Radiation Effect on Thermal Explosion in Combustible Gas Containing Fuel Droplets

Igor Goldfarb [1], Vladimir Gol'dshtein [1], Grigory Kuzmenko [1], Sergei Sazhin [2]

[1]Department of Mathematics and Computer Sciences, Ben-Gurion University of the Negev, P.O.B. 653, Beer-Sheva 84105, Israel, goldfarb@cs.bgu.ac.il

[2]School of Engineering, Faculty of Science and Engineering, The University of Brighton, Brighton BN2 4GJ, UK, S.Sazhin@bton.ac.uk

Introduction

The problem of thermal explosion in a combustible gas mixture containing fuel droplets is a long-standing one and has numerous applications to furnaces, gas turbines and internal combustion engines [1,2]. Over the recent years the theoretical analysis of this problem has been mainly based on the CFD packages [2]. This approach has a number of attractive features since it potentially allows to take into account various heat transfer and combustion processes in a self-consistent way. The downside of this approach, however, is that it does not allow to obtain detailed qualitative information and to separate the contribution of the different physical processes. As a result it can not be particulary helpful in understanding of the relative contribution of these processes.

An alternative approach to this problem is based on analytical analysis of the underlying equations in different limiting cases. This approach cannot replace the CFD but can effectively complement it. One of these asimptotic tools is based on the geometrical version of integral manifolds method [3]. This method has been successfully applied to the number of problems of thermal explosion [4-6].

An original physical model of self-ignition in combustible gas mixture containing evaporating liquid droplets is developed in the present paper. The main attention is concentrated on the situations where delays might occur before final ignition. We aim primarily to study an impact of thermal radiation on delay time.

Problem Statement

The main physical assumptions of the suggested model are the following. The combustible gas mixture contains evaporating ideal spherical droplets of fuel. The mixture is placed in a limited volume. We presuppose that all droplets have the same size (radius). All droplets are of the same constant temperature (on the saturation line). We suppose the chemical reaction is taking place in gas phase only. Spatially homogeneous approach is applied. Pressure changes influence is negligible. Heat flux from the burning gas to the droplets is perceived to be composed from two components: conventional conductive flux and radiant flux. The term responsible for conductive flux is supposed to be proportional to the phases temperature difference. The contribution of the thermal radiation is taken into account based on the P-1 approximation [7] for the thermal radiation transfer with Marshak boundary conditions [8]. We assume that fuel drops are not transparent and their surfaces are gray and the radiative heat fluxes at these surfaces may be described according to the Stefan-Boltzman law with a given emissivity at the droplets' surface. It is assumed that the burning gas is optically thick, the walls of the volume are ideal reflectors and the radiation temperature is equal to the gas temperature.

Under these assumptions the system of governing equations reads as follows

$$\mathbf{c_{pg}\rho_g\alpha_g\frac{dT_g}{dt}=C_fQ_f\alpha_gA\mu_f\exp\left(-\frac{E}{RT_g}\right)-4\pi R_d\lambda_g n_d\left(T_g-T_s\right)-4\pi R_d^2\sigma_1 n_d\left(T_g^4-T_s^4\right)} \quad (1)$$

$$\mathbf{\frac{d\left(R_d^2\right)}{dt}=-\frac{2\lambda_g}{\rho_L L}\left(T_g-T_s\right)-\frac{4\pi R_d\sigma_1}{L\rho_L}\left(T_g^{\,4}-T_s^{\,4}\right)} \quad (2)$$

$$\mathbf{\frac{dC_f}{dt}=-C_fA\exp\left(-\frac{E}{RT_g}\right)+\frac{4\pi R_d\lambda_g n_d}{L\mu_g\alpha_g}\left(T_g-T_s\right)+\frac{4\pi R_d^2\sigma_1 n_d}{L\mu_g\alpha_g}\left(T_g^{\,4}-T_s^{\,4}\right)} \quad (3)$$

The system (1)-(3) includes an energy equation for the reacting gas (1), a mass equation for a liquid droplet (2) and a concentration equation for the reacting gas mixture (3). Initial conditions for the system:

$$\mathbf{T_g = T_{g0};\ \ C_f = C_{f0};\ \ R_d = R_{d0};\ \ T_s = T_{g0}}$$

Here we use the following notation: $\mathbf{T}$ - temperature; $\mathbf{E}$ - activation energy; $\mathbf{L}$ - liquid evaporation energy; $\mathbf{C}$ - concentration; $\mathbf{R_d}$ -radius of the drops; $\mathbf{Q}$ - combustion energy; $\sigma_1 = 2\sigma\varepsilon_d/(2-\varepsilon_d)$, σ is the Stefan-Boltzman constant, ε_d is the emissivity of the droplet's surface; μ - molar mass; ρ - density; α - volumetric phase content; λ - thermal conductivity; $\mathbf{n}$ - number of drops per unit volume; $\mathbf{A}$ - preexponential factor; $\mathbf{R}$ - universal gas constant. Subscripts: $\mathbf{g}$ - gas mixture; $\mathbf{L}$ - liquid; $\mathbf{f}$ - combustible gas component of the mixture; $\mathbf{d}$ - liquid drops; $\mathbf{p}$ - under constant pressure; $\mathbf{s}$ - on the saturation line.

The same nondimensionalising of temperature, concentration, radius and time as in [4-6] is used in order to distinguish the impact of the processes with various characteristic times. Thus we introduce the following dimensionless variables:

$$\theta = \frac{\mathbf{T_g - T_{g0}}}{\mathbf{T_{g0}}}\frac{\mathbf{E}}{\mathbf{RT_{g0}}};\ \ \eta = \frac{\mathbf{C_f}}{\mathbf{C_{f0}}};\ \ \mathbf{r} = \frac{\mathbf{R_d}}{\mathbf{R_{d0}}};\ \ \tau = \frac{\mathbf{t}}{\mathbf{t_{react}}};\ \ \mathbf{t_{react}} = \mathbf{A^{-1}}\exp\left(\frac{\mathbf{E}}{\mathbf{RT_{g0}}}\right)$$

The dimensionless system reads

$$\gamma\frac{\mathbf{d}\theta}{\mathbf{d}\tau} = \eta\exp\left(\frac{\theta}{1+\beta\theta}\right) - \varepsilon_1\mathbf{r}\theta - \varepsilon_1\varepsilon_3\mathbf{r}^2\theta \tag{4}$$

$$\frac{\mathbf{d}\left(\mathbf{r}^2\right)}{\mathbf{d}\tau} = -\frac{2\varepsilon_1\varepsilon_2}{3}\theta - \frac{2\varepsilon_1\varepsilon_3\varepsilon_2}{3}\mathbf{r}\theta \tag{5}$$

$$\frac{\mathbf{d}\eta}{\mathbf{d}\tau} = -\eta\exp\left(\frac{\theta}{1+\beta\theta}\right) + \varepsilon_1\psi\mathbf{r}\theta + \varepsilon_1\varepsilon_3\psi\mathbf{r}^2\theta \tag{6}$$

In equations (4)-(6) the following parameters are used:

$$\beta = \frac{\mathbf{RT_{g0}}}{\mathbf{E}};\quad \gamma = \frac{\mathbf{c_{pg}T_{g0}}\rho_{g0}}{\mathbf{C_{f0}Q_f}\mu_f}\beta;\quad \varepsilon_1 = \frac{4\pi\mathbf{R_{d0}}\lambda_g\beta\mathbf{T_{g0}n_d}}{\mathbf{AC_{f0}Q_f}\alpha_g\mu_F}\exp\left(\frac{\mathbf{E}}{\mathbf{RT_{g0}}}\right)$$

$$\varepsilon_2 = \frac{\mathbf{Q_fC_{f0}}\alpha_g\mu_f}{\rho_L\mathbf{L}\alpha_L};\quad \psi = \frac{\mathbf{Q_f}}{\mathbf{L}};\quad \varepsilon_3 = 4\frac{\mathbf{T_{g0}^3}\sigma_1\mathbf{R_{d0}}}{\lambda_{g0}}$$

Parameters β and γ are small for highly exothermic reactions (this is the assumption used in the classical thermal explosion theory) and hence equations (4)-(6) can be considered as singularly perturbed system. Parameters $\varepsilon_1, \varepsilon_2$ are similar to those introduced in the previous papers [4-6] and have the same physical meaning. The parameter ε_3 is a new one and it describes the relation between the radiant heat flux from burning gas to a droplet and conventional conductive heat flux.

We deal with the adiabatic system and hence the number of equation in the system (4)-(6) may be reduced by one using the integral of the energy. The reduced system contains equations (4) and (6) where the expression for the radius as a function of concentration and temperature is substituted instead of independent variable **r**.

Analysis and Discussion

To investigate qualitatively the typical system behaviour, we use the zeroth order approximation ($\gamma = \mathbf{0}$) of the geometrical asymptotic method of integral manifolds [3]. Steady state analysis of the system (4)-(6) shows that the system behaviour is explosive. Nevertheless, there can be a delay before the ignition event eventualy takes place. This phenomenon exists because heat losses (conductive and radiant) are balancing the system before exothermic oxidation finally dominates. The characteristic dynamical regimes are investigated qualitatively on the phase plane ($\eta - \theta$). An arbitrary trajectory (solution of the reduced system depicted on the plane ($\eta - \theta$)) starts from the initial point ($\eta = \mathbf{1};\quad \theta = \mathbf{0}$). The trajectory may be subdivided into fast and slow parts. The slow part of the trajectory lies within γ-neighbourhood of the slow curve $\Omega(\theta,\eta)$ (the terms of the order $\beta\theta$ are neglected in equation (7) for the slow curve $\Omega(\theta,\eta)$)

$$\Omega(\theta,\eta)=\eta\exp(\frac{\theta}{1+\beta\theta})-\varepsilon_1\theta\left(1+\frac{\varepsilon_2(\eta-1)}{1-\psi}\right)^{1/3}-\varepsilon_1\varepsilon_3\theta\left(1+\frac{\varepsilon_2(\eta-1)}{1-\psi}\right)^{2/3}=0 \qquad (7)$$

Fast temperature variations and slow concentration variations are comparable on the slow integral manifold, which is given in the zeroth order approximation by the equation (7). It turns out that there are three main dynamical regimes of the system, namely, slow regimes, conventional fast explosive regimes and delayed thermal explosion. In its turn, delayed thermal explosion may be subdivided into three different sub-types: regimes, when the concentration of the combustible gas decreases or increases, and the so called regime with freeze delay [4]. Peculiarities of these dynamical regimes are investigated and their dependence on physical system parameters is analyzed.

The delay phenomenon is described by the system dynamics on the slow curve. The delay time may be naturally defined as the period when the trajectory moves along the slow curve [4,6]. The so-called turning point on the slow curve is defined by the relations $\Omega(\theta,\eta)=\partial\Omega(\theta,\eta)/\partial\theta=0$. It gives us the θ coordinate of the turning point ($\theta=1$). This allows us to conclude that during the slow motion dimensionless temperature θ changes from approximately zero to unity. Hence the delay time can be estimated as:

$$\frac{\mathrm{Ln}(\eta_{\max})}{\mathrm{e}(\psi-1)}<\tau_{\mathrm{delay}}<\frac{\mathrm{Ln}(\eta_{\max})}{(\psi-1)}$$

where $\eta_{\max}$ is the value of the concentration of the gaseous fuel on the slow curve at the turning point. To find this value we should solve (numerically or analytically) the following equation

$$\mathrm{a}_0\mathrm{s}^3+\mathrm{a}_1\mathrm{s}^2+\mathrm{a}_2\mathrm{s}^1+\mathrm{a}_3\mathrm{s}^0=0$$

$$\eta=\frac{1}{\varepsilon_2}(\mathrm{s}^3-1)(1-\psi)+1 \qquad (8)$$

$$\mathrm{a}_0=\frac{\mathrm{e}}{\varepsilon_2}(1-\psi);\quad \mathrm{a}_1=-\varepsilon_1\varepsilon_3;\quad \mathrm{a}_2=-\varepsilon_1;\quad \mathrm{a}_3=\mathrm{e}\left(1-\frac{1-\psi}{\varepsilon_2}\right)$$

Preliminary analysis allows us to conclude that the parameter ε_3 is responsible for the contribution of the thermal radiation into system dynamics. The data presented in the Table 1 demostrated the impact of the thermal radiation on the delay time in the framework of the suggested model for some particular sets of parameters (initial temperature of the droplets is $\mathrm{T_{g0}}=490\mathrm{K}$, initial concentration $\mathrm{C_{f0}}=10^{-4}\,\mathrm{kmol/m^3}$, gas pressure $\mathrm{P}=100\mathrm{kPa}$). Data comparison (with and without radiant effects) allows us to conclude that the radiation effect on the delay time can be large enough (up to 15% of the total delay time under the presented system parameters) but its relative contribution decreases when a number of droplets per unit volume increases.

Table 1: Analytical upper and lower limits of the delay times for n-decane

Radius of droplets R_{d0}, (m)	Number of droplets n_d, $(1/m^3)$	Lower τ_{delay}, seconds		Upper τ_{delay}, seconds		Relative difference percents
		Without radiation	With radiation	Without radiation	With radiation	
10E-5	10E+4	No delay	No delay	No delay	No delay	
10E-5	5*10E+4	0.0272	0.0278	0.07404	0.07562	2.1
10E-5	10E+5	0.07398	0.07405	0.201	0.201	0.1
10E-5	10E+6	0.7676	0.7676	2.087	2.087	10E-5
10E-4	10E+3	No delay	No delay	No delay	No delay	
10E-4	5*10E+3	2.720	3.118	7.394	8.475	12.8
10E-4	10E+4	7.389	7.449	20.085	20.249	0.8
10E-4	10E+5	75.956	75.956	206.469	206.469	10E-4

The radiation effect on the delay time may be studied analytically further using appropriate approximation for the roots of the equation (8). Such approach can allow to investigate the impact of the thermal radiation on other important characteristics of delays such as values of independent variables (concentration, radius and temperature) just before ignition.

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References

[1] Kuo K.K., Principles of Combustion, 1986, John Wiley & Sons.

[2] Aggarwal S.K., A review of spray ignition phenomena: present status and future research, *Progress of Energy Combustion Science*, 1998, V.24, pp.565-600.

[3] Gol'dshtein V.M., Sobolev V.A., Singularity Theory and Some Problems of Functional Analysis, *AMS Translations*, 1992, Series 2, V. 153, pp.73-92.

[4] Goldfarb, I., Gol'dshtein, V., Kuzmenko, G. and Greenberg, B., 1997, Monodisperse Spray Effects on Thermal Explosion in a Gas, HTD-352, *Proceedings of ASME Heat Transfer Division*, Vol.2, pp.199-206, ASME International Congress and Exposition, Dallas (USA).

[5] McIntosh A. C., Gol'dshtein V., Goldfarb I. and Zinoviev A., Thermal explosion in a combustible gas containing fuel droplets. *Combustion Theory and Modelling*, 1998, V.2, pp.153-165.

[6] Goldfarb, I., Gol'dshtein, V., Kuzmenko, G. and Greenberg, B., On Thermal Explosion of a Cool Spray in a Hot Gas, Twenty-Sixth Symposium (International) on Combustion, 1998, The Combustion Institute, Pittsburgh, PA, to be published.

[7] Sazhin, S.S., Sazhina, E.M., Faltsi-Saravelou, O. and Wild, P.,1996, The P-1 model for thermal radiation transfer (advantages and limitations). *Fuel*, V.75, No.3, pp.289-294.

[8] Marshak, R.E. (1947) Note on the spherical harmonic method as applied to the Milne problem for a sphere, *Physical Review*, 1947, V.71, No.7, pp. 443--446.