Detonation Initiation in Dispersed Fuel-Air Mixtures

N.N. Smirnov¹, V.F. Nikitin¹, J. Khadem¹, V.M. Shevtsova², J.C.Legros² ¹Moscow M.V. Lomonosov State University, Moscow 119899, Russia ²Free University of Brussels, Brussels 1050, Belgium

Corresponding author: N.N. Smirnov: ebifsun1@mech.math.msu.su

Introduction

The paper presents the results of theoretical and experimental investigations of the detonation initiation in heterogeneous polydispersed mixtures of liquid hydrocarbon fuels with air. Mathematical models able to predict the onset of detonation in turbulized polydispersed and homogeneous mixtures were developed. 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. Experimental investigations carried out taking diesel oil or vaporized gasoline as fuel and air as an oxidant. Two types of initiation: initiation by a shock wave and by a spark ignition, – were investigated.

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 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.

Averaging by Favre with the $\alpha \rho$ weight (α – volumetric fraction of the gas phase, ρ – gas density) we obtain the system for the gas phase in a multiphase flow [1] 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 equations (2) was modeled using the Gaussian quadrature technique [2].

The dynamic interaction of liquid droplets with the gaseous flow could bring to an instability of the interface and atomization of droplets. The criterion for liquid droplets instability is that of the critical Weber number [4]: $\mathbf{W}\mathbf{e} = \frac{\rho v_{rel}^2 d}{\sigma}$, 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. These main characteristics of the atomization process could be taken into account by the following approximate formula [2, 3] determining mean diameters of droplets d_a originating in breakups of initial droplets (diameter d):

$$d_{a} = \begin{cases} d = \left(\frac{6\alpha_{2}}{\pi n}\right)^{\frac{1}{3}}, & \mathbf{We} < \mathbf{We}_{*}; \\ \frac{d\mathbf{We}_{*}}{\mathbf{We}}, & \mathbf{We}_{*} \le \mathbf{We} \le \mathbf{We}_{**}; \\ d_{*} = \frac{d\mathbf{We}_{*}}{\frac{1}{8}C_{d}(\mathbf{We} - \mathbf{We}_{**})\mathbf{We}_{*} + \mathbf{We}_{**}}, & \mathbf{We} > \mathbf{We}_{**}; \end{cases}$$

(

where n is the number of droplets per volume unit, α_2 – volumetric fraction of the droplet phase, the critical Weber numbers are determined as follows:

> $\mathbf{We}_* = 12(1 + \mathbf{Lp}^{-0.8}), \mathbf{We}_{**} = 350,$ where the Laplace number $Lp = \frac{d\rho_c \sigma}{\mu_c^2}$,

 ρ_c , μ_c - liquid density and viscosity.

Onset of Detonation in Polydispersed Mixtures of Air with Liquid Hydrocarbons.

Numerical investigations of detonation initiation in dispersed hydrocarbon fuel - air mixtures by shock waves of different intensities were performed. To simulate hydrocarbons parameters for diesel fuel were taken: $\rho = 850 \text{ kg/m}^3$; $\Delta H = 43 \text{ MJ/kg}$; $h_L = 200 \text{ kJ/kg}$; W = 140 kg/kmol. The share of water in hydrocarbon decomposition was assumed to be $\zeta = 0.2$. The mean droplets diameter was assumed 50 µm, minimal diameter - 10 µm, maximal - 100 µm. The droplets size distribution function was assumed to be a triangular one. The initial droplets volume concentration $\alpha = 0.001$.

The tube diameter was 20 mm, the tube length for numerical modeling was chosen equal to 1 m, but only the zone of 350 mm length was occupied by the polydispersed mixture at ambient pressure temperature 300 K. The rest of the tube was used for a plate shock wave to get formed. 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. The number of model particles used in calculations was 15000.

The results show that on entering the dispersed mixture strong attenuation of the initiating shock wave takes place. Behind the shock wave there originates a zone of high concentration of dispersed phase. A profile of condensed phase concentration behind the shock wave is shown in Fig.1. The initial volume concentration of condensed phase was uniform starting from $x=x_0$. The zone of increased density of solid particles behind shock waves was first discovered numerically by Korobeinikov [5] and named the p-layer. Later, the formation of p-layers in dusty gases was confirmed experimentally. The present results show that for liquid droplets p-layers are formed as well behind shock waves despite droplets atomization. The density maximum is more close to the



Fig. 1. Condensed phase mean volume share profiles for successive times in shock wave ignition of dispersed fuelair mixture. Shock wave propagates from left to right.

atomizing droplets is stronger than for solid particles of the same initial size due to the increase of integral drag forces. Combustion of droplets promotes evaporation thus decreasing the volume fraction of condensed phase behind the shock wave. Nevertheless, the structure of the p-layer behind the shock remains the same, but concentration maximums are much lower and essentially more close to the shock wave. The reason for such a behavior of the player is the ignition delay. Combustion does not begin simultaneously behind the shock wave, but starts after a some delay. Thus, concentration profiles just behind the shock are similar to that for unburned droplets.

Later combustion brings to a rapid decrease of condensed phase concentration. Thus, the combination of the opposite effects shifts the concentration maximum more close to the shock wave.

Energy release in combustion of dispersed mixture decreases the attenuation of the initiating shock wave and can bring in the long run to its acceleration. Fig. 2 illustrates droplets size and temperature distributions in the tube for successive times after the shock wave entered the zone of dispersed mixture. Atomization and heating of small droplets take place behind the shock wave. Atomization is non-uniform in the cross-section of the tube: large droplets are still present near the wall being suspended later into the core, of the shock induced flow. The rate of heating of atomized droplets decreases gradually on penetrating the shock deeper into the dispersed mixture due to a rapid attenuation of the shock wave.

The example illustrated in Fig. 2 shows the onset of the detonation wave in the atomized and pre-heated mixture compressed by the primary shock wave. The detonation wave is characterized by a very narrow reaction zone, wherein most of small droplets burn out.



t=0.163 ms



Fig. 2. Shock wave ignition of dispersed fuel-air mixture. *a* - scheme of the computational domain; *b* - droplet size and temperature maps for successive times

Successive axial pressure profiles on shock wave entering the combustible dispersed mixture are shown in Fig. 3*a*. The initiating shock wave was obtained due to initial pressure and temperature discontinuity. A strong attenuation of the shock wave on entering the dispersed mixture takes place. In some time hot spots are formed in the zone of mixture compressed by the primary shock wave. The additional chemical energy release in the hot spots brings to a local pressure increase (Fig.3*a*, curve 1). Among two "hot spots" having appeared behind the primary shock wave only one brings to a rapid pressure increase and formation of an overdriven irregular detonation wave that overtakes the primary shock wave and then slows down.



Leading shock velocity variation on entering the zone occupied by disperse mixture are illustrated in Fig. 3b for different velocities of initiating shock wave. Depending on the intensity of the initiating shock wave different scenarios of the process are possible. On relatively low intensity of the initiating shock wave ignition delay is long and combustion does not begin due to shock wave rapid attenuation. Shock waves of higher intensity could initiate combustion in the dispersed mixture. The induced combustion brings to acceleration of the shock wave. The increase of its velocity causes the increase of losses in the dispersed mixture. Thus, after ignition of dispersed mixture either turbulent combustion wave is formed lagging behind the attenuating shock wave, or a self-sustaining

detonation wave. The initial attenuation of shock wave in dispersed mixtures is much stronger than that taking place in initiating a self-sustained detonation in gas-film systems [6].

Initiation of heterogeneous detonations via DDT



It is seen that after ignition heated reaction products penetrate the twophase mixture causing heating and evaporation of droplets (Fig. 4). The zone of chemical reaction penetrated not very deeply into the vessel, while convective flow of heated reaction products had already caused heating of a large portion of droplets ahead of the flame zone. Evaporation of droplets and combustion of vapors take place more rapidly in the center of the tube due to the higher rate of filtration of hot gases there. While some droplets still remain unburned near the walls. On acceleration of the leading disturbance the length of zone wherein evaporation and combustion of droplets take place decreases. After combustion wave propagates along the tube there is still some unburned fuel left near the walls of the tube. The curvature of the reaction zone appearing in Fig.4 is due to decoupling of the leading shock and the reaction zone. Multidimensional effects have a stronger manifestation during the decoupling because of initial curvature of the leading shock in the tube. Fig.5 illustrates the flame front trajectory in the tube. The dark curve was obtained by tracing the maximal average temperature in the cross-section. The gray curve was obtained by tracing the maximal reaction rate. Mean velocities are also shown in the figure.

Fig. 4. Convective combustion propagation in dispersed mixtures, t=6.26 ms.



Fig. 5. Flame trajectory in convective combustion propagation in dispersed mixtures as obtained in numerical simulations.

Conclusions

Investigations of the detonation initiation in two-phase dispersed mixtures showed that:

Prior to ignition the process of mixture formation consumes a lot of initiation energy to heat, evaporate and set to motion fuel droplets.

To initiate a self-sustaining detonation process one needs to have a strong shock wave with velocity sometimes higher than that of the self-sustaining regime.

On entering the dispersed mixture the shock wave forms behind it a zone of increased concentration of the dispersed phase — the so-called ρ -layer. In combustible dispersed mixture the ρ -layer is thinner than that formed in inert dispersed mixture.

On igniting liquid hydrocarbon fuel-air dispersed mixtures (mean droplet diameter $d \ge 50 \mu m$) at ambient pressures and temperatures the galloping combustion mode was attained.

Acknowledgements

Russian Foundation for Basic Research (Project code 05-03-32232), INTAS (00-0706) and Office of Naval Research (are acknowledged for financial support.

References

[1] N.N. Smirnov, V.F. Nikitin, J.C. Legros, Combust. Flame, 123, (1/2), (2000), 46 – 67.

[2] N.N. Smirnov, V.F. Nikitin, A.V. Kulchitskiy, J.C. Legros, V.M. Shevtsova in G.D.Roy, P.J.Strikowski (Eds.) *Proc. Thirteenth ONR Propulsion meeting*, Univ. of Minnesota, Minneapolis, 2000, p. 213-232.

[3] Smirnov N.N., Zverev I.N. *Heterogeneous combustion*, Moscow University Publishers, Moscow, 1992, 446 p.

[4] B.J. Azzopardi, G.F. Hewitt, Multiphase Sci. & Tech., 9, (1997), 109-204.

[5] V.P. Korobeinikov, Archivum Combustionis, 9, (¼), (1989), 149-152.

[6] N.N. Smirnov, Int.J.Heat Mass Transfer, 1988, vol. 31, No 4, pp. 779--793.