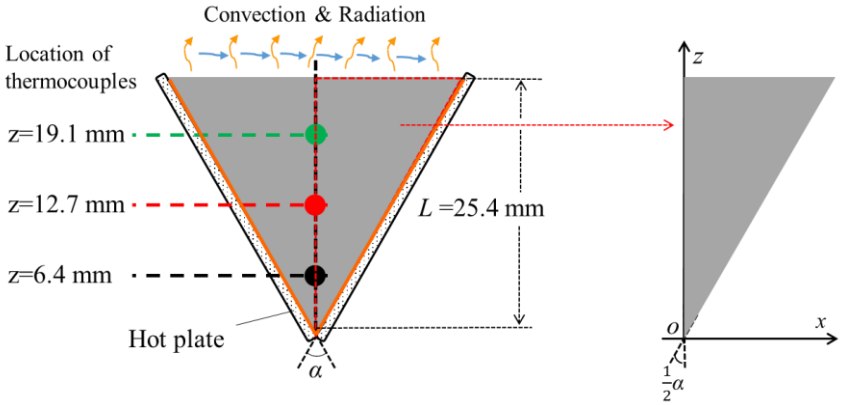

Figure 8 2D Computational domain of hot plate experiment in wedge configuration; Red triangle indicates the half of geometry used in simulations.

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The wedge configuration is used for investigating the influence of geometry. The schematic for the wedge configuration experiment is shown in Figure 7. This configuration uses two hot plates to form a wedge-like geometry. In the experiments [9], the height of the sample is fixed at 25.4 mm with two different wedge angles (α = 60^{o} and 90 ^{o}) investigated. Three thermocouples were mounted evenly at the central line (z = 6.4 mm, 12.7 mm, and 19.1 mm).

Sahu, et al. [12] developed a two-dimensional computational model to simulate the wedge configuration experiment using FLUENT. They focused on the location of hot spot at onset of ignition at supercritical conditions and predicted the trend that the location of hot spot rises as wedge angle increases. It was the first computational study to simulate the wedge configuration and predict the formation of hot spot at onset of ignition. In their study, a one-step reaction scheme was used and the reaction rate was assumed to be independent of oxygen. These assumptions are commonly used for simulating the onset of self-heating ignition in previous studies [1, 7]. However, our study focuses on the formation and movement of the hot spot during self-heating and smouldering combustion, a transient process where oxygen diffusion and consumption plays an important role. Thus, in this work we use a two-step scheme with the influence of oxygen diffusion and consumption taken into account.

The two-dimensional computational domain (in x-z plane) used here is the cross-sectional area in the middle of the sample (as indicated in Figure 7). Taking advantage of symmetry, the computational domain is half of the real geometry to save computational time as shown in Figure 8. The dimension perpendicular to the x-z plane is not included in the domain. In this experiment setup, the sample has similar sizes in all dimensions. Take the case wedge angle = 90 ^{o} as an example, the sample has a size of 76.2 mm in the *y* direction (L_y) (See Figure 7) and size of 50.4 mm in *x* direction(L_x). The ratio of L_y to L_x is 1.5 and both sides are of the same order of magnitude. Therefore the heat transfer through y direction is considered by

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incorporating a volumetric heat loss coefficient (h_{vl}) into the energy conservation equation Eq.(3). This coefficient has been used before [10, 18, 43] to accomplish dimensionality reduction by only including the main dimension(s) in the computational domain and the heat losses through un-included dimension(s) are calculated through h_{vl} . We studied the effect of h_{vl} and found that using h_{vl} = 80 W/m^{3}K (within the order of magnitude reported in previous studies [10, 18]) simulations show a good agreement with the experimental measurements.

The boundary conditions for wedge configuration are as follows: At plane of symmetry (i.e x=0), we impose an adiabatic condition (Eq.(22)) and permeable conditions (Eqs(23)& (24)). At z=L, both convective and radiative heat transfers (Eq. (25)) are considered and boundary conditions for gas transport are Eqs.(26) &(27). At the hot plate surface (z = x·cot(α/2)), the boundary conditions are the same as those in the flat configuration as shown in Eq.(28), (29), and (30).

$$-k\left.\frac{\partial T}{\partial x}\right|_{x=0}=0 \tag{22}$$

$$-\bar{\psi}\rho_g D\left.\frac{\partial Y_j}{\partial x}\right|_{x=0}=0 \tag{23}$$

$$\left.\frac{\partial P}{\partial x}\right|_{x=0}=0 \tag{24}$$

$$k\left.\frac{\partial T}{\partial z}\right|_{z=L}=h_c\left(T\big|_{z=L}-T_\infty\right)+\varepsilon\sigma\left[\left(T\big|_{z=L}\right)^4-T_\infty^4\right] \tag{25}$$

$$-\bar{\psi}\rho_g D\left.\frac{\partial Y_j}{\partial z}\right|_{z=L}=h_m\left(Y_j^\infty-Y_j\big|_{z=L}\right) \tag{26}$$

$$P\big|_{z=L}=P_\infty \tag{27}$$

$$T\big|_{z=x\cdot\cot(\alpha/2)}=T_{hp} \tag{28}$$

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$$-\bar{\psi}\rho_g D\left.\frac{\partial Y_j}{\partial z}\right|_{z=x\cdot\cot(\alpha/2)}=0 \tag{29}$$

$$\left.\frac{\partial P}{\partial x}\right|_{z=x\cdot\cot(\alpha/2)}=0 \tag{30}$$

5.2 Validation

The model is first validated against the experimental measurements of T_{ig} at different wedge angles as shown in Figure 9. The measurements are predicted accurately by the model with a margin of error smaller than the experimental uncertainty.

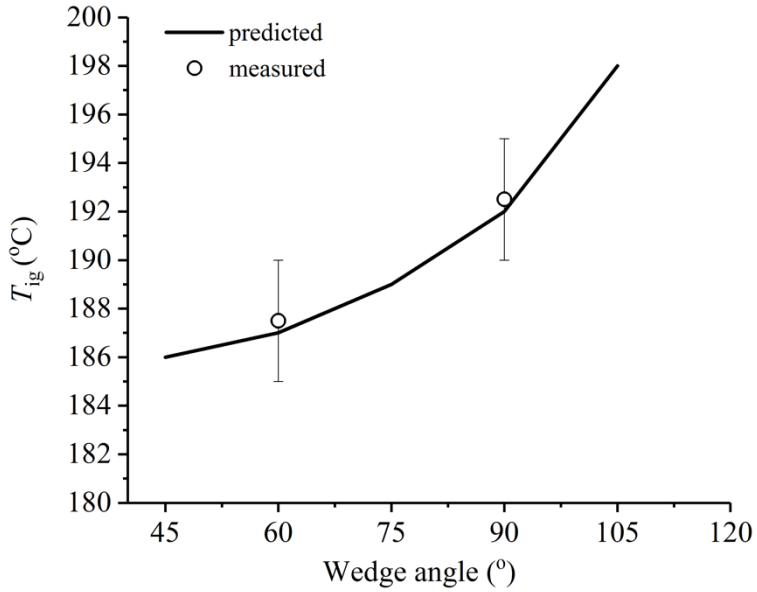

Figure 9 Comparison between predicted and measured [9] minimun ignition temperature for samples with different wedge angles.

The model is further validated by comparing predicted centreline temperature profiles with the experimental data. Simulations show good agreement with the experiment. The simulation of angle α=90° is shown in Figure 10 to present the details. At subcritical condition (T_{hp} = 190 °C), ignition does not occur. The maximum temperature point is located near the bottom and the temperature profile reaches steady state after 60 min. At supercritical condition (T_{hp}= 195 °C), the temperature profile changes significantly after ignition. According to the simulation, the hot spot moves from 11 mm (at 60 min) to 16 mm (at 70 min) with an average spread rate

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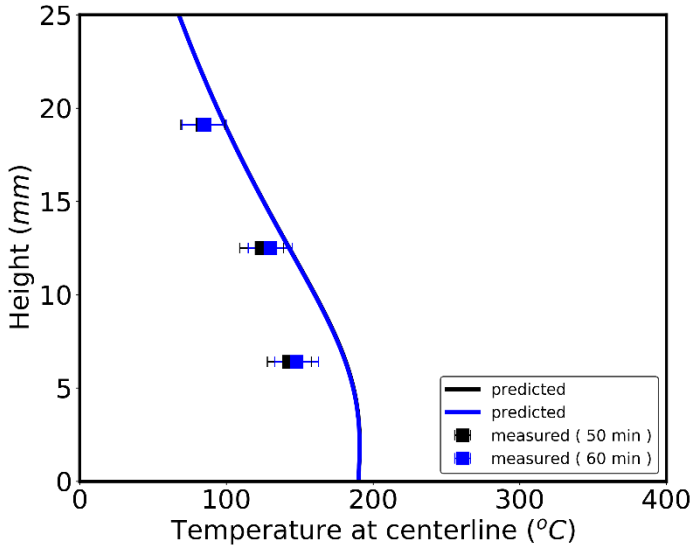
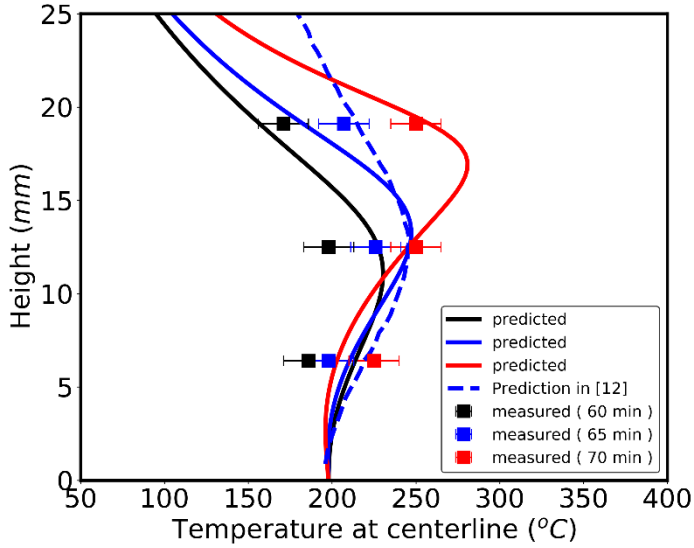
of 0.5mm/min, and with the maximum temperature rising from 220 ºC to 270 ºC.



(a)



(b)

Figure 10 The comparison of predicted centerline temperature and experimental measurements [9] for wedge configurations at different time steps for α=90º; (a) subcritical condition T_{hp}=190 ºC; (b) supercritical condition T_{hp}=195 ºC.

The predicted temperature profile by Sahu, et al. [12] is also compared with the present model in Figure 10. It is seen that both models have a similar prediction for the location of hot spot at the moment of formation. With respect to [12], our model has a better agreement with the experimental data at the bottom whereas [12] has a better prediction near the top surface. This might be because Fluent has a stronger solver of fluid mechanics and hence a more

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accurate calculation for the convective heat transfer at the free surface, which lead to a good prediction near the top surface. Based on Gpyro, our model focuses more on the transport phenomena and chemistry inside the porous media and it includes two oxidative reactions as well as the consumption and diffusion of the oxygen. Therefore we can simulate transient behaviour of formation and spread of hot spot during self-heating ignition and smouldering spread. This is the main contribution of the present model that distinguishes it from previous studies.

The 2D profiles of temperature, oxygen, and reaction rates are shown in Figure 11-Figure 13. At t=60 min, a hot spot starts to form at the lower part. After that, it moves upward to the upper part at 80 min. It is seen in Figure 12 that oxygen is consumed rapidly after t = 60 min and the oxygen at the bottom has been depleted by t = 80 min, leading to the upward spread of smouldering. Figure 13 shows the transient evolution of reaction rate for both adsorption and smouldering combustion. Both reactions show a similar trend. At t = 60 min, the reaction peak zone is at the lower part. After ignition, reaction accelerates and the reaction zone moves upward to seek oxygen supply. This characteristic is similar to what has been discussed for flat configuration in Section 4.3.

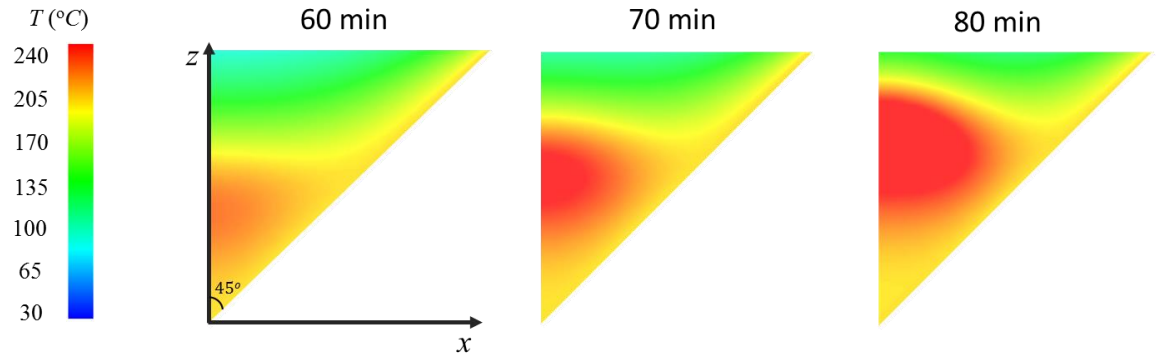

Figure 11 Predicted temperature profiles at different times (60min, 70min, and 80min) for α =90° at supercritical condition (T_{hp} = 195°C).

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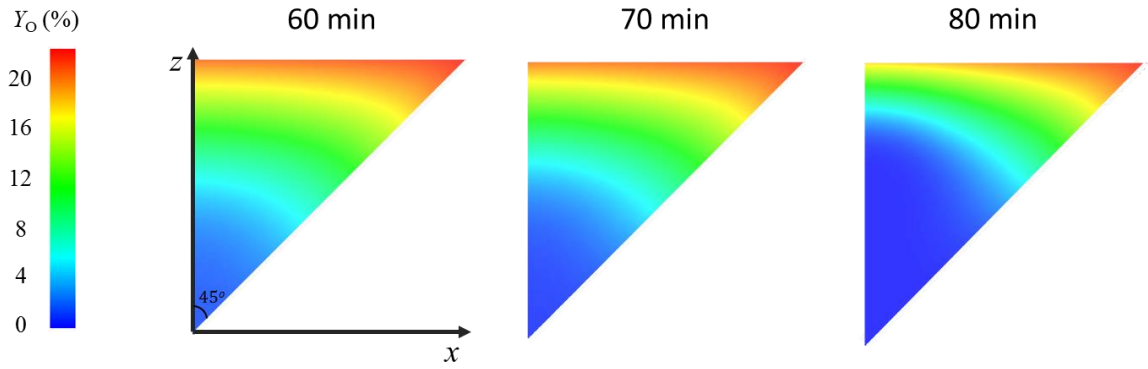
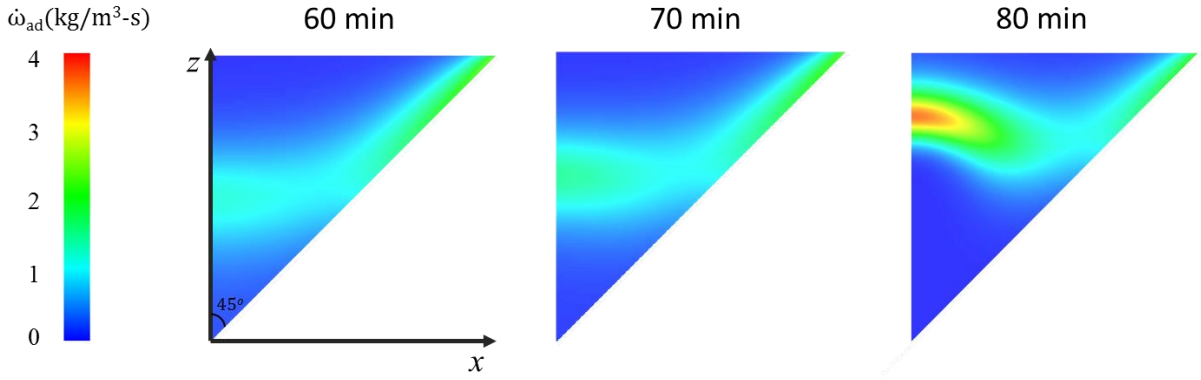
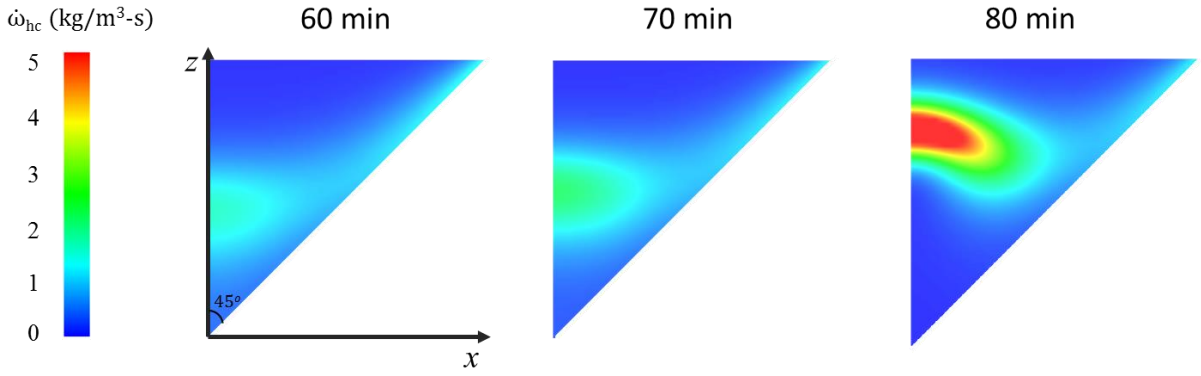


Figure 12 Predicted oxygen profiles at different times (60min, 70min, and 80min) for α =90° at supercritical condition (T_{hp} = 195°C).



(a)



(b)

Figure 13 Predicted reaction rate profiles at different times (60min, 70min, and 80min) for α =90° at supercritical condition (T_{hp} = 195°C): (a) Adsorption reaction (b) Heterogeneous combustion.

5.3 Influence of wedge angle on the location of maximum temperature

Previous studies have investigated the influence of hot plate temperature [36] and wedge angle [12, 13] on the location of the hot spot at the onset of ignition under supercritical condition.

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This location is referred to as ignition location in the literature [12, 13]. However, as already discussed in this paper, the hot spot always originates at the contact of the hot plate and then spreads upward after ignition. It is hard to define the exact ignition location due to the movement of the hot spot. To better investigate the influence of geometry on the location of hot region in the sample, here we focus on subcritical conditions. At subcritical conditions, a steady state is eventually reached. The maximum temperature point (maximum temperature point is used for subcritical conditions to distinguish the hot spot in supercritical conditions) stays at a specific location and does not change once steady state is reached (as shown in Figure 10). Nevertheless, since the subcritical condition is very close to the criticality, the location (z_{max}) of max temperature point at steady state indicates the position where ignition is about to occur.

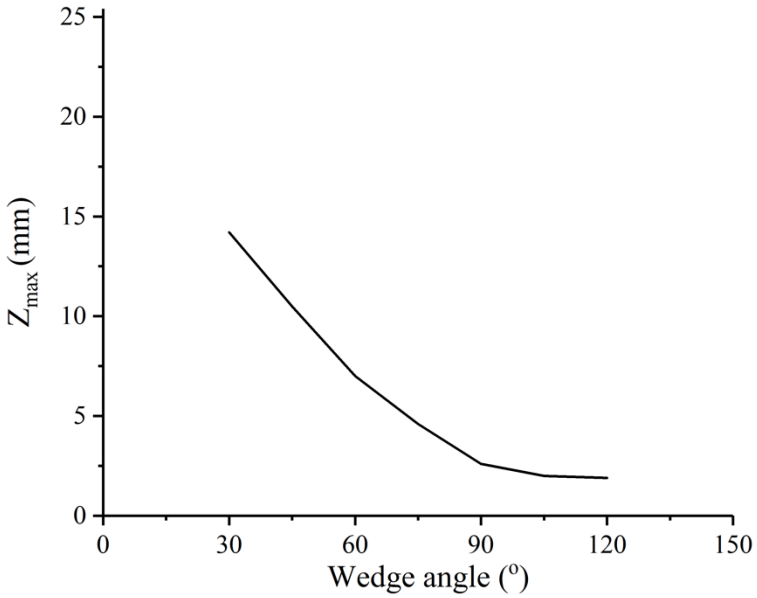

Figure 14 Height of maximum temperature point at the steady state versus wedge angle.

The maximum temperature point is at centreline due to symmetry. Therefore, here we focus on the temperature profile of centreline. The height of the maximum temperature (Z_{max}) in the sample is defined as the vertical distance from the apex of the wedge to the maximum temperature point. Z_{max} is predicted for different wedge angles as shown in Figure 14. It is seen that wedge angle has a large influence on the temperature profile. Z_{max} decreases significantly with the wedge angle. The decrease can be more than 12 mm (from 14.3 mm to 1.9 mm) when

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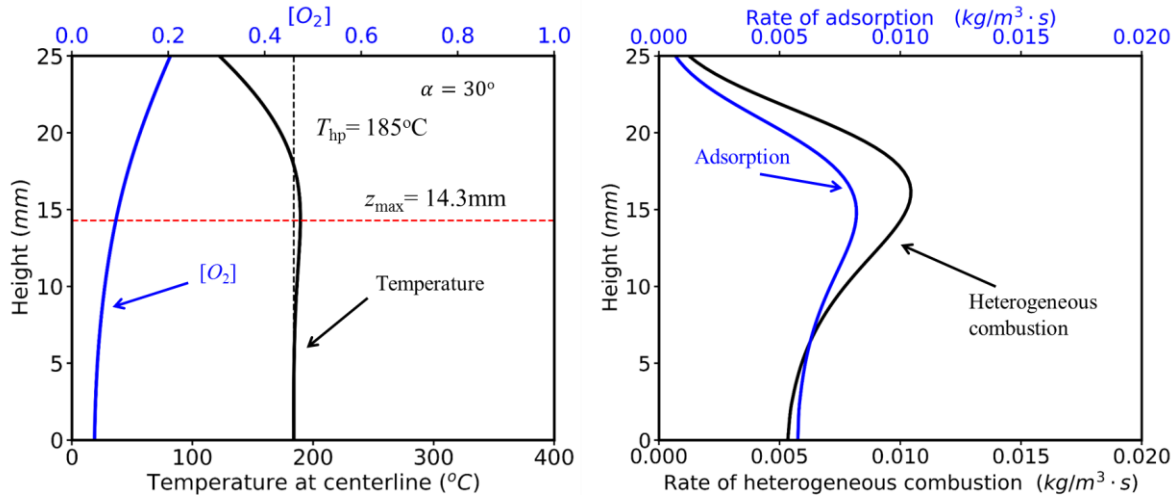
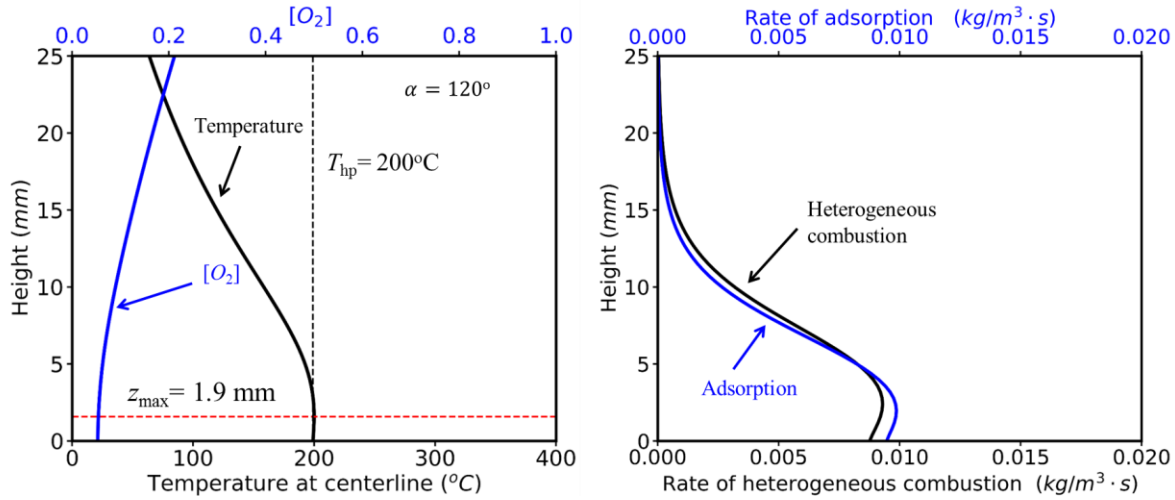
wedge angle increases from 30 ° to 120°.



(a)



(b)

Figure 15 The predicted centreline profiles of temperature, oxygen concentration, and reaction rates for wedge configuration at subcritical condition. (a) α =30° (T_{hp} = 185 °C) and (b) α =120° (T_{hp} = 200 °C).

The predicted profiles of temperature, oxygen concentration, and reaction rates for α =30° and α =120 ° are shown in Figure 15 as examples. The sample with a smaller α tends to have a more uniform profile and the location of the maximum temperature is higher. This trend can be expained by the influence of geometry on heat tranfer, which would be discussed in detail later using Figure 16. In terms of oxygen concentration, at steady state, there is still a certain amount (7-8%) of oxygen left at the lower part of sample layer. The oxygen diffused from the ambient and the oxygen consumed by reactions reaches a balance at steady state. In terms of reaction rates, two reactions have similar reaction rates at subcritical condition (close to the criticality).

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Similar to the supercritical condition, the maximum temperature point indicates the location of peak reaction zone.

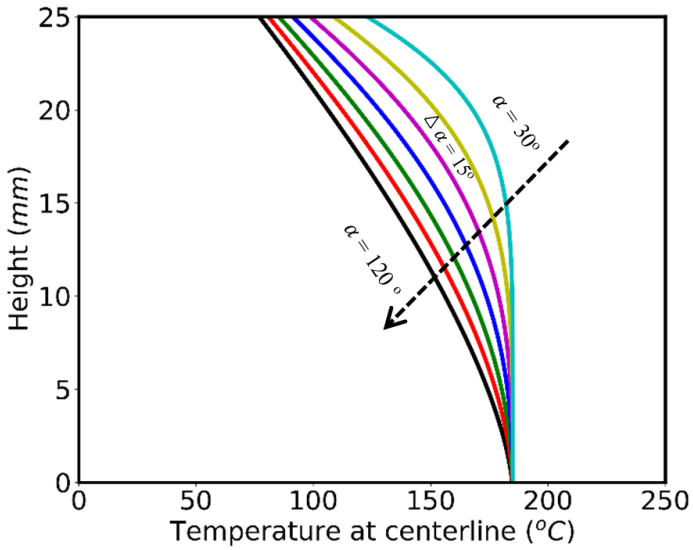

Figure 16 The predicted centerline temperature profiles for ideal heat transfer cases (T_{hp} = 190 °C); different colors refer to different wedge angles ranging from 30° to 120 °; The increment of wedge angle between two adjacent line is 15 °.

To explain the influence of wedge angle on heat transfer, we decouple the influence of chemistry by simulating the case of heat transfer process for an inert sample, which is not reactive but with all the thermo-physical properties the same as those in Table 3. For convenience of comparison, the hot plate temperature is set as a constant of 190 °C for all wedge angles. The boundary conditions are the same as listed in (22)-(29). We calculate the centreline temperature profiles for different wedge angles and the comparison is shown in Figure 15. It is seen that the smaller the angle is, the more uniform the temperature distribution is. For example, at α =30° the lower half part of the sample has almost the same temperature as the hot plate, whereas at α =120° the temperature distribution alone the centerline is almost linear. In other words, when α is smaller the temperature gradient is smaller. Under this circumstance, the maximum temperature point tends to appear at a higher location. This is because when the tempearture distribution is relatively uniform, reaction rate is not limited by temperature but the oxygen concentration (Eq. (9)). Therefore, the peak of reaction rate tends to occur at a higher

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position, where more oxygen is available. For the wedge with a larger α, the temperature gradient is larger. In this case, the maximum temperature point tends to be located at a lower position, as temperature at the upper part is too low to allow the peak of reaction rate.

6 Conclusions

This paper develops a two-dimensional computational model to simulate self-heating ignition and smouldering spread by adopting a two-step kinetic scheme. The model is first validated against a classical flat configuration experiment for coal. The simulation shows a good agreement with transient temperature measurements: At the supercritical condition (T = 215^{o}C), a hot spot forms and then spreads towards the free surface with an averaging spread rate of 0.5mm/min after ignition. Bowes hypothesized this upward movement of hot spot in [1]. In this paper the hypothesis is tested and confirmed using a validated computational model. Further analysis demonstrates that the movement of the hot spot reflects that the smouldering spreads upwards to seek for oxygen supply after the oxygen at the bottom has been depleted.

The model is then validated against the wedge configuration experiment to investigate the characteristics under more complex geometries. In wedge configurations, the hot spot lies at the centreline due to the geometrical symmetry and it shows a similar transient characteristics as that in flat configuration: The influence of wedge angle on location of hot region is investigated by focusing the subcritical condition. Simulations show that the height of maximum temperature decreases with wedge angle. This is because when wedge angle is smaller the temperature gradient along the centreline of the sample is lower. Therefore, reaction peak tends to appear at higher positions to seek for more oxygen as reaction rate is not limited by temperature.

This computational study investigates the transient characteristics of hot spot in different configurations, confirms the Bowes's hypothesis, explains the reason for the upward movement

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of hot spot and links it to smouldering combustion. It deepens our understanding of self-heating ignition and can help mitigate relevant fire hazards.

Acknowledgement

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