Radiative heat loss impact modelling on thermal decomposition analysis in a reactive slab of variable thermal conductivity

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Abstract

In this article, an investigation into the impact of radiative heat loss in a stockpile of combustible material is considered. The heat loss is due to exothermic chemical reaction when carbon containing material of the stockpile reacts automatically with oxygen trapped within the system. The study is modelled in a rectangular slab of thermal conductivity that varies with temperature and loses heat to the surrounding environment by radiation. The differential equations governing the problem are solved numerically using Runge-Kutta-Fehlberg (RKF) method coupled with shooting technique. The behaviour of each embedded kinetic parameter of the system due to variation with temperature, oxygen depletion (O_2) and carbon dioxide emission (CO_2), is analysed and results are graphically expressed and discussed appropriately. The results show that kinetic parameters which enhance exothermic chemical reaction correspondingly increase the temperature and CO_2 emission of the combustion process. Copyright © 2018 VBRI Press.

Keywords: Radiative heat loss, exothermic chemical reaction, reactive slab, oxygen depletion, carbon dioxide emission.

Introduction

A detailed introduction is required here with proper emphasis about: (i) Importance of the addressed subject in general, (ii) importance of addressed subject in particular, (iii) related aspects covered in the literature, (iv) at the end a clear motivation about what is uniqueness about the present work (what is new here or how it differs from the previous works). It must be written in such a way that readers can get a detailed overview about the addressed subject (past, present and future perspectives and challenges). References should be listed as: [**1**] wherever needed Analysis of impact of radiative heat loss in a stockpile of combustible material is considered in this study. This study is motivated by spontaneous ignition of stockpiles of combustible materials. A combustible material is the one that contains carbon or hydrocarbon compound that readily reacts with oxygen trapped within the reactive stockpile. An example of a reactive stockpile is a heap of coal or rubbish containing hay, cotton or wool, or a mixture thereof. Spontaneous reaction between the material carbon and oxygen is due to exothermic chemical reaction, also called low-temperature oxidation. The spontaneous reaction between the carbon and oxygen results with carbon dioxide and heat as part of products. Accumulation of heat within the stockpile results with temperature raise, and should the heat loss to the surrounding environment be exceeded by heat production due to continued exothermic chemical reaction, thermal runaway that leads to self-ignition may take place [**1, 2, 3**]. Exothermic chemical reaction taking place within a stockpile of combustible material is of environmental importance. The previous studies highlighted that almost 80% of carbon dioxide contributing to Greenhouse effect is due to self-ignited fires from neglected stockpiles of combustible materials [**4, 5**]. The emission of carbon dioxide and heat from ignition processes such as coal burning including other reactive materials in households and particularly industries, contributed so much to climate change and global warming [**6, 7**]. This is evidenced by possible collapse of the Totten Glaciers due to warmth of the climate [**8**]. Spontaneous ignition of combustible materials that are not attended to, is one of the main causes of veld fires which are hazardous to living species and the environment at large. (**Fig. 1**) below is an example of veld fire that remains a great challenge and cause of harm to natural resources, forests and animal habitats including, sometimes, loss of life and property [**9**].

Fig. 1. Veld fire

The combustion process due to spontaneous reaction between combustible material and oxygen results with very complicated reaction mechanism. An elaborate chemical kinetics model for the reaction mechanism involving combustible material and oxygen is outlined in [**10**]. The combustion reaction mechanism is very complicated and involves many radicals, and in order to study radiative heat loss impact of the system, mathematical modelling is necessary [**11**]. The impact of radiative heat loss on combustible material with constant thermal conductivity was studied in [**12**]. The objective of this study is to investigate behaviors of temperature, oxygen depletion and carbon dioxide emission in a combusting stockpile of reactive material of variable thermal conductivity subjected to radiative heat loss. The article outlay is as follows, mathematical modelling is given is section 2, section 3 elaborates on the numerical method applied to solve the nonlinear differential equations governing the problem, graphical results and discussion thereof are done in section 4.

Experimental

It should be noted that this is a theoretical study that involved application of mathematics to investigate the impact of radiative heat loss on heat transfer, oxygen depletion and carbon dioxide emission during a combustion process. The investigation is done by varying kinetic parameters using suitable arbitrary values understand the behavior of temperature, oxygen depletion and carbon dioxide emission. For example, in order to study the effect of the activation energy parameter (ε) in this investigation, the following values, 0.1, 0.4, 0.7 and 1 were applied whilst other parameters were kept constant. The effect of each parameter used was done similarly. The partial differential equations for energy, to investigate the temperature, and for mass transfer, to investigate both oxygen depletion and carbon dioxide emission, are given under mathematical modelling subsection. The equations were converted into dimensionless state in order to allow a form that can be easily solved using numerical methods, as shown by equations 6. The numerical form of dimensionless equation are shown under the numerical method subsection. The numerical algorithms to solve nonlinear systems are embedded in many mathematical software, and in this investigation, Maple software was applied to solve the equations. Appropriate Maple programming for each parameter was drawn to give graphical solutions to the equations. The plotted graph depicts the effect of a particular parameter on the temperature, oxygen depletion and carbon dioxide emission behaviors. More explanation on effects of parameters is done under results and discussion section.

Mathematical modelling

Exothermic chemical reaction taking place within a stockpile of combustible material is modelled in a rectangular slab. It is assumed that the slab undergoes an n^{th} order oxidation chemical reaction and the complicated reaction is simplified by a one-step finite irreversible process [3,4,12] expressed as:

$$\mathrm{C}_i\mathrm{H}_j + \left(i + \frac{j}{4}\right)\mathrm{O}_2 \rightarrow i\mathrm{CO}_2 + \left(\frac{j}{2}\right)\mathrm{H}_2\mathrm{O} + \text{heat.}$$

The reactive slab is also assumed to lose heat to the surrounding environment by radiation, and the heat loss is expressed as $q = \mu\sigma(T^4 - T_w^4)$, following Stefan-Boltzmann's law. In this case μ is the solid slab's surface emissivity $(0 < \mu < 1)$, σ is the Stefan-Boltzmann constant ($5.6703\times 10^{-8} W/m^2K^4$), T is the slab's absolute temperature and T_w is the ambient temperature. The slab's material is of thermal conductivity k, that varies with temperature at $t > 0$ and it has the expression $k = \tau e^{b(T-T_w)}$, where τ is the material thermal conductivity at the ambient temperature T_w and b is the thermal conductivity variation parameter. The geometry of the problem is given by (**Fig. 2**) below.

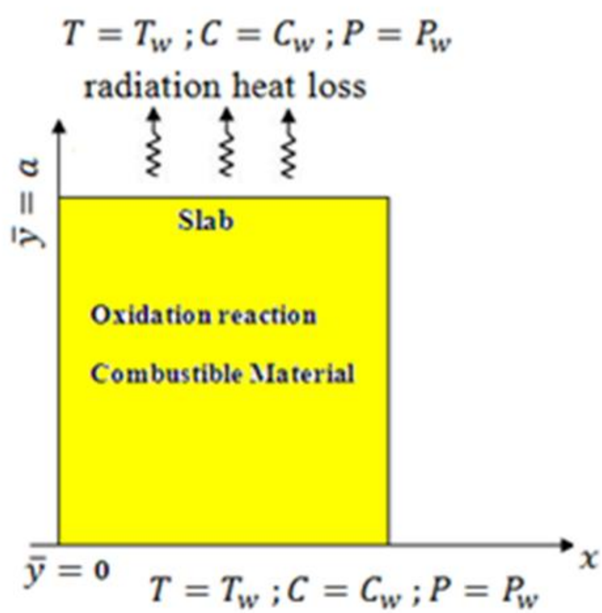

Fig. 2. Geometry of the problem.

Following [**3,4,12**] the nonlinear ordinary differential equations governing the problem are expressed as:

$$k\frac{d^2T}{d\bar{y}^2} + QA\left(\frac{KT}{vl}\right)^m C^n exp\left(-\frac{E}{RT}\right) - \mu\sigma(T^4 - T_w^4) = 0 \quad (1)$$

$$D\frac{d^2C}{d\bar{y}^2} - A\left(\frac{KT}{vl}\right)^m C^n exp\left(-\frac{E}{RT}\right) = 0 \quad (2)$$

$$\gamma\frac{d^2P}{d\bar{y}^2} + A\left(\frac{KT}{vl}\right)^m C^n exp\left(-\frac{E}{RT}\right) = 0, \quad (3)$$

with boundary conditions:

$$\bar{y} = 0,\ T = T_w,\ C = C_w,\ P = P_w, \quad (4)$$

$$\bar{y} = a,\ T = T_w,\ C = C_w,\ P = P_w \quad (5)$$

where C is the oxygen concentration, P is the carbon dioxide emission concentration, C_w is the oxygen concentration at the slab surface, P_w is the carbon dioxide concentration at the slab surface, D is the diffusivity of oxygen in the slab, γ is the diffusivity of carbon dioxide in the slab, Q is the heat of reaction, A is the rate constant, E is the activation energy, R is the universal gas constant, l is the Planck number, v is the vibration frequency, K is the Boltzmann constant, n is the order of exothermic chemical reaction, and m is the numerical exponent such that $m = -2$ is for Sensitized (laser induced) kinetics, $m = 0$ represents Arrhenius kinetics and $m = 0.5$ is for Bimolecular kinetics, following [**3,4,12**]. The following dimensionless parameters are introduced to equations (1) – (5)

$$\theta = \frac{E(T-T_w)}{RT_w^2},\ \Phi = \frac{C}{C_w},\ \Psi = \frac{P}{P_w}, \beta = \frac{bRT_w^2}{E},$$

$$\beta_1 = \frac{kRT_w^2}{QEDC_w}, \beta_2 = \frac{kRT_w^2}{QE\gamma P_w},$$

$$\lambda = \left(\frac{KT_w}{vl}\right)^m \frac{QAEa^2(C_w)^n}{kRT_w^2} exp\left(-\frac{E}{RT_w}\right),$$

$$y = \frac{\bar{y}}{a}, \varepsilon = \frac{RT_w}{E}, Ra = \frac{\mu\sigma E a^2 T_w^2}{kR}. \quad (6)$$

Equations (1) – (5) take the dimensionless form

$$\frac{d^2\theta}{dy^2} + \beta\left(\frac{d\theta}{dy}\right)^2 + \lambda(1+\varepsilon\theta)^m \Phi^n e^{\theta/(1+\varepsilon\theta)} e^{-\beta\theta} - Ra[(\varepsilon\theta+1)^4 - 1]e^{-\beta\theta} = 0, \quad (7)$$

$$\frac{d^2\Phi}{dy^2} - \lambda\beta_1(1+\varepsilon\theta)^m \Phi^n e^{\theta/(1+\varepsilon\theta)} e^{-\beta\theta} = 0, \quad (8)$$

$$\frac{d^2\Psi}{dy^2} + \lambda\beta_2(1+\varepsilon\theta)^m \Phi^n e^{\theta/(1+\varepsilon\theta)} e^{-\beta\theta} = 0, \quad (9)$$

$$y = 0,\ \theta = 0,\quad \Phi = 1,\quad \Psi = 1, \quad (10)$$

$$y = 1,\ \theta = 0,\quad \Phi = 1,\quad \Psi = 1, \quad (11)$$

where λ is the Frank-Kamenetski parameter, ε is the activation energy parameter, β is the variable thermal conductivity parameter, β_1 is the oxygen consumption rate parameter, β_2 is the carbon dioxide emission rate parameter, Ra is the radiation parameter. It should be noted further that if the rate of heat generation in the slab exceeds the rate of heat loss to its surrounding, ignition can take place.

Numerical method

The set of equations (7) – (9) together with the boundary conditions (10) – (11) were solved numerically using the Runge-Kutta-Fehlberg method coupled with shooting technique [9]. The following is the numerical algorithm used to convert second order differential equations into first order form, where we consider:

$$\theta = s_1,\ \theta' = s_2,\ \Phi = s_3,\ \Phi' = s_4,\ \Psi = s_5, \Psi' = s_6.$$

Equations (6) – (11) are transformed into first order differential equations as follows:

$$s'_1 = s_2$$

$$s'_2 = -\lambda(1+\varepsilon s_1)^m (s_3)^n e^{s_1/(1+\varepsilon s_1)} e^{-\beta s_1} - Ra[(\varepsilon s_1 + 1)^4 - 1]e^{-\beta s_1}$$

$$s'_3 = s_4$$

$$s'_4 = \lambda(1+\varepsilon s_1)^m (s_3)^n e^{s_1/(1+\varepsilon s_1)} e^{-\beta s_1}$$

$$s'_5 = s_6$$

$$s'_6 = -\lambda(1+\varepsilon s_1)^m (s_3)^n e^{s_1/(1+\varepsilon s_1)} e^{-\beta s_1}, \quad (13)$$

subject to the initial conditions

$$s_1(0) = 0,\ s_3(0) = 1,\ \ s_5(0) = 1,\ s_1(1) = 0,\ s_3(1) = 1,\ s_5(1) = 1 \quad (14)$$

The shooting method is coupled with RKF45 to give results to expected accuracy.

Results and discussion

In this section variation of some thermo-physical parameters with temperature, oxygen depletion and carbon dioxide emission of the system are investigated and discussed appropriately. Thermo-physical parameters analysed are $\lambda, m, n, Ra, \varepsilon, \beta, \beta_1$ and β_2. The following parameter values were used: $\lambda = 1, m = 0.5, n = 1, Ra = 1, \beta = 0.1, \beta_1 = 0.1, \beta_2 = 0.1, \varepsilon = 0.1$. The value of $\varepsilon = 10$ was applied only in (**Fig. 8**), (**Fig. 13**) and (**Fig. 18**).

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Conclusion

Appropriate conclusion needs to written here which reflects the exact finding demonstrated in the paper.

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Author's contributions

Conceived the plan: xx, xy, yz; Performed the expeirments: xx, xy; Data analysis: xx yz; Wrote the paper: xx, xy, yz (xx, xy, yz are the initials of authors). Authors have no competing financial interests.

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