

Shock Wave Ignition of Multi-phase Fuel-oxidant Mixtures Numerical Simulations

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1 Introduction

The paper presents the results of developing of physical and mathematical model making it possible to take into account the effect of droplets density on ignition conditions for aerosols. The problems of particulate phase dynamics are regarded accounting for the interaction with gas phase atomization, evaporation and combustion.

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]. Investigations of acute problems of heat and mass exchange accompanied by phase transitions need adequate modeling of evaporation, which is extremely important for small droplets and sprays [2]. Combustion of hydrocarbon fuels takes place mostly in a gas-phase regime. Thus, evaporation of fuel from the surface of droplets turns to be one of the limiting factors of the process.

2 Mathematical Model

The mathematical models for simulating turbulent chemically reacting flows in heterogeneous mixtures were described in details in [3, 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 [5], 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 polydispersed 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.

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 [3, 4].

The effect of the gas mean stream and pulsations of parameters in the gas phase on the motion of droplets is considered. Gas flow properties (the mean kinetic energy and the rate of pulsations decay) make it possible to model the droplets stochastic motion determining the pulsations change frequency under assumptions of the Poisson flow of events.

We model a great amount of real droplets by assembling model droplets (their number is of the order of thousands). Each model droplet is characterized by a vector of values, representing its location, velocity, mass and other properties. The following vector is determined for each model droplet:

$$\{N, m, \vec{r}, \vec{v}, \vec{w}, \phi, T_s, \psi, R\}_i, \quad i = 1, \dots, N_p.$$

where N – number of real droplets represented by a model one, m – mass of a real droplet, \vec{r} – droplet coordinate, \vec{v} – droplet velocity, \vec{w} – stochastic component of surrounding gas velocity, ϕ – droplet volume, T_s – droplet temperature, ψ – index characterizing droplet life, which is equal to 1 until the model droplet is taken into account in simulations, and which is equal to 0 on droplet total evaporating, R_i – radius of a spherical neighborhood of a model droplet, wherein all real droplets are distributed represented by the model one. When a droplet is burnt out, its mass $m_i = 0$, and this droplet is excluded from calculations. The parameter \vec{w}_i is used to model dispersed phase turbulent pulsations. It represents the pulsation velocity vector added to the gas velocity vector \vec{u} , thus a stochastic force resulting from the interaction with turbulized gas is calculated jointly with a resistance force.

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

$$m \frac{d\vec{v}}{dt} = m\vec{g} - \phi \cdot \nabla p + \vec{f}_r, \quad \frac{d\vec{r}}{dt} = \vec{v}, \quad (1)$$

where the drag force could be expressed as follows:

$$\vec{f}_r = \frac{1}{2} C_f(\text{Re}) \rho S (\vec{v} + \vec{w} - \vec{u}) |\vec{v} + \vec{w} - \vec{u}|, \quad (2)$$

the drag coefficient being the function of Reynolds number [5]

$$C_f = \left(\frac{24}{\text{Re}} + \frac{4,4}{\sqrt{\text{Re}}} + 0,42 \right) \beta \cdot k, \quad \text{Re} = \frac{\rho |\vec{v} + \vec{w} - \vec{u}| d}{\mu}, \quad \beta = \sqrt{\frac{\rho}{\rho_s} \left(2 - \frac{\rho}{\rho_s} \right)}, \quad k = \left(\frac{T}{T_s} \right)^{4/5} \quad (3)$$

$$\frac{\rho_s}{\rho} = \begin{cases} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{1/(\gamma-1)}, & M < 1; \\ \frac{(\gamma+1)M^2}{(\gamma-1)M^2+2} \left(1 + \frac{\gamma-1}{2} \cdot \frac{(\gamma-1)M^2+2}{2\gamma M^2 - (\gamma-1)} \right)^{1/(\gamma-1)}, & M \geq 1. \end{cases} \quad M = \frac{|\vec{v} + \vec{w} - \vec{u}|}{c}, \quad c = \sqrt{\gamma p / \rho} \quad (4)$$

Formulas (2-4) illustrate drag force in streaming flows of rarefied mixtures, when condensed phase volume fraction is small ($\alpha_s \ll 1$). Accounting for the effect of neighboring droplets on interaction of each droplet with a streaming flow provide different formulas.

For high density & low Reynolds limit the formula for drag force takes the form:

$$\vec{f}_r = -\frac{\alpha \mu \vec{v}_{rel}}{K}, \quad K = \frac{\alpha^3 d^2}{180(1-\alpha)^2}, \quad C_f(\text{Re}, \alpha) = \frac{10(1-\alpha)}{\alpha^2} \cdot \frac{24}{\text{Re}} \quad (5)$$

For the case of low density & low Reynolds limit the formulas (2, 3) take the form

$$\tilde{f}_r = 3\pi d \mu \tilde{\nu}_{rel} \left(1 + 3\sqrt{\frac{1-\alpha}{2}}\right), \quad C_f(\text{Re}, \alpha) = \left(1 + 3\sqrt{\frac{1-\alpha}{2}}\right) \cdot \frac{24}{\text{Re}} \quad (6)$$

And interpolation formula, which would be used in our simulations, has the following form

$$C_f(\text{Re}, \alpha) = \frac{24}{\text{Re}} \left(\left(1 + \sqrt{\frac{1-\alpha}{2}}\right) \cdot e^{-8.72(1-\alpha)} + \frac{10(1-\alpha)}{\alpha^2} \right) \cdot (1 + 0.183\sqrt{\text{Re}} + 0.0172 \text{Re}) \quad (7)$$

The energy equation for a droplet has the following form

$$m \frac{de}{dt} = q + Q_s, \text{ where } e = c_{vs} T_s + h_f^0. \quad (8)$$

The energy of phase transitions could be determined by the formula:

$$Q_s = \frac{dm}{dt} h_L, \quad (9)$$

where h_L is the latent heat of evaporation. Heat flux to a single droplet from the surrounding gas flow is determined as follows [5]

$$q = \begin{cases} \pi d \lambda \cdot \text{Nu} \cdot (T - T_s), & \text{Re} < 1000; \\ \pi d^2 \rho |\vec{v} - \vec{u}| \cdot \text{St} \cdot (H_r - H_w), & \text{Re} \geq 1000. \end{cases} \quad \text{Nu} = 2 + 0.16 \cdot \text{Re}^{2/3} \cdot \text{Pr}^{1/3} \quad \text{St} = \frac{C_f}{2} \text{Pr}^{-2/3} \quad (10)$$

For dense particulate phase Nusselt number in (11) should be multiplied by a special coefficient accounting for the presence of surrounding particles.

$$\text{Nu}^* = \frac{\text{Nu}}{1 - (\alpha_s)^{1/3}} \quad (11)$$

As it follows from equations (10), (11), the heat flux going inside droplet and heating it q_f is determined as a difference between heat flux coming to a droplet from surrounding gas, and energy consumed for surface evaporation:

$$q_s = q - \dot{m} h_L; \quad \dot{m} = -\frac{dm}{dt} - \text{evaporation rate.}$$

This heat flux is responsible for droplet gradual mean temperature increase as determined by the equation (9). While the effect of heat conductivity coefficient in fluid could manifest only on calculating temperature profile inside droplet.

The non-equilibrium evaporation model is used to determine the evaporation rate [6]

$$\dot{m} = \pi d \cdot \rho D \cdot \text{Nu} \cdot \log \left(\frac{1 - Y_e}{1 - Y_w} \right), \quad Y_w = \frac{W_N P_0}{W_p} \exp \left[\frac{H_b}{R} \left(\frac{1}{T_b(P_0)} - \frac{1}{T_s} \right) \right] - \dot{m} \frac{\sqrt{2\pi R T_s}}{\pi \delta_e p d^2} \quad (12)$$

On approaching by the droplet surface temperature the value of boiling temperature T_b integration of system of equations becomes time consuming due to enormous increase of time steps necessary to resolve the system. Then surface temperature could be assigned the boiling value and a simplified formula could be used to determine evaporation rate on the last stages of droplet life:

$$\frac{dm}{dt} = \frac{q_s - q}{h_L}, \quad q_s = \dot{m} c_s (T_b - T_s), \text{ which yields } \frac{dm}{dt} \left(1 + \frac{c_s (T_b - T_s)}{h_L} \right) = -\frac{q}{h_L} \quad (13)$$

Joint integration of (13) and (9) shows that internal temperature on decreasing droplet size tends to surface one exponentially: $\frac{T_b - T_s}{T_b - T_{s0}} \sim e^{-t/t_0}$. Thus on the last stages of droplet life the mean temperature could be assigned the boiling value.

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]: $We = \frac{\rho v_{rel}^2 d}{\sigma}$, 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.

3 An example 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 $l = 0.01$ m, 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 [4]. 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 droplet diameter was assumed 100 μ m, minimal diameter – 10 μ m, maximal – 200 μ m. The droplet size distribution function was assumed to be a triangular one, aerosol density 1 kg/m³.

Initial discontinuity gives birth to a shock wave generated in the system, which on entering dispersed mixture cloud could ignite it and bring to the onset of either deflagration, or detonation, or some intermediate galloping mode.

Fig.1 shows pressure fields in the vessel for successive times. Fig.2 illustrates droplet temperature fields in K. Fig. 3 illustrates cross-section averaged temperature profiles for gaseous phase (green curves), and for droplet phase (red curves). The results show that under the conditions regarded shock wave does not initiate combustion process just behind its front. Rather slow evaporation takes place, then after a definite induction time heat release begins non-uniformly: at the front edge of the cloud, and somewhere inside behind the shock wave. Active mixture combustion could be initiated by a reflected wave.

After shock wave falling on dilute aerosol cloud ignition delays caused by chemical and physical inductions (chemical delay and delay of mixture formation due to atomization and evaporation of droplets) bring to formation of two exothermic centers: one at the front edge of cloud, and the other inside the cloud behind the attenuating shock wave. The reason for such a scenario is the following. Ignition delay decreases with an increase of temperature of the surrounding gas as well as with an increase of droplet exposition time in the high temperature region. As one could see from figure 3, temperature peak is very narrow on shock wave entering aerosol cloud, then due to gas interaction with cloud the temperature peak becomes wider, while its maximal value slightly decreases. Thus droplets located inside the cloud have more favorable conditions for ignition due to smaller induction time, because those droplets are exposed to elevated temperature for the longest period. On the other hand, droplets being at front edge of the cloud are exposed to a higher temperature, but for a shorter time, and then the ambient gas temperature decreases, which increases induction time. However, this makes ignition in the front zone also probable.

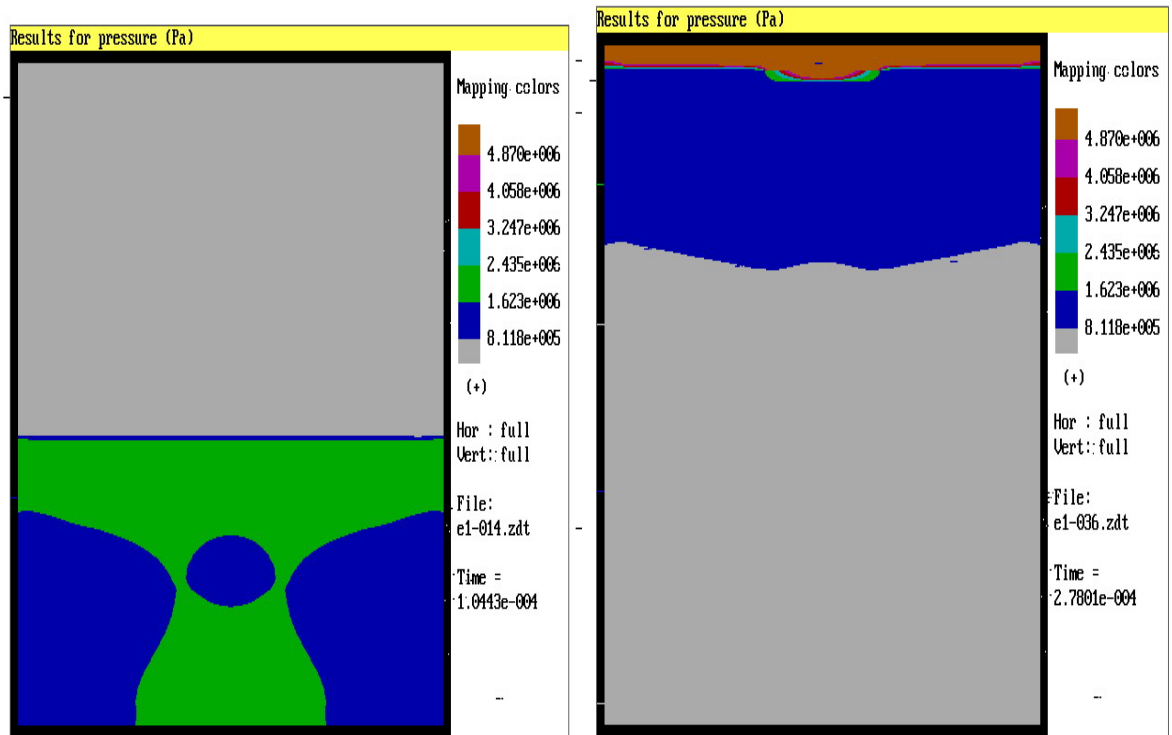


Fig.1. Pressure field in gas for successive times.

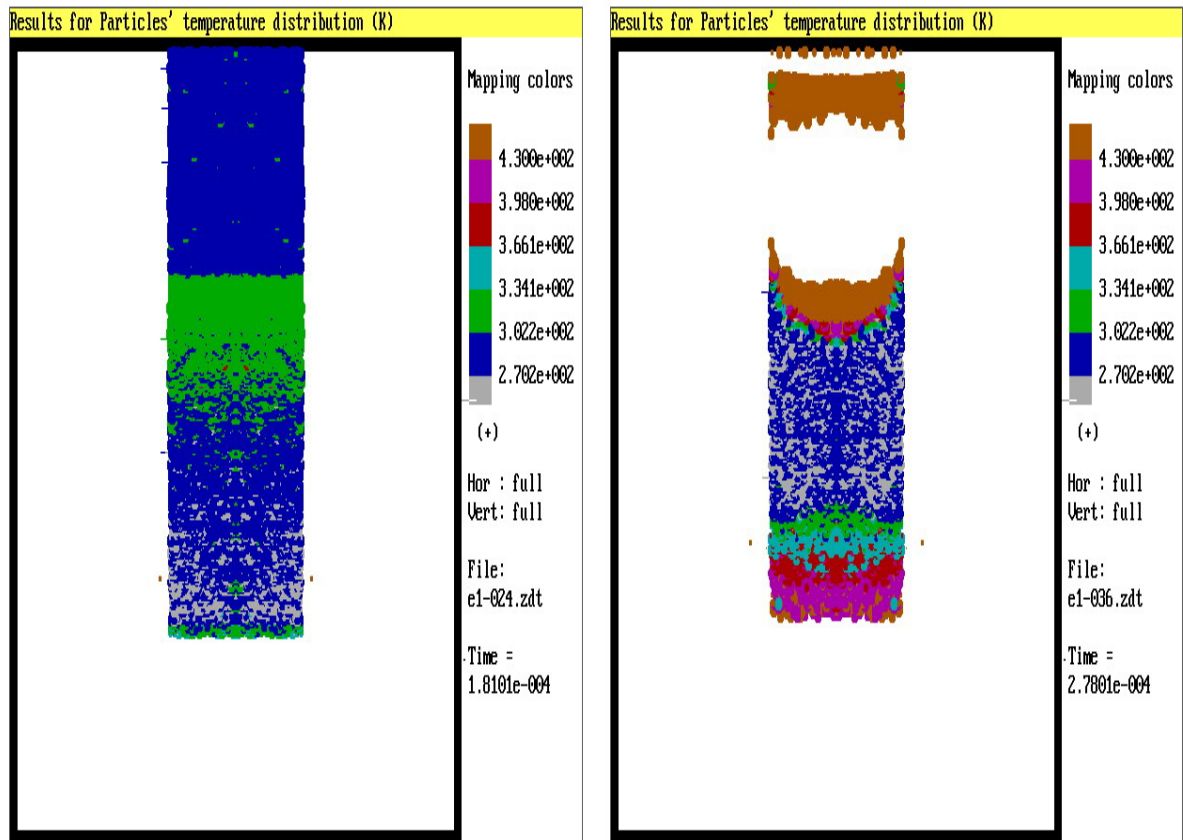


Fig.2. Droplet temperature field for successive times in shock wave meeting the combustible aerosol. Shock wave propagates from bottom to top.

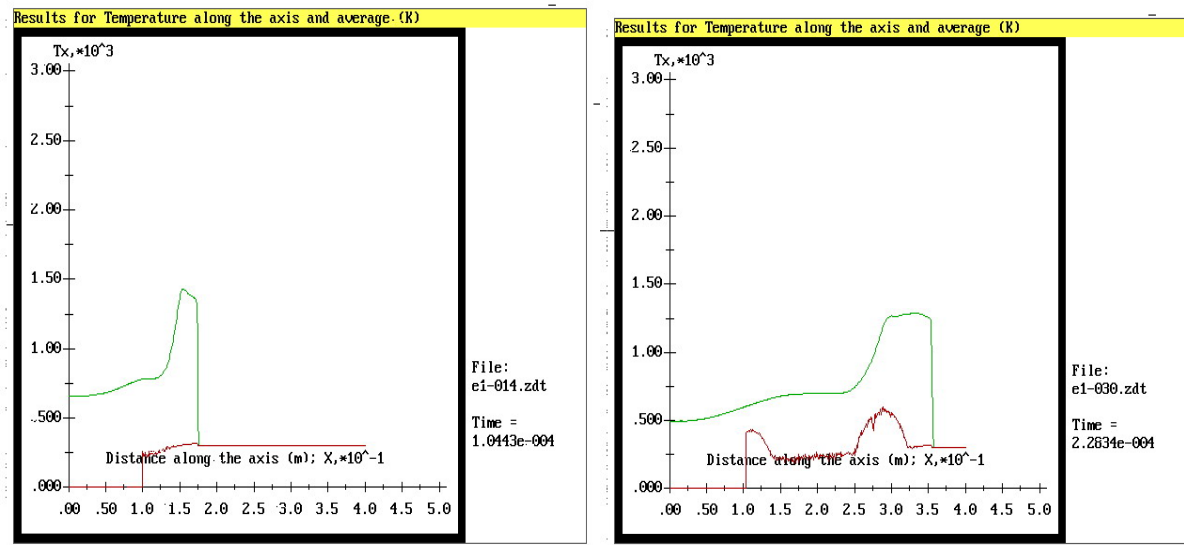


Fig.3. Cross-section averaged temperature profile in gas (green curves) and droplets (red) for successive times in shock wave meeting the combustible aerosol.

4 Conclusions

It was shown that depending on droplet size distribution and aerosol cloud density different flow scenario were possible.

Several ignition zones could be formed behind incident shock wave depending on mixture properties and initiation parameters. The possibility of numerical simulation permitting variation of definite parameters only made it possible to explain this fact.

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