Combustion of poly-dispersed Reactive Systems

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1 Abstract

The paper presents the results of theoretical investigations of combustion and detonation initiation in heterogeneous polydispersed mixtures. A mathematical model for ignition and turbulent combustion of polydispersed mixtures incorporating solid dust and liquid droplets in cylindrical vessel is developed. The equations of motions for particles consider the influence of random turbulence pulsations in gas flow. Thermal destruction of dust particles, vent of volatiles, chemical reactions in the gas phase, carbon skeleton heterogeneous oxidation by O_2 , CO_2 and chemical reaction with H_2O are the processes essential for describing dust and particulate phases. The problems of liquid droplets atomization, evaporation and combustion being the key factors for ignition delays and shock waves attenuation evaluation in heterogeneous mixtures and the non-equilibrium effects in droplets atomization and phase transitions were taken into account. The effects of droplets size non-uniformity and spatial distribution non-uniformity on mixture ignition and flame acceleration were investigated. Dispersed mixtures having been formed by different pulverizers could not be spatially uniform. However, in most experimental and theoretical investigations the ignition characteristics of uniformly distributed in space mixtures were studied. To achieve uniform droplet distribution and to avoid gravitational separation of the mixture having been formed investigations under microgravity conditions are performed [1]. The goal of the present research was, however, to investigate sensitivity of detonation onset to mixture parameters non-uniformity (spatial non-uniformity of dispersed phase, size distribution function, etc.).

2 Mathematical model for poly-dispersed mixture combustion

The mathematical models for simulating turbulent chemically reacting flows in heterogeneous mixtures were described in details in [2 - 4]. Combustion processes in heterogeneous mixtures differ greatly from that in homogeneous mixtures, because they are governed not only by chemistry but also by physical processes of combustible mixture formation, such as droplet atomization [3, 4], evaporation and diffusive mixing of fuel vapor with an oxidant.

The motion of polydispersed droplets (particles) is modeled making use of a stochastic approach. A group of representative model particles is distinguished each of them representing a number of real particles. Motion of these particles is simulated directly taking into account the influence of the mean stream of gas and pulsations of parameters in gas phase [2, 3], as well as evaporation and atimization. Thus a great amount of real particles (liquid droplets) was modeled by an ensemble of model particles. Each model particle was characterized by a vector of values, representing its location, velocity, mass,

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number of real particles represented by the given model one and other properties. The number of model particles was 25000 each representing up to hundred thousand real particles (depending on mass fraction of fuel). The number of cells was of the order of thousand. Thus the minimal average number of model particles per a grid node was provided guaranteeing sufficient accuracy of fluxes between phases evaluation. To perform recalculation of fluxes from model particles to that from the real ones the following procedure was used. All model particles were considered to have a definite spatial distribution around the model one. Different distributions were tried the results being compared for different grid size, initial and boundary conditions: uniform, Gaussian, triangular – the latter having been found an optimal one.

The momentum equation for a single droplet motion in the gas flow has the following form

$$m\frac{d\vec{u}}{dt} = m\vec{g} - \phi \cdot \nabla p + \vec{f}_d, \quad \frac{d\vec{r}}{dt} = \vec{u}, \qquad \qquad \vec{f}_d = \frac{C_d}{2} \rho_g \frac{\pi d^2}{4} (\vec{v} - \vec{u}) |\vec{v} - \vec{u}|, \qquad (1)$$

the drag coefficient being the function of Reynolds number

$$C_{d} = \left(\frac{24}{\text{Re}} + \frac{44}{\sqrt{\text{Re}}} + 0.42\right) \beta K, \text{Re} = \frac{\rho |\vec{v} - \vec{u}| d}{\mu}, \beta = \sqrt{\frac{\rho}{\rho_{s}} \left(2 - \frac{\rho}{\rho_{s}}\right)}, K = \left(\frac{T}{T_{s}}\right)^{45}, \frac{\rho_{s}}{\rho} = \begin{cases} \left(1 + \frac{\gamma - 1}{2}M^{2}\right)^{1/\gamma - 1}, & M < 1; \\ \frac{(\gamma + 1)M^{2}}{(\gamma - 1)M^{2} + 2} \left(1 + \frac{\gamma - 1}{2} \cdot \frac{(\gamma - 1)M^{2} + 2}{2\gamma M^{2} - (\gamma - 1)}\right)^{1/\gamma - 1}, & M > 1. \end{cases}$$

The energy equation for a droplet has the following form

$$m\frac{de}{dt} = q + Q_s$$
, where $e = c_{vs}T_s + h_f^0$. $Q_s = \frac{dm}{dt}h_L$ (3)

where h_L is the latent heat of evaporation, Q_s - the energy of phase transitions. Heat flux to a single droplet from the surrounding gas flow is determined as follows

$$q = \begin{cases} \pi d\lambda \cdot \operatorname{Nu} \cdot (T - T_s), & \operatorname{Re} < 1000; \\ \pi d^2 \rho |\vec{v} - \vec{u}| \cdot \operatorname{St} \cdot (H_r - H_w), & \operatorname{Re} \ge 1000. \end{cases} \quad \operatorname{Nu} = 2 + 0.16 \cdot \operatorname{Re}^{2/3} \cdot \operatorname{Pr}^{1/3}, \quad \operatorname{St} = \frac{C_d}{2} \operatorname{Pr}^{-2/3}, \quad (4)$$

The non-equilibrium evaporation model is used to determine the evaporation rate

$$\dot{m} = \pi d \cdot \rho D \cdot \operatorname{Nu} \cdot \log\left(\frac{1 - Y_e}{1 - Y_w}\right), \qquad \qquad Y_w = \frac{W_N P_0}{W p} \exp\left[\frac{H_b}{R}\left(\frac{1}{T_b(P_0)} - \frac{1}{T_s}\right)\right] - \dot{m} \frac{\sqrt{2\pi R T_s}}{\pi \delta_e p d^2}.$$
(5)

The dynamic interaction of liquid droplets with the gaseous flow could bring to instability of the interface and atomization of droplets. The criterion for liquid droplets instability is that of the critical Weber number [5]:, where σ is the surface tension at the interface, v_{rel} is relative velocity of a droplet versus gas. On exceeding the critical value of the Weber number droplets breakup due to vibrational instability takes place. On essentially surpassing the critical Weber number other mechanisms start playing essential roles in the breakup process that brings to formation of fine mist. These main characteristics of the atomization process could be taken into account by the following approximate formula [3] determining mean diameters of droplets d_a originating in breakups of initial droplets (diameter d):

$$d_{a} = \begin{cases} d = \left(\frac{6\alpha_{2}}{\pi n}\right)^{\frac{1}{3}}, & \mathbf{We} < \mathbf{We}_{*}; \\ \frac{d\mathbf{We}_{*}}{\mathbf{We}}, & \mathbf{We}_{*} \le \mathbf{We} \le \mathbf{We}_{**}; \\ d_{*}, & \mathbf{We} > \mathbf{We}_{*}; \end{cases} \qquad \mathbf{We} = \frac{\rho v_{rel}^{2} d}{\sigma} \quad \mathbf{We}_{*} = 12(1 + \mathbf{Lp}^{-0.8}), \quad (6)$$

where *n* is the number of droplets per volume unit, α_2 – volumetric fraction of the droplet phase, **We**_{*} - the critical Weber number, $Lp = \frac{d\rho_c \sigma}{\mu_c^2}$ - the Laplace number, ρ_c , μ_c - liquid density and

viscosity.

To determine the mean diameter of droplets d_* after the breakup of a type of an explosion $(\mathbf{We} > \mathbf{We}_{**})$ one needs to evaluate the part of the accumulated by a droplet elastic energy spent for the breakup. The assumption, that the breakup energy was spent for the formation of new free surface makes it possible to evaluate the number N and the mean diameter d_* of the formed droplets. The breakup energy is evaluated as the difference between the work of the drag forces separating small droplets from the initial one, and the kinetic energy of fragments' scattering.

Assuming that the initial droplet is split into N_* equal droplets ($N_* = \frac{d^3}{d_*^3}$) having equal velocities of

radial expansion of the cloud v_* and the separation of droplets takes place after the droplet is moved away at a distance $\sim d_*$, one obtains the formula for d_* versus Weber number and cloud expansion velocity. The mean velocity of the cloud expansion v_* could be evaluated based on the condition of matching the two formulas for d_a at $We = We_{**}$. The reason to perform that matching is that both formulas for breakup regimes were obtained from experiments, thus, indirectly the expansion of the cloud of droplets after the breakup should have been taken into account. On the other hand, the dependence of characteristic droplets diameters on the Weber number should be continuous. In modeling droplets breakup in a gas flow the inertia of the process should be taken into account. Fragmentation does not take place instantaneously: it needs time for small droplets to be established, elongated and broken [3]. Then, finally the first order estimates give the following formula:

$$d_* = \frac{d\mathbf{W}\mathbf{e}_*}{\frac{1}{8}C_d(\mathbf{W}\mathbf{e} - \mathbf{W}\mathbf{e}_{**})\mathbf{W}\mathbf{e}_* + \mathbf{W}\mathbf{e}_{**}}, \quad t_* = \frac{d}{v_{rel}}\frac{\mathbf{W}\mathbf{e}_*}{\mathbf{W}\mathbf{e}}\left(1 + \frac{3}{8}C_d\frac{\rho}{\rho_c}\left(1 - \frac{4}{C_d\mathbf{W}\mathbf{e}_*}\right)\right). \tag{7}$$

3 Results of numerical simulations

Numerical investigations of detonation initiation in dispersed hydrocarbon fuel - air mixtures after mild ignition via DDT and by shock waves of different intensities were performed. The vessel was 0.5 m long and 0.05m diameter. The aerosol occupied the cylindrical coaxial zone beginning from 0.1 m along the axis its diameter being equal to 0.015 m. The flow was assumed to have the following initial turbulence characteristics: energy k = 0.1 J/kg, the mixing length l = 0.01m, mean velocity u = 0, initial temperature 300 K. The number of model particles used in calculations was 20000. Validation of numerical scheme was performed based on comparing the obtained results of numerical simulations for the detonation wave velocities in dispersed mixtures with available experimental data [7]. To simulate hydrocarbons the following parameters were taken: $\rho = 850$ kg/m³; $\Delta H = 43$ MJ/kg; $h_L = 200$ kJ/kg; W = 140 kg/kmol. The share of water in hydrocarbon decomposition was assumed to be $\zeta = 0.2$. The mean droplets diameter was assumed 100 µm, minimal diameter -10 µm, maximal -200 µm. The droplets size distribution function was assumed to be a triangular one. The initial droplets density was varied from 5 to 20 kg/m³.

The results of simulations show that for different fuel concentration and intensity of shock wave initiation different scenarios of the process are possible. There could be formed a combustion wave lagging behind attenuating shock. There could be onset of detonation, or galloping detonation in the dispersed layer. For high average density of fuel droplets within the layer combustion does not take place inside layer, where pressure is maximal, however high speed detonation type process onset on

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the periphery is observed supported by the piston effect due to induced vapor combustion in the zones within the concentration limits.



Figure 1. Hydrocarbon concentration for successive times of shock wave propagation in dispersed mixture (top figures - initial fuel density 5 kg/m³; bottom - initial fuel density 20 kg/m³).



Figure 2. Temperature maps (K) for successive stages of shock wave propagation in dispersed mixture (top figures - initial fuel density 5 kg/m^3 ; bottom - initial fuel density 20 kg/m^3).

Thus the results illustrate the fact, that increase of droplet concentration above definite value inhibits the onset of detonation in dispersed mixtures and gives birth to a detonation mode typical for non-premixed systems.

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