Journal of the Nigerian Association of Mathematical Physics
Volume **11 (November 2007), 95 - 102**

A free-boundary value problem related to auto ignition of combustible fluid in insulation materials.

A. O. Popoola* and R. O. Ayeni**
Department of Pure and Applied Mathematics
Ladoke Akintola University of Technology, Ogbomoso Nigeria.
e-mails: * bobdee11@yahoo.com, ** ayeni_ro@yahoo.com,

Abstract

We examine a free boundary value problem related to auto ignition of combustible fluid in insulation materials. The criteria for the existence of similarity solution of the model equations are established. The conditions for the existence of unique solution are also stated. The numerical results which show the influence of activation energies on the three-component model of the chain reaction also identify the ignition point of the combustible fluids.

Keywords**:** Free boundary value problem, auto ignition, combustible fluids, similarity solution.

1.0 Introduction

Auto ignition of combustible fluids in insulation materials is one of the major problems facing the processing industries and many developing nations and this leads to a serious environmental problem. The fact is that auto ignition can lead to catastrophic damage of lives and properties (Truscott et.al [10]). Apart from the unhealthy criminal actions of pipeline vandals that cause fire outbreak in various economic developing nations. The leakage of combustible fluids into the insulation materials is also hazardous as a result of the oxidation of the 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.

Models of combustion are characterized by two phenomena; ignition and explosion [1, 2, 5, 9]. Truscott et.al [10] examined an initial value problem which represents the model of auto ignition of combustible fluids in insulation materials and investigated the effect of diffusion on the system. They identified the behaviour of the system parameters such as size and the endothermicity. The combustion zone is assumed fixed.

Following the approach of Cannon and Matheson [3], we extend the model of Truscott et.al [10] to a free boundary value problem by assuming the reactant is not confined to a fixed space. We also assumed that the order of reaction is greater than zero. Following Popoola and Ayeni [8], we investigate the effect of activation energies of the chain reaction on the temperature, fuel concentration and oxygen concentration of the system. A similarity solution is sought using the standard procedure [7]. We assumed that the initial temperature of the system, initial fuel concentration and initial concentration of oxygen are known and investigate the behaviour of the thermal system at any subsequent time.

2.0 Mathematical formulation

Extending the model of Truscott et.al [10] to a free boundary value problem, we obtain

$$\rho\ell\frac{\partial T}{\partial t}=k\frac{\partial^2 T}{\partial x^2}+Q_1A_1CZT^n e^{\frac{-E_1}{RT}}-Q_2A_2CZT^m e^{\frac{-E_2}{RT}} \qquad (2.1)$$

$$\frac{\partial C}{\partial t}=D_x\frac{\partial^2 C}{\partial x^2}-1A_1CZe^{\frac{-E_1}{RT}}-A_2Ce^{\frac{-E_2}{RT}} \qquad (2.2)$$

$$\frac{\partial Z}{\partial t}=-A_1CZe^{\frac{-E_1}{RT}}+D_o\frac{\partial^2 Z}{\partial x^2} \qquad (2.3)$$

with the conditions

$$T(0,t)=T_0,\quad C(0,t)=C_0,\; Z(0,t)=Z_0, \qquad (2.4)$$

$$\left.\begin{aligned} &kT_x(s(t),t)=(T_o-T(s(t),t))\dot{s}(t),\\ &D_xC_x(s(t),t)=-\mu(C_o+C(s(t),t))\dot{s}(t),\\ &D_0Z_x(s(t),t)=-\lambda(Z_o+Z(s(t),t))\dot{s}(t),\\ &\dot{s}(t)=\frac{1}{t^\gamma} \qquad 0<x<s(t)\end{aligned}\right\} \qquad (2.5)$$

where ρ is the density of the reactant,

ℓ is the heat capacity and k is the thermal conductivity of the medium.

Q_1 and Q_2 are enthalpies of oxidation and endothermic evaporation respectively

A_1 & A_2 are pre-exponential factors of the first and second steps reaction respectively.

E_1 and E_2 are activation energies of the first and second steps reaction respectively

R is the universal gas constant; n and m are orders of first and second steps reaction respectively. T is the temperature of the reaction while T_0 denotes the initial temperature of the system

C denotes the fuel concentration while Z is the oxygen concentration

D_x denotes the diffusion coefficient for fuel while D_0 is the diffusion coefficient for oxygen.

$s(t)$ is the moving boundary,

$T(s(t),t).\dot{s}(t)$ represents the energy flux induced by the motion of the boundary to preserve energy conservation while

$T_o\dot{s}(t)$ is the heat energy released per unit time by the reaction.

$\mu C_o.\dot{s}(t)$ represents the number of moles per unit time of fuel while

$\mu C(s(t),t).\dot{s}(t)$ is the mass flux of fuel induced by the motion of the boundary to preserve mass conservation.

$\lambda Z_o.\dot{s}(t)$ represents the number of moles per unit time of oxidizer that diffused to the system for the reaction and

$\lambda Z(s(t),t).\dot{s}(t)$ is the mass flux of oxidizer.

3.0 Non-Dimensionalization

The following parameters are assumed for non-dimensionalization.

$$T=T_o+\frac{RT_o^2\theta}{E_1},\quad \varepsilon=\frac{RT_o}{E_1},\quad E_2=\alpha E_1,\quad C=C_oc,\; Z=Z_oz$$

Then the equations (2.1) and (2.3) subject to conditions (2.4) and (2.5) become

$$\frac{\partial\theta}{\partial t}=æ\frac{\partial^2\theta}{\partial x^2}+a(1+\varepsilon\theta)^n cze^{\frac{\theta}{1+\varepsilon\theta}}-b(1+\varepsilon\theta)^m ce^{\frac{\alpha\theta}{1+\varepsilon\theta}} \tag{3.1}$$

$$\frac{\partial c}{\partial t}=D_x\frac{\partial^2 c}{\partial x^2}-F_1cze^{\frac{\theta}{1+\varepsilon\theta}}-F_2ce^{\frac{\alpha\theta}{1+\varepsilon\theta}} \tag{3.2}$$

$$\frac{\partial z}{\partial t}=-F_3cze^{\frac{\theta}{1+\varepsilon\theta}}+D_0\frac{\partial^2 z}{\partial x^2} \tag{3.3}$$

satisfying

$$\left.\begin{array}{l}\theta(0,t)=0,\ c(0,t)=1,\ z(0,t)=1,\\ k\frac{\partial\theta}{\partial x}(s(t),t)=-\theta(s(t),t)\dot{s}(t),\\ D_x\frac{\partial c(s(t),t)}{\partial x}=-\mu(1+c(s(t),t))\dot{s}(t),\\ D_0\frac{\partial z(s(t),t)}{\partial x}=-\lambda(1+z(s(t),t))\dot{s}(t),\\ \dot{s}(t)=\frac{1}{t^{\gamma}},\ t>0,\ \gamma\neq 0, D_x, D_0, \lambda, \mu \text{ are positive constants}\end{array}\right\} \tag{3.4}$$

where

$$æ=\frac{k}{\rho c_p},\ a=a(t)=\frac{Q_1A_1czC_oZ_oT_0^{\,n-1}}{\varepsilon\rho\,\ell}e^{\frac{-1}{\varepsilon}},\ b=b(t)=\frac{Q_2A_2cC_oT_0^{\,m-1}}{\varepsilon\rho\,\ell}e^{\frac{-\alpha}{\varepsilon}}$$

$$F_1=F_1(t)=A_1Z_0e^{\frac{-1}{\varepsilon}},\quad F_2=F_2(t)=A_2e^{\frac{-\alpha}{\varepsilon}},\quad F_3=F_3(t)=A_1C_0e^{\frac{-1}{\varepsilon}}.$$

Let $\theta(x,t)=f(\eta),\ c(x,t)=g(\eta),\ z(x,t)=h(\eta),$

such that $\eta=\frac{x}{t^{\sigma}}$ [6, 7]. The criteria for the similarity solution are

$$\sigma=\frac{1}{2},\ \gamma=\frac{1}{2},\ A_1=\frac{1}{t},\ A_2=\frac{1}{t}. \tag{3.5}$$

The resulting equations for the similarity transformation as $\varepsilon\to 0$, are

$$æf''+\frac{\eta}{2}f'+\delta_1ghe^{f}-\delta_2ge^{\alpha f}=0 \tag{3.6}$$

$$D_xg''+\frac{\eta}{2}g'-\delta_3ghe^{f}-\delta_4ge^{\alpha f}=0 \tag{3.7}$$

$$D_0h''+\frac{\eta}{2}h'-\delta_5ghe^{f}=0 \tag{3.8}$$

Considering the free boundary conditions(3.4), at $x=s(t)$, $\eta=2$ then we obtain

$$\left.\begin{array}{l} f(0)=0, \quad g(0)=1, \quad h(0)=1, \\ kf'(2)=-f(2), \\ D_X g'(2)=-\mu(1+g(2)), \\ D_0 h'(2)=-\lambda(1+h(2)), \end{array}\right\} \tag{3.9}$$

4.0 Existence and Uniqueness of Solution

***Theorem* 4.1**

For $0 \le \alpha \le N,\ 0 \le \eta \le 2,$, $æ, D_x, D_o, \delta_1, \delta_2, \delta_3, \delta_4, \delta_5, N > 0$, *problem* (3.6-3.8) *which satisfies conditions* (3.9) *and for which* $f'(0),\ g'(0)$ *and* $h'(0)$ *are fixed, has a unique solution.*

Remark

The existence of unique solution of problem (3.6-3.8) which satisfies (3.9) implies the existence of unique solution of problem (3.1-3.3) satisfying (3.4).

Let
$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \end{pmatrix} = \begin{pmatrix} \eta \\ f \\ g \\ h \\ f' \\ g' \\ h' \end{pmatrix} \tag{4.1}$$

$$\begin{pmatrix} y_1' \\ y_2' \\ y_3' \\ y_4' \\ y_5' \\ y_6' \\ y_7' \end{pmatrix} = \begin{pmatrix} 1 \\ y_5 \\ y_6 \\ y_7 \\ -\frac{y_1 y_5}{2æ} - \frac{\delta_1}{æ} y_3 y_4 e^{y_2} + \frac{\delta_2}{æ} y_3 e^{\alpha y_2} \\ -\frac{y_1 y_6}{2D_x} + \frac{\delta_3}{D_x} y_3 y_4 e^{y_2} + \frac{\delta_4}{D_x} y_3 e^{\alpha y_2} \\ -\frac{y_1 y_7}{2Do} + \frac{\delta_5}{Do} y_3 y_4 e^{y_2} \end{pmatrix} = \begin{pmatrix} f_1(y_1, y_2, y_3, y_4, y_5, y_6, y_7) \\ f_2(y_1, y_2, y_3, y_4, y_5, y_6, y_7) \\ f_3(y_1, y_2, y_3, y_4, y_5, y_6, y_7) \\ f_4(y_1, y_2, y_3, y_4, y_5, y_6, y_7) \\ f_5(y_1, y_2, y_3, y_4, y_5, y_6, y_7) \\ f_6(y_1, y_2, y_3, y_4, y_5, y_6, y_7) \\ f_7(y_1, y_2, y_3, y_4, y_5, y_6, y_7) \end{pmatrix} \tag{4.2}$$

$æ, D_x, D_0 > 0$

subject to the initial conditions

$$\begin{pmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \\ y_4(0) \\ y_5(0) \\ y_6(0) \\ y_7(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} \tag{4.3}$$

$0 \le \alpha \le N,\ 0 \le y_1 \le 2, 0 \le y_2 \le M_1, 0 \le y_3 \le M_2, 0 \le y_4 \le M_3, 0 < y_5 \le \omega_1,\ 0 < y_6 \le \omega_2,$
$0 < y_7 \le \omega_3,\ \omega_1, \omega_2, \omega_3, M_1, M_2, M_3, N > 0$

***Theorem* 4.2**

For $0 \le \alpha \le N,\ 0 \le y_1 \le 2, 0 \le y_2 \le M_1, 0 \le y_3 \le M_2, 0 \le y_4 \le M_3,\ 0 < y_5 \le \omega_1,$

$0 < y_6 \le \omega_2, 0 < y_7 \le \omega_3,\ \omega_1, \omega_2, \omega_3, M_1, M_2, M_3 > 0$, *the functions* $f_i (i = 1,2,3,4,5,6,7)$ are *Lipschitz continuous.*

Proof

It is observed that $\frac{\partial f_i}{\partial y_j}, i, j = 1,2,3,4,5,6,7$ are bounded since there exists a constant

$K > 0$, such that $\left|\frac{\partial f_i}{\partial y_j}\right| \le K, \quad i, j = 1, 2, 3,4,5,6,7$ where K is the Lipschitz constant.

Hence $f_i(y_1, y_2, y_3, y_4, y_5, y_6, y_7), i = 1,2,3,4,5,6,7$ are Lipschitz continuous and so (4.2) which satisfies (4.3) is Lipschitz continuous. ■

***Proof of Theorem* 4.1**

By theorem 11.7 [4], the existence of Lipschitz constant in the proof of theorem 2 implies the existence of unique solution of (4.2) satisfying (4.3). And this implies the existence of unique solution of problem (3.6-3.8) satisfying the boundary conditions (3.9). This completes the proof. ■

5.0 Numerical Results

The problem (4.2) subject to initial conditions (4.3) is solved by shooting method where the values of $\omega, \omega_2 \omega_3$ are guessed such that

$$y_5(2) = -\frac{y_2(2)}{k}, y_6(2) = -\mu\left(\frac{1 + y_3(2)}{Dx}\right), y_7(2) = -\lambda\left(\frac{1 + y_4(2)}{Do}\right), \mu, \lambda, k, D_x, D_o > 0.$$

The numerical results are presented in the figures 1 to 5.

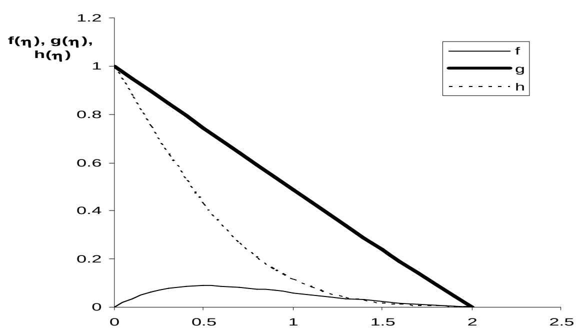

FIGURE 1:The graphs show the temperature f(η), fuel concentration g(η) and oxygen concentration h(η) against the position η when α=0.25

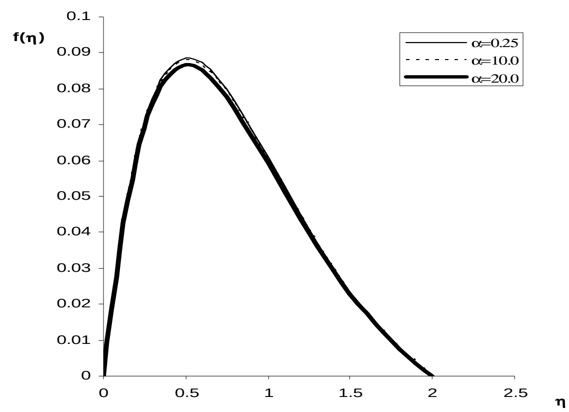

FIGURE 2:The graphs show the temperature f(η) against η for various values of α

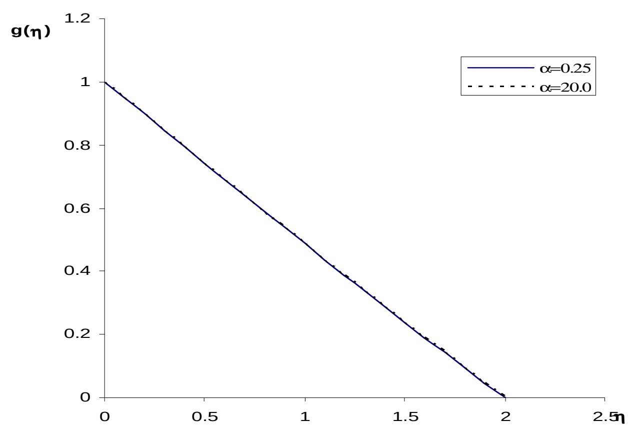

FIGURE 3: The graphs show the fuel concentration g(η) against η for various values of α

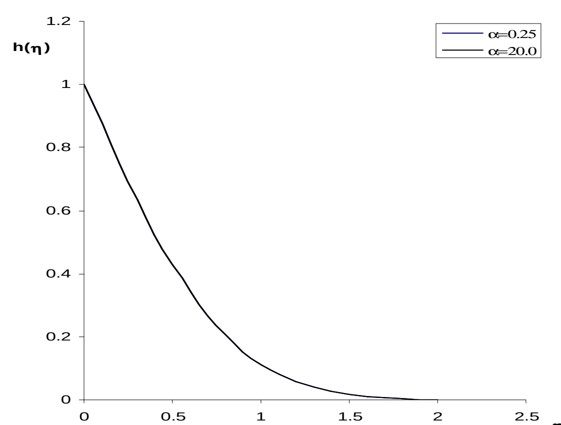

FIGURE 4: The graph shows the oxygen concentration h(η) for various values of α

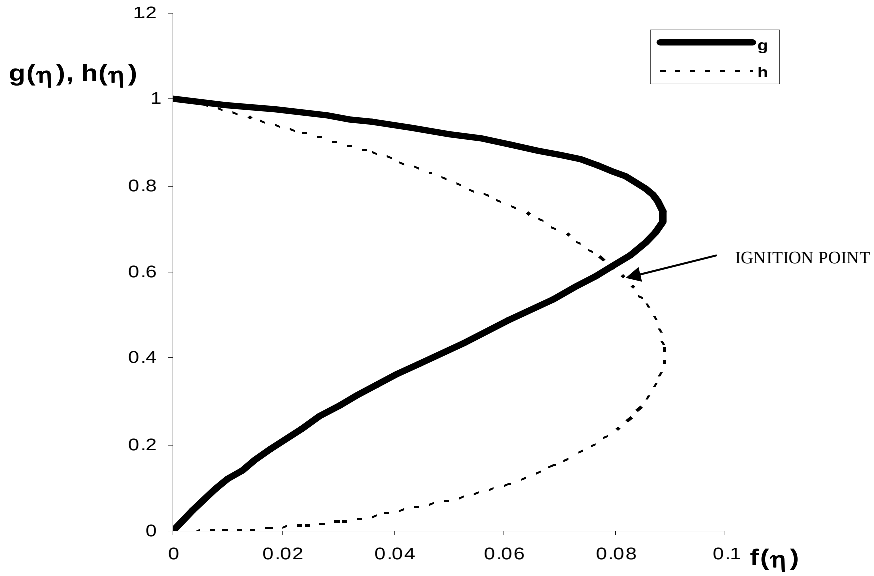

Figure 5: The profiles of fuel concentration g(η) and oxygen concentration h(η) against the temperature f(η) when α =0.25

6.0 Discussion of results

The work of Truscott et al. [10] was extended to a free boundary by assuming the reactant is not confined to a fixed space, and we studied the behaviour of the system under specified conditions. The criteria for the similarity solution were established in (3.5) and in theorems 1 and 2, the conditions for the existence of unique solution were stated and proved. The numerical results show the influence of activation energies ratio α on the three-component model and identified the ignition point of the reaction.

The figure 1 shows the temperature, fuel and oxygen concentrations profiles. It is observed that the temperature of the system rises and reaches maximum as the fuel concentration decreases linearly along the spatial domain, while the oxygen concentration also decreases at a slow rate. The figure 2 shows the effect of activation energies ratio on the maximum temperature of the chain reaction, and as α increases the maximum temperature of the system lowers. The figures 3 and 4 respectively show that α has little effect on the fuel concentration but none on the oxygen concentration. Figure 5 shows the ignition temperature $f(\eta) = 0.0765$ which is the temperature at which the combustible fluid begins to burn.

7.0 Conclusion

The existence of a solution of the free boundary problem implies that the problem represents a physical problem under specified conditions. Therefore the established conditions and results are not only expected to guide insulation materials manufacturers but provide safety precautions during storage and usage.

References

[1] Ayeni R.O., Akinpelu F.O. and Popoola A.O.: Some Remarks on Thermal Explosion in the Early Evolutions of the Earth *Science Focus1* **12***(1):1-3*. (2007)

[2] Ayeni R.O., Akinpelu F.O. and Popoola A.O.: Effect of radioactive heat source and Gravitational Differentiation on Thermal Explosions in the Early Evolution of the Earth *Science Focus1* **12***(1):136-138*. (2007)

[3] Cannon, J.R. and A.I Matheson: A Free Boundary value Problem related to the Combustion of a Solid: Flux Boundary Conditions *Quarterly of Applied Mathematics* **LV** *(4):687-705*. (1997)

[4] W. R. Derrick and S.I. Grossman: Elementary Differential Equations, Addison Wesley, Readings (1976).

[5] O. D. Makinde: Thermal Ignition in a Reactive Viscous Flow through a Channel filled with a Porous Medium, *Journal of Heat transfer* **128***:601-604* (2006).

[6] B. I. Olajuwon and A. O. Popoola: On Self Similar Solution of Non-Linear Diffusion Equation with Convection Term, *Journal of Mathematics and Statistic* **2***(4): 453-456* (2006).

[7] Popoola, A.O. and R.O. Ayeni: On a Stefan Problem Arising from the Theory of Combustion, *Science Focus* **2***:103-107*. (2003)

[8] Popoola, A.O. and R.O. Ayeni: On the Dependency of Activation Energies of a Two-Step Arrhenius Reaction *Journal of Mathematical Association of Nigeria (abacus)* **32**(2a):79-86. (2005)

[9] V.G. Prokof'ev and V. K. Smolyakov: Unsteady Combustion of a Binary Gasless Mixture Ignited by a hot wall *Combustion Explosion and Shock Waves* **41***(2):158-163 (2005).*

[10] Truscott, J. E., Brindley, J., McIntosh, A. and J. Griffiths:, The Effect of Diffusion on the Auto Ignition of Combustible Fluids in insulation Materials. *IMA. J. of Applied Maths* **61,** 231-271. (1996)