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Mathematical Modelling of Polydisperse Fuel Spray Applied to Engineering Science

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Abstract: In this paper, we investigate the problem of thermal explosion in two-phases polydisperse combustible mixtures of gas with fuel droplets. The size distribution of the fuel droplets is assumed to be continuous. The system of the polydisperse fuel spray takes into account the effects of the thermal radiation and convection. We applied numerical simulation to the full model in order to find the time of the explosion of the droplets after evaporation process. We compared our numerical results to experimental data for different type of fuels and for different type of PDF function as: Rosin-Rammler, Nukiyama-Tanasawa, Log-Normal distribution and Normal distribution. Our results show that the relative error of the Rosin-Rammler PDF compared to the experimental is the smallest one in compared to the other PDF functions.

Keywords: nonlinear differential equations, thermal explosion, polydisperse fuel spray evaporation of droplets

Nomenclature:

A pre-exponential rate factor (s^{-1})
B universal gas constant ($Jkmol^{-1}K^{-1}$)
C molar concentration ($kmolm^{-3}$)
c specific heat capacity ($Jkg^{-1}K^{-1}$))
E activation energy ($Jkmol^{-1}$)
L liquid evaporation energy (i.e., latent heat of evaporation, Enthalpy of evaporation) (Jkg^{-1})
n number of droplets per unit volume (m^{-3})
$P(\cdot)$ probability density function (PDF), also defined as P_R, and for dimensionless form as $\tilde{P}_r$
Q combustion energy (Jkg^{-1})
q heat flux (Wm^{-2})
R radius of droplet (m)
r dimensionless radius
T temperature (K)
t time (s)
t_{react} characteristic reaction time (s) defined in Equation (14)

Greek symbols:

α dimensionless volumetric phase content
β dimensionless reduced initial temperature (with respect to the so-called activation temperature E/B)
γ dimensionless parameter that represents the reciprocal of the final dimensionless adiabatic temperature of the thermally insulated system after the explosion has been completed
ε_i i=1,...,3 dimensionless parameters defined in Equation (14)
η dimensionless fuel concentration
θ dimensionless temperature
λ thermal conductivity ($Wm^{-1}K^{-1}$)
μ molar mass ($kgkmol^{-1}$)
ρ density (kgm^{-3})
σ Stefan-Boltzmann constant ($W\,m^{-2}K^{-4}$)
τ dimensionless time
ψ represents the internal characteristics of the fuel (the ratio of the specific combustion energy and the latent heat of evaporation) defined in Equation (14) and for diesel fuel $\psi >> 1$
Υ dimensionless parameters defined in Equation (14)

Subscripts:

c convection
d liquid fuel droplets
f combustible gas component of the mixture
g gas mixture
l liquid phase

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p under constant pressure
r radiation
s saturation
0 initial state

1 Introduction

Most physical and engineering phenomena are modeled by non-linear differential equations. Such models are nonlinear and involve different time scales. In this paper we focused on the auto-ignition of polydisperse fuel spray. The research is motivated by a large number of industrial applications. For example, internal combustion and diesel engines, homogeneous chemical reactors, spontaneous insulation fires occurrence etc.

Thermo-chemical processes demonstrate a rich variety of complicated dynamical phenomena, which are not completely understood despite the relatively long history of combustion theory. Even in a relatively simple practical situation a large number of different chemical and thermo-physical processes are involved simultaneously. Therefore, attempts to give a detailed description of this processes lead to extremely complicated system of non-linear partial differential equations. Such models are almost useless for analytical extraction of main conceptual information about the dynamics of the processes, but the history of the thermal explosion theory shows that the main peculiarities of self-ignition in homogeneous case may be roughly described by simple Semenov's type model [1]. Semenov was the first who suggested a mathematical description of the thermal explosion phenomenon for highly exothermic chemical reaction. In his model the reactant consumption was neglected, which lead to the absence of energy conservation law, and the critical condition (i.e., thermal explosion limit) was described analytically as the loss of stability for the unique singular point of the single ODE. Stability means that the temperature is bounded at any time. The thermal explosion is an infinite increase of the temperature. In the Semenov's model, there are only two possible type of dynamical behavior : explosive and slow non-explosive regimes. Semenov's model become physically more realistic if the reactant concentration is taken into account. In this case the system is closed, which means that the mass and the energy conservation laws are valid.

In this paper we investigate the problem of thermal explosion in two-phases polydisperse combustible mixtures of gas with fuel droplets. The droplets are described by using PDF function which means that they assumed to be in continuous form. In addition, the model of the polydisperse fuel spray takes into account the effects of the thermal radiation and convection. We solve the full model by applying numerical simulation, Runge Kutta method using MATLAB software using PDE Solver package.

2 The PDF Function Describing the Size Distribution of Droplets, the Model of Polydisperse Fuel Spray that Take into Account the Convection and Radiation, Relative Error, Experimental Data

In this section we describe in details the model with taking into account the convection and radiation processes, the droplets size distribution, the relative error between different type of fuel and the experimental data: $n-decane$, $n-heptane$ and $Tetralin$.

2.1 The time evolution of PDF function

The time evolution of a two-phase medium consisting of the gas and evaporating droplets of fuel is examined. The volume concentration of droplets is assumed to be low. The size distribution of droplets is taken to be continuous and characterized by the normalized PDF P_R. The model takes into account both the density of convective heat flux and the density of integral flux of thermal radiation to the droplets surface. The entire heat flux that is delivered to the droplet surface is spent for evaporation i.e.,

$$q_c + q_r = L j_m \tag{1}$$

The density of convective heat flux to the droplet surface according to the "film model" is represented as [2]:

$$q_c = \frac{c_{pg} j_m (T_g - T_s)}{e^{\frac{2 j_m B c_{pg}}{Nu \lambda_g}} - 1}, \tag{2}$$

where Nu is the Nusselt number disregarding the effect of the evaporation process and is given by the known relation $Nu = 2 + 0.6\sqrt{Re}\sqrt[3]{Pr}$ and where Re and Pr are the Reynolds and Prandtl numbers. In the case when $2 j_m R c_{pg} / Nu \lambda_g << 1$, Equation (2) is reduced to:

$$q_c = \frac{Nu \lambda_g (T_g - T_s)}{2R}. \tag{3}$$

In our paper the thermal conductivity is taken to be in the form of:

$$\lambda_g = \lambda_{g0} \sqrt{\frac{T_g}{T_{g0}}}. \tag{4}$$

The flux density of the thermal radiation to the droplet surface in the limit of low concentration of droplets and for droplets of diesel fuel is given by:

$$q_r = \left(1 - e^{-2K_a R}\right) \sigma \left(T_g^4 - T_s^4\right). \tag{5}$$

In our analysis we assume that K_a is constant.
The evolution of the size distribution of droplets due to the evaporation process is described by the kinetic equation for the PDF [3],

$$\frac{\partial P_R}{\partial t} = \frac{\partial}{\partial R}\left(\frac{j_m}{\rho_l}P_R\right). \quad (6)$$

The approximation of this equation as suggested in [4] is:

$$\frac{\partial P_R}{\partial t} = \frac{\partial}{\partial R}\left(\frac{J_m}{\rho_l}P_R\right), \quad (7)$$

where:

$$J_m = \frac{\int_0^\infty R^2 j_m P_R dR}{\int_0^\infty R^2 P_R dR}. \quad (8)$$

Equation (7) coincides with Equation (6) in the case when the rate of evaporation does not depend on the droplet radius, as well as when the droplets are treated as a monodisperse system. However, the averaging of j_m is performed in such a manner that Equation (7) would yield the same balance equation for the mass of the liquid equation. The integro-differential equation (7) with (8) has a self-similar solution that satisfies the initial distribution $P_R(0,R) = P_{R0}(R)$,

$$P_R = P_{R0}(R+\delta),\ \delta = \int_0^t \frac{J_m}{\rho_l}dt, \quad (9)$$

and δ is found from the solution of the equation:

$$\frac{d\delta}{dt} = \frac{J_m}{\rho_l},\ \delta(0) = 0. \quad (10)$$

2.2 PDF function

In our analysis we compared between four different PDF functions as described below:
1: The Rosin-Rammler distribution [5] is:

$$f(2R) = \frac{a}{b}\left(\frac{2R}{b}\right)^{a-1} e^{-\left(\frac{2R}{b}\right)^a}, \quad (A.2)$$

where a, b are free parameters.
2: The Nukiyama-Tanasawa distribution [5] is:

$$f(2R) = \frac{a(2R)^5}{b^6\Gamma(\frac{6}{a})} e^{-\left(\frac{2R}{b}\right)^a}, \quad (A.3)$$

where Γ is the Gamma function: $\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}dx$.
3: The log-normal distribution [6] is:

$$f(2R) = \frac{1}{2Rln(\sigma)\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{ln(2R/D)}{ln(\sigma)}\right)^2}, \quad (A.4)$$

where $\sigma > 0$ represent the width of the distribution and D is the logarithmic mean size of the distribution.
4: The normal distribution [7] is:

$$f(2R) = \frac{1}{s_n\sqrt{2\pi}} e^{-\frac{1}{2s_n^2}(2R-\bar{D})^2}. \quad (A.5)$$

where s_n is a measure of the deviation of the value $2R$ from a mean value $\bar{D}$.

2.3 The model of polydisperse fuel spray

According to the above assumption the following non-dimensional Cauchy problem for the gas temperature, mass and concentration with the approximation of the Frank-Kamenetskii has the form of:

$$\gamma\frac{d\theta_g}{d\tau} = \eta e^{\theta_g} - \varepsilon_1\theta_g\int_0^\infty r\tilde{P}_{r0}(r+\Upsilon)dr - \varepsilon_1\varepsilon_3\theta_g\int_0^\infty r^2\tilde{P}_{r0}(r+\Upsilon)dr - \varepsilon_1\varepsilon_3\theta_g\int_0^\infty r^2 e^{-2K_a r}\tilde{P}_{r0}(r+\Upsilon)dr, \quad (11)$$

$$\frac{d\Upsilon}{d\tau} = \frac{\varepsilon_1\varepsilon_2\theta_g\int_0^\infty \tilde{P}_{r0}(r+\Upsilon)dr}{3\int_0^\infty r^2\tilde{P}_{r0}(r+\Upsilon)dr} + \frac{1}{3}\varepsilon_1\varepsilon_2\varepsilon_3\theta_g\left(1 - \frac{\int_0^\infty r^2 e^{-2K_a r}\tilde{P}_{r0}(r+\Upsilon)dr}{\int_0^\infty r^2\tilde{P}_{r0}(r+\Upsilon)dr}\right) \quad (12)$$

$$\frac{d\eta}{d\tau} = -\eta e^{\theta_g} + \Psi\varepsilon_1\theta_g\int_0^\infty r\tilde{P}_{r0}(r+\Upsilon)dr + \Psi\varepsilon_1\varepsilon_3\theta_g\int_0^\infty r^2\tilde{P}_{r0}(r+\Upsilon)dr - \Psi\varepsilon_1\varepsilon_3\theta_g\int_0^\infty r^2 e^{-2K_a r}\tilde{P}_{r0}(r+\Upsilon)dr, \quad (13)$$

where the non-dimension parameters are as follows

$$\beta = \frac{BT_{g0}}{E},\ \tau = \frac{t}{t_{react}},\ t_{react} = \frac{e^{1/\beta}}{A}, r = \frac{R}{R_0}, \tilde{P}_{r0} = \frac{R_0}{n_{d0}}P_{R0},$$
$$\gamma = \beta\frac{c_{pg}T_{g0}\rho_g}{C_{f0}Q_f\mu_f},\ \Psi = \frac{Q_f}{L}, R_0 = \frac{\int_0^\infty R^3 P_{R0}dR}{\int_0^\infty P_{R0}dR},\ \theta_g = \frac{1}{\beta}\frac{T_g - T_{g0}}{T_{g0}}$$
$$\eta = \frac{C_f}{C_{f0}},\ \varepsilon_1 = \frac{4\pi\lambda_{g0}R_0\beta T_{g0}n_{d0}}{AQ_f C_{f0}\alpha_g\mu_f}e^{\left(\frac{1}{\beta}\right)},\ \varepsilon_2 = \frac{Q_f\mu_f\alpha_g C_{f0}}{\frac{4\pi}{3}R_0^3 n_{d0}\rho_l L}$$
$$\varepsilon_3 = \frac{4\sigma T_{g0}^4 R_0}{\lambda_{g0}},\ \Upsilon = \frac{\delta}{R_0}. \quad (14)$$

We compared the following methods: the full model (11)-(13) that has been solved using numerical method Runge-Kutta for four different type of PDF function: The Log-Normal distribution, Rosin-Rammler PDF, Normal distribution and Nukiyama-Tanasawa PDF. The results are presented in Figures $1-3$. Figure 1 relates to the solution profile of the gas temperature vs. the dimensionless time, Figure 2 relates to the solution profile of the PDF vs. the dimensionless time and Figure 3 relates to the solution profile of the concentration vs. the dimensionless time. According to these figures the Rosin-Rammler PDF is closed to the experimental data.
Our aim in this paper is to find the time when the droplets are evaporated completely and after this process the thermal explosion occurs immediately. As we can see from Figures $1,3$ the time for explosion, $t_{explosion} \approx 0.03$

2.4 Relative error

Let us define the relative error in percent of the solution profiles of the gas temperature, PDF and concentration

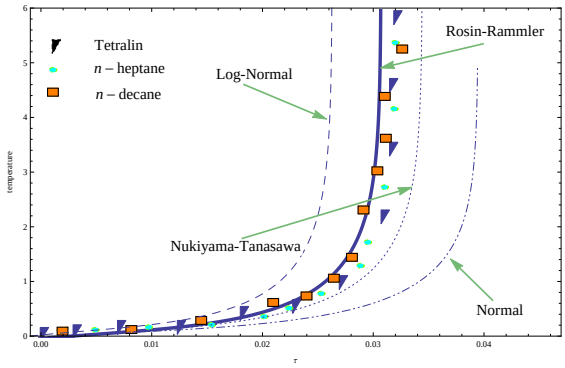

Fig. 1: Solution profiles of the temperature. The initial radius is $R_0 = 10^{-4}$ for $n-decane$, $R_0 = 10^{-3}$ for $n-heptane$, and $R_0 = 10^{-4}$ for $tetralin$

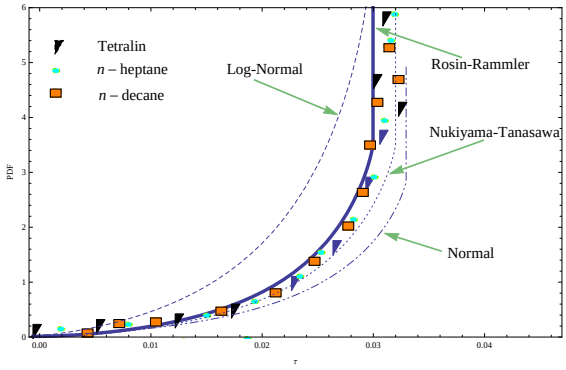

Fig. 2: Solution profiles of the distribution parameter $\Upsilon - \tau$. The initial radius is $R_0 = 10^{-4}$ for $n-decane$, $R_0 = 10^{-3}$ for $n-heptane$, and $R_0 = 10^{-4}$ for $tetralin$

from the experimental data as:

$$\Delta_1 = \frac{\left|\tau_{Rosin-Rammler} - \tau_{exp.}\right|}{\tau_{exp.}} \cdot 100\%$$
$$\Delta_2 = \frac{\left|\tau_{Log-Normal} - \tau_{exp.}\right|}{\tau_{exp.}} \cdot 100\% \qquad (15)$$
$$\Delta_3 = \frac{\left|\tau_{Normal} - \tau_{exp.}\right|}{\tau_{exp.}} \cdot 100\%$$
$$\Delta_4 = \frac{\left|\tau_{Nukiyama-Tanasawa} - \tau_{exp.}\right|}{\tau_{exp.}} \cdot 100\%$$

where the dimensionless time τ refers to the time until the thermal explosion occurs. The results are as follows: $\Delta_1 \approx 3.25\%$, $\Delta_2 \approx 9.76\%$, $\Delta_3 \approx 11.85\%$ and $\Delta_4 \approx 4.95\%$.

2.5 Experimental data

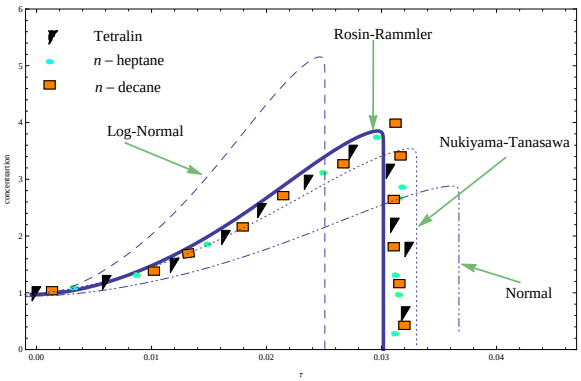

Fig. 3: Solution profiles of the concentration. The initial radius is $R_0 = 10^{-4}$ for $n-decane$, $R_0 = 10^{-3}$ for $n-heptane$, and $R_0 = 10^{-4}$ for $tetralin$

Table 1: Thermophysical experimental data applied to the model (11)-(13)

Property	n-decane	n-heptane	tetralin	units
c_{pg}	1050	1256	1256	$J\,kg^{-1}K^{-1}$
ρ_g	0.712	0.621	0.842	kg m^{-3}
L	3.21E+05	3.2E+05	3.17E+05	$J\,kg^{-1}$
T_{g0}	450	460	580	K
T_{d0}	450	460	580	K
μ_f	142	145	153	kg $kmol^{-1}$
Q_f	4.42E+07	4.54E+07	1.266E+07	J kg^{-1}
E	1.257E+08	1.257+08	2.8E+08	$J\,kg^{-1}$
λ	0.0193	0.0193	0.084	$Wm^{-1}K^{-1}$
A	0.95E+07	0.95E+07	1.15E+08	s^{-1}
α_g	0.25	0.28	0.37	dimensionless
C_{f0}	5E-4	7E-4	9E-4	$kmol\,m^{-3}$
ρ_l	730	750	725	$kg\ m^{-3}$

3 Conclusion

In this paper we solve numerically (Runge-Kutta method) the problem of thermal explosion in two-phases polydisperse combustible mixture of gas with fuel droplets. The size distribution of the fuel droplets is assumed to be continuous in four different experimental form. The Log-Normal distribution, the Normal distribution, Rosin-Ramler and Nukiyama-Tanasawa PDF.

We introduced the terms Δ_i $(i = 1,..,4)$ that express the relative error between the different PDF from the experimental data. According to our results the Rosin-Rammler has the smallest relative error from the experimental data for the solution profile of the temperature, the PDF and the concentration solution.

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Ophir Nave research area is focused on all aspects of combustion of polydisperse and monodisperse fuel spray. The models that describe the physical phenomena of these processes are systems of non-linear partial differential equations. In order to investigate these models, we applied a semi-analytical and asymptotic methods such as the homotopy analysis method (HAM), the method of integral invariant method (MIM), and singular perturbad homotopy analysis method (SPHAM).