Combustion onset in non-uniform dispersed mixtures

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Abstract

The paper presents the results of theoretical investigations of combustion and detonation initiation in heterogeneous polydispersed mixtures. The problems of fuel 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 for strong and mild initiation of detonation: by a shock wave and spark ignition followed by deflagration to detonation transition (DDT).

Keywords: spray, detonation, combustion, onset, droplet.

Introduction

Most of rocket and aviation engines have pulverized in air fuels combustion serving the base of their working cycle. Thus combustible mixtures formation and deflagration or detonation initiation in poly-dispersed fuel – air mixtures are the key aspects providing different limitations for operation of those engines. Onset of detonation being very dangerous for conventional engines could, however, serve the basis for creating new generation of engines - pulse detonating engines (PDE). 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.) for both strong and mild initiation. Special attention was paid to peculiarities of droplet interaction with a high enthalpy flow.

Mathematical model for polydispersed 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 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 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 atomization. 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, 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.

The momentum equation for a single droplet motion in the gas flow has the following form [2, 3]

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

the drag coefficient being the function of Reynolds number

$$C_d = \left(\frac{24}{Re} + \frac{4,4}{\sqrt{Re}} + 0,42\right)\beta \cdot K, \quad Re = \frac{\rho\,|\underline{v} - \underline{u}|\,d}{\mu},$$

$$\beta = \sqrt{\frac{\rho}{\rho_s}\left(2 - \frac{\rho}{\rho_s}\right)} \quad K = \left(\frac{T}{T_s}\right)^{4/5}$$

$$\frac{\rho_s}{\rho} = \begin{cases} \left(1 + \frac{\gamma-1}{2}M^2\right)^{1/(\gamma-1)}, & M < 1 \\ \frac{(\gamma+1)M^2}{(\gamma-1)M^2+2}\left(1 + \frac{\gamma-1}{2}\frac{(\gamma-1)M^2+2}{2\gamma M^2-(\gamma-1)}\right)^{1/(\gamma-1)}, & M \geq 1 \end{cases} \quad (2)$$

The energy equation for a droplet has the following form [2]

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

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 [7]:

$$q = \begin{cases} \pi d\lambda \cdot Nu \cdot (T - T_s), & Re < 1000, \\ \pi d^2\rho|\underline{v} - \underline{u}| \cdot St \cdot (H_r - H_w), & Re \geq 1000, \end{cases} \quad (4)$$

$$Nu = 2 + 0.16 \cdot Re^{2/3} \cdot Pr^{1/3}, \quad St = \frac{C_d}{2}Pr^{-2/3}$$

The non-equilibrium evaporation model is used to determine the evaporation rate [3]

$$\dot{m} = \pi d \cdot \rho D \cdot Nu \cdot \log\left(\frac{1 - Y_e}{1 - Y_w}\right) \quad Y_w = \frac{W_N P_0}{W_p}\exp\left[\frac{H_b}{R}\left(\frac{1}{T_b(P_0)} - \frac{1}{T_s}\right)\right] - \dot{m}\frac{\sqrt{2\pi RT_s}}{\pi\delta_e pd^2} \quad (5)$$

The dynamic interaction of liquid droplets with the gaseous flow could bring to instability of the interface in the shear flow 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 break up due to vibrational instability takes place. On essentially surpassing the critical Weber number other mechanisms start playing essential roles in the break up process that brings to formation of fine mist [3, 5, 7]. 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 atomization of initial droplets (diameter d):

$$d_a = \begin{cases} d = \left(\frac{6\alpha_2}{\pi n}\right)^{1/3}, & We < We_* \\ \frac{dWe_*}{We}, & We_* \leq We \leq We_{**} \\ d_*, & We > We_{**} \end{cases} \quad We_* = 12(1 + Lp^{-0.8}), We_{**} = 350 \quad (6)$$

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 ($We > We_{**}$) one needs to evaluate the part of the accumulated by a droplet 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:

$$N = \left(1 + \frac{E_*}{\sigma\pi d^2}\right)^3 \quad d_* = \frac{d}{1 + \frac{E_*}{\sigma\pi d^2}} \quad E_* = A_{drag} - \sum_{i=1}^{N_*} \frac{m_i v_{i*}^2}{2} \quad (7)$$

Where 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. Thus main assumption of the model is the following: work of drag forces in separating pieces of droplets is spent for additional free surface formation and relative kinetic energy of fragments.

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 following formulas:

$$A_{drag} = \frac{1}{8} N_* \rho C_d v_{rel}^2 \pi d_*^2 d_* \quad d_* = \frac{d}{1 + \frac{1}{4}\left(\frac{1}{2}C_d\rho v_{rel}^2 - \frac{1}{3}\rho_c v_*^2\right)\frac{d}{\sigma}} \quad (8)$$

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 separate from the initial one, i. e. it needs a definite time for the liquid bridges between the droplets to be established, elongated and broken [3]. Then, finally the first order estimates give the following formula:

$$d_* = \frac{dWe_*}{\frac{1}{8}C_d(We - We_{**})We_* + We_{**}} \quad t_* = \frac{d}{v_{rel}}\frac{We_*}{We}\left(1 + \frac{3}{8}C_d\frac{\rho}{\rho_c}\left(1 - \frac{4}{C_dWe_*}\right)\right) \quad (9)$$
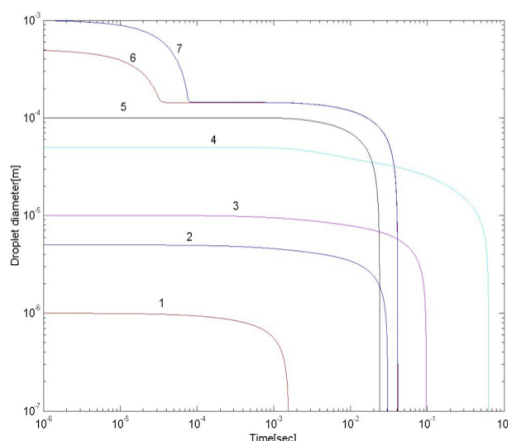
Figure 1: Droplet diameter variation versus time for droplets of different initial diameters. $V_0 = 50m/s$, taking into account atomization.
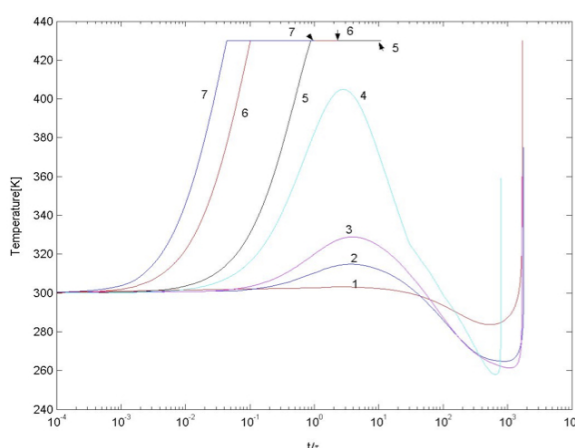
Figure 2: Mean droplet temperature variation versus dimensionless time for droplets of different diameters. $V_0 = 50m/s$, taking into account atomization.

Coalescence of droplets due to collisions is neglected. This assumption is valid for rarefied mixtures. In present simulations we'll study mixtures, wherein volume fraction of fluid is 10^{-3}, which provides the probability of collision 10^{-6}.

Numerical investigation of gas-droplet interaction in streaming flows

In order to evaluate the influence of different factors on the rate of droplet evaporation and mixture formation in heterogeneous detonation, let us investigate the problem of droplet interaction with the streaming gas flow taking into account mechanical drag, atomization of droplets, non-equilibrium heat and mass transfer. A series of model problems was regarded, in which gas flow and droplet initially had different relative velocities and temperatures, and then relaxation took place. Those model problems are similar to that encountered in shock wave initiation of detonation in combustible dispersed fuel-air mixtures. The two-phase flow becomes strongly non-equilibrium behind the shock wave, because due to mechanical inertia droplets keep their speed practically constant and gas accelerates on passing the shock wave. Besides, due to thermal inertia, temperature inside droplets practically does not change, while gas temperature increases instantaneously behind the shock wave. Due to that reason gas temperature in all the numerical experiments was assumed to be higher than the boiling temperature for liquid droplets.

The thermophysical properties for gas and droplets were assumed similar for all numerical experiments: ambient pressure $p = 1.013bar$, temperature $T = 1000K$, gaseous phase – air, liquid – n-decane ($C_{10}H_{22}$). Initial droplet temperature was assumed to be $T = 300K$.

The relaxation processes for droplets of different diameters were regarded. Numbered lines on the successive figures correspond to the following initial diameters of droplets: $1 - 1 \mu m$; $2 - 5\mu m$; $3 - 10 \mu m$; $4 - 50 \mu m$; $5 - 100 \mu m$; $6 - 500 \mu m$; $7 - 1000 \mu m$.

Figs. 1-2 illustrate parameters of droplets variation in the process of mechanical and thermal relaxation for the set of numerical experiments assuming initial velocity difference to be equal to 50 m/s. Fig. 1 illustrates droplet diameter variation due to evaporation. Large droplets undergo atomization until their diameter gets smaller. That is the reason for the 6-th and 7-th curves in Fig. 1 to converge into one, because atomization terminates

on reaching by all droplets one and the same diameter. It is seen from the figure that evaporation time increases with the increase of initial droplet diameter, but the increase does not take place monotonically: the increase of life time (curves 1, 2, 3, 4) changes for a decrease (curves 4, 5) and then comes back to an increase (curves 5, 6, 7). That testifies the effect of manifestation of different mechanisms depending on the characteristic size of droplets.

One could distinguish the characteristic deceleration time τ (velocity decreases e times) for each droplet. This time depends on droplet initial mass m_0, relative gas velocity v_0 and drag f_d.

$$\tau = \frac{v_0}{a_0} \quad \text{where} \quad a_0 = \frac{f_d(t=0)}{m_0} \tag{10}$$

The time being normalized to this value, and droplet diameter being normalized to its initial value allow us to obtain the dependences for a droplet temperature versus normalized time, which is present in Fig. 2. The dynamics of droplet heating is the following. For small droplets (curves 1, 2, 3, 4) in the very beginning the temperature increases due to external heating. On rapid decrease of droplet relative velocity evaporation in the stream of gas brings to a decrease of temperature. Then on decreasing droplet radius heat fluxes growth brings to an increase of temperature until the droplet disappears. The first increase of temperature is higher for larger droplets, which relative velocity decreases much slower than for small droplets. Very large droplets follow different scenario. The first increase of their temperature goes as high as up to the critical value. Then evaporation takes place at a critical temperature very rapidly. Arrows with numbers in Fig. 2 indicate the end of droplet life time. That is the reason for a larger droplet (curves 5 in Figs. 1 and 2) to have a shorter life time.

Non-uniform sprays combustion

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 in tubes of cylindrical geometry. 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 25000. 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. Fig. 6a illustrates detonation velocities in hydrocarbon-oxygen two-phase mixtures developed in numerical simulations and in experiments [8-10]. Liquid n-decane ($C_{10}H_{22}$) fuel was used. Fig. 6b illustrates turbulent flame propagation velocities versus velocity pulsation in gaseous mixtures of CH_3OH, O_2 and N_2. (Curves – experiments [11], dots – numerical computations). Satisfactory coincidence of theoretical and experimental data could serve a macroscopical validation for the developed model.

To simulate hydrocarbons the following parameters were taken: $\rho = 850 kg/m^3$; $\Delta H = 43 MJ/kg$; $h_L = 200 kJ/kg$; $W = 140 kg/kmol$. The reduced kinetic model is provided in [7]. The share of water in hydrocarbon decomposition was assumed to be $\zeta = 0.2$.

Initiation of combustion by a shock wave was studied in a tube 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 mean droplets diameter was assumed $100 \mu m$, minimal diameter - $10 \mu m$, maximal- $200 \mu m$. The droplets size distribution function was assumed to be a triangular one. The initial droplets density was varied from 5 to $20 kg/m^3$. The results of simulations (Figs. 3 and 4) show that for different fuel concentration and
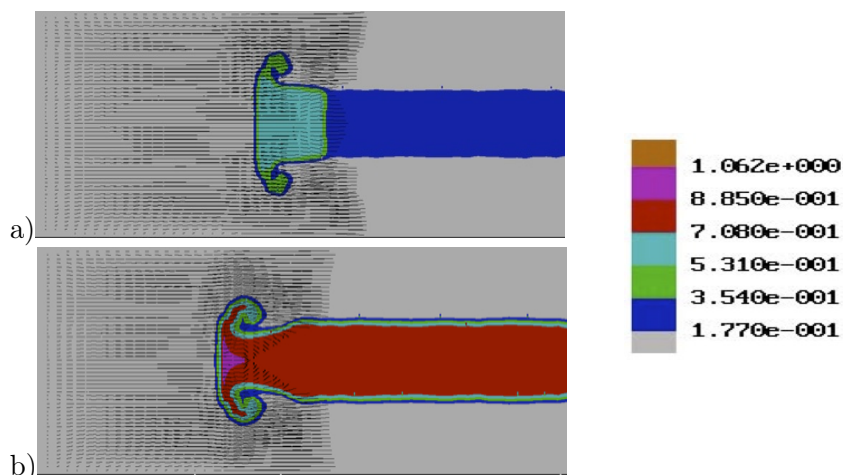
Figure 3: Hydrocarbon concentration for shock wave propagation in dispersed mixture (a - initial fuel density 5 kg/m^3; b - initial fuel density $20 kg/m^3$).
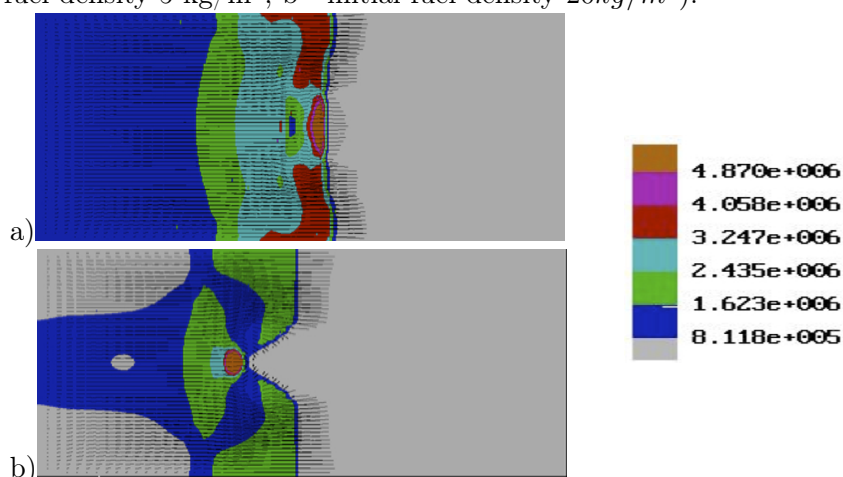

Figure 4: Pressure maps (Pa) for shock wave propagation in dispersed mixture (a - initial fuel density $5 kg/m^3$; b - initial fuel density $20 kg/m^3$).

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

Mild ignition and detonation onset via DDT was simulated in a tube, which diameter was 20 mm, the tube length was 2 m (Fig. 5), the mean droplet diameter was assumed $50 \mu m$, minimal diameter - $10 \mu m$, maximal - $100 \mu m$. The droplet size distribution function was assumed to be a triangular one. The mixture filled the whole tube, initial droplet volume concentration being equal $\alpha = 0.001$.

Numerical modeling of two phase mixture ignition and combustion was carried out to understand better the deflagration to detonation transition (DDT) processes. Submicron particles did not play any role in the present study, as their lifetime was negligibly small being below the limit of accuracy of numeric scheme. The size of droplets accounted by the

Figure 5: Computational domain for DDT simulations.
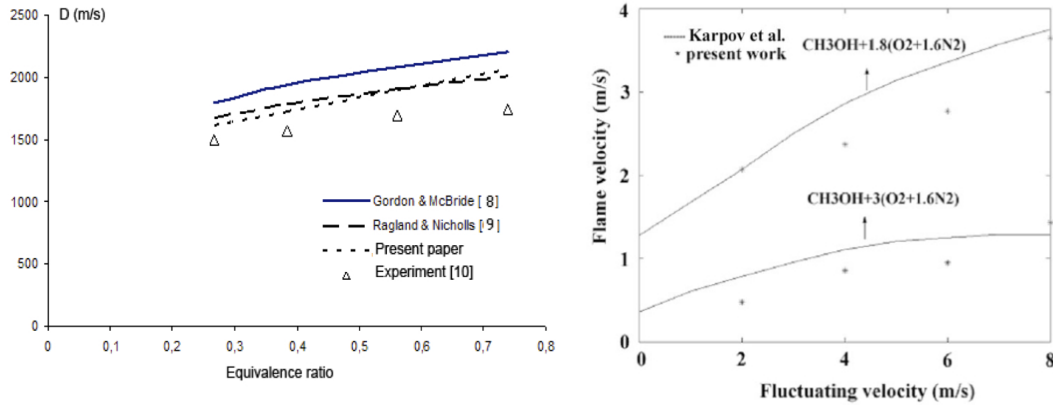
Figure 6: Detonation velocities in n-decane ($C_{10}H_{22}$)-oxygen two-phase mixture (a) and turbulent flame velocity in one-phase (b) mixture developed in numerical simulations and in physical experiments.

model is the one larger then minimal size evaporating within one time step. Reaction rate of smaller (submicron) particles cannot influence simulations, as the total energy release of their burning out is distributed within the computational cell within one time step. The effect of droplet size distribution function on the DDT process was investigated in [4]. Here we'll study the effect of droplet spatial distribution on the onset of detonation. As it was shown in [2] droplet spatial non-uniformity promotes ignition and combustion onset. In particular, the presence of concentration gradient in droplet spatial distribution lowers the minimal ignition concentration in the zone of energy release. The successive results illustrate the combustion zone averaged axial velocity variation versus time and tube length for different spatial distributions of droplets.

For one and the same fuel content ($\bar{\rho} = 0.8$kg/m³) and similar droplet size distribution function the spatial non-uniformity along the longitudinal co-ordinate was investigated. The values of other ignition characteristics were also similar: $T_0 = 300K, p_0 = 1bar, k_0 = 0.1j/kg, E_{ign} = 3.5j, t_{ign} = 100\mu s$ Fig. 7 presents the comparison of results obtained for homogeneous (a) and non-homogeneous (b) spatial distribution of droplets. In case (b) mean fuel concentration is decreasing along x-axis.

For the case (a) the turbulent flame propagation in the mixture is very non-monotonic. Velocity first stays at the level of 200 m/s, then it increases up to 700 m/s, again decreases to 600 m/s then increases to 1100 m/s and decreases to 500 m/s again, and then increases up to 1800 m/s and decreases to an average self-sustaining velocity of 1600 m/s with periodical oscillations near that value. It is seen, that in the beginning some galloping combustion mode is established, which turns to be unstable with increasing amplitude of
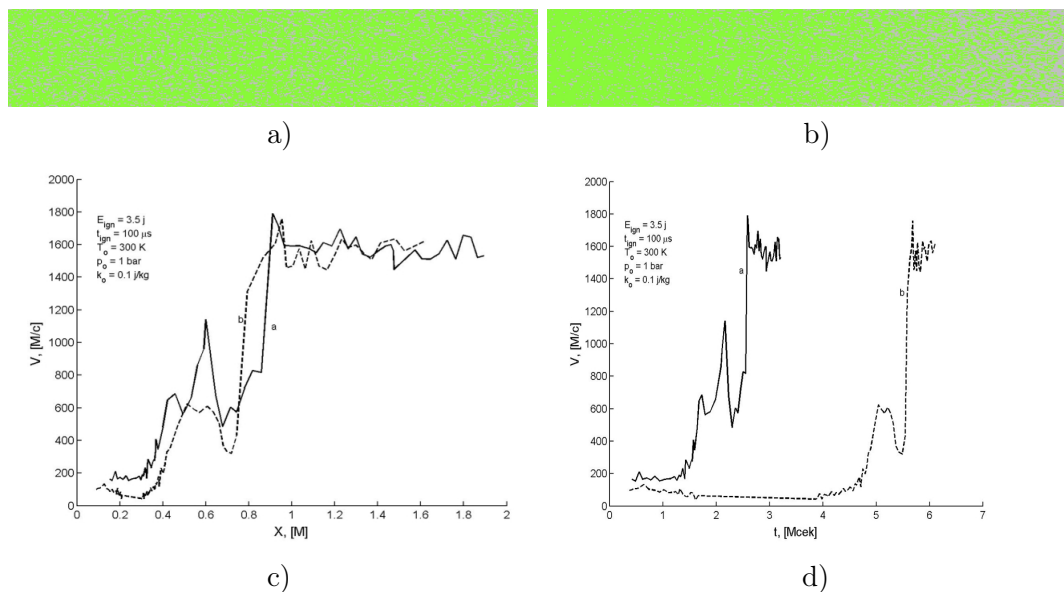
Figure 7: The effect of spatial non-uniformity of mean droplet concentration distribution (a – uniform, b – non-uniform) on the onset of detonation in polydispersed mixtures. Velocity versus axial coordinate (c) and versus time (d) diagrams.
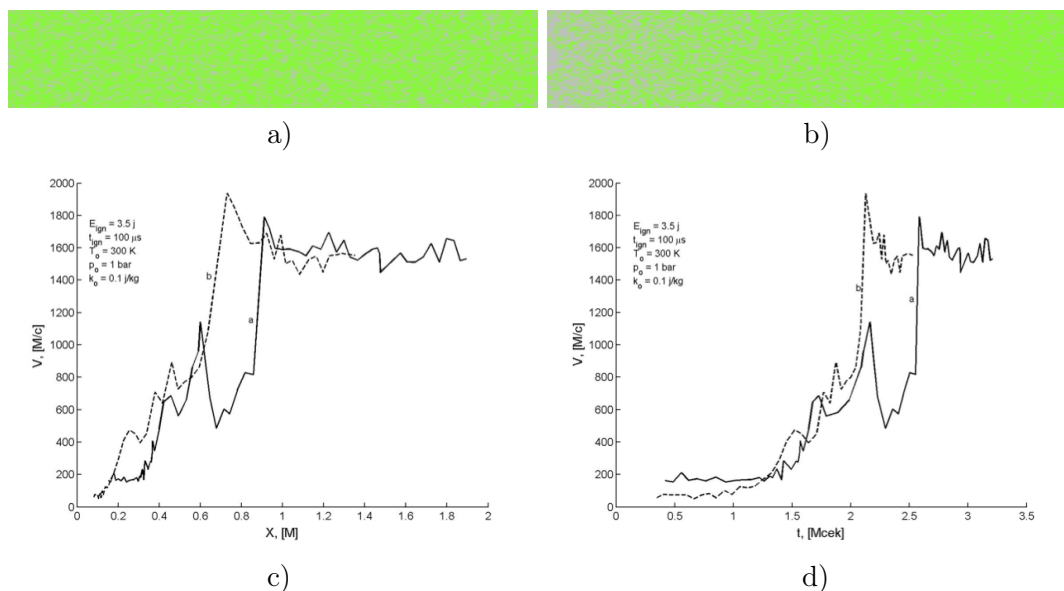

Figure 8: The effect of increasing along the axis mean droplet concentration (a – uniform, b – non-uniform) on the onset of detonation in polydispersed mixtures. Velocity versus axial coordinate (c) and versus time (d) diagrams.

a)   b)

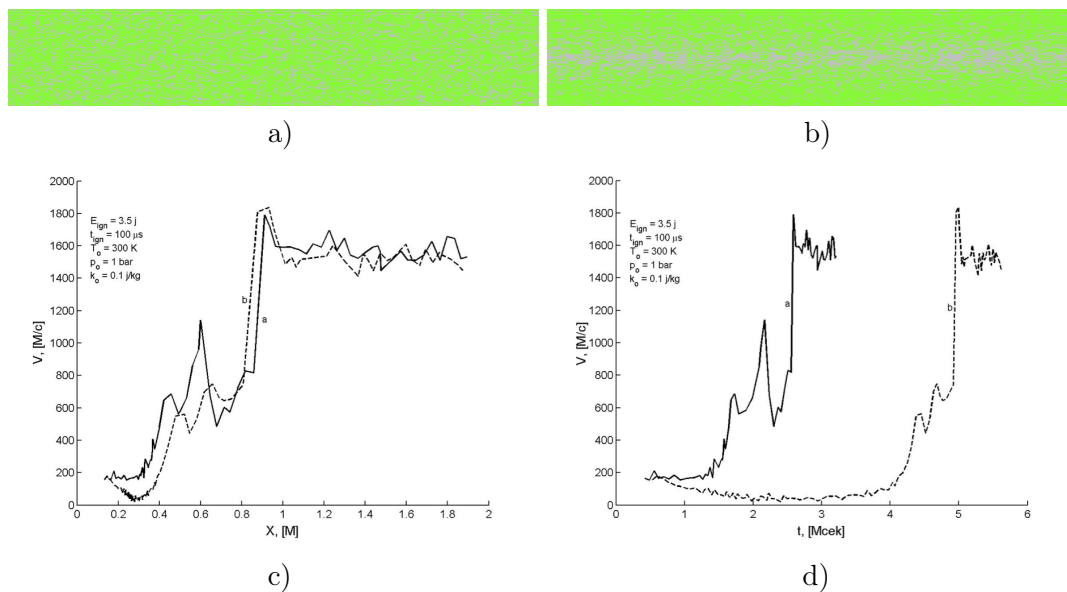c)   d)

Figure 9: The effect of spatial non-uniformity of mean droplet concentration distribution in radial direction (a – uniform, b – minimum on the axis) on the onset of detonation in polydispersed mixtures. Velocity versus axial coordinate (c) and versus time (d) diagrams.

oscillations until finally an overdriven regime is formed, after which mean velocity cannot go down below the self-sustaining one. Detonation in poly-dispersed fuel-air mixture is named a self-sustaining propagation of shock induced ignition. Comparison with cellular gaseous detonation does not seem legible, because cellular structure is an attribute of gaseous detonation, but by no means its definition.

Results of numerical simulations show that pre-detonation length remains practically the same for different spatial distribution of condensed matter (Figure 7 c). It seems to be even a little shorter for the case of the increased fuel concentration in the beginning of the tube. While velocity versus time diagrams show essential increase of pre-detonation time. This effect is due to a serious decrease of flame propagation velocity in the ignition section (50 – 100 m/s), which takes place because of the increased heat losses to heat the increased mass of droplets.

Figs. 8-9 illustrate DDT process after ignition in the non-uniform mixture with increasing along the axis mean fuel content (Fig. 8), decreasing in the radial direction (minimal in the center – Fig. 9). Comparison of results shows, that for the increasing fuel concentration along the axis pre-detonation length and time practically do not depend on such type of non-uniformity, while for radial non-uniformity pre-detonation time grows due to initial decrease of mean axial flame propagation velocity. When fuel concentration is maximal in the ignition zone more time is needed to heat all the droplets, which increases ignition delay, when fuel concentration is minimal in the ignition zone at the axis, propagation velocity is limited by lean conditions, which brings to ignition delay due to the increase of evaporation time to guarantee the necessary vapor concentration.

The results of simulations based on the developed model show that the zone of increased density of droplets behind shock waves appear, which was first discovered numerically by Korobeinikov [6] and named the ρ-layer. Later, the formation of ρ-layers in dusty gases was confirmed experimentally. The present results show that for liquid droplets ρ-layers are formed as well behind shock waves despite droplets atomization. After ignition of dispersed mixture either turbulent combustion wave is formed lagging behind the atten-

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uating shock wave, or a self-sustaining detonation wave. The spatial non-uniformity of droplet distribution in the radial direction for this type of initiation also inhibits the onset of detonation.

Conclusions

Investigating the behavior of individual droplets in a heated air flow allowed distinguishing two scenarios for droplet heating and evaporation. Small droplets undergo successively heating, then cooling due to heat losses for evaporation, and then rapid heating till the end of their life time. Larger droplets could directly be heated up to a critical temperature and then evaporate rapidly. Atomization of droplets interferes heating and evaporation scenario.

Investigating droplet cloud strong ignition by a shock wave showed 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, when chemical reaction takes place only in a thin border layer of the cloud from thus supporting the shock wave in pure gas propagation.

The onset of detonation in case of a mild ignition of dispersed mixtures at ambient pressures and temperatures comes via galloping combustion mode with increasing amplitude finally bringing to an overdriven detonation regime, which then evolves into a self-sustaining one. Generally speaking, convective combustion in dispersed mixture could lead either to a galloping mode, or to onset of detonation. For large droplets and small ignition energy only galloping combustion modes could be attained.

Non-uniform spatial distribution of droplets has a strong influence on predetonation time (in most cases time is increasing) and much smaller effect on predetonation length. Different types of spatial non-uniformity inhibit deflagration to detonation transition, or direct initiation of detonation, while in case of turbulent flame initiation by spark ignition spatial non-uniformity could serve a promoting factor [2].

Acknowledgments

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