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STABILITY ANALYSIS OF TWO -VARIABLE MODEL
FOR COMBUSTION IN SEALED CONTAINER

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Abstract: The paper studies a model for combustion of self heating chemicals which are in drums inside a sealed shipping container. The stability of interacting drums of chemicals is a problem of great importance for the safety of manufacturers, users and handlers of the energetic material. Since the rate of reaction varies rapidly with temperature, the paper objectively examines the role of temperature on stability of the energetic materials and specifically investigates the effect of temperature broadening exponent called numerical exponent on its stability. The criteria for which stable focus, unstable focus and Hopf's bifurcation may occur in the new model are established. Of major interest is a criterion on the numerical exponent for which maximum ambient temperature could be attained.

Key Words: stability, reaction order, temperature broadening exponent, sealed container

1. Introduction

Many industrials chemical are heat-producing substances that are frequently blamed for causing fires. During shipping the temperature change from one

place to the other thus, overheating to the point of ignition of those combustibles is a potential hazard. Because of that potential hazard, industrialist incorporate engineering safeguards such as high-limit thermostats to prevent fires. Yet many fires involving industrial chemicals occur where these engineering safeguards operated properly, and the cause appears to have been ignition of the chemicals in the drum. Several researchers have performed investigations on chemical in sealed container but the one that really dealt changes in temperature accounted for the numerical exponent which is the objective of this study are scarce in literature. The knowledge of the variation in the temperature of the chemical in sealed containers is essential for the economics viability of the shipping and storage in industries and to prevent an unexpected ignition. Similarly, safety for personnel can be enhanced during handling and shipping of these substances.

Spontaneous explosion of self heating substance stored in drums inside a sealed shipping container, remains a problem of interest to researchers. This problem has attracted many researchers who have developed interesting models in combustion theory and other relevant fields in order to resolve the problem.

Researchers [1-10] have shown that to assess the thermal stability of energetic materials, thermal analyses are inevitable. The analyses of equilibrium, stability and Hopf's bifurcation (if any), and the investigation of the significance of some sensitive factors in this kind of model, are helpful to rely on self heating substances. In a thermal explosive reaction the rate of reaction varies rapidly with temperature and the moment of explosion occurs at some finite temperature [2].

Gray [5] in his work on the critical conditions for an assembly of interacting thermons derived under various assumptions, the critical conditions for the complete assembly of interacting heat producers (thermons) and identified the modes of ignition. Following Gray [5], Trenham and Forbes [10] discussed a model for combustion of a self-heating chemical (such as pool chlorine), stored in drums within a shipping container. Self-sustained oscillations are found to occur, as a result of Hopf bifurcation. Their result showed the period of oscillation and its variation with respect to the ambient temperature and the reaction parameter. In their contributions to this research worked on a comparison of two-and three- variable model for combustion in sealed containers. Having compared the two-and three- variable model, they established the conditions for stable focus, unstable focus and Hopf's bifurcation to occur.

Luangwilai et. al [6] examined a one-dimensional model for self-heating in compost piles, where self-heating occurs through a combination of biological and chemical mechanisms. They showed that at sufficiently low temperatures, the heat release rate due to biological activity is modelled by a function which is a

monotonic increasing function of temperature and at higher temperatures, it is a monotonic decreasing function of temperature. Nelson and Chen [7] presented the survey of experimental work on the self-heating and spontaneous combustion of coal. They showed among other investigations the frequent weakness in the literature about the kinetic data of self-heating systems, which is the absence of error estimates from regression analysis and the associated constraints on the reliability of the data for modeling.

Nelson et. al [8] used the singularity theory to investigate the generic properties of the thermal behaviour of cellulosic materials in the presence of microorganisms undergoing exothermic reactions.

The objective of this paper is to investigate the role of temperature on stability of the energetic materials. This paper therefore introduces a temperature broadening factor known as numerical exponent to the Arrhenius term in the paper of Trenham and Forbes [10]. The stability of the equilibrium solution of the resulting model is discussed and a criterion for Hopf's bifurcation to occur is established. The paper also formulates a theorem that establishes a bound to the value of the exponent for which the maximum ambient temperature could be attained.

2. Mathematical Formulation

Following Trenham and Forbes [10] and Popoola [9], we consider a two-step reaction of the form $A \xrightarrow{k_0} X \xrightarrow{ZT^m e^{\frac{-E}{RT}}} B$ which occurs during the decay of a precursor chemical substance A which forms an intermediate X and final product B. It is assumed that the decomposition process takes place at constant reaction rate k_0 while the combustion process depends on Arrhenius chemical reaction rate.

We define

$$k(T) = ZT^m e^{\frac{-E}{RT}}, \tag{1}$$

where m is the numerical exponent.

We remark that the case $m = 0$ corresponds to the model considered by Trenham and Forbes [6]. Since the reaction rate varies rapidly with temperature, the numerical exponent m is a temperature broadening parameter that also accounts for this variation.

Meanwhile, the process for a system of n- drums is described by the following equations

$$\frac{d[X_1]}{dt} = K_{j0}[A_j] - K_{j1}(T_j)[X_j], \tag{2}$$

$$\rho_j c_j V_j \frac{dT_j}{dt} = Q_j m_j^w V_j [X_j] K_{j1}(T_j) + X_j S_j (T_D - T_j), \quad j = 1, 2, 3, ..., n, \quad (3)$$

and for the entire container, the above is supplemented by conservation energy equation

$$\rho_D c_D V_D \frac{dT_D}{dt} = \sum_{j=1}^{n} X_j S_j (T_1 - T_D) - X_D S_D (T_D - T_a), \quad (4)$$

where the parameters in the equations are defined as follow:

$|A_j|$ Concentration of the pool chemical A;
ρ_D Density of the entire container;
ρ_j Density for each drum;
Q_j Exothermic heating term;
$k_{j1}(T_j)$ Exothermic rate;
λ_1 Heat transfer coefficient between drums and the entire container;
m_j^w Molecular weight;
χ_j Newtonian cooling coefficient representing energy/degree/area/time.;
n Number of drums;
k_{j0} Rate of constant step for each drum;
c_D Specific heat capacity of the entire container;
c_j Specific heat capacity of the material for each drum;
S_j Surface area of each drum;
S_D Surface area of the entire container;
β_D Surface area ratio between the container and the drums;
T_j Temperature of each drum;
T_D Temperature of the entire container;
V_j Volume of each drum;
V_D Volume of the entire container.

    The dimensionless equations for the equations (1)-(4) for identical drums are

$$k_1(T_1) = Z_1(\theta_a T_1)^m e^{\frac{-1}{T_1}}, \quad (5)$$

$$\frac{dX_1}{dt} = \mu_1 - X_1(\theta_a T_1)^m e^{\frac{-1}{T_1}}, \quad (6)$$

$$\frac{dT_1}{dt} = X_1(\theta_a T_1)^m e^{\frac{-1}{T_1}} + \lambda_1(T_D - T_1), \quad (7)$$

$$\alpha_g \frac{dT_D}{dt} = n\lambda_1(T_1 - T_D) - \beta\lambda_1(T_D - \theta_a), \quad (8)$$

where the dimensionless parameter $\alpha_g = \frac{\rho_D c_D V_D}{\rho_1 c_1 V_1}$ represents a volume and specific heat ratio between the container and any of the drums, $\beta_D = \frac{X_D S_D}{X_1 S_1}$

represents a surface area ratio between the container and the drums, and $\mu_1 = k_{10}\tau$ represents a non-dimensional rate term dependent on the reaction. The scaled ambient temperature $\theta_a = \frac{RT_a}{E_1}$ is a non-dimensional temperature of the environment outside the container, $\lambda_1 = \frac{X_1 S_1 E_1}{V_1 Q_1 m_1^w [A_1] Z_1 R}$ is the heat transfer coefficient between the drums and the container, n is the number of drums in the container, and the reference time $\tau_s = \frac{\rho_1 c_1 E_1}{Q_1 m_1^w [A_1] Z_1 R}$.

By Quasi-equilibrium assumption for T_D, $T_D \approx \left(\frac{n}{n+\beta_D}\right) T_1 + \frac{\beta_D \theta_a}{n+\beta_D}$ and the model becomes the system of equations

$$\frac{dX_1}{dt} = \mu_1 - X_1(\theta_a T_1)^m e^{\frac{-1}{T_1}}, \tag{9}$$

$$\frac{dT_1}{dt} = X_1(\theta_a T_1)^m e^{\frac{-1}{T_1}} - \frac{\beta_D \lambda_1}{n + \beta_D}(T_1 - \theta_a), \tag{10}$$

The critical point is

$$(X_{1e}, T_{1e}) = \left(\mu_1 \exp\left(\frac{\beta_D \lambda_1}{\theta_a \beta_D \lambda_1 + \mu_1(n + \beta_D)} \right) \left(\theta_a^2 + \frac{\mu_1(n + \beta_D)\theta_a}{\beta_D \lambda_1} \right)^{-m}, \right.$$

$$\left. \theta_a + \frac{\mu_1(n + \beta_D)}{\beta_D \lambda_1} \right). \tag{11}$$

3. Stability Analysis of (X_{1e}, T_{1e})

Let equations (9) and (10) be

$$\left.\begin{array}{l} \dfrac{dX_1}{dt} = f(X_1, T_1), \\ \dfrac{dT_1}{dt} = g(X_1, T_1), \end{array}\right\} \tag{12}$$

where

$$\left.\begin{array}{l} f(X_1, T_1) = \mu_1 - X_1(\theta_a T_1)^m e^{\frac{-1}{T_1}}, \\ g(X_1, T_1) = X_1(\theta_a T_1)^m e^{\frac{-1}{T_1}} - \frac{\beta_D \lambda_1}{n + \beta_D}(T_1 - \theta_a). \end{array}\right\} \tag{13}$$

It is easy to show that the Taylor's expansions of $f(X_1, T_1)$ and $g(X_1, T_1)$

$$f(X_1, T_1) = f(X_{1e}, T_{1e}) + \frac{\partial f}{\partial X_1}(X_{1e}, T_{1e})X_1 + \frac{\partial f}{\partial T_1}(X_{1e}, T_{1e})T_1 + \cdots \tag{14}$$

$$g(X_1, T_1) = g(X_{1e}, T_{1e}) + \frac{\partial g}{\partial X_1}(X_{1e}, T_{1e})X_1 + \frac{\partial g}{\partial T_1}(X_{1e}, T_{1e})T_1 + \ldots \quad (15)$$

And at equilibrium:

$$f(X_{1e}, T_{1e}) = g(X_{1e}, T_{1e}) = 0. \quad (16)$$

Then (14) and (15) imply

$$\left(\begin{array}{c} f(X_1, T_1) \\ g(X_1, T_1) \end{array} \right) = \left(\begin{array}{c} -(\theta_a T_{1e})^m \, e^{\frac{-1}{T_{1e}}} - X_{1e}\theta_a^m T_{1e}^{m-1}\left(m + \frac{1}{T_{1e}}\right) e^{\frac{-1}{T_{1e}}} \\ (\theta_a T_{1e})^m \, e^{\frac{-1}{T_{1e}}} X_{1e}\theta_a^m T_{1e}^{m-1}\left(m + \frac{1}{T_{1e}}\right) e^{\frac{-1}{T_{1e}}} - \frac{\beta_D \lambda_1}{n+\beta_D} \end{array} \right)$$

$$\times \left(\begin{array}{c} X_1 \\ T_1 \end{array} \right) + \left(\begin{array}{c} f_1(X_{1e}, T_{1e}) \\ g_1(X_{1e}, T_{1e}) \end{array} \right). \quad (17)$$

The eigenvalue σ of the coefficient matrix satisfies the quadratic equation

$$\sigma^2 - T_j \sigma + D_j = 0 \quad (18)$$

for which the trace T_j and determinant D_j are expressed as

$$T_j = (\theta_a T_{1e})^m \, e^{\frac{-1}{T_{1e}}} \left(\frac{X_{1e}}{T_{1e}}\left(m + \frac{1}{T_{1e}}\right) - 1 \right) - \frac{\beta_D \lambda_1}{n + \beta_D}, \quad (19)$$

$$D_j = (\theta_a T_{1e})^m \, e^{\frac{-1}{T_{1e}}} \frac{X_{1e}}{T_{1e}}\left(m + \frac{1}{T_{1e}}\right) + \frac{\beta_D \lambda_1}{n + \beta_D} - X_{1e}\theta_a^m T_{1e}^{m-1}\left(m + \frac{1}{T_{1e}}\right). \quad (20)$$

The quadratic equation (18) therefore has the solution

$$\sigma = \frac{1}{2}\left(T_j \pm \sqrt{T_j^2 - 4D_j} \right). \quad (21)$$

If $D_j > 0$ and $T_j^2 < 4D_j$ then the stability of equilibrium solution is determined by the sign of T_j

$$\left. \begin{array}{l} \text{1. Stable focus occurs for } T_j < 0; \\ \text{2. Unstable focus occurs for } T_j > 0; \\ \text{3. Hopf's bifurcation occurs for } T_j = 0. \end{array} \right\} \quad (22)$$

The Hopf's condition $T_j = 0$ below describes the point at which the stability changes

$$\left(\theta_a^2 + \frac{\mu_1(n + \beta_D)\theta a}{\beta_D \lambda_1} \right)^m e^{\frac{-\beta_D \lambda_1}{\mu_1(n+\beta_D)+\theta_a \beta_D \lambda_1}}$$

$$-\frac{m\mu_1\beta_D\lambda_1}{\mu_1(n+\beta_D)+\theta_a\beta_D\lambda_1}-\frac{\mu_1\left(\beta_D\lambda_1\right)^2}{\left(\mu_1(n+\beta_D)+\theta_a\beta_D\lambda_1\right)^2}+\frac{\beta_D\lambda_1}{n+\beta_D}=0. \quad (23)$$

Theorem. *For $m < 1$, there exists $\mu_1 e(m)$ such that $\theta_a\left(\mu_1 e\right)$ is maximum.*

Proof. Consider the Hofp's condition (23).
It is obvious that

$$\left(\theta_a^2+\frac{\mu_1(n+\beta_D)\theta a}{\beta_D\lambda_1}\right)^m e^{\frac{-\beta_D\lambda_1}{\mu_1(n+\beta_D)+\theta_a\beta\beta_D\lambda_1}} \to 0 \quad (24)$$

$$\Rightarrow \theta_a^2+\frac{\mu_1}{\lambda_1\beta_D}\left(n+\beta_D\right)\left(2-m\right)\theta_a-\frac{\mu_1\left(n+\beta_D\right)}{\lambda_1\beta_D}+\frac{\mu_1^2\left(1-m\right)\left(n+\beta_D\right)^2}{\left(\lambda_1\beta_D\right)^2}$$
$$= 0. \quad (25)$$

Differentiating (25) implicitly with respect to μ_1

$$\frac{d\theta_a}{d\mu_1}=\frac{\frac{q}{2}\left(m^2+\frac{2}{\mu_1 q}\right)}{\pm\sqrt{\left(m^2+\frac{4}{\mu_1 q}\right)}}+\frac{q}{2}(m-2). \quad (26)$$

Here

$$q=\frac{(n+\beta_D)}{\lambda_1\beta_D}, \quad (27)$$

$$\frac{d^2\theta_a}{d\mu_1^2}=\frac{-2}{\mu_1^3 q\left(m^2+\frac{4}{\mu_1 q}\right)^{\frac{3}{2}}}. \quad (28)$$

At turning point: $\frac{d\theta_a}{d\mu_1}=0$, and the two conditions

$$\mu_1 a=\frac{2}{m^2 q}\left(-1+\sqrt{\left(1-\frac{m^2}{4(m-1)}\right)}\right), \quad (29)$$

$$and \mu_1 b=\frac{2}{m^2 q}\left(-1-\sqrt{\left(1-\frac{m^2}{4(m-1)}\right)}\right) \quad (30)$$

must hold. It is obvious that $\frac{d^2\theta_a}{d\mu_1^2}$ is negative at the point $\mu_1=\mu_{1a}$.
This therefore implies that $\theta_a\left(\mu_1 e\right)$ has a maximum at the point μ_{1a}.
Hence, by equation (29), $m < 1$.

4. Numerical Solution of Hopf's Condition

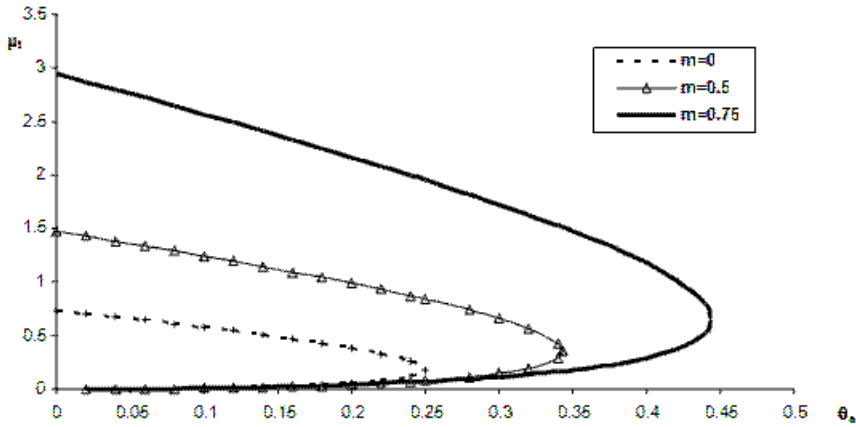The numerical result of Hopf's condition is presented on Figure 1.

Figure 1

4.1. Results and Conclusion

The stability analysis of a two-variable model for combustion in sealed shipping container has been examined. It is obvious that the numerical exponent for temperature has appreciable effects on stability of the self heating chemical.

Equation (11) shows that even when the numerical exponent is non-zero, problems (9) and (10) have a critical point. The criteria for which stable focus, unstable focus and for which Hopf's bifurcation may occur in the system are established in equation (22). The Hopf's condition (23) for $m = 0$ agrees with the result obtained by Trenham and Forbes [6]. The proof of the theorem has equally shown that for a maximum ambient temperature, the reaction order $m < 1$, and this implies that $0 \leq m < 1$. Figure 1 shows that the region of instability increases as the numerical exponent m ($m < 1$) increases.

In conclusion, the paper has shown that the self heating chemical gradually looses stability as the numerical exponent rises and reaches maximum. And also equation (30) which determines the maximum ambient temperature shows that a blow up occurs when $m = 1$.

This research work has important applications storage and shipping situations, where drums of chemical materials are shipped inside containers which

generally poor heat transfer characteristics and cause significant interactions

Acknowledgments

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