Poly-dispersed Droplets in Streaming Flows: Atomization, Evaporation, Combustion

Nikolay N. Smirnov[1,2](✉)

[1] Faculty of Mechanics and Mathematics Moscow M.V, Lomonosov State University,
Leninskie Gory 1, Moscow 119992, Russia
`ebifsun1@mech.math.msu.su`, `ebifsun1mech.math.msu@inbox.ru`
[2] Federal Science Center "Scientific Research Institute for System Analysis of Russian
Academy of Sciences, Nakhimovskiy pr. 36-1, Moscow 117218, Russia

Abstract. The paper presents the survey of results of theoretical, numerical and experimental investigations of combustion and detonation initiation in heterogeneous polydispersed mixtures. The problems of fuel droplets atomization, evaporation and combustion and the non-equilibrium effects in droplets atomization and phase transitions are discussed. The effects of droplets size non-uniformity and spatial distribution non-uniformity on mixture ignition and flame acceleration were investigated for strong and mild initiation of detonation: by a shock wave and spark ignition followed by deflagration to detonation transition (DDT). Peculiarities of jet injection and ignition in reaction chamber are studied.

Keywords: Combustion · Aerosol · Poly-dispersed · Non-equilibrium effects · Non-uniformity

1 Mathematical Model

The mathematical models for simulating turbulent chemically reacting flows in heterogeneous mixtures were described in details in [1, 2]. 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 model applies both deterministic methods of continuous mechanics of multiphase flows to determine the mean values of parameters of the gaseous phase and stochastic methods to describe the evolution of poly-dispersed particles in it and fluctuations of parameters. Thus the influence of chaotic pulsations on the rate of energy release and mean values of flow parameters can be estimated. The transport of kinetic energy of turbulent pulsations at the same time obeys the deterministic laws being the macroscopic characteristic.

Averaging by Favre with the $\alpha\rho$ weight (α – volumetric fraction of the gas phase, ρ – gas density) we obtain the following system for the gas phase in a multiphase flow [5]

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(the averaging bars are removed for simplicity):

$$\partial_t(\alpha\rho) + \nabla \cdot (\alpha\rho\vec{u}) = \dot{M}, \tag{1}$$

$$\partial_t(\alpha\rho Y_k) + \nabla \cdot (\alpha\rho Y_k\vec{u}) = -\nabla \cdot \vec{\mathrm{I}}_{\mathrm{k}} + \dot{M}_k + \dot{\omega}_k, \tag{2}$$

$$\partial_t(\alpha\rho\vec{u}) + \nabla \cdot (\alpha\rho\vec{u} \otimes \vec{u}) = \alpha\rho\vec{g} - \alpha\nabla p + \nabla \cdot \tau + \dot{\vec{K}}, \tag{3}$$

$$\partial_t(\alpha\rho E) + \nabla \cdot (\alpha\rho E\vec{u}) = \alpha\rho\vec{u} \cdot \vec{g} - \nabla \cdot p\vec{u} - \nabla \cdot \vec{I}_q + \nabla \cdot (\tau \cdot \vec{u}) + \dot{E}. \tag{4}$$

The Eqs. (1)–(4) include mass balance in the gas phase, mass balance of k-th component, momentum balance and energy balance respectively (p – pressure, $\vec{u}$ – fluid velocity vector, $\vec{g}$ – gravity acceleration vector, E – specific energy, $\dot{\vec{K}}$ – specific momentum flux to gas phase, $\dot{M}$ – specific mass flux, $\dot{E}$ – specific energy flux, τ – turbulent stress tensor), $\vec{\mathrm{I}}_k$ is the turbulent diffusion flux of the k-th component. We have the following relationships between the terms in the Eqs. (1) and (2):

$$\sum_k Y_k = 1, \sum_k \dot{M}_k = \dot{M}, \sum_k \vec{\mathrm{I}}_k = 0, \sum_k \dot{\omega}_k = 0.$$

The state equations for gaseous mixture are the following:
$p = R_g\rho T \sum\limits_k Y_k/W_k,$

$$E = \sum_k Y_k(c_{vk}T + h_{0k}) + \frac{\vec{u}^2}{2} + k, \tag{5}$$

where E – gas energy, k – turbulent kinetic energy, W_k - molar mass of k-th gas component, h_{0k} – specific chemical energy, c_{pk},c_{vk} – specific heat capacity, Y_k - mass concentration of k-th gas component, T – gas temperature, R_g - universal gas constant. The term responsible for chemical transformations, $\dot{\omega}_k$ is very sensitive to temperature variations, as it is usually the Arrhenius law type function for the reactions' rates. To take into account temperature variations the source term $\dot{\omega}_k$ in the Eq. (2) was modeled using the Gaussian quadrature technique.

Let us regard the temperature being a stochastic function T with mean $\overline{T}$ and mean squared deviate $\theta = \overline{T'T'}$. Then, the mean value of a function having T as independent variable could be determined as follows:

$$\overline{f(T)} = \int f(\overline{T} + \zeta\sqrt{\theta})P_d(\zeta)d\zeta,$$

where ζ is a random value with zero expectation and unit deviate; its probability density function is $P_d(\zeta)$. To estimate the integral, the minimal number of terms is used(namely, three) and $P_d(\zeta)$ is assumed to be even. In this case, the formula for *f(T)* averaging is:

$$\overline{f(T)} = \frac{1}{2\chi^2}f(\overline{T} - \chi\sqrt{\theta}) + \left(1 - \frac{1}{\chi^2}\right)f(\overline{T}) + \frac{1}{2\chi^2}f(\overline{T} + \chi\sqrt{\theta}).$$

In case of normal (Gaussian) deviate, the value of χ is equal to $\sqrt{3}$ (Gauss-Hermite case). Therefore, the formula above could be transformed as follows:

$$\overline{f(T)} = \frac{1}{6}f(\overline{T} - \sqrt{3\theta}) + \frac{2}{3}f(\overline{T}) + \frac{1}{6}f(\overline{T} + \sqrt{3\theta}).$$

In our case, the function *f(T)* is the Arrhenius temperature dependence; the whole average for $\dot{\omega}_k$ is constructed using combinations of these dependencies. Averaged magnitudes for mass fractions and density were used in the Arrhenius law for $\dot{\omega}_k$ as the dependence of these functions is not as strong as the dependence of temperature.

The turbulent heat flux $\vec{\mathrm{I}}_q$ in the Eq. (4) is a sum of two terms:

$$\vec{I}_q = \vec{J}_q + \sum_k (c_{pk}T + h_{0k})\vec{I}_k, \tag{6}$$

where $\vec{\mathrm{J}}_q$ could be interpreted as turbulent conductive heat flux. The eddy kinematic viscosity ν^t is expressed according to k-epsilon model as $\nu^t = C_\mu \frac{k^2}{\varepsilon}$. The turbulent fluxes are:

$$\tau = \alpha(\mu + \rho\nu^t)(\nabla\vec{u} + \nabla\vec{u}^T - (2/3)(\nabla\cdot\vec{u})U) - (2/3)\alpha\rho k U, \tag{7}$$

$$\vec{I}_k = -\alpha\rho(D + (\nu^t/\sigma_d))\nabla Y_k, \tag{8}$$

$$\vec{J}_q = -\alpha(\lambda + \sum_k c_{pk}\rho(\nu^t/\sigma_t))\nabla T. \tag{9}$$

The model is closed then by the equations for *k*, θ and ε*:*

$$\partial_t(\alpha\rho k) + \nabla\cdot(\alpha\rho\vec{u}k) = \nabla\cdot(\alpha(\mu + \rho(\nu^t/\sigma_k))\nabla k) + \tau^t{:}\nabla\vec{u} - \alpha\rho\varepsilon, \tag{10}$$

$$\begin{aligned}&\partial_t(\alpha\rho\varepsilon) + \nabla\cdot(\alpha\rho\vec{u}\varepsilon) = \\ &\nabla\cdot(\alpha(\mu + \rho(\nu^t/\sigma_\varepsilon))\nabla\varepsilon) + (\varepsilon/k)(C_{1\varepsilon}\tau^t{:}\nabla\vec{u} - C_{2\varepsilon}\alpha\rho\varepsilon),\end{aligned} \tag{11}$$

$$\partial_\mathrm{t}(\alpha\rho\theta) + \nabla\cdot(\alpha\rho\vec{\mathrm{u}}\theta) = \nabla\cdot(\alpha(\mathrm{\mu} + \sum_k c_{pk}\rho(\nu^\mathrm{t}/\sigma_\mathrm{k}))\nabla\theta) + \mathrm{P}_\theta + \mathrm{W}_\theta - \mathrm{D}_\theta, \tag{12}$$

where the production terms P_θ,W_θ and the dissipation term D_θ are:
$\mathrm{P}_\theta = 2\alpha\rho\tilde{c}_p\frac{\nu_t}{\sigma_k}|\nabla T|^2$, $\mathrm{W}_\theta = -\sum_k \overline{\omega_k T'}h_{0k}$,

$$\mathrm{D}_\theta = \mathrm{C_g}\alpha\rho\sum_k c_{pk}\frac{\varepsilon}{\mathrm{k}}\frac{\theta}{\theta_m - \theta}. \tag{13}$$

The constants take the following values [5]:

$$C_\mu = 0.09, C_{1\varepsilon} = 1.45, C_{2\varepsilon} = 1.92, \sigma_d = 1, \sigma_t = 0.9,$$

$$\sigma_k = 1, \sigma_\varepsilon = 1.13,\ \theta_m = \overline{T}^2/4, \mathrm{C_g} = 2.8.$$

One could see that the Eqs. (10)–(12) do not contain terms responsible for particulate phase contribution to turbulence energy growth. This is due to the direct stochastic modeling of the particulate phase: the influence of the last on the gas phase leads to stochastic behavior of the momentum source terms $\dot{\vec{K}}$. These terms affect the averaged gas phase velocity in the stochastic manner and therefore the source term $\tau^t{:}\nabla\vec{u}$ is also affected. The motion of polydispersed droplets (particles) is modeled making use of a stochastic approach. A group of representative model particles is distinguished. 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. The procedure is described in details in papers [1, 2, 5].

The non-equilibrium effects in gas – droplet interaction for evaporating droplets and for burning droplets were taken into account based on a single fuel droplet interaction with heated streaming flow of oxidant [6–8]. The effectiveness of numerical scheme was linear: computation time was directly proportional to the increase of cells in a gas phase and number of model droplets.

2 Results of Numerical Investigations

Using a single droplet dynamics model, we simulated the interaction of a strong shock wave in the air with an aerosol consisting of fuel droplets. Aerosol droplets are small in size and spherical in shape. The initial state of the aerosol is poly-disperse, that is, it is possible to consider the simultaneous existence of droplets of different initial diameters [4, 5].

When considering the interaction of a shock wave with an aerosol, the following hierarchy of models is considered sequentially:

1. taking into account only the resistance force,
2. taking into account the resistance force and heat exchange,
3. accounting for resistance, heat transfer and evaporation,
4. taking into account the resistance force, heat transfer, evaporation and atomization of droplets,
5. accounting for resistance, heat transfer, evaporation, droplet atomization and combustion.

Numerical simulation of two-dimensional flow in a cylindrical tube was performed. The pipe consists of two parts. Pressure and temperature on the left side $x \le b$ are elevated ($P_1 = 10 \div 100$ bar, $T_1 = 1500$ K,) as compared with conditions in the right hand side ($P_0 = 1$ bar, $T_0 = 300$ K). Left hand side is filled with air, while the right hand side for $b < x < x_0$ is also filled with air, and for $x \ge x_0$ aerosol is added (Fig. 1). The tube length $L = 2$ m, diameter $D = 8$ cm. Aerosol density 0.8 kg/m^3, which corresponds to a volume concentration 10^{-3}.

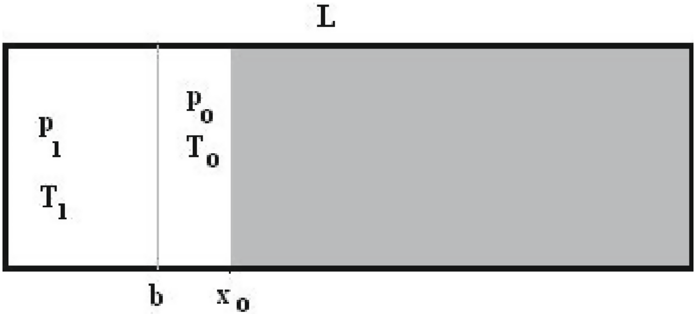

Fig. 1. A schematic representation of the problem statement.

In Figs. 2, 3, 4, 5 and 6 the diagrams for the shock wave velocity along the tube axis are presented for different values of initial pressure ratios P_1/P_0. Different curves numbered from 1 to 5 correspond to different models of gas – droplet interaction described above.

Figure 2 presents results for initial pressure ratio $P_1/P_0 = 10$. It can be seen that when the shock wave enters the area filled with aerosol, the wave speed decreases. The most intensive speed reduction occurs when only resistance and heat transfer are taken into account (curve 2), the least intensive wave speed reduction – when only resistance is taken into account (curve 1). Other, more complex models correspond to intermediate results. Accounting for evaporation brings to lower reduction of shock wave velocity as compared with accounting for only thermal and mechanical losses. The reason is the following: evaporation brings to formation of additional gas volume behind the shock wave, which supports its propagation (curve 3).

With an increase in the initial intensity of the shock wave ($P_1/P_0 = 25$, Fig. 3), the greatest decrease in its intensity also occurs when taking into account resistance and heat exchange (curve 2), but the smallest – when taking into account resistance, heat exchange and evaporation (curve 3). This is due to the fact that the intensity of evaporation of drops increases the volume of gas. Accounting for droplets atomization brings to a more rapid decrease of shock wave velocity as compared to accounting for thermos-mechanical interaction and evaporation (curve 4). The explanation of this fact is the following: atomization of droplets brings to formation of new free surface, which increases momentum and energy exchange between gas and condensed phase; small droplets decelerate and warm up much faster, thus, increasing the momentum and energy losses in the gas flow, which brings to shock wave slowing down. When combustion is taken into account (curve 5), near the right end of the pipe, the wave velocity increases to 1500–1700 m/s, which corresponds to the ignition of the gas mixture and the transition of combustion to the detonation mode.

In Fig. 4, the results correspond to the intensity of the shock wave $P_1/P_0 = 50$. The general character of the shock wave intensity decrease in the aerosol-filled area remains similar to the previous results, but when taking combustion into account (curve 5), the transition to detonation occurs at a distance of 1.2–1.5 m from the beginning of the pipe; after that, the wave intensity decreases slightly. This behavior can be interpreted as the transition of deflagration to detonation via an overdriven regime with successive slowing down to a self-sustained stationary velocity.

Figure 5 corresponds to initial pressure ratio $P_1/P_0 = 75$, and Fig. 6 corresponds to initial pressure ratio $P_1/P_0 = 100$. From these figures, we can see the nature of the decrease in the intensity of the initial shock wave for interaction models of various complexity. When combustion is taken into account (curve 5), the acceleration of combustion and the transition to detonation occurs at 1.2–1.3 m ($P_1/P_0 = 75$) – at 0.7–1.1 m ($P_1/P_0 = 100$). Figure 6 shows that the detonation propagates in an overdriven mode (strong detonation) at 1.2–1.3 m, and then slows down to the stationary mode (Chapman-Jouget detonation) Fig. 7 shows examples for droplets fragmentation scenarios on interaction with shock waves moving from left to right.

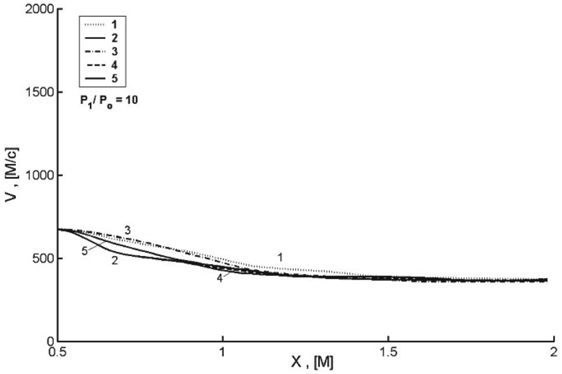

Fig. 2. Evolution of shock wave velocity along the tube axis on entering dispersed mixture for different models of gas – droplet interactions. $P_1/P_0 = 10$.

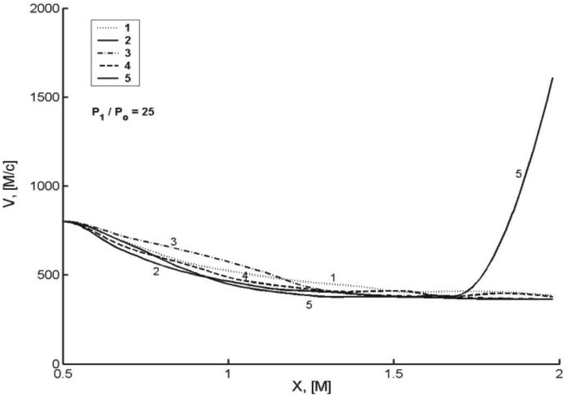

Fig. 3. Evolution of shock wave velocity along the tube axis on entering dispersed mixture for different models of gas – droplet interactions. $P_1/P_0 = 25$.

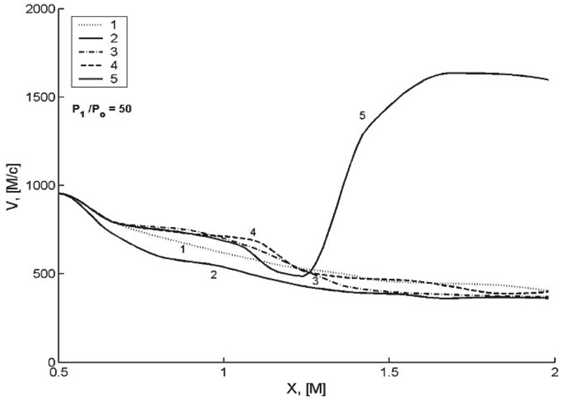

Fig. 4. Evolution of shock wave velocity along the tube axis on entering dispersed mixture for different models of gas – droplet interactions. $P_1/P_0 = 50$.

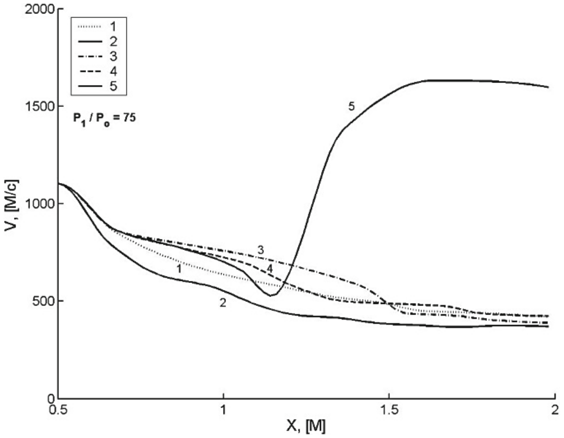

Fig. 5. Evolution of shock wave velocity along the tube axis on entering dispersed mixture for different models of gas – droplet interactions. $P_1/P_0 = 75$.

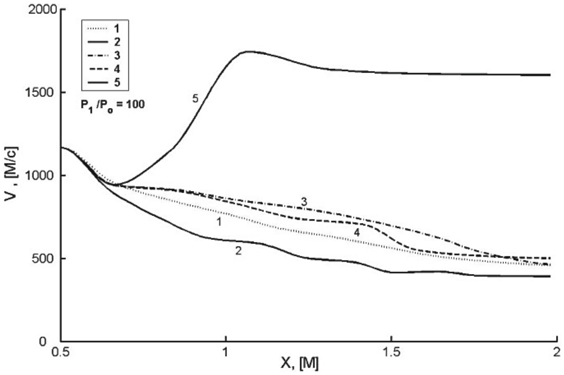

Fig. 6. Evolution of shock wave velocity along the tube axis on entering dispersed mixture for different models of gas – droplet interactions. $P_1/P_0 = 100$.

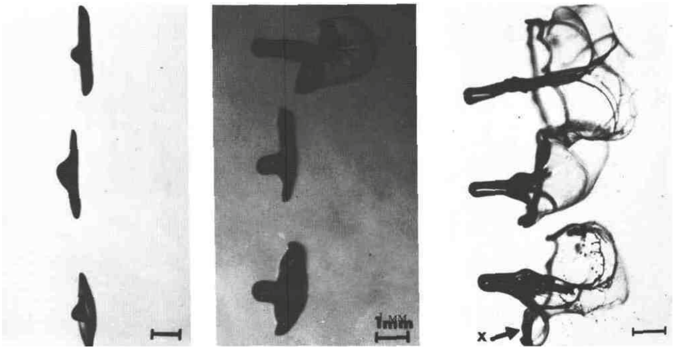

Fig. 7. An example of shock wave-droplet interaction.

3 Conclusions

Investigating different models for gas – droplet interaction made it possible evaluating the role of different effects on shock wave behavior: mechanical losses, thermal losses, evaporation, of droplets, atomization, ignition and burning of fuel vapor.

It was demonstrated that when the shock wave enters the area filled with aerosol, the wave speed decreases. The most intensive speed reduction occurs when only resistance and heat transfer are taken into account, the least intensive wave speed reduction – when only resistance is taken into account.

Accounting for evaporation brings to lower reduction of shock wave velocity as compared with accounting for only thermal and mechanical losses. The reason is the following: evaporation brings to formation of additional gas volume behind the shock wave, which supports its propagation.

Accounting for droplets atomization brings to a more rapid decrease of shock wave velocity as compared to accounting for thermos-mechanical interaction and evaporation. The explanation of this fact is the following: atomization of droplets brings to formation of new free surface, which increases momentum and energy exchange between gas and condensed phase; small droplets decelerate and warm up much faster, thus, increasing the momentum and energy losses in the gas flow, which brings to shock wave slowing down.

When combustion is taken into account, after some period of deceleration in the aerosol, the shock wave velocity increases to 1500–1700 m/s, which corresponds to the ignition of the gas mixture and the transition of deflagration to the detonation mode.

The transition of deflagration to detonation takes place via an overdriven regime (strong detonation mode characterized by an elevated velocity and pressure) with successive slowing down to a self-sustained stationary velocity of the Chapman-Jouget mode.

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