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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 mild initiation of detonation by spark ignition followed by deflagration to detonation transition (DDT).

1. 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) [1–3]. 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 [4]. While in RAM engines thrust is formed essentially by the nozzle, wherein reaction products are already homogeneous [5,6], thrust in pulse detonation engine essentially depends on detonation onset process, which is strongly affected by mixture heterogeneity and spatial non-uniformity. The goal of the present research was, however, investigating sensitivity of detonation onset to mixture parameters non-uniformity (spatial non-uniformity of dispersed phase, size distribution function, etc.) for mild initiation. Special attention was paid to peculiarities of droplet interaction with a high enthalpy flow.

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 [7–9]. 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 [8,9], evaporation and diffusive mixing of fuel vapor with an oxidant.

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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 poly-dispersed 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 [7,8], 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 25,000 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 [7,8]:

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

the drag coefficient being the function of Reynolds number

$$C_d = \left(\tfrac{24}{Re} + \tfrac{4.4}{\sqrt{Re}} + 0.42\right)\beta\cdot K, \quad Re = \frac{\rho\left|\vec{v} - \vec{u}\right|d}{\mu},$$
$$\beta = \sqrt{\frac{\rho}{\rho_s}\left(2 - \frac{\rho}{\rho_s}\right)}, \quad K = \left(\frac{T}{T_s}\right)^{4/5},$$
$$\frac{\rho_s}{\rho} = \begin{cases} \left(1 + \tfrac{\gamma-1}{2}M^2\right)^{1/(\gamma-1)}, & M < 1; \\ \tfrac{(\gamma+1)M^2}{(\gamma-1)M^2+2}\left(1 + \tfrac{\gamma-1}{2}\cdot\tfrac{(\gamma-1)M^2+2}{2\gamma M^2-(\gamma-1)}\right)^{1/(\gamma-1)}, & M \geq 1. \end{cases} \tag{2}$$

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

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

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 [12]:

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

The non-equilibrium evaporation model is used to determine the evaporation rate [8]

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

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 [10]: $We = \frac{\rho v_{rel}^2 d}{\sigma}$, 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 [8,10,12]. These main characteristics of the atomization process could be taken into account by the following approximate formula [8] determining mean diameters of droplets d_a originating in atomization of initial droplets (diameter d):

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

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 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

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

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 $\left(N_* = d^3/d_*^3\right)$ 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:

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

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