

Thermal Explosion in a Droplet-Gas Cloud with Chemical Reaction of General Order

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Introduction

There is some compelling experimental evidence to indicate that the combustion of a spray of liquid fuel droplets in a combustible mixture can be strikingly different than that of an equivalent purely gaseous mixture. The complexity of these two-phase systems makes their mathematical analysis rather difficult. In a realistic system one is concerned with simultaneous heat, mass and momentum transfer of a multi-component, multi-phase mixture. Mathematically, one has to contend with a set of strongly non-linear coupled partial differential equations. In order to disentangle the many physico-chemical processes at play, and to attempt to identify their realms of relevance and importance it is reasonable to adopt an approach that focuses on singling out the key driving mechanisms. These are analyzed separately as a preliminary stage before building up an integrated picture of their interaction. In this paper we follow this line of thought in order to carry out a qualitative investigation of the thermal explosion dynamics in a fuel droplet + gas cloud, with a general order chemical reaction describing the chemistry. By “thermal explosion” we exclusively refer to the initial stages of the behaviour of a combustible medium as its temperature begins to rise (by about 100-200K) and various competing physical and chemical processes are called into play. It is what takes place at this initial evolutionary period that sets the stage for the ultimate behaviour of the system. Thus, we only focus on this particular episode in the spray’s lifetime, rather than on its entire life history. The subsequent evolution of the spray-gas cloud’s behavior is of no concern to us in this work, and indeed, cannot be described by the equations we consider here.

Problem Statement

The mutual effect of oxidizer and fuel concentrations on the thermal explosion of a flammable spray in a pre-heated combustible gas mixture is the new feature included in the simplified physical model suggested earlier by the authors. The model involves the following main physical assumptions. Evaporating fuel droplets in a combustible gas mixture comprise a mono-disperse spray, whose effect on the blow-up process is investigated qualitatively. All droplets are of the same constant temperature (on the saturation line), which differs from that of the hot gas. The mixture is placed in a thermally insulated enclosure (adiabatic approximation). Heat flux from the burning gas to the droplets is supposed to be proportional to the temperature difference between the liquid and gas phases. The chemistry is modeled as a one-step highly exothermic chemical reaction. The order of the chemical reaction is taken in accordance with the results suggested by Westbrook and Dryer (1982): the reaction rate contains the multiple of non-integer powers of the fuel and oxidizer concentrations in addition to the conventional Arrhenius exponential term. A mathematical model is developed as a system of four highly non-linear ordinary differential equations (ODEs): temperature equation (1), mass equation for the single droplet (2) and two concentration equations (for both fuel

and oxidizer 3-4). The initial system of equation is non-dimensionalized along the lines of Semenov's classical approach (Semenov, 1928, Frank-Kamenetskii, 1969) to the analysis of thermal explosion, which based on the initial values of the key parameters of the considered system. Under the above mentioned assumptions the dimensionless set of governing equations reads as follows

$$\gamma \frac{du}{d\tau} = \eta^a \xi^b \exp\left(\frac{u}{1 + \beta u}\right) - \varepsilon_1 r(u + \theta_0) \quad (1)$$

$$\tilde{\varepsilon}_2 \frac{d(r^3)}{d\tau} = -\varepsilon_1 r(u + \theta_0) \quad (2)$$

$$\tilde{v}_f \frac{d\eta}{d\tau} = -\eta^a \xi^b \exp\left(\frac{u}{1 + \beta u}\right) + \tilde{v}_f \psi \varepsilon_1 r(u + \theta_0) \quad (3)$$

$$\tilde{v}_o \frac{d\xi}{d\tau} = -\eta^a \xi^b \exp\left(\frac{u}{1 + \beta u}\right) \quad (4)$$

where the following dimensionless parameters appear

$$\beta = \frac{RT_{g0}}{E} \quad \gamma = \frac{c_{pg} \rho_g T_{g0}}{(C_{ff} C_{ox0})^{0.5} Q_f \mu_f} \beta \quad \varepsilon_1 = \frac{4\pi R_{d0} \lambda_g \beta T_{g0} n_d}{AC_{ox0}^b C_{ff}^a Q_f \alpha_g \mu_f} \exp(1/\beta) \quad (5)$$

$$\tilde{\varepsilon}_2 = \frac{\rho_L L \alpha_L}{(C_{ff} C_{ox0})^{0.5} Q_f \alpha_g \mu_f}; \quad \psi = \frac{Q_f}{L} \left(\frac{C_{ox0}}{C_{ff}}\right)^{0.5} \quad K = \frac{v_o C_{ff}}{v_f C_{ox0}} \quad (6)$$

$$\tilde{v}_f = \frac{1}{v_f} \left(\frac{C_{ff}}{C_{ox0}}\right)^{0.5}; \quad \tilde{v}_o = \frac{1}{v_o} \left(\frac{C_{ox0}}{C_{ff}}\right)^{0.5}$$

The following notations are used here: **A** - pre-exponential factor ($\text{m}^{3(a+b-1)} / \text{s} / \text{kmol}^{a+b-1}$); **C**- concentration (kmol / m^3); **E**- activation energy; **L**- latent heat (J/kg); **Q** - combustion energy (J/kg); **R**- universal gas constant; **R_d** - radius of the drops (**m**); **T** - temperature (**K**); **n_d** - number of drops per unit volume; **α** - volumetric phase content, **λ**- thermal conductivity; **v** - stoichiometric coefficient (dimensionless); **ρ** - density (kg / m^3); **t**- time (**s**); **μ**-molar mass (kg/kmol); subscripts are related to: **d**- liquid droplets; **f**- combustible component (fuel); **g**- gas mixture; **o** - oxidizer; **ff** - overall fuel (i.e. liquid +vapor) concentration; **p** - under constant pressure; **0** - undisturbed (initial) state.

The system (1) - (4) has two partial integrals, one of which represents an energy integral. The existence of these integrals permits us to exclude two of the four dependent variables in (1) - (4). The reduced set of equations is

$$\gamma \frac{du}{d\tau} = \eta(u, r)^a \xi(u, r)^b \exp\left(\frac{u}{1 + \beta u}\right) - \varepsilon_1 r(u + \theta_0) \quad (7)$$

$$\tilde{\varepsilon}_2 \frac{d(r^3)}{d\tau} = -\varepsilon_1 r(u + \theta_0) \quad (8)$$

Main Results

The dimensionless model (both (1)-(4) and (7)-(8)) represents a multi-scale system (with a small parameter) due to the great difference in characteristic times of the processes involved (highly exothermic chemical reaction, droplets evaporation). Due to this scale hierarchy the system can be considered as singularly perturbed and the well-known method of integral manifolds can be applied (MIM, Gol'dshtein and Sobolev, 1992). The technique of asymptotic analysis on invariant manifolds has proved its high efficiency in numerous previous works of the authors (a rather more comprehensive description of the procedure can be found, for example, in the paper by Goldfarb *et al* 2000).

The conventional thermal explosion theory (Semenov, 1928, Frank-Kamenetskii, 1969) is based on consideration of the balance between the rate of heat generation due to chemical

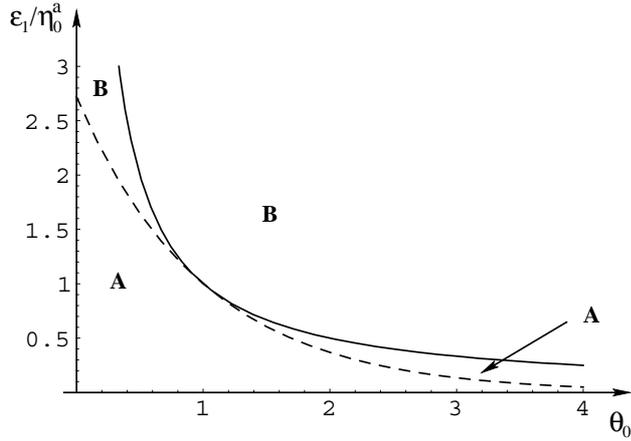


Fig.1. Parametric map of main dynamic regimes.

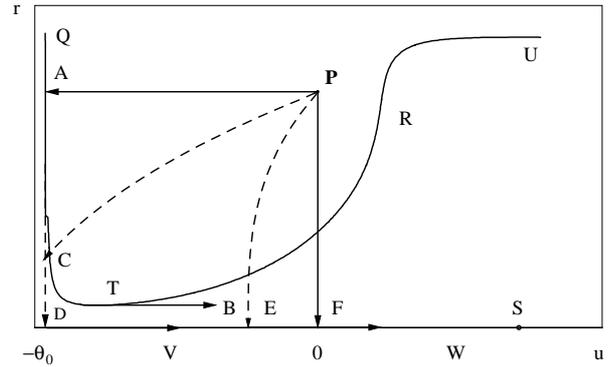


Fig.2. Plane u-r and possible delayed trajectories of the system.

reaction and the rate of heat loss to the surroundings. Ignition is normally associated with conditions under which a fine steady-state becomes impossible and the temperature rises to high values associated with active combustion (final explosion). Prior to this, a temporary balance arises between chemical heat release and *internal* heat losses due to intensive liquid fuel (droplets) evaporation. The delay time is defined as the time during which such a balance exists.

Analysis of the relative location of the slow curve and initial point allows one to obtain a critical expression for the physical parameter $\varepsilon_1 = (\eta_0)^a \exp(1 - \theta_0)$. This critical value of ε_1 collapses to that of Semenov's classical theory of thermal explosion (when $\eta_0 = 1$ and $\theta_0 = 0$) it. If $\varepsilon_1 < e$ only conventional thermal explosion can be expected, if $\varepsilon_1 > e$ a more complicated set of scenarios is anticipated. Here the possible dynamical regimes that are determined by the slow curves are as follows (see figure 1)

A. When (i) $\varepsilon_1 < (\eta_0)^a \exp(1 - \theta_0)$

$$(ii) \frac{(\eta_0)^a}{\theta_0} > \varepsilon_1 > (\eta_0)^a \exp(1 - \theta_0), \theta_0 > 1$$

the conventional fast explosive regime results - the chemical reaction dominates the evaporation process, the system explodes and the gas temperature rises sharply.

EMBEDEMBEDEM B. When (i) $\varepsilon_1 > \frac{(\eta_0)^a}{\theta_0}$

$$(ii) \frac{(\eta_0)^a}{\theta_0} > \varepsilon_1 > (\eta_0)^a \exp(1 - \theta_0), \theta_0 < 1$$

a delay regime results - the fast trajectory reaches the stable branch of the slow curve. The next part of the trajectory adheres to the slow curve and describes decreasing droplets radii, until the turning point or adiabatic point of the system is reached. Essentially what happens is that following a rapid temperature change, the two processes of heat release and heat loss become balanced and the droplets radii begin to decrease. This fine balance is responsible for the existence of the delay effect.

Here, the aforementioned approach (MIM) is applied to carry out a qualitative analysis of the possible regimes of thermal explosion. The detailed dynamical picture is defined by the shape and location of the slow curve and by the location of the initial point relative to it (delayed regimes are depicted in Fig.2, case **B**). The curve **QTRU** represents the slow curve for the case, when temperature is the fast variable, the straight line **VW** serves as slow curve in the opposite case (radius is fast, temperature is slow). **PATBS** represents a trajectory of delayed regime, where the part **AT** is responsible for the delay itself (as it lies on the slow curve). **PFS** is a trajectory corresponding to the process when total evaporation of the droplets (asymptotically no changes of temperature occurs) precedes final explosion (**FS**).

The MIM approach allows analytical expressions for the delay time to be derived for cases of practical interest. Figure 3 represents dependence of the delay time on the initial radius of the droplets. It is readily seen that the theoretical estimations match the results of direct numerical simulations rather well (Fig.3b).EMBEDEMBEDEM

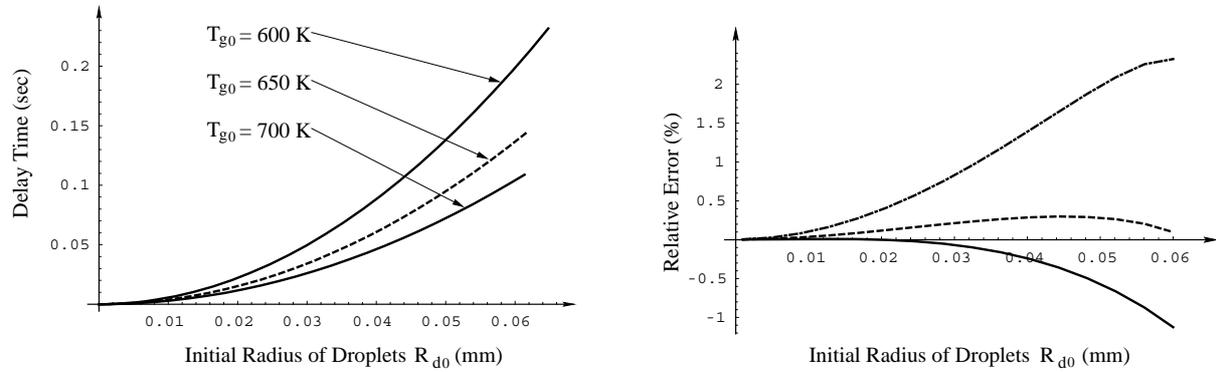


Fig.3. a (left) predicted (theoretical) delay time dependence on the initial radius of droplets for three different initial temperatures; **b (right)** relative error of the predicted delay time with respect to direct numerical simulations of the original system. The simulations were conducted for n-decane mixture with parameters: $n_d=10^7$ (m^{-3}), $T_d=490$ (K), $P_{g0}=10^5$ (Pa), $K=0.2$

Conclusions

The purpose of this paper was to study theoretically the input of oxidizer presence to the phenomenon of thermal explosion in combustible gaseous mixture with evaporating fuel droplets. The essential results may be formulated as follows. A mathematical description of the suggested physical model includes four highly non-linear ODEs. The analysis of the model was performed analytically on the basis of the method of integral manifolds (MIM). The accepted mathematical approach permits to the study of thermal explosion in both fuel rich and fuel lean mixtures. Possible types of dynamical behavior of the system are studied and parametric regions of their existence are determined analytically. It is pointed out that the present model generalizes previous results for fuel lean combustible mixtures, which are a particular case of the current model. Two main types of regimes (conventional explosive and delayed) were uncovered in the fuel rich case. Peculiarities of these dynamical regimes are investigated and their dependence on physical system parameters analyzed. In particular, explicit formulae for the total ignition and delay times are developed and found to agree with the predictions of direct numerical simulations.

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