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PARAMETRIC STUDY OF SINGLE SODIUM DROPLET TEMPERATURE WITH GENERIC REACTION RATE AND VARIABLE THERMAL CONDUCTIVITY

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ABSTRACT
The main objective of this parametric study was to examine influence of pertinent thermo-physical parameters on sodium droplet temperature. The generic reaction rate and thermal conductivity of the single droplet are varied as non-linear functions of temperature, whereas the contribution of heat loss mechanisms are based on Newton law of cooling and P-1 approximation for thermal radiation transfer. An extension of existing models was obtained which was non-linear initial value problem. Theorem on existence and uniqueness of solution was formulated and proved to validate the new model based on some criteria. The differential equation was not amenable to analytical solution due to its non-linearity. Therefore, the non-linear problem was tackled numerically, using a finite difference procedure based on a small step-size. Parametric studies were performed to investigate significant effects of thermo-physical parameters on temperature of the single droplet for typical reaction rates such as Sensitized, Arrhenius and Bimolecular reaction rates. The results show the impacts of different thermo-physical parameters on the single sodium temperature of sensitized, Arrhenius and bimolecular reaction rates.

Keywords: Sodium droplet, non-linear problem, variable thermal conductivity, critical temperature, explosion time, sensitized, Arrhenius and bimolecular reaction rates.

INTRODUCTION

Several researchers have delved into the problems of thermal explosion of combustible droplets in the literature. One of the utmost concerns is that of ignition of sodium droplet because of its extensive use as a working fluid in the design of nuclear facilities. Goldfarb *et al*. (1999) performed the study of thermal radiation effect on thermal explosion in gas containing fuel droplets; they presented an original physical model of self-ignition in combustible gas mixture containing evaporating liquid droplets. The main attention of this paper was focused on the situation where delays might occur before final ignition. Sazhin *et al*. (2001) considered thermal ignition analysis of a mono-disperse spray with radiation. The chemical term was presented in the Arrhenius form with the pre-exponential factor calculated from the enthalpy equation, using the shell auto-ignition model. In Okano and Yamaguchi (2003), a single sodium droplet combustion in steady-airflow was simulated using the COMET. Goldfarb *et al*. (2004) studied the problem of delayed thermal explosion in a flammable gas mixture with addition of volatile fuel droplets based on the asymptotic method of integral manifolds. The results of the analysis were applied to the modelling of thermal explosion in diesel engines. Sazhin (2006) reviewed recent developments in modelling the heating and evaporation of fuel droplets and identified unsolved problems. The numerical analysis of droplets heating using the effective thermal conductivity model was based on the analytical solution of the heat conduction equation inside the droplet. This approach was shown to have advantages compared with the approach based on the numerical solution of the same equation both from the point of view of accuracy and computer efficiency. Goldfarb *et al*. (2007) investigated the dynamics of thermal explosion in a fuel droplets/air mixture using the geometrical version of the method of integral manifolds. The relevant parametric regions of the system were analysed, and explicit analytical formulae for the ignition delay in the presence of thermal radiation were derived. It was shown that the effect of thermal radiation could lead to considerable reduction of the total ignition delay time.

Although basic research on droplet combustion has been conducted, some questions that arose from these previous studies (Makino, 2003; Makino and Fudaka, 2005; Makino, 2006; Alao *et al*., 2011) suggested the need for further investigations. Makino (2003) examined the theory and experimental comparisons of the ignition delay and limit of ignitability of a single sodium droplet. He concluded that, the ignitable range expand with increasing temperature and decreasing Nusselt number. Makino and Fudaka (2005) studied ignition and combustion of a single sodium droplet experimentally by using a falling droplet. It was established that the ignition delay time increases first gradually and then rapidly, with decreasing initial temperature and/or oxygen concentration and reached the limit of ignitability. Okoya (2006) considered the effect of heat loss on the problem studied by Varatharajan and Williams (2000). Mostly analytical investigations of the simplified model using standard Semenov' techniques were presented. The analytical method provided expressions for criticality and the transition points. Also, the different qualitative effects of varying the dimensionless parameters were investigated. In addition, Makino (2006) considered both theoretical and experimental analyses on ignition delay and limit of ignitability for sodium pool. In order to evaluate the appropriateness of the theory, experimental comparisons were conduced, using experimental data in the literature. It was demonstrated that there exists a fair degree of agreement between the experimental and analytical results, as far as the trend and approximate magnitude are concerned, in spite of difference in experimental conditions and several assumptions made in the analysis. Adegbie (2008) studied the properties of solutions to a system of coupled non-linear ordinary differential equations arising from thermal explosion in a combustible gas containing fuel droplets with generalized temperature dependent reaction rate. Theorems on the properties of solutions to the new physical model problem such as existence and uniqueness, concavity and convexity were formulated based on some criteria and the proofs of the theorems were established accordingly. Analytical solutions for combustible gas temperature and fuel droplet radius were obtained based on some reasonable assumptions and approximations. The results revealed effects of varying different dimensionless parameters and different dynamic behaviours are reported. Adegbie (2009) examined property of solutions to a system of ordinary differential equations arising from thermal explosion of combustible dusty gas containing fuel droplet with generic reaction rate. Theorems on the qualitative properties of new system of equations governing the physical model were stated and proved respectively. Closed-form solutions were obtained based on quadratic approximations to the Arrhenius terms under realistic conditions. The results revealed that the delay before ignition depend significantly on interphase heat exchange parameter and energy needed to transfer heat from gas phase to solid phase parameter. In another development, Alao *et al*. (2011) investigated the effect of thermal radiation on ignition time and critical temperature of a single sodium droplet. The results showed that the inclusion of additional heat sink mechanism, i.e. radiative heat loss, significantly delayed the ignition time and reduced the critical temperature with respect to results of Makino (2003). Saravanan *et al*. (2012) investigated ignition behaviour of sodium droplets in the atmospheric air numerically with two available models of pre–ignition stage combustion. Rao *et al*. (2012) analysed quasi-steady sodium droplet combustion in convective environment using the Finite Volume Method (FVM). Adegbie (2013) extended the problem of thermal explosion in combustible gas mixtures containing fuel droplets to permit a more general temperature dependent rate of reaction for most typical practical reactions under physically reasonable assumptions. The results revealed that the existence of thermal radiation and numeric exponent play significant roles in the thermal stability of combustible gas mixture, which is of great importance for combustion and explosion industry safety. Recently, Sathiah and Roelofs (2014) considered numerical modelling of single sodium droplet combustion. The model predictions of falling velocity and burned mass were in good agreement with experimental data. Additionally, parametric studies were performed to investigate the effects of initial droplet diameter, temperature and oxygen concentration on burning rate and on ignition time delay.

This present study examines parametric analysis of new model for sodium droplet temperature accounting for generic reaction rate and variable thermal conductivity in the presence of convective and radiative heat losses, which none of the previous studies took into consideration. The resulting governing equation is highly non-linear ordinary differential equation. Theorem on existence and uniqueness of solution to validate the new model is adequately formulated and proved respectively based on some criteria. Consequently, a numerical technique known as a finite difference procedure based on a small step-size is employed to solve the governing equation due to its non-linearity. Parametric studies are performed to investigate the effects of thermo-physical parameters on temperature of the single droplet for typical reaction rates such as Sensitized, Arrhenius and Bimolecular reaction rates.

MATHEMATICAL FORMULATION OF THE PROBLEM

Recent advancement in reactor design is focused on construct of sodium cooled fast reactor. The novel development is essential because liquid sodium has excellent thermo-physical properties which are responsible for its extensive use as a coolant in the design of nuclear reactor facilities. However, hazardously reaction can occur when liquid sodium droplet is exposed to air or water. The surface reaction is considered between Na (subscript F) and O_2 (subscript o), producing Na_2O, according to $v_F F + v_O O \rightarrow v_p P$ with generating heat q^o per unit mass of Na, where v_i is the stoichiometric coefficient. For the safety of a sodium cooled fast reactor, sodium-air reactions should be prevented. To prevent and to mitigate the consequences, thermal explosion of sodium droplet, it is essential to understand various physical phenomena involved in a sodium-air reactions. The present study extends the problem on ignition of a single sodium droplet taken into account generic reaction rate and variable thermal conductivity in the presence of convective and radiative heat losses. The contributions of the convective and radiative heat losses are based on Newton law of cooling and P-1 approximation for thermal radiation transfer respectively. The resulting governing equation is highly non-linear differential equation, which is extension of previous models Makino (2003) and Alao *et al*. (2011), is given as

$$\frac{4}{3}\pi r_s^3 \rho_F c_p \frac{dT}{dt} = 4\pi r_s^2 q^0 V_F W_F \left(\frac{\rho_g Y_0}{W_0}\right)^n B_s(T) - Q_C - Q_R, \qquad (1)$$

$$T(0) = T_0, \qquad (2)$$

where, r_s is the radius of single sodium droplet, ρ is the density, c_p is the specific heat, T is the droplet temperature, T_0 is the temperature in an oxidizing atmosphere with

T_∞ $(\le T_0)$ and oxygen mass fraction Y_0. t is the time, q^0 is the heat generated per unit mass of Na, V is the stoichiometric coefficient, W is the molecular weight, B_s is the pre-exponential or frequency factor of the "global" surface reaction with the activation energy E, R is the universal gas constant, Q_C and Q_R are convective and radiative heat loss respectively. The generic reaction rate, which is varied and only considered as non-linear function of temperature, is presented in the form (see Adegbie (2013) and Okoya (2006))

$$B_s(T) = B_{s0}\left(\frac{T}{T_0}\right)^m \exp\left(\frac{-E}{RT}\right), \quad (3)$$

where B_{s0} is pre-exponential factor at initial, E is the activation energy, R is the universal gas constant, m is the numeric exponent depicting typical reaction rate. The contribution of convective heat loss is due to Newton law of cooling which is given as (see Adegbie (2013))

$$Q_C = 4\pi r_s^2 h(T - T_\infty), \quad \text{where} \quad h = \frac{Nu\lambda_g}{2r_s}. \quad (4)$$

It is pertinent to note that thermal conductivity of both monatomic and polyatomic gases is proportional to $\sqrt{T}$ (see Adegbie, 2008; 2013 for details). Therefore, in this study we assume thermal conductivity of sodium gas as non-linear function of temperature in the form

$$\lambda_g(T) = \lambda_{g0}\left(\frac{T}{T_0}\right)^r. \quad (5)$$

where λ_{g0} is thermal conductivity at initial temperature and r is numeric exponent.
Hence, the convective heat loss term can be written as

$$Q_C = 4\pi r_s^2 h(T - T_\infty) = 2\pi r_s Nu\lambda_{g0}\left(\frac{T}{T_0}\right)^r (T - T_\infty), \quad (6)$$

where h is the heat transfer coefficient, Nu is the Nusselt Number. Likewise, the radiative heat loss is given as (see Adegbie (2013) and Alao *et al*. (2011))

$$Q_r = 4\pi r_s^2 \sigma\left(T^4 - T_\infty^4\right), \quad (7)$$

where σ is the Stefan-Boltzmann's constant.

Now, iintroducing the following dimensionless variables:

$$\theta = \frac{T - T_0}{\varepsilon T_0}, \quad \varepsilon = \frac{RT_0}{E}, \quad \tau = \Delta t \quad \text{where}$$

$$\frac{1}{\Delta} = \frac{2r_s\rho_F c_p T_0}{6B_s q^0 V_F W_F}\cdot\left(\frac{W_0}{\rho_g Y_o}\right)^n\cdot\left(\frac{RT_0}{E}\right)\exp\left(E/RT_0\right). \quad (8)$$

Here θ, ε and τ are dimensionless temperature, reduced activation energy and time respectively. The dimensionless form of equations (1) and (2) in conjunction with equations (3), (6) and (7) are obtained as

$$\frac{d\theta}{d\tau} = (1+\varepsilon\theta)^m \exp\left(\frac{\theta}{1+\varepsilon\theta}\right) - (1+\varepsilon\theta)^r(\gamma + \alpha\theta) - \left(\beta^*(1+\varepsilon\theta)^4 - \delta^*\right), \quad (9)$$

$$\theta(0) = 0. \quad (10)$$

The dimensionless governing equation is defined by four dimensionless parameters:

$$\left.\begin{aligned} \gamma &= \frac{6Nu}{(2r_s)^2\Delta}\frac{\lambda_{g0}}{\rho_F c_p}\frac{T_0 - T_\infty}{T_0}\left(\frac{E}{RT_0}\right), & \alpha &= \frac{6Nu}{(2r_s)^2\Delta}\frac{\lambda_{g0}}{\rho_F c_p}, \\ \beta^* &= \frac{6\sigma}{(2r_s)\Delta}\frac{ET_0^3}{\rho_F c_p R}, & \delta^* &= \frac{6\sigma}{(2r_s)\Delta}\frac{ET_\infty^4}{\rho_F c_p R T_0^2} \end{aligned}\right\} \quad (11)$$

Here, γ is convective heat loss parameters, α is the heat loss parameter via thermal conductivity, β^* and δ^* are modified parameters responsible for the contribution of the thermal radiation, Nusselt number $Nu = 2r_s h/\lambda_{g0}$. In the limit of large activation energy (i.e. $\varepsilon \to 0$), it is imperative to note that equation (9) without γ, β^* and δ^* coincides with that of Semenov's classical thermal explosion problem, Frank-Kamenetskii (1969). Whenever $\beta^* = \delta^* = 0$ (i.e. radiative heat loss is neglected) and $\varepsilon \to 0$ equation (9) is similar to the model in Makino (2003). Likewise, when $m = 0$ and θ is asymptotically expanded to $o(\varepsilon^2)$ with constant thermal conductivity, we obtain equation (2.2) in Alao *et al*. (2011).

EXISTENCE AND UNIQUENESS OF SOLUTION

The aim of this section is to show that the initial value non-linear differential equation (9) and (10) governing the new model is well-posed. This is done by formulating theorem on existence and uniqueness of solution based on some criteria and adequately delineated the proof to validate the model see Adegbie (2008) for details.

THEOREM:

Let

$$G=\{(\tau,\theta):0\le\tau\le a,0\le\theta\le b\} \quad (12)$$

and

$$H=\{0\le\alpha\le c_1,0\le\beta^*\le c_2,0\le\delta^*\le c_3,0\le\gamma\le c_4\} \quad (13)$$

If G and H hold where a,b and $c_i, i=1,2,3,4$ are finite real constants. Then for $\varepsilon\ge 0$ and $m,\ r\,\varepsilon\,\Re$, there exists a unique solution of non-linear differential equation (9) which satisfies the initial condition (10).

PROOF:

Let

$$f(\tau,\theta)=(1+\varepsilon\theta)^m\exp\left(\frac{\theta}{1+\varepsilon\theta}\right)-(1+\varepsilon\theta)^r(\gamma+\alpha\theta)-\left(\beta^*(1+\varepsilon\theta)^4-\delta^*\right). \quad (14)$$

It is obvious that $f(\tau,\theta)$ is continuous in D and bounded on D. This implies that there exists a real number $\mathrm{M}>0$ such that

$$\mathrm{M}=\sup_D f(\tau,\theta)$$

$$=(1+\varepsilon b)^m\exp\left(\frac{b}{1+\varepsilon b}\right)-(1+\varepsilon b)^r(c_4+c_1 b)-\left(c_2(1+\varepsilon b)^4-c_3\right). \quad (15)$$

That is

$$|f(\tau,\theta)|\le\mathrm{M}. \quad (16)$$

Now, $f(\tau,\theta)$ is continuously differentiable in D and bounded there. Then there exists a real number $\mathrm{K}, 0\le\mathrm{K}<\infty,$ such that

$$\left|\frac{\partial f(\tau,\theta)}{\partial\theta}\right|\le\mathrm{K}, \quad (17)$$

where

$$\mathrm{K}=\sup_D\left|\frac{\partial f(\tau,\theta)}{\partial\theta}\right|=(1+m\varepsilon+m\varepsilon^2 b)(1+\varepsilon b)^{m-2}-\exp\left(\frac{b}{1+\varepsilon b}\right)$$

$$-\left((r+1)c_1\varepsilon b+(c_1+r\varepsilon c_4)\right)(1+\varepsilon b)^{r-1}-4c_2\varepsilon(1+\varepsilon b)^4\ge 0 \quad (18)$$

Therefore, $f(\tau,\theta)$ is Lipschitz continuous in D. Hence, there exists a unique solution of non-linear differential equation (9) which satisfies initial condition (10).

NUMERICAL COMPUTATION

The equations (9)-(10) arising from ignition of a combustible single sodium droplet is non-linear initial value problem and does not possess closed form solutions. Therefore, we investigate temperature behaviour of the model numerically using a finite difference procedure based on a small step-size. Consequently, parametric studies are performed from the numerical results obtained to investigate the effects of pertinent thermo-physical parameters on temperature of the single sodium droplet as shown in Figures below.

NUMERICAL RESULTS

The results in Figures 1-5 reveal the effects of pertinent thermo-physical parameters on single sodium droplet temperature for sensitized, Arrhenius and bimolecular reaction rates. In Figures 1- 4, we observe significant reduction in the sodium droplet temperature for typical sensitized, Arrhenius and bimolecular reaction rates whenever thermo-physical parameters are increasingly varied whereas in Figure 5 it is obvious that increase in modified radiative heat loss parameter δ^* causes a noticeable increment in sodium droplet temperature.

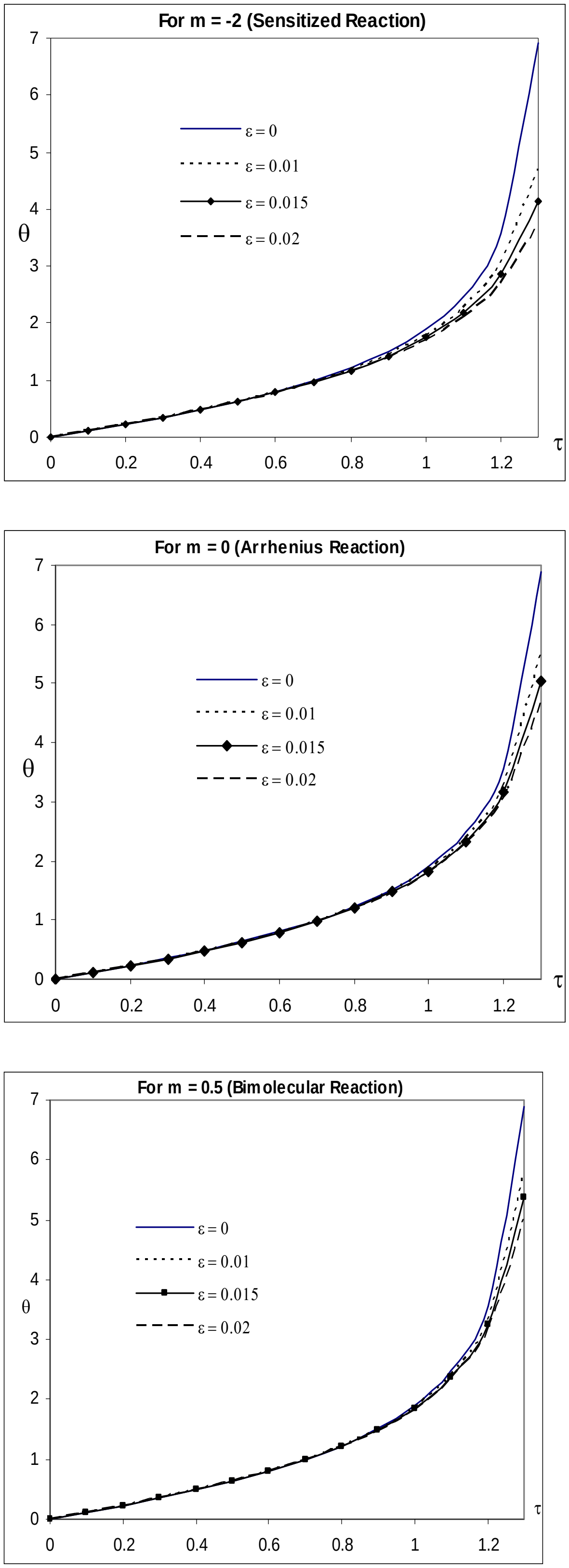

Fig.1. Variation of reduced activation energy ε on sodium droplet temperature when $m = (-2, 0, 0.5)$.

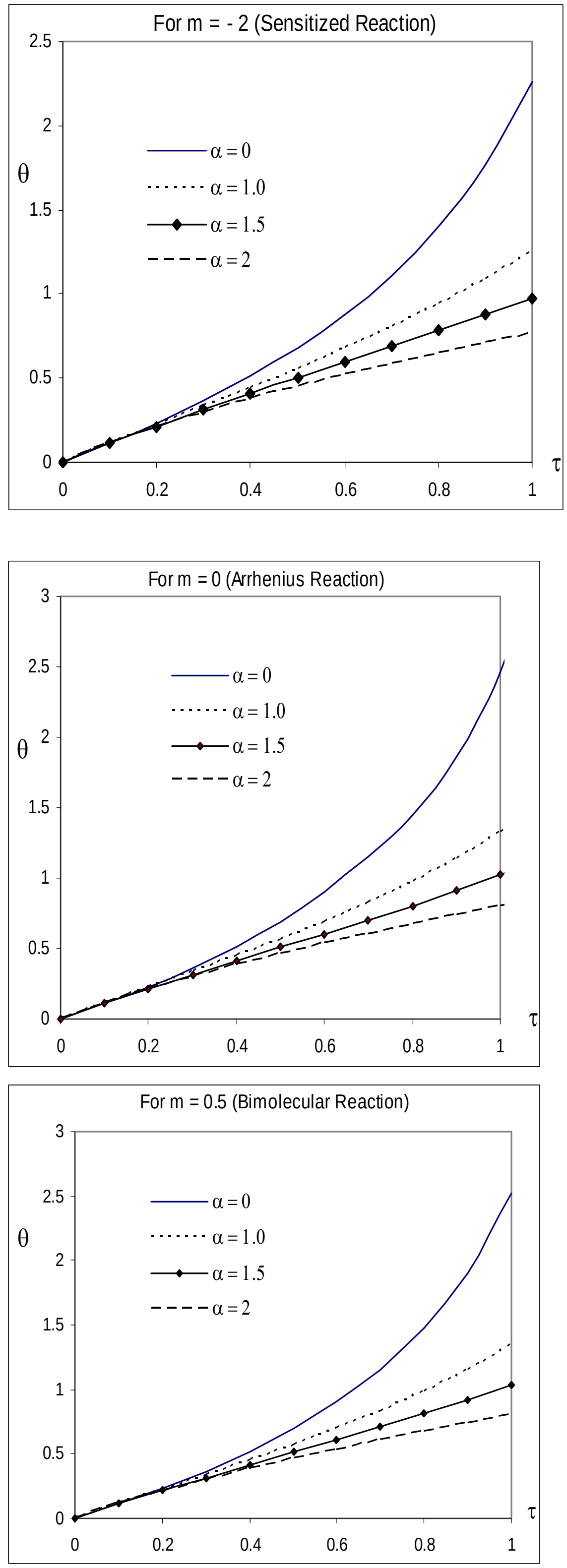

Fig. 2. Variation of convective heat loss parameter α on sodium droplet temperature when $m = (-2, 0, 0.5)$

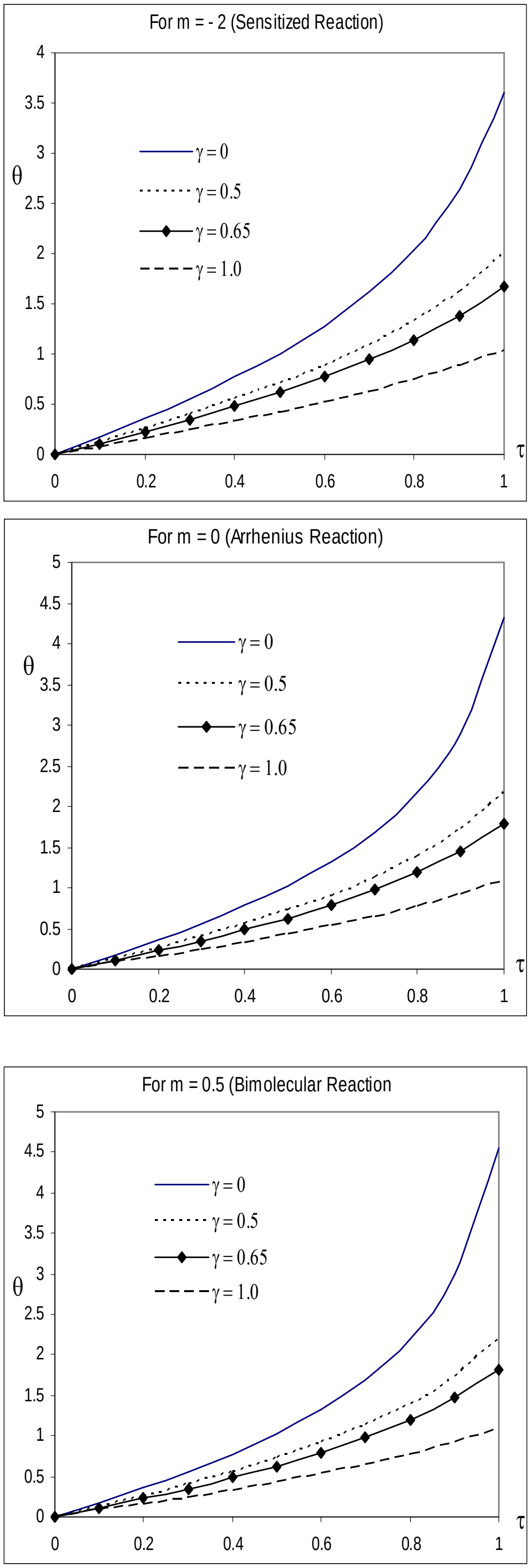

Fig. 3. Variation of convective heat loss parameter γ on sodium droplet temperature when $m = (-2, 0, 0.5)$

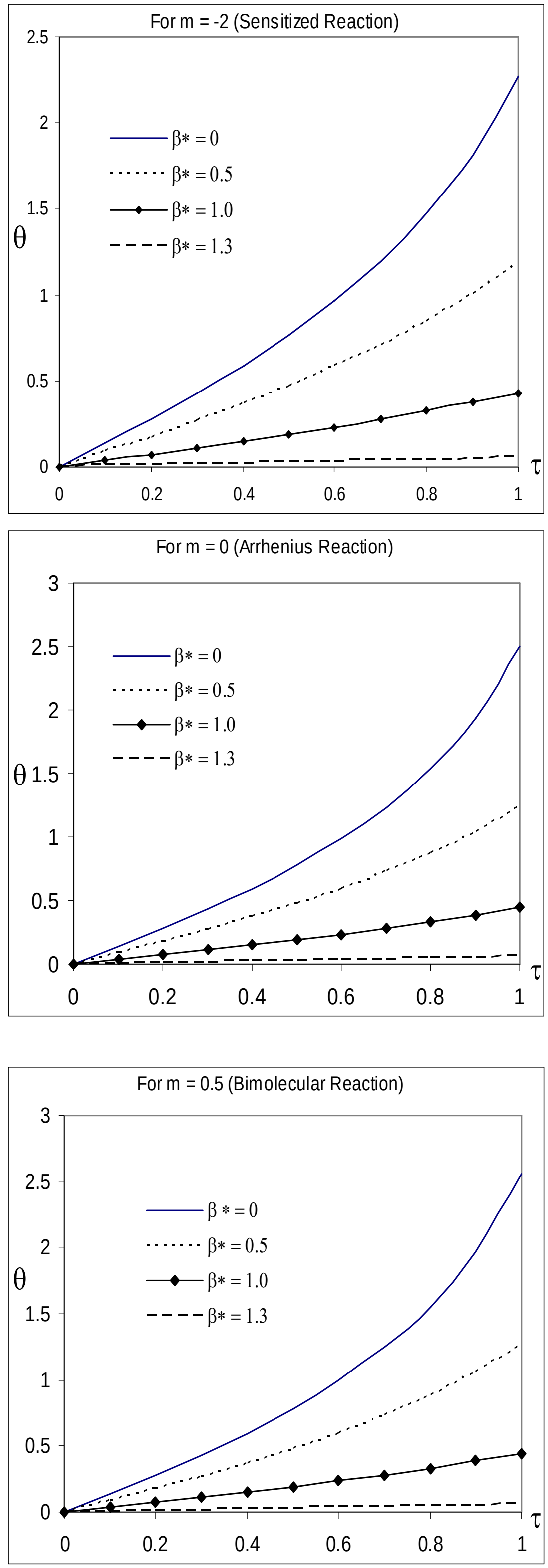

Fig. 4. Variation of radiative heat loss parameter β^* on sodium droplet temperature when $m = (-2, 0, 0.5)$

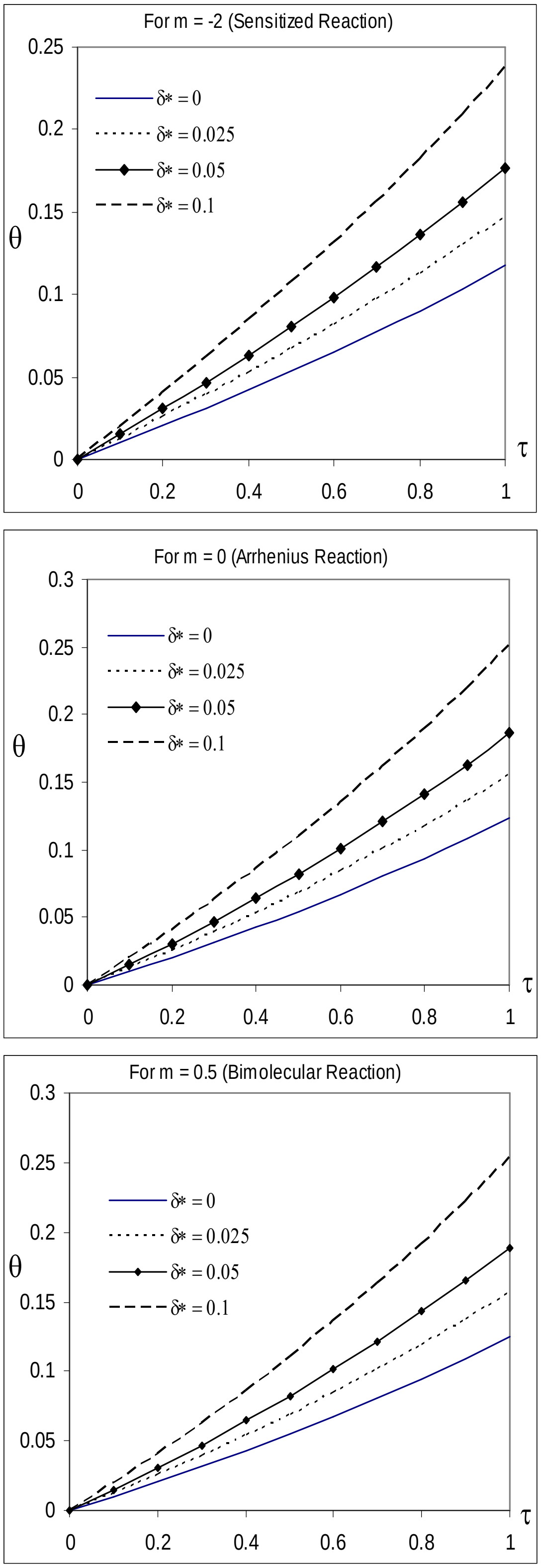

Fig. 5. Variation of radiative heat loss parameter δ^* on sodium droplet temperature when $m=(-2,0,0.5)$

CONCLUSION

In this study, the problems on ignition of a single sodium droplet have been extended to permit a more general reaction rates and variable thermal conductivity in the presence of both convective and radiative heat losses. The new model was considered under physically reasonable assumptions in order to obtain information which is useful for safety measures in nuclear reactor facilities. The mathematical formulation involves a highly non-linear ordinary differential equation. The questions relating to properties of solution such as existence and uniqueness of solution to validate the model was adequately answered by formulating theorem and establishing the proof respectively. The non-linear initial value problem governing the dynamical model was solved numerically. Numerical results were presented graphically for sensitized, Arrhenius and bimolecular reaction rates respectively. The effects of varying pertinent dimensionless thermo-physical parameters were also reported. The study revealed the importance of thermo-physical parameters in regulating the temperature of sodium droplet as coolant in nuclear reactor facilities to prevent and to mitigate the consequences of hazardous events. Likewise, the study is essential to understand various physical phenomena involved in a sodium-air reactions.

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