Some New Results on a Free Boundary Value Problem Related to Auto Ignition of Combustible Fluid in Insulation Materials

Olayiwola, R. O.; Cole, A. T.; Shehu, M. D.; Oguntolu, F. A.; Fadepo J. T., Okoosi F. E.

Department of Mathematics,
Federal University of Technology, Minna, Nigeria.
olayiwola.rasaq@futminna.edu.ng

Abstract. Auto ignition of combustible fluids in insulation materials is one of the major problems facing the processing industries and many developing nations because it leads to serious environmental problem. This paper presents an analytical solution to a free boundary value problem related to auto ignition of combustible fluids in insulation materials. The aim is to ascertain whether such a system is safe or if it will undergo ignition for a particular set of conditions. The conditions for the existence of unique solution of the model is established by actual solution method. The properties of solution is examined. The analytical solution is obtained via polynomial approximation method, which show the influence of the parameters involved on the system. The effect of changes in parameters such as the Lewis number and Nusselt number are presented graphically and discussed.

Keywords: Auto ignition, combustible fluids, free boundary value problem, polynomial approximation method

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Introduction

Apart from the unhealthy criminal actions of pipeline vandals that cause fire outbreak in various economic nations. The leakage of combustible fluids into the insulation materials is

also hazardous as a result of the oxidation of a fluid which generates heat, and the resulting exothermic reaction can lead to ignition which consequently damages the pipe, lives and other valuable properties in the area (Popoola and Ayeni, 2007).

Models of combustion are characterized by two phenomena; ignition and explosion (Ayeni *et al.*, 2007; Makinde, 2006). Truscott *et al.* (1996) examined an initial value problem related to auto ignition of combustible fluids in insulation materials and investigated the effect of diffusion on the system. Popoola and Ayeni (2007) extended the model of Truscott *et al.* (1996) to a free boundary value problem by assuming that the reactant is not confined to a fixed space. Brindley *et al.* (1999) developed the theoretical background and the limiting criteria for safe operation on auto ignition of combustible fluids in insulation materials and discussed the magnitudes of the parameters that may be used to compare theory with experiment.

In this paper, the aim is to establish an approximate analytical solution capable of predicting the temperature distribution in a process of auto ignition of combustible fluids in insulation materials. For this we shall follow the method proposed in Prakash and Mahmood (2013).

Model Formulation

Extending the work of Popoola and Ayeni (2007) by considering the model geometry which may be represented by a single characteristic dimension to be sphere, the respective conservation equations in spherical coordinate system are thus:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r} \right) + \frac{QA}{\rho c} C_f^\alpha C_{ox}^\beta e^{-\frac{E}{RT}} - \frac{Q_v F}{\rho c} C_f e^{-\frac{E_v}{RT}} \tag{1}$$

$$\frac{\partial C_f}{\partial t} = \frac{D_f}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial C_f}{\partial r} \right) - A C_f^\alpha C_{ox}^\beta e^{-\frac{E}{RT}} - F C_f e^{-\frac{E_v}{RT}} \tag{2}$$

$$\frac{\partial C_{ox}}{\partial t} = \frac{D_0}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial C_{ox}}{\partial r} \right) - v A C_f^\alpha C_{ox}^\beta e^{-\frac{E}{RT}} \tag{3}$$

with the initial and boundary conditions:

$$T(r,0)=T_s, \qquad \left.\frac{\partial T}{\partial r}\right|_{r=0}=0, \qquad \left. k^*\frac{\partial T}{\partial r}\right|_{r=s(t)}=h(T_s-T)|_{r=s(t)}\dot s(t)$$

$$C_f(r,0)=C_{fs}, \qquad \left.\frac{\partial C_f}{\partial r}\right|_{r=0}=0, \qquad \left.D_f'\frac{\partial C_f}{\partial r}\right|_{r=s(t)}=-k_{mf}(C_{fs}+C_f)|_{r=s(t)}\dot s(t) \qquad (4)$$

$$C_{ox}(r,0)=C_{oxs}, \qquad \left.\frac{\partial C_{ox}}{\partial r}\right|_{r=0}=0, \qquad \left.D_s'\frac{\partial C_{ox}}{\partial r}\right|_{r=s(t)}=-k_{mox}(C_{oxs}+C_{ox})|_{r=s(t)}\dot s(t)$$

$$\dot s(t)=\frac{1}{t^2}, \qquad 0<r<s(t)$$

where C_{ox} is the concentration of Oxygen, C_f is the concentration of condensed reactant, D_s is the Oxygen diffusion coefficient, D_f is the condensed reactant diffusion coefficient, ρ is the density of the reactant, k is the thermal conductivity of the medium, c is the heat capacity of the medium, Q is the enthalpy of oxidation (exothermicity), Q_v is the enthalpy of vaporization (endothermicity), R is the universal gas constant, T is the temperature of the medium, E is the activation energy (reaction), E_v is the activation energy (vaporization), T_s is the initial temperature of the medium, v is the stoichiometry coefficient, C_{oxs} is the initial oxygen concentration within the insulation block, C_{fs} is the initial concentration of the uniformly distributed fluid, t is the time, A is the pre-exponent factor (reaction), F is the pre-exponent factor (vaporization), α and β are the order of reaction, r is the spatial coordinate, $s(t)$ is the moving boundary, D_0^* is the effective Oxygen diffusion coefficient, D_f^* is the effective condensed reactant diffusion coefficient, k^* is the effective thermal conductivity of the medium, k_{mf} is the condensed reactant convective mass transfer coefficient, k_{mox} is the Oxygen convective mass transfer coefficient, h is the convective heat transfer coefficient, $hT_0\dot s(t)$ is the heat energy released per unit time by the reaction, $hT|_{r=s(t)}\dot s(t)$ is the energy flux induced by the motion of the boundary preserve energy conservation, $k_{mf}C_{f0}\dot s(t)$ is the number of moles per unit time of condensed fluid, $k_{mf}C_f|_{r=s(t)}\dot s(t)$ is the mass flux of condensed fluid induced by the motion of the boundary preserve mass conservation, $k_{mox}C_{ox0}\dot s(t)$ is the number of moles per unit time of oxidizer that diffused into the system for the reaction, $k_{mox}C_{ox}|_{r=s(t)}\dot s(t)$ is the mass flux of oxidizer.

Method of Solution

Non-dimensionalisation

Dimensionless variables for space, time, medium temperature, condensed fluid concentration and oxygen concentration is been introduced as follows:

$$r' = \frac{2r}{\sqrt{D_f} s(t)}, \quad t' = \frac{4t}{s(t)^2}, \quad \theta = \frac{E}{RT_0^2}(T - T_0), \quad \psi = \frac{C_f}{C_{f0}},$$

$$\phi = \frac{C_{ox}}{C_{ox0}}, \quad E_v = nE, \quad \epsilon = \frac{RT_0}{E}, \quad (5)$$

where $s(t) = (1-\gamma)^{-1} t^{1-\gamma}$ is moving boundary. Here, we choose $\gamma = \frac{1}{2}$ as in Popoola and Ayeni (2007).

Using (5), and after dropping the prime, equations (1) - (4) become

$$\frac{\partial \theta}{\partial t} = \frac{Le}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \theta}{\partial r}\right) + \delta \psi^\alpha \phi^\beta e^{\frac{\theta}{1+\epsilon\theta}} - \delta_1 \psi e^{\frac{n\theta}{1+\epsilon\theta}} \qquad (6)$$

$$\frac{\partial \psi}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) - \sigma_1 \psi^\alpha \phi^\beta e^{\frac{\theta}{1+\epsilon\theta}} - \sigma_2 \psi e^{\frac{n\theta}{1+\epsilon\theta}} \qquad (7)$$

$$\frac{\partial \phi}{\partial t} = \frac{\alpha_1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) - \beta_1 \psi^\alpha \phi^\beta e^{\frac{\theta}{1+\epsilon\theta}} \qquad (8)$$

$$\left. \begin{array}{l} \theta(r,0) = 0, \quad \left.\frac{\partial \theta}{\partial r}\right|_{r=0} = 0, \quad \left.\frac{\partial \theta}{\partial r}\right|_{r=\frac{2}{\sqrt{D_f}}} = -Nu\theta\big|_{r=\frac{2}{\sqrt{D_f}}} \\[4mm] \psi(r,0) = 1, \quad \left.\frac{\partial \psi}{\partial r}\right|_{r=0} = 0, \quad \left.\frac{\partial \psi}{\partial r}\right|_{r=\frac{2}{\sqrt{D_f}}} = -Sh_f\left(1 + \psi\big|_{r=\frac{2}{\sqrt{D_f}}}\right) \\[4mm] \phi(r,0) = 1, \quad \left.\frac{\partial \phi}{\partial r}\right|_{r=0} = 0, \quad \left.\frac{\partial \phi}{\partial r}\right|_{r=\frac{2}{\sqrt{D_f}}} = -Sh_{ox}\left(1 + \phi\big|_{r=\frac{2}{\sqrt{D_f}}}\right), \quad 0 < r < \frac{2}{\sqrt{D_f}} \end{array} \right\}, (9)$$

where

$Le = \dfrac{k}{\rho c D_f}$ is the Lewis number, $\delta = \dfrac{QA(s(t))^2 C_{fo}^{\alpha} C_{ox0}^{\beta} e^{-\frac{E}{RT_0}}}{4 \in T_0 \rho c}$ is the Frank-Kamenetskii

number (reaction), $\delta_1 = \dfrac{Q_v F(s(t))^2 C_{fo} e^{-\frac{E}{RT_0}}}{4 \in T_0 \rho c}$ is the Frank-Kamenetskii number

(vaporization), $\alpha_1 = \dfrac{D_0}{D_f}$, $\sigma_1 = \dfrac{A(s(t))^2 C_{fo}^{\alpha-1} C_{ox0}^{\beta} e^{-\frac{E}{RT_0}}}{4}$, $\sigma_2 = \dfrac{F(s(t))^2 e^{-\frac{E}{RT_0}}}{4}$,

$\beta_1 = \dfrac{vA(s(t))^2 C_{fo}^{\alpha} C_{ox0}^{\beta-1} e^{-\frac{E}{RT_0}}}{4}$, $Sh_f = \dfrac{k_{mf}\sqrt{D_f}}{D_f^{\cdot}}$ is the Sherwood number (condensed fluid),

$Sh_{ox} = \dfrac{k_{mox}\sqrt{D_f}}{D_0^{\cdot}}$ is the Sherwood number (oxidizer), $Nu = \dfrac{h\sqrt{D_f}}{k^{\cdot}}$ is the Nusselt number.

Existence and Uniqueness of Solution

Theorem 1: Let $Le = \alpha_1 = \sigma_1 = \sigma_2 = \beta_1 = Nu = Sh_f = Sh_{ox} = 1$ and $\delta_1 = -\dfrac{\delta}{2}$. Then there

exists a solution of (6) – (8) which satisfies (9).

Proof: Multiply (7) and (8) by $\dfrac{\delta}{2}$ and adding the resulting equations, we obtain

$$\frac{\partial \varphi}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \varphi}{\partial r}\right) \tag{20}$$

$$\varphi(r,0) = \delta, \quad \left.\frac{\partial \varphi}{\partial r}\right|_{r=0}, \quad \left.\frac{\partial \varphi}{\partial r}\right|_{r=\frac{2}{\sqrt{D_f}}} = -\left(\delta + \left.\varphi\right|_{r=\frac{2}{\sqrt{D_f}}}\right) \tag{31}$$

where

$$\varphi(r,t) = \theta(r,t) + \frac{\delta}{2}(\psi(r,t) + \phi(r,t))$$

Assuming a polynomial solution of the form (see, Prakash and Mahmood (2013)):

$$\varphi(r,t) = c_0(t) + c_1(t)r + c_2(t)r^2 \tag{42}$$

we obtain the approximated solution of equations (10) and (11) as

$$\varphi(r,t) = \frac{\delta\sqrt{D_f}}{4} + \left(1 + \frac{\sqrt{D_f}}{4}\right)\left(b + (\delta - b)e^{-at}\right) - \frac{\sqrt{D_f}}{4}\left(\delta + \left(b + (\delta - b)e^{-at}\right)\right)r^2 \quad (53)$$

where

$$a = \frac{240 D_f}{40 D_f + 8\sqrt{D_f} - 32}, \qquad b = -\frac{12}{D_f}\delta$$

Then, we obtain

$$\psi(r,t) = \frac{2}{\delta}\left(\left(\frac{\delta\sqrt{D_f}}{4} + \left(1 + \frac{\sqrt{D_f}}{4}\right)\left(b + (\delta - b)e^{-at}\right) - \frac{\sqrt{D_f}}{4}\left(\delta + \left(b + (\delta - b)e^{-at}\right)\right)\right) - \theta(r,t)\right) - \phi(r,t) \quad (64)$$

$$\phi(r,t) = \frac{2}{\delta}\left(\left(\frac{\delta\sqrt{D_f}}{4} + \left(1 + \frac{\sqrt{D_f}}{4}\right)\left(b + (\delta - b)e^{-at}\right) - \frac{\sqrt{D_f}}{4}\left(\delta + \left(b + (\delta - b)e^{-at}\right)\right)\right) - \theta(r,t)\right) - \psi(r,t) \quad (75)$$

$$\theta(r,t) = \left(\frac{\delta\sqrt{D_f}}{4} + \left(1 + \frac{\sqrt{D_f}}{4}\right)\left(b + (\delta - b)e^{-at}\right) - \frac{\sqrt{D_f}}{4}\left(\delta + \left(b + (\delta - b)e^{-at}\right)\right)\right) - \frac{2}{\delta}\left(\psi(r,t) + \phi(r,t)\right) \quad (86)$$

Hence, there exists a solution of problem (6) – (9). This completes the proof.

Properties of Solution

Following thermal ignition theory, it is necessary to assume that there is always sufficient oxygen and fuel present in subcritical conditions so that the behaviour of the system is then governed solely by the energy conservation equation (6). That is ψ and ϕ are assumed constant.

Lemma 1: Let $\epsilon \to 0$. Then the parabolic differential equation (6) with initial and boundary conditions (9) has a unique solution.

Proof: It suffices to show that the Lipschitz condition is satisfied. That is if we are able to show that $|f(r,t,\theta_1) - f(r,t,\theta_2)| \le k|\theta_1 - \theta_2|$

From (6), $f(r,t,\theta) = \delta\psi^a\phi^\beta e^\theta - \delta_1\psi e^{n\theta}$

By mean value theorem $\dfrac{\partial f}{\partial\theta} = \delta\psi^a\phi^\beta e^\theta - \delta_1 n\psi e^{n\theta}$

But $\max \dfrac{\partial f}{\partial\theta}$ is achieved when $n = 0$ and $e^\theta = 1$ i.e. $n = 0$ and $\theta = 0$

Hence, $k = \max \dfrac{\partial f}{\partial\theta} = \delta\psi^a\phi^\beta$

Therefore, $|f(r,t,\theta_1) - f(r,t,\theta_2)| \le \delta\psi^a\phi^\beta|\theta_1 - \theta_2|$

Since the Lipschitz condition is satisfied, equation (6) has a unique solution. This completes the proof.

For a well stirred reaction when the activation energy for reaction is the same as activation energy for vaporization, i.e. $n = 1$ and in a high activation energy situation $\epsilon \to 0$, equation (6) reduces to

$$\frac{d\theta}{dt} = \delta\psi^a\phi^\beta e^\theta - \delta_1\psi e^\theta, \qquad \theta(0) = 0 \qquad\qquad (97)$$

Solving (17), we obtain

$$\theta(t) = \ln\left(\frac{1}{\left(1 - \left(\delta\psi^a\phi^\beta - \delta_1\psi\right)t\right)}\right) \to \infty \quad \text{as} \quad t = \frac{1}{\left(\delta\psi^a\phi^\beta - \delta_1\psi\right)} \qquad (108)$$

Hence, $\theta(t) \to \infty$ is thermal runaway and $t = \dfrac{1}{\left(\delta\psi^a\phi^\beta - \delta_1\psi\right)}$ is actually the time of thermal runaway.

Analytical Solution by Polynomial Approximation Method

In the presence of diffusion, assuming constant ψ and ϕ, equation (6) can be solve analytically in the limit $\epsilon \to 0$. Following Ayeni (1982), we assume the expression for $\exp(\theta)$, that is,

$$\exp(\theta) \approx 1 + (e - 2)\theta \qquad\qquad (119)$$

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Then (6) and (9) can be written as:

$$\frac{\partial \theta}{\partial t} = \frac{Le}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \theta}{\partial r}\right) + \delta \psi'' \phi''(1 + (e-2)\theta) - \delta_1 \psi(1 + (e-2)\theta)^2 \quad (20)$$

$$\theta(r,0) = 0, \qquad \left.\frac{\partial \theta}{\partial r}\right|_{r=0} = 0, \qquad \left.\frac{\partial \theta}{\partial r}\right|_{r=\frac{2}{\sqrt{D_f}}} = -Nu\theta\big|_{r=\frac{2}{\sqrt{D_f}}} \quad (21)$$

Here, we assume polynomial solution of the form (see, Prakash and Mahmood (2013)):

$$\theta(r,t) = a_0(t) + a_1(t)r + a_2(t)r^2 \quad (22)$$

Applying the boundary conditions as given in (21), we obtain

$$a_1(t) = 0, \qquad a_2(t) = -\frac{Nu\sqrt{D_f}}{4}\theta\big|_{r=\frac{2}{\sqrt{D_f}}}, \qquad a_0(t) = \left(1 + \frac{Nu\sqrt{D_f}}{4}\right)\theta\big|_{r=\frac{2}{\sqrt{D_f}}} \quad (23)$$

Then, equation (22) becomes

$$\theta(r,t) = \left(1 + \frac{Nu\sqrt{D_f}}{4}\right)\theta\big|_{r=\frac{2}{\sqrt{D_f}}} - \frac{Nu\sqrt{D_f}}{4}\theta\big|_{r=\frac{2}{\sqrt{D_f}}}r^2 \quad (24)$$

For long spherical shape (see, Keshavart and Taheri (2007)), we have

$$\bar{\theta} = 3\int_0^1 r^2\theta dr, \quad (25)$$

where $\bar{\theta}$ is the average temperature.

Equations (25) gives the relations

$$\bar{\theta} = \frac{8}{D_f\sqrt{D_f}}\left(1 + \frac{Nu\sqrt{D_f}}{4} - \frac{12Nu}{20\sqrt{D_f}}\right)\theta\big|_{r=\frac{2}{\sqrt{D_f}}} \quad \text{and} \quad \frac{\partial}{\partial t}\bar{\theta} = \frac{8}{D_f\sqrt{D_f}}\left(1 + \frac{Nu\sqrt{D_f}}{4} - \frac{12Nu}{20\sqrt{D_f}}\right)\frac{\partial}{\partial t}\theta\big|_{r=\frac{2}{\sqrt{D_f}}} \quad (26)$$

Integrating (20) with respect to x, yield the following equation

$$\left.\frac{\partial}{\partial t}\theta\right|_{r=\frac{2}{\sqrt{D_f}}} + p\theta\big|_{r=\frac{2}{\sqrt{D_f}}} = q \quad (27)$$

Solving (27) gives

$$\theta\Big|_{r=\frac{2}{\sqrt{D_r}}} = \frac{q}{p}\left(1-e^{-pt}\right) \tag{28}$$

Substituting equation (28) into equation (24) gives

$$\theta(r,t) = \frac{q}{p}\left(1+\frac{Nu\sqrt{D_f}}{4}\right)\left(1-e^{-pt}\right) - \frac{qNu\sqrt{D_f}}{4p}\left(1-e^{-pt}\right)r^2 \tag{29}$$

where

$$p = \frac{\left[\frac{12LeNu}{D_f} + \frac{8\delta\psi''\phi''(e-2)}{D_f\sqrt{D_f}}\right]\left[\frac{3Nu}{5\sqrt{D_f}} - \left(1+\frac{Nu\sqrt{D_f}}{4}\right)\right] + \delta\psi n(e-2)\left[\left(1+\frac{Nu\sqrt{D_f}}{4}\right) - \frac{12Nu}{5D_f^2}\right]}{\left[\frac{8}{D_f\sqrt{D_f}}\left(1+\frac{Nu\sqrt{D_f}}{4}\right) - \frac{96Nu}{20D_f^2}\right]},$$

$$q = \frac{\frac{8}{D_f\sqrt{D_f}}\left(\delta\psi''\phi'' - \delta_t\psi\right)}{\left[\frac{8}{D_f\sqrt{D_f}}\left(1+\frac{Nu\sqrt{D_f}}{4}\right) - \frac{96Nu}{20D_f^2}\right]}$$

The computations were done on equations (29) using computer symbolic algebraic package MAPLE 16.

Results and Discussion

To conclude this analysis we examine the relationship between the Nusselt and Lewis numbers and the transient state temperature $\theta(r,t)$. Figure 1 depicts the graph of temperature $\theta(r,t)$ against spatial co-ordinate r and time t for different values of Nusselt number Nu. It is observed that the temperature increases with time and decreases along spatial co-ordinate but decreases as Nusselt number increases. Figure 2 displays the graph of temperature $\theta(r,t)$ against spatial co-ordinate r and time t for different values of Lewis number Le. It is observed that the temperature increases with time and decreases along spatial co-ordinate but increases as Lewis number increases.
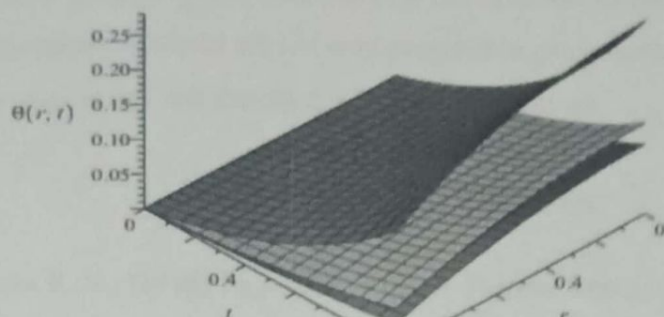
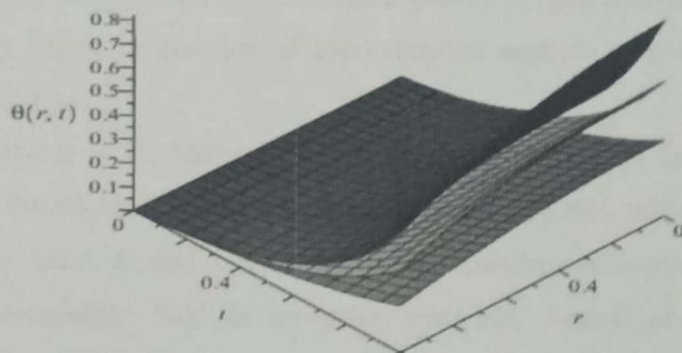Figure 1: Relation among temperature, time and spatial co-odinate for various values of Nusselt number *Nu*

Figure 2: Relation among temperature, time and spatial co-odinate for various values of Lewis number *Le*

It is worth pointing out that the effects observed in Figures 1 and 2, are important to guide insulation materials manufacturers so as to provide safety precautions during storage and usage.

Conclusion

For a well stirred reaction and in a high activation energy situation $\epsilon \rightarrow 0$, we have found that thermal runaway could still occur when the activation energy for reaction is the same as

activation energy for vaporization, i.e. $n = 1$. That is $\theta(t) \to \infty$ as $t \to \dfrac{1}{\left(\delta\psi^{\alpha}\phi^{\beta} - \delta_1\psi\right)}$.

Therefore the established conditions for the existence of the unique solution of the problem and the results obtained are not only expected to guide manufacturers of insulation materials but provide safety precautions during storage and usage.

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