

**On delay-type behaviour of thermal explosion in a combustible gas mixture containing fuel droplets with Arrhenius power-law model**

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*Abstract*

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*The problem of thermal explosion in combustible gas mixtures containing fuel droplets is extended to permit a more general temperature dependent rate of reaction for most typical practical reactions based on Arrhenius equation under physically reasonable assumptions. A detailed numerical analysis of the resulting system of coupled non-linear ordinary differential equations is performed to account for numeric exponent effects relating to most typical practical reactions such as sensitized, Arrhenius and bimolecular reactions respectively. The computed results reveal different dynamic delay-type behaviours and are illustrated graphically in this study.*

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**NOMENCLATURE**

**English symbols**

$A$	pre-exponential factor ( $1/s$ )
$C_f$	molar concentration combustible gaseous mixture ( $kmol / m^3$ )
$C_{pg}$	specific heat capacity of the gas phase at constant pressure ( $JK^{-1}kg^{-1}$ ).
$E$	activation energy ( $J/kmol$ )
$L$	latent heat of evaporation ( $J/kg$ )
$m_f$	molar mass ( $kg/kmol$ )
$n$	numerical exponent
$n_d$	number of droplets per unit volume ( $m^{-3}$ ),
$Q$	specific combustion energy ( $J/kg$ )
$R_d$	droplet radius ( $m$ )
$R_u$	universal gas constant $Jkmol^{-1}K^{-1}$
$t$	time ( $s$ )
$T_{g0}$	combustible gas initial temperature ( $K$ )
$T_g$	combustible gas temperature ( $K$ )

**Greek Symbols**

$\rho$	density of the combustible gaseous mixture ( $kg/m^3$ )
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$\lambda$  thermal conductivity ( $Wm^{-1}K^{-1}$ )

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$\varphi$  volumetric phase content (dimensionless)

$\sigma$  Stefan-Boltzmann's constant

$\beta$  dimensionless activation energy

$\gamma$  dimensionless adiabatic temperature

$\mathcal{E}_1$  dimensionless parameter expressing competition between the combustion and evaporation processes

$\mathcal{E}_2$  dimensionless parameter expressing impact of thermal radiation

$\mathcal{E}_3$  dimensionless parameter expressing heat released during combustion and energy needed to evaporate all fuel droplets

$\Psi$  dimensionless parameter expressing ratio of specific combustion energy and latent heat of vaporization

$\tau$  dimensionless time

#### Subscripts

0: initial

*g*: gas mixture,

*f*: combustible gas component of the mixture (fuel);

*d*: liquid droplets.

## 1.0 Introduction

The phase of research on combustion and explosions that began at the end of the nineteenth century and continues to this day is associated with the invention of the internal combustion engine, with the development of explosive technology and of internal ballistics for artillery, and, in recent decade, with the extensive introduction of jet and diesel engines. In many respects, these have stimulated the rapid development of combustion science [31]. The procedure for thermal explosion in gases, which contain fuel droplets, has been of much interest. After Semenov [25] developed the basic theory of phenomenon of thermal explosion, models that are more complicated have been suggested in [20] and [29].

The focus of this research work is therefore on the long standing problem of thermal explosion and ignition in a combustible gas containing fuel droplets and its numerous applications to furnaces, gas turbines and internal combustion engines [18, 20, and 27, 29, 30]. Over recent years, the theoretical analysis of this problem has been performed mainly by the use of modern computers. In this regard, there exist many computational packages that have proved useful. These packages have been developed to take into account heat and mass transfer and combustion processes in the mixture of gas and fuel droplets in a self-consistent manner [7 and 21-23]. This approach, however, is not particularly helpful in aiding and understanding the relative contribution of various processes. An alternative approach to the problem is to analyse the equations in some limiting cases. This cannot replace computational methods but can complement them. One of these analyses is based on the geometrical asymptotic method of integral manifolds [9-17].

In view of the physical problem under consideration, none of these papers examined generalised temperature dependent rate of reaction based on Arrhenius equation for combustion phenomenon. Therefore, a generalised physical model for thermal explosion in combustible gas mixture containing fuel droplets is developed in the present paper. The major interest is focused on numerical solutions to the new system of coupled non-linear ordinary differential equations governing the physical model. Moreover, effects of numeric exponent and dimensional parameters on gas temperature, gas concentration and droplet radius are reported for the following cases: sensitised, Arrhenius and bimolecular reactions, and delay-type behaviours of thermal explosions also feature promptly.

## 2.0 Mathematical formulation of the problem

The problem of thermal explosion in combustible gas mixture containing fuel droplets is studied. The problem is therefore extended to investigate spatially homogeneous combustible gas containing evaporating ideal spherical fuel droplets while taking into account generalised temperature dependent rate of reaction made of

chemical reactive species for most practical reactions (see [1] for details). The generalised temperature dependence of the reaction rate (i.e. Arrhenius Power-law model equation [1, 19]) is given as

$$K(T_g) = A(T_g/T_{g0})^n \exp\left(\frac{-E}{R_u T_g}\right) \quad (2.1)$$

where  $T_{g0}$  is initial temperature. In previous analyses, we note that  $n=0$  coincides with the models in literatures (see for example [9-17, 22-24] and the references therein). Fitted rate of reaction typically lie in the range  $-1 < n < 1$ . Classically  $n \in \{-2, 0, 0.5\}$  for most practical reactions which correspond to sensitised, Arrhenius and bimolecular rates of reaction respectively [1, 4 and 6]. Theoretical analyses yield various predictions for  $n$ . Thus, the system of equations for spatially homogeneous case of the physical model problem taking assumptions in [1] into account is

$$C_{pg} \phi_g \rho_{g0} T_{g0} T_g^{-1} \frac{dT_g}{dt} = Q_f m_f \phi_g c_f A T_{g0}^{-n} T_g^n \exp\left(\frac{-E}{R_u T_g}\right) - 4\pi R_d n_d \lambda_{g0} \sqrt{\frac{T_g}{T_{g0}}} (T_g - T_{g0}) - 4\pi R_d^2 n_d \sigma (T_g^4 - T_{g0}^4) \quad (2.2)$$

$$\frac{dR_d}{dt} = -\frac{1}{L\rho_d} \frac{\lambda_{g0}}{R_d} \sqrt{\frac{T_g}{T_{g0}}} (T_g - T_{g0}) - \frac{1}{L\rho_d} \sigma (T_g^4 - T_{g0}^4) \quad (2.3)$$

$$\phi_g \frac{dc_f}{dt} = -\phi_g c_f A T_{g0}^{-n} T_g^n \exp\left(\frac{-E}{R_u T_g}\right) + \frac{4\pi R_d n_d \lambda_{g0}}{Lm_f} \sqrt{\frac{T_g}{T_{g0}}} (T_g - T_{g0}) + \frac{4\pi R_d^2 n_d \sigma}{Lm_f} (T_g^4 - T_{g0}^4) \quad (2.4)$$

The systems (2.2) - (2.4) includes an energy equation for reacting gas, a mass equation for a liquid droplet and a concentration equation for the reacting gas mixture respectively. Initial conditions for the system:

$$T_g(0) = T_{g0}, c_f(0) = c_{f0}, R_d(0) = R_{d0}, \quad (2.5)$$

## 2.1 Non-Dimensional Analysis

In this study, we introduce the following dimensionless variables before attempting to make any approximations:

$$\theta_g = \frac{(T_g - T_{g0})E}{R_u T_{g0}^2}, r = \frac{R_d}{R_{d0}}, \eta = \frac{c_f}{c_{f0}}, \tau = \frac{t}{t_{react}}, t_{react} = A_0^{-1} \exp(1/\beta). \quad (2.6)$$

Using (2.6) in (2.2) - (2.5), the dimensionless system of governing equations reads as:

$$\gamma(1 + \beta\theta_g)^{-1} \frac{d\theta_g}{d\tau} = \eta(1 + \beta\theta_g)^n \exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right) - \varepsilon_1 r \left\{ \theta_g \sqrt{(1 + \beta\theta_g)} + \varepsilon_2 r [(1 + \beta\theta_d)^4 - 1] \right\} \quad (2.7)$$

$$\frac{dr}{d\tau} = -\frac{\varepsilon_3}{r} \left\{ \theta_g \sqrt{(1 + \beta\theta_g)} + \varepsilon_2 r [(1 + \beta\theta_g)^4 - 1] \right\} \quad (2.8)$$

$$\frac{d\eta}{d\tau} = -\eta(1 + \beta\theta_g)^n \exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right) + \varepsilon_1 \psi r \left\{ \theta_g \sqrt{(1 + \beta\theta_g)} + \varepsilon_2 r \left[ (1 + \beta\theta_g)^4 - 1 \right] \right\} \quad (2.9)$$

with the initial conditions:

$$\theta_g(0) = 0, \quad r(0) = 1 \quad \text{and} \quad \eta(0) = 1. \quad (2.10)$$

In equations (7)–(9) the following dimensionless parameters have been introduced:

$$\gamma = \frac{C_{pg} \rho_{g0} T_{g0}}{Q_f m_f c_{f0}} \beta, \quad \beta = \frac{R_u T_{g0}}{E}, \quad \varepsilon_1 = \frac{4\pi R_{d0} n_d \lambda_{g0} T_{g0} \beta \exp(1/\beta)}{Q_f \phi_g m_f c_{f0} A_0}, \quad \varepsilon_2 = \frac{R_{d0} \sigma^* T_{g0}^3}{\beta \lambda_{g0}},$$

$$\varepsilon_3 = \frac{\lambda_{g0} T_{g0} \beta \exp(1/\beta)}{\rho_d A_0 R_{d0}^2 L}, \quad \psi = \frac{Q_f}{L}.$$

The dimensionless system of equations (2.7) - (2.9) is defined by the six dimensionless parameters  $\gamma, \beta, \varepsilon_1, \varepsilon_2, \varepsilon_3$  and  $\psi$ . Remarks on the properties of solutions to the problems (7) - (10) are reported in [3]. Some special cases of the system of coupled non-linear ordinary differential equations (7) - (9) and initial conditions (2.10) and related problems have been studied analytically and numerically for  $n = 0$  (see for example [1] and the references therein). In the events that  $n = 0, \varepsilon_1 = \varepsilon_2 = 0$  and  $n = 0, \varepsilon_2 = 0$ , analyses have been performed both analytically and numerically in ([8, 22-25, 31] and references cited therein).

### 3.0 Numerical computation

The dynamic system of highly coupled nonlinear differential equations (2.7) - (2.9) with the initial conditions (2.10) arising from the problem of thermal explosion in a combustible gas containing fuel droplets is not amenable to analytical solutions. Therefore, numerical solutions based on finite difference scheme are presented.

The finite difference forward approximation for first derivative of  $\theta_g, r$  and  $\eta$  with respect to time  $\tau$  are given as

$$\frac{d\theta_g}{d\tau} = \frac{\theta_{g,i+1} - \theta_{g,i}}{h}, \quad (3.1)$$

$$\frac{dr}{d\tau} = \frac{r_{i+1} - r_i}{h}, \quad (3.2)$$

and 
$$\frac{d\eta}{d\tau} = \frac{\eta_{i+1} - \eta_i}{h} \quad (3.3)$$

respectively, where  $h$  is step length.

Substituting equations (3.1), (3.2) and (3.3) into equations (2.7) - (2.10)), we obtain the following approximation schemes for  $\theta_g, r$  and  $\eta$  respectively:

$$\theta_{g,i+1} = \theta_{g,i} + \frac{h}{\gamma} \eta_i (1 + \beta\theta_{g,i})^{n+1} \exp\left(\frac{\theta_{g,i}}{1 + \beta\theta_{g,i}}\right) - \frac{h}{\gamma} \varepsilon_1 r_i (1 + \beta\theta_{g,i}) \left\{ \theta_{g,i} \sqrt{(1 + \beta\theta_{g,i})} + \varepsilon_2 r_i \left[ (1 + \beta\theta_{g,i})^4 - 1 \right] \right\} \quad (3.4)$$

$$r_{i+1} = r_i - \frac{h}{r_i} \varepsilon_3 \left\{ \theta_{gi} \sqrt{(1 + \beta \theta_{gi})} + \varepsilon_2 r_i [(1 + \beta \theta_{gi})^4 - 1] \right\} \quad (3.5)$$

$$\eta_{i+1} = \eta_i - h \eta_i (1 + \beta \theta_{gi})^n \exp\left(\frac{\theta_{gi}}{1 + \theta_{gi}}\right) + h \varepsilon_1 \psi r_i \left\{ \theta_{gi} \sqrt{(1 + \beta \theta_{gi})} + \varepsilon_2 r_i [(1 + \theta_{gi})^4 - 1] \right\} \quad (3.6)$$

with the initial values

$$\theta_0 = 0, \quad r_0 = 1 \quad \text{and} \quad \eta_0 = 1 \quad (3.7)$$

The numerical approximation schemes above are compute for time histories of dimensionless gas mixture temperature  $\theta_g$ , gas concentration  $\eta$  and droplet radius  $r$  for sensitized, Arrhenius and bimolecular reactions respectively for various values of dimensionless parameters:  $\varepsilon_1, \varepsilon_2, \varepsilon_3, \psi, \beta, \gamma$ .

#### 4.0 Discussion of results

We present in Figure 4.1, convectonal thermal explosions which occurs without delay for sensitized, Arrhenius and bimolecular reactions when  $\varepsilon_1 = 2.3, \varepsilon_2 = 0.048, \varepsilon_3 = 2, \psi = 15, \beta = 0.005$  and  $\gamma = 0.001$ . We note that with  $n$  increasing, dimensionless temperature  $\theta_g$  and gas concentration  $\eta$  increasing, whereas dimensionless droplet radius  $r$  decreases.

Figure 4.2 and Figure 4.3 describe thermal explosions with cases of delay-type behaviour. It is seen that initially there is a small yet sharp temperature increase, followed by a moderate temperature rise until explosion occur. In these cases, it is observed that the delay is more pronounced as  $\psi$  decreases. However, in

Figure 4.1a

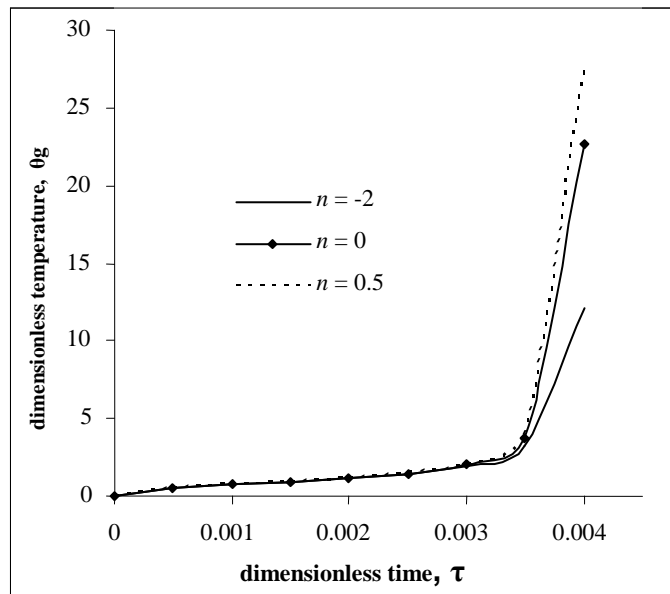


Figure 4.1b

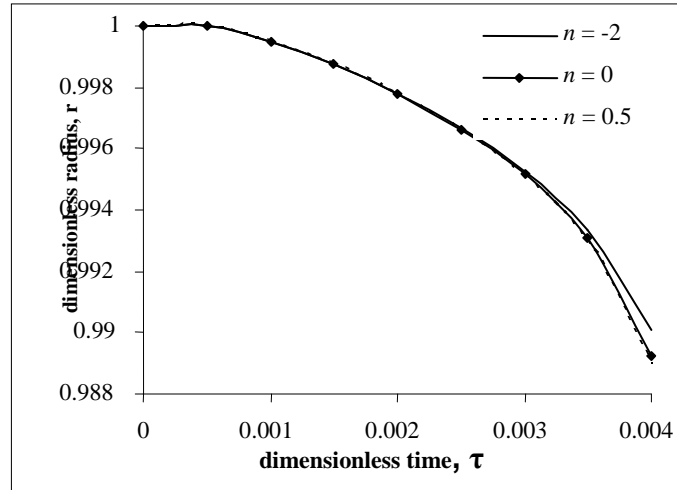


Figure 4.1

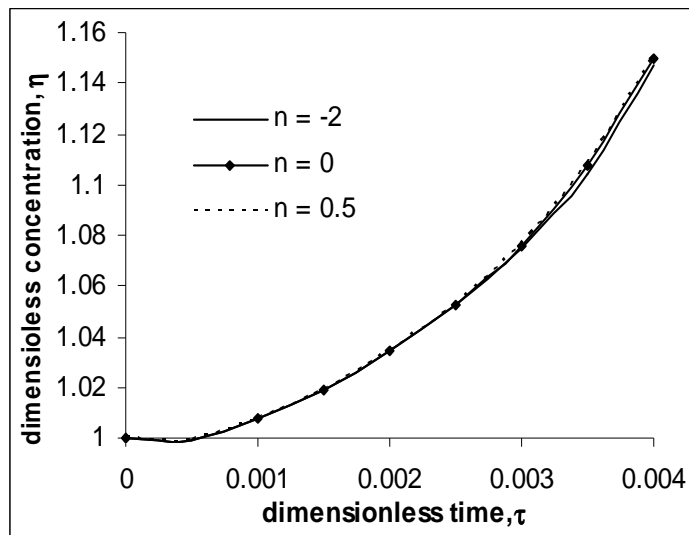


Figure 4.1: Convectonal thermal explosion when  $\epsilon_1 = 2.3$ ,  $\epsilon_2 = 0.048$ ,  $\epsilon_3 = 2$ ,  
 $\psi = 15$ ,  $\beta = 0.005$ ,  $\gamma = 0.001$ .

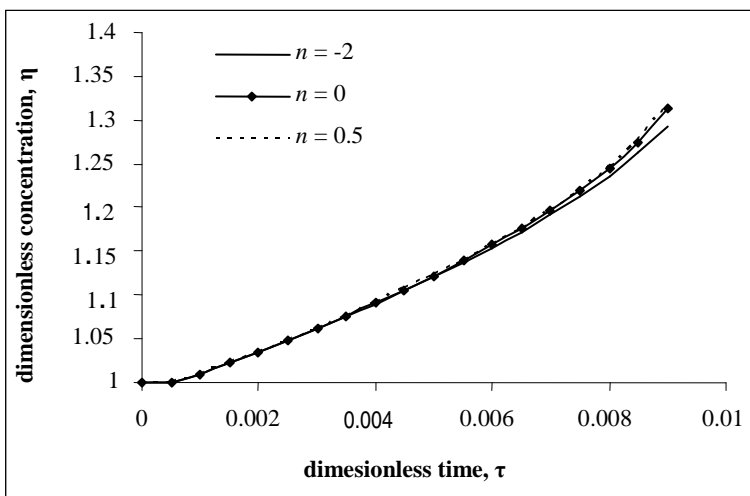
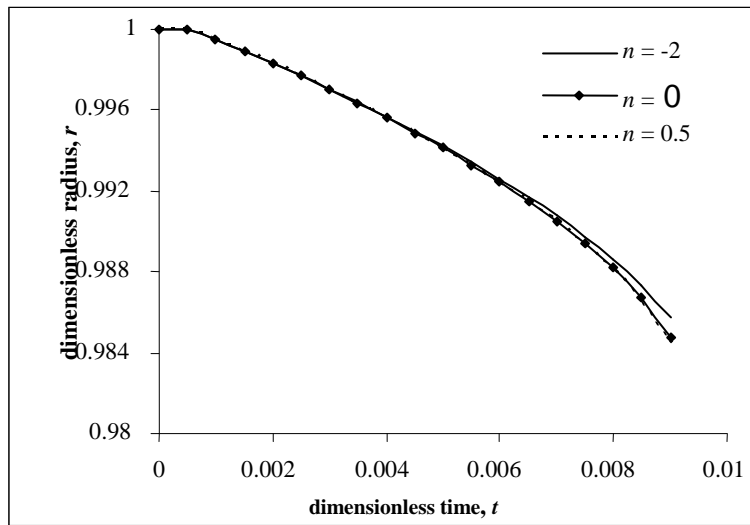
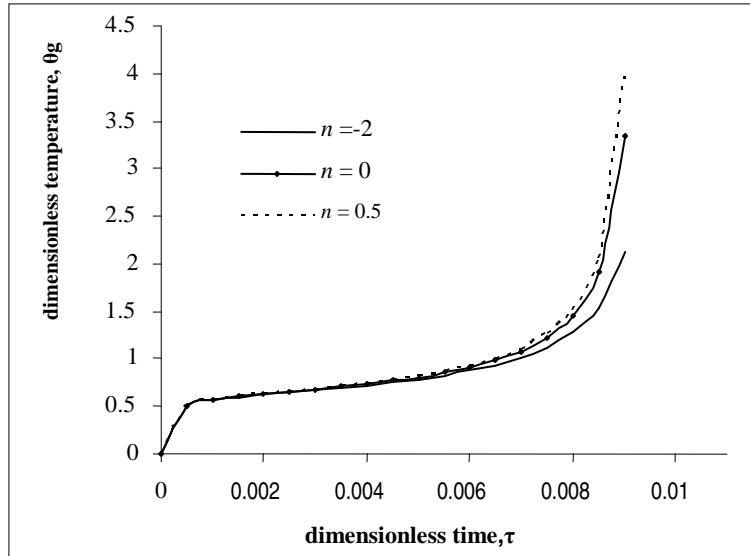
the former case it is accomplished by a concentration increase, whereas in the latter concentration decrease is observed. It is seen from Figures 4.2 and 4.3 that as  $n$  increasing, dimensionless gas concentration  $\eta$  increases;

dimensionless temperature  $\theta_g$  increases and decreases respectively, whereas dimensionless droplet radius  $r$  decreases and increases respectively.

In Figures 4.4 and 4.5, analysis reveals that dimensionless temperature  $\theta_g$ , gas concentration  $\eta$  and droplet radius  $r$  oscillate before thermal explosions occur. After initially increasing up to the maximum value of  $\theta_g$  the temperature starts to oscillate and then reveals steadiness before final explosion. The oscillations are due to the effect which is associated with heat losses in our system. The phenomenon is characterized by increase and decrease in gas concentration after oscillations respectively. It is worth noting that as  $n$  increasing, dimensionless temperature  $\theta_g$  and droplet radius  $r$  increases and decreases respectively, whereas dimensionless gas concentration  $\eta$  increases and decreases respectively in Figures 4.4 and 4.5.

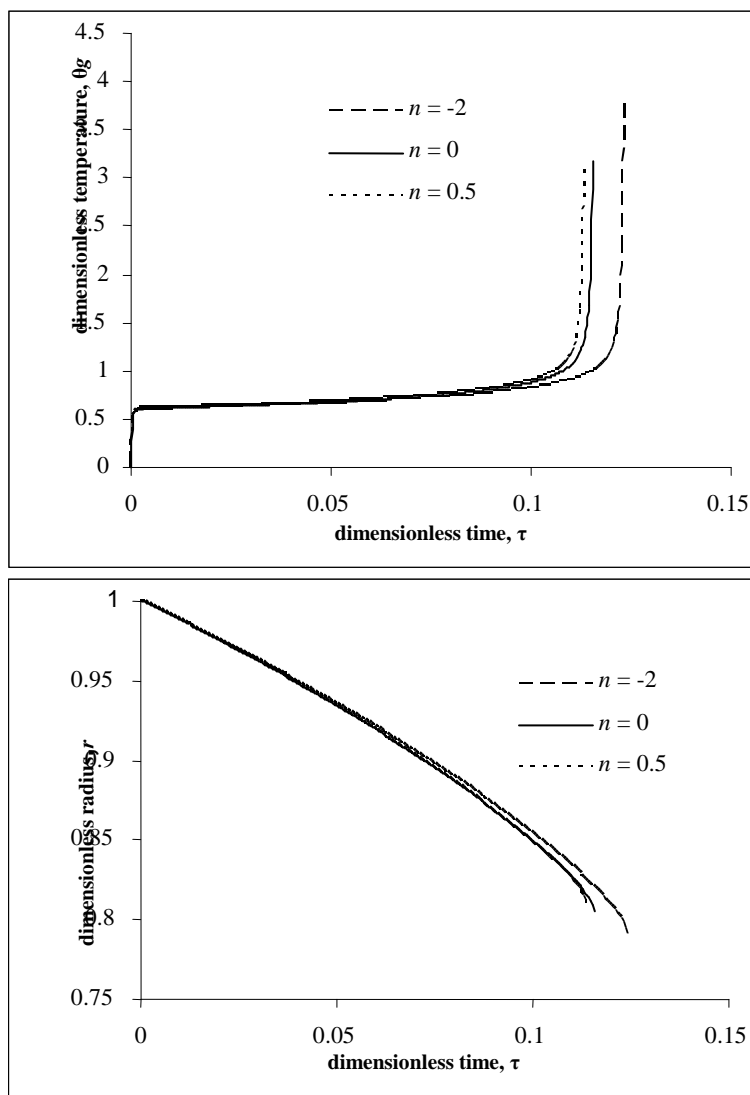
Figures 4.6 and 4.7 illustrate thermal explosions with cases of freeze delay-type behaviour. After initial increase in temperature there is a sharp decrease before final explosive increase. The entire process involves a decrease and increase in gas concentration respectively. It is obvious from Figure 4.6 and g that as  $n$  increasing, dimensionless droplet radius  $r$  and dimensionless temperature  $\theta_g$  increases respectively, whereas dimensionless gas concentration  $\eta$  increases and decreases respectively.

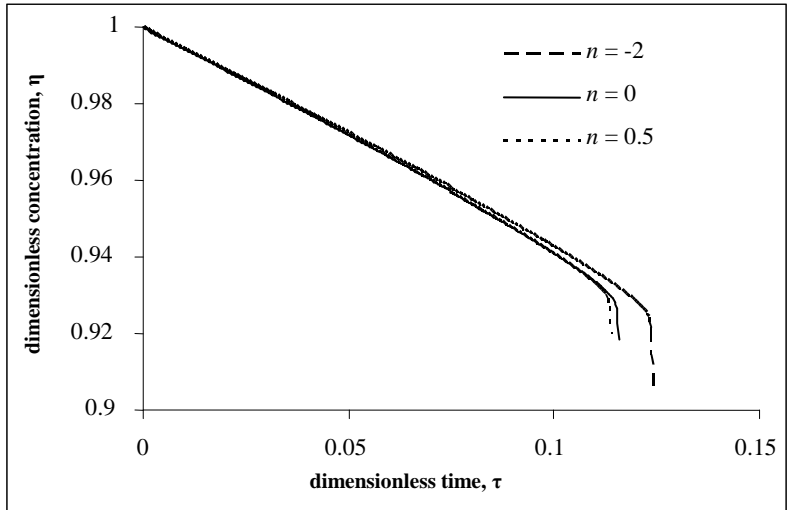
Figure 4.8 shows the slow non-explosive case of the dynamic system. Note the initial sharp jump in the temperature followed by the decay, the decay in the concentration and final non-zero value of the droplet radius.



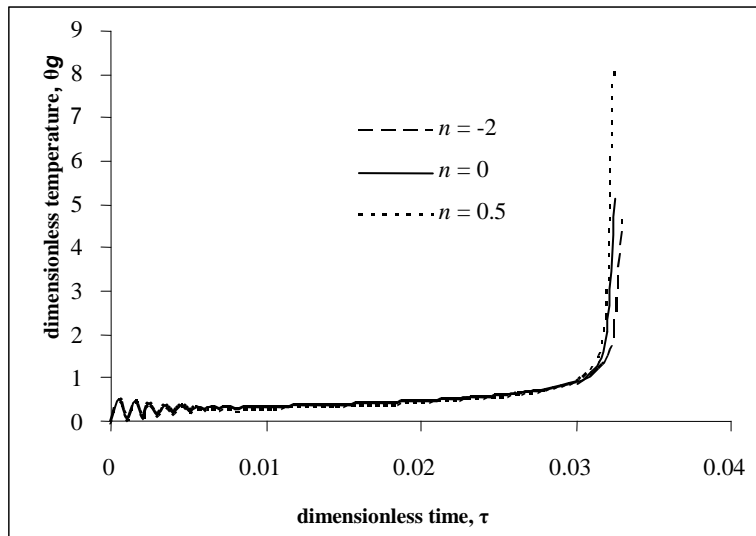


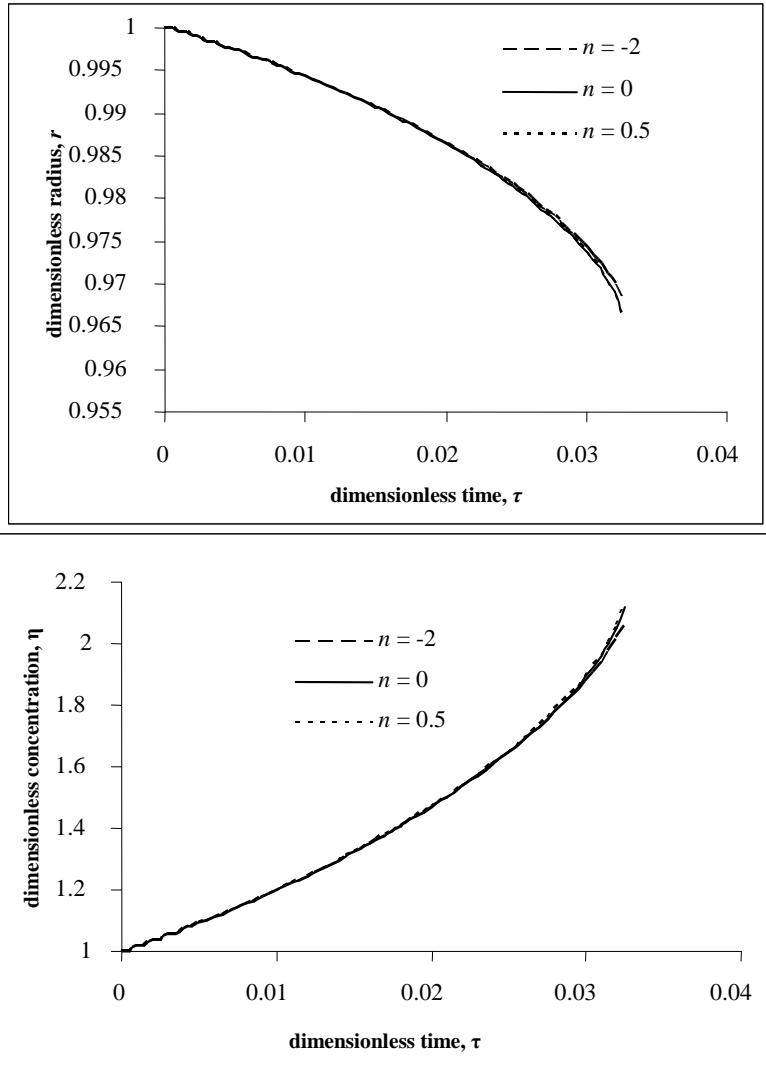
**Figure 4.2:** Thermal explosion with delay and gas concentration increases when  $\varepsilon_1 = 3$ ,  $\varepsilon_2 = 0.048$ ,  $\varepsilon_3 = 2$ ,  $\psi = 15$ ,  $\beta = 0.005$ ,  $\gamma = 0.001$ .



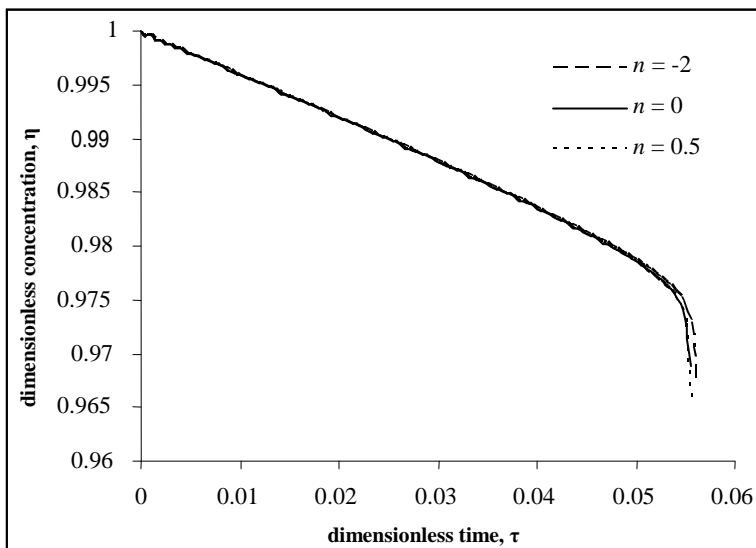
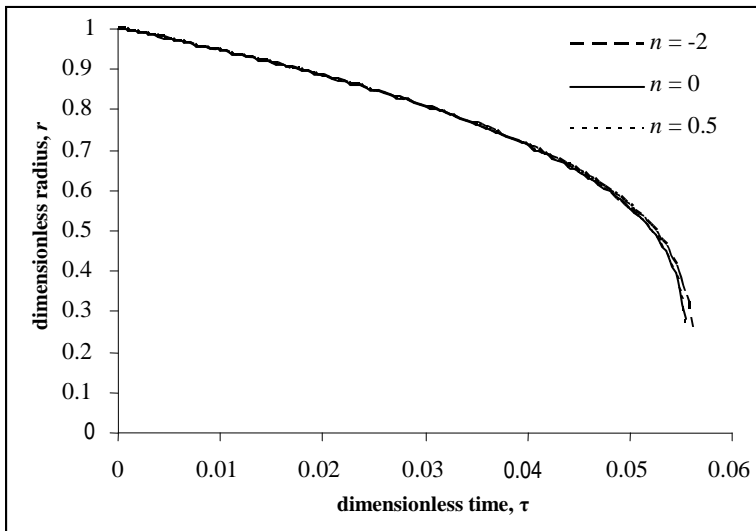
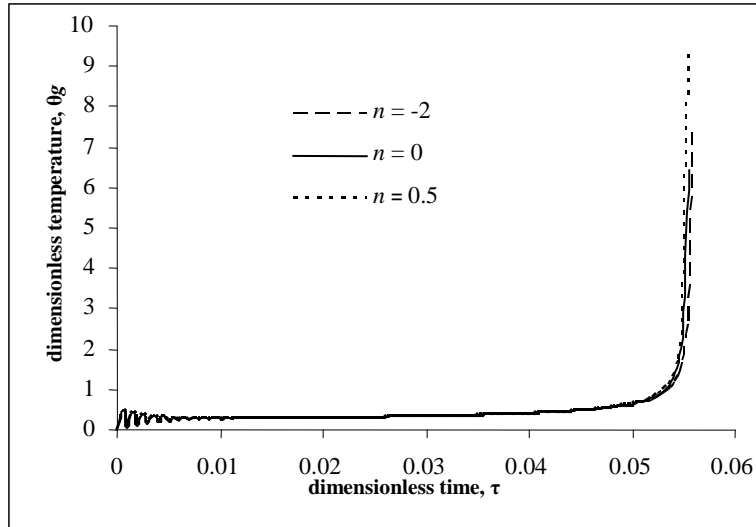


**Figure 4.3:** Thermal explosion with delay and gas concentration decreases when  $\varepsilon_1 = 3, \varepsilon_2 = 0.048, \varepsilon_3 = 2, \psi = 0.7, \beta = 0.005, \gamma = 0.001$ .

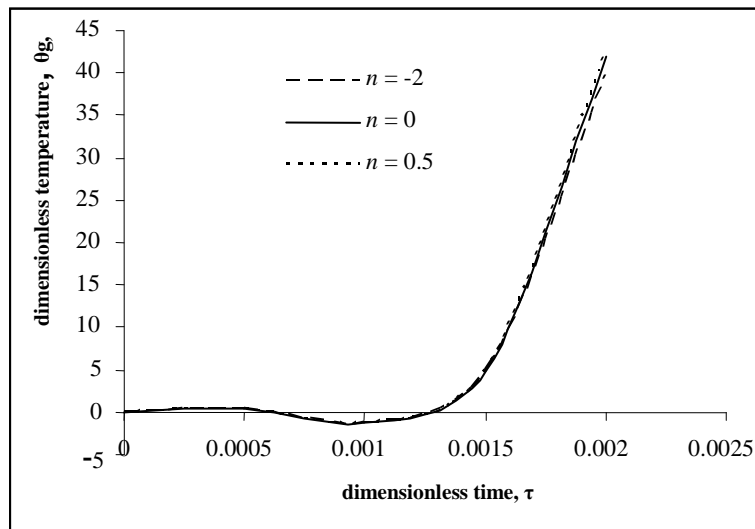


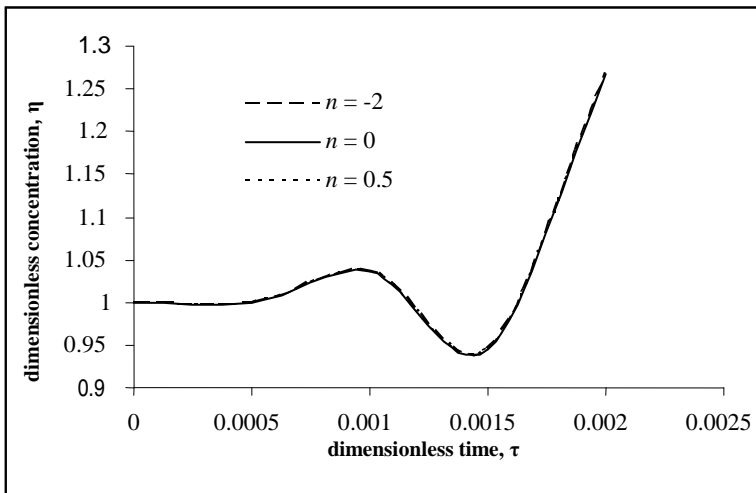
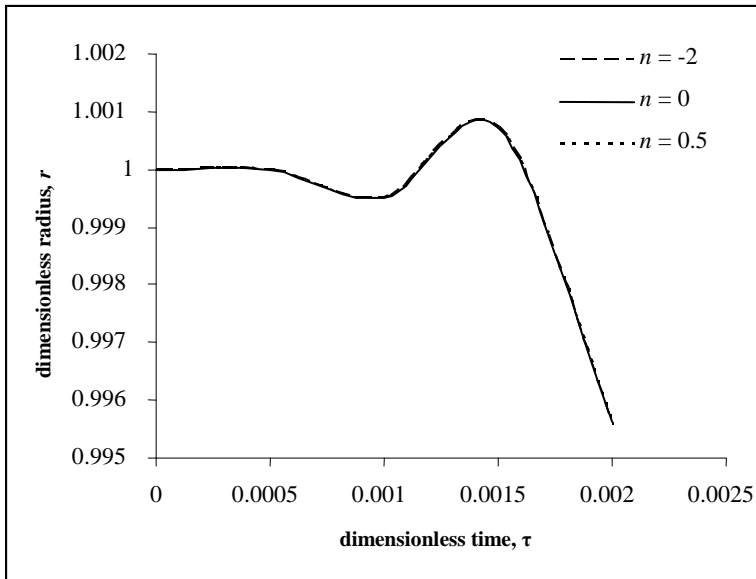


**Figure 4.4:** Thermal explosion with oscillating delay and concentration increases when  $\varepsilon_1 = 5, \varepsilon_2 = 0.5, \varepsilon_3 = 2, \psi = 15, \beta = 0.005, \gamma = 0.001$ .

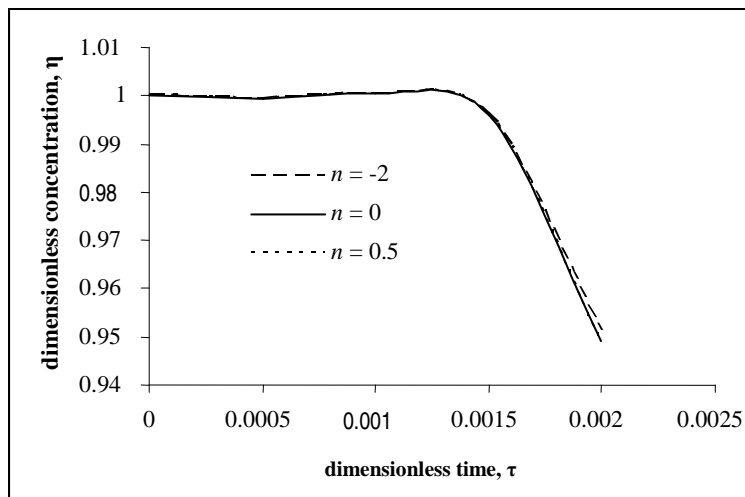
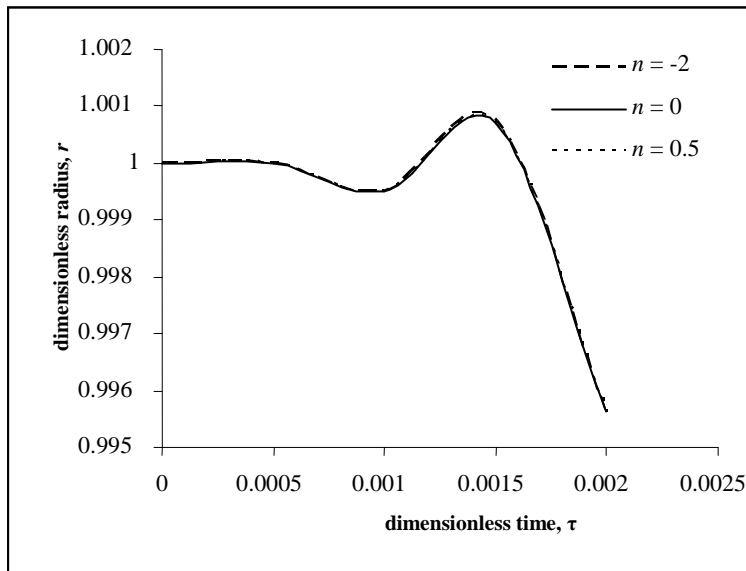
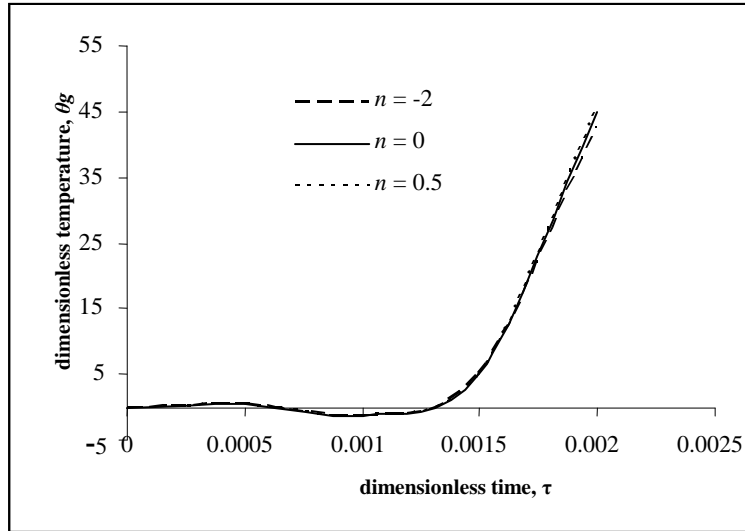


**Figure 4.5:** Thermal explosion with oscillating delay and concentration decreases when  $\varepsilon_1 = 5$ ,  $\varepsilon_2 = 0.5$ ,  $\varepsilon_3 = 20$ ,  $\psi = 0.7$ ,  $\beta = 0.005$ ,  $\gamma = 0.001$ .

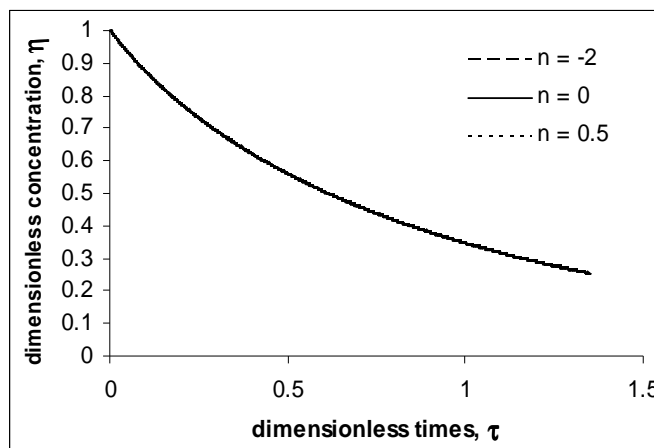
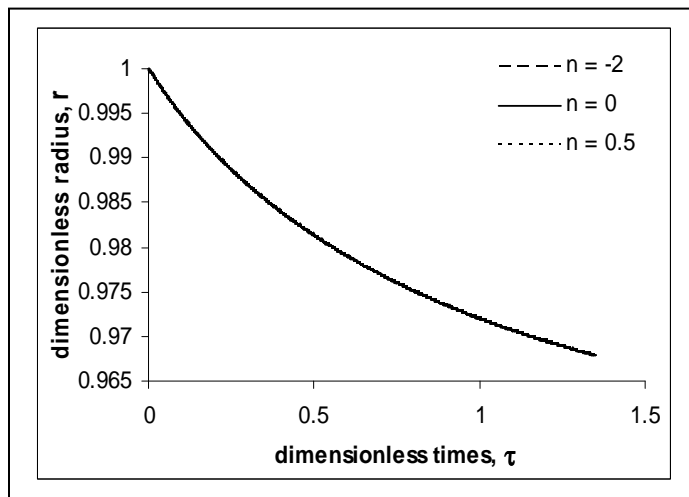
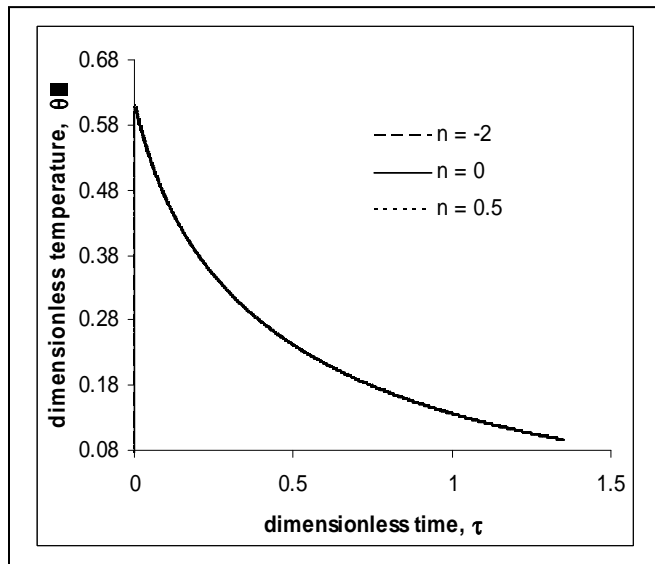




**Figure 4.6:** Thermal explosion with freeze delay and concentration increases when  $\varepsilon_1 = 10, \varepsilon_2 = 0.5, \varepsilon_3 = 2, \psi = 15, \beta = 0.005, \gamma = 0.001$ .



**Figure 4.7:** Thermal explosion with freeze delay and concentration decreases when  $\varepsilon_1 = 10, \varepsilon_2 = 0.5, \varepsilon_3 = 2, \psi = 0.7, \beta = 0.005, \gamma = 0.001$ .





**Figure 4.8:** Slow non-explosive system when

$$\varepsilon_1 = 3, \varepsilon_2 = 0.048, \varepsilon_3 = 0.1, \psi = 0.2, \beta = 0.005, \gamma = 0.001.$$

## 5.0 Conclusion

It was found that the dynamical behaviour of the system can be classified for different values of four key dimensionless parameters  $(\varepsilon_1, \varepsilon_2, \varepsilon_3, \psi)$  that arise in the analysis. Eight main dynamical behaviours were identified: convective thermal explosion, thermal explosion with delay (the concentration of the combustible gas decreases and increases), and thermal explosion with oscillating delay (the concentration of the combustible gas decreases and increases), thermal explosion with freeze delay (the concentration of the combustible gas decreases and increases) and slow non-explosive behaviours.

It is significant to note that the phenomenon of delay before the onset of explosion is very important from a practical point of view. Its dependence on physicochemical properties of the liquid fuel droplets under consideration can be critical in assessing safety features of a given dynamic system.

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