Full Length Article

A computational model to simulate self-heating ignition across scales, configurations, and coal origins

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ABSTRACT

Self-heating of fuel layers can trigger ignition when the temperature of the surroundings is sufficiently high. Self-heating ignition has been a hazard and safety concern in raw materials production, transportation, and storage facilities for centuries. Hot plate and oven-basket experiments are the two most used lab-scale experiments to assess the hazard of self-heating ignition. While extensive experiments have been done to study this phenomenon, modelling of the experiments is substantially lagging behind. A computational model that can accurately simulate self-heating ignition under the two experimental configurations has not been developed yet. In this study, we build such a model by coupling heat transfer, mass transfer, and chemistry using the open-source code Gpyro. Due to the accessibility of large amount of experimental data, coal is chosen as the material for model validation. A literature review of the kinetic parameters for coal samples from different origins reveals that there is a compensation effect between the activation energy and exponential factor. Combining the compensation effect with our model, we simulate 6 different experimental studies covering the two experimental configurations, a wide range of sample sizes (heights ranging from 5 mm to 126 mm), and various coal origins (6 countries). The model accurately predicts critical ignition temperature (T_{ig}) for all 24 experiments with an error below 7 °C. This computational model unifies for the first time the two most used self-heating ignition experiments and provides theoretical insights to understand self-ignition for different fuels under different conditions.

1. Introduction

Self-heating is the temperature rise tendency of a material due to heat generated by exothermic processes taking place within the body of material [1]. Self-heating can lead to ignition when the rate of heat generation is greater than the rate at which the heat dissipated to the surrounding. In many industrial processes, fuel dust is often produced as main or by-product. Fuel dust can unintentionally accumulate or be intentionally stored in layers. A fuel layer has self-heating propensity, because exothermic low-temperature oxidation can occur between solid phase fuel dust and the oxygen diffusing from ambient atmosphere inside the fuel layer. Self-heating of a fuel layer can lead to ignition when the surrounding that the layer is exposed to is sufficiently hot. Self-heating ignition of coal layers has been a safety concern in fuel production, transportation, and storage facilities for centuries.

Hot plate experiment and oven-basket experiment are the two most commonly used experimental techniques to assess the self-heating and ignition hazard of fuel dusts. The hot plate experiment is particularly relevant for the situation where dust can accumulate on hot surfaces [2]. In this experiment, a uniform thin layer of dust is placed on a hot plate that is maintained at a constant temperature, while the top face of the layer is exposed to the ambient air with side faces framed by a metal ring [3,4]. The hot plate temperature is increased between different experimental runs until ignition is observed. The experiment aims to measure the critical temperature of the hot plate that triggers the ignition of a dust layer. This critical temperature is referred as minimum ignition temperature [5].

The oven-basket experiment is used to classify self-heating substances for the transport of dangerous goods [6]. In the oven-basket experiment [4,7], the bulk dust is packed inside a basket which is then hung in an isothermal oven with constant temperature. The oven temperature is increased between runs until ignition occurs. This experiment aims to measure the critical oven temperature that triggers the ignition of the dust bulk. This critical temperature is referred as self-ignition temperature [8].

It is seen that both experiments aim to measure the critical surrounding temperature (either hot plate or oven temperature) that triggers ignition. This temperature is one of the most important indicators to assess the self-heating and ignition hazard for fuel layers. For the convenience of notation, the minimum ignition temperature in

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	mass-transfer coefficient, kg/m^2-s
h_{vl}	volumetric heat loss coefficient, W/m^3-k
ΔH	change in enthalpy, MJ/kg
k	thermal conductivity, W/m-k
L	the thickness of sample, mm
$\dot{m}''$	mass flux, kg/m^2-s
n	heterogeneous reaction order
P	pressure, Pa
Ra	Rayleigh number
Pr	Prandtl number
s	sensitivity coefficient
t	time, s
T	temperature, °C
Y	mass fraction
z	height, mm

Greeks

ε	emissivity
κ	permeability, m^2
$\bar{\rho}$	bulk density, kg/m^3
ν	stoichiometric coefficient
ϕ	porosity
$\dot{\omega}''$	volumetric reaction rate, kg/m^3-s

Subscripts

0	initial
c	coal
cr	critical
f	formation
d	destruction
g	gas
hp	hot plate
ig	ignition
j	gaseous species number
k	reaction number
N	nitrogen
O	oxygen
∞	ambient

hot plate experiment and the self-ignition temperature in oven-basket experiment are denoted uniformly as T_{ig} in this paper.

Both types of experiments have been conducted extensively to evaluate the self-heating and ignition hazard of various fuels, such as coals [7,9–13], carbon-rich soils [14], shale rocks [15,55], and biomass [16–19]. Janes et al. [2] tested 14 different materials and reported a correlation between the two experiments. Based on the correlation, a procedure is proposed to estimate the minimum ignition temperature of a dust layer using the oven-basket experiment when it is not possible to carry out hot plate experiment.

To gain more insights into these two experiments, theoretical studies have also been conducted. Frank-Kamenetskii [20] established the fundamental self-heating ignition theory for porous solid materials. He proposed a dimensionless number, the Frank-Kamenetskii (F-K) parameter, to determine the critical ignition condition. Bowes and Thomas [1,21] advanced Frank-Kamenetskii's theory by taking the convection on the boundary into consideration and obtained a corrected F-K parameter which includes the Biot number. From the perspective of

these fundamental theories, the self-heating ignition that occurs in these two experimental configurations is the same phenomenon and the mechanisms (heat transfer, mass transfer, and chemistry) that control self-heating ignition do not change with experimental configurations. The main difference between these two experiments is the boundary condition: Oven-basket experiments have a symmetrical boundary condition whereas hot plate experiments have an unsymmetrical one. By modifying the boundary condition, the ignition criterion for two different experimental configurations can be analytically determined within the same theoretical frame [1]. However, these theories assume steady-state and mainly focus on the criticality. The transient behavior of self-heating ignition, such as the evolution of temperature, the time to ignition, and transient temperature profile cannot be obtained. To better understand this phenomenon, we need computational models that can conduct transient simulation.

So far a number of computational models have been built for various types of materials, covering coal [9,22–27], metal [28,29], and biomass [30,31]. However, all of these computational models were
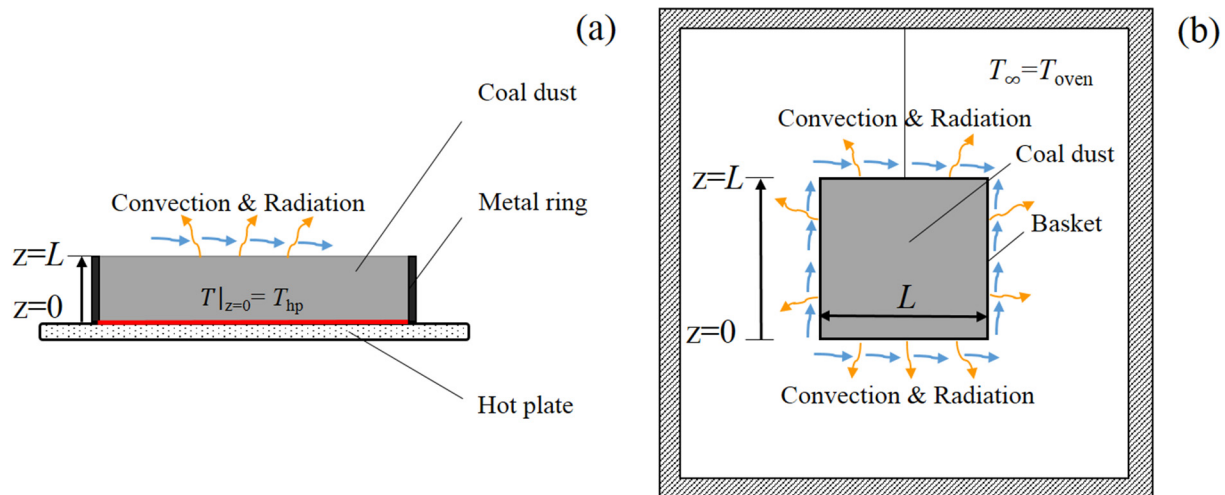

Fig. 1. Schematics for two types of experiments; (a) hot plate experiment, (b) oven-basket experiment.