Thermal explosion characteristics in the presence of an additional heat source

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Abstract.

The present work is focussed on the analysis of the thermal explosion characteristics associated with an additional source of heat released due to forces of internal friction(mechanical heat source), which is important in connection with the motion of highly viscous reactive system.

By using the quasi-stationary state procedure, an approximate criterion was derived for a finite activation energy. We used some experimental data to determine the extent contributions of this additional heat source on the criterion of thermal explosion by comparing with known results.

1 Introduction

The calssical problem of thermal explosion for an exothermic chemical reaction with heat loss was first discussed by Semenov in 1928. Based on some assumptions (an exothermic heat source, large activation energy, initial temperature (T_0) , etc.), the critical thermal explosion parameter (Semenov number (ϕ)), necessary for thermal explosion was derived.

In addition to the exothermic reaction, the inclusion of an additional source of heat has also been considered. Dik [1] considered the influence of an additional heat source(not dependent on temperature), on the critical ignition parameter. They showed that there is no additive behaviour of the contribution of the additional heat source to the critical temperature and critical semenov parameter. Stolin and Merzhanov [2 examined the thermal explosion associated with an additional heat released due to forces of internal friction(mechanical heat), which is

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important in connection with the motion of highly viscous fluids. They showed that the critical value of the Frank-Kamenetskii parameter decreases as the strength of the mechanical heat source increases.

In this work, we intend to examine the effect of an additional heat source due to forces of internal friction and a temperature dependent pre-exponential parameter, on the thermal explosion parameter. We also intend to use experimental data to examine the behaviour of these results and compare with existing ones in literature.

2 Model description

We consider a one step reaction of the form

$$A \to P,$$
 (I)

where A and P refers to the fuel and product respectively.

The spatially homogeneous dimensionless equations corresponding to the above exothermic reaction are

$$\frac{d\eta}{dt} = -\eta (1 + \beta\theta)^m \exp\left(\frac{\theta}{1 + \beta\theta}\right),\tag{1}$$

$$\gamma \frac{d\theta}{dt} = \eta (1 + \beta \theta)^m \exp\left(\frac{\theta}{1 + \beta \theta}\right) + \frac{1}{\phi_M} \exp\left(\frac{\theta}{1 + \beta \theta}\right) - \frac{1}{\phi_S} \theta = q^+ - q^-, (2)$$
$$\eta(0) = 1, \quad \theta(0) = 0, \tag{3}$$

where

$$\gamma = \frac{\rho C_p R T_0^2}{A_0 Q E}, \ \beta = \frac{R T_0}{E}, \ \hat{\phi}_S = \phi_S^{-1} = \frac{S \chi R T^{2-m}}{V E Q k_0 A_0} \exp(\frac{1}{\beta}), \ \hat{\phi}_M = \hat{\phi}_M^{-1} = \frac{G \exp\left(\frac{E-U}{R T_0}\right)}{A Q k_0 A_0 T_0^m} \exp(\frac{1}{\beta}).$$

Here θ and η are the dimensionless temperature and reactant concentration respectively, α is the heat loss parameter, β is the reduced ambient temperature, while γ is the reciporcal of the adiabatic temperature rise and χ is the coefficient of heat transfer, A_0 is the concentration of fuel, q^+ refers to heat source and q^- refers to heat loss to the surrounding. The presence of γ in (1) - (2) makes it a multi-scale system, with γ as the small parameter. Thus, the system (1) - (3) can be studied using different asymptotic methods. Based on the Semenov criterion, the critical conditions for runaway(thermal explosion) are identified by the relations;

$$q^+ = q^-, \tag{4}$$

and

$$\frac{dq^+}{d\theta} = \frac{dq^-}{d\theta}.$$
(5)

From equation (4) and (5), the quasi-stationary state temperature θ_c is determined. From the preliminary calculation, the critical(ignition) temperature is given as;

$$\theta_c = 1 + (1+B) \left[B + (B^2 - 1)\hat{\phi}_M \right] \hat{\phi}_M + \left[(2-m)(1+\hat{\phi}_M) - mB\hat{\phi}_M \right] \left[1 + \hat{\phi}_M (1+B) \right] \beta + O(\beta^2).$$
(6)

and

$$\hat{\phi}_{S} = e^{-1} \frac{1 - B\left\{1 + (1+B)\left[B + (B^{2} - 1)\hat{\phi}_{M}\right]\hat{\phi}_{M}\right\}}{(1+m\beta - B)} + e^{-1} \frac{\left\{2 - B\left[(2-m)(1+\hat{\phi}_{M}) - mB\hat{\phi}_{M}\right]\left[1 + (1+B)\hat{\phi}_{M}\right] - 2(1+B)\left[B + (B^{2} - 1)\hat{\phi}_{M}\right]\hat{\phi}_{M}\right\}}{(1+m\beta - B)}$$
(7)

3 Conclusion

We have investigated the effect of an additional heat source on the ignition temperature(θ_c) and the Semenov parameters ($\hat{\phi}_S$). The solutions obtained here are generalization of known results, as known previous works(Okoya [3], Ajadi and Gol'dshtein [4]) are special cases. Further analysis of these results were carried out using some established experimental data.

References

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