SIMULATION OF THE EXPLOSION BEHAVIOR OF BUBBLES IN ORGANIC SOLVENTS

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In the present work theoretical investigations of the explosion behavior of hydrocarbon-oxygen bubbly media under shock wave impact have been performed. A model of dynamics and ignition of a single bubble in a liquid taking into account the compressibility and viscosity of the liquid, the mechanical agitation of phases, the induction period of the chemical reaction, the shift of chemical equilibrium and possible soot formation has been suggested. It allows the simulation of detonation processes in a wide range of bubble systems, where the liquid and the initial gas have the following chemical compositions: $b_1C_{n1}H_{n2} + b_2H_2O$ and $a_0C_{m1}H_{m2} + a_1H_2 + a_2O_2 + a_3N_2 + a_4Ar$ respectively. Here a_i, b_i are the stoichiometric coefficients and m_i, n_i correspond to the chemical composition of hydrocarbons.

The bubble dynamics is described by the generally accepted Rayleigh-type equation, which takes into account losses owing to acoustic radiation of the bubble. In this case it is assumed, that the bubble does not lose its spherical shape.

Inter-phase transfer processes are simulated by an instant injection of liquid micro-droplets with total mass M_L and initial diameter D_0 into the gas at the point in time t_{inj} and for their subsequent evaporation.

During the induction period of chemical reaction the vapor-gas mixture is assumed to be non-reactive. At the moment of the end of the induction period the bubble ignition takes place and the vapor-gas mixture instantaneously reaches the state of chemical equilibrium. The chemical equilibrium is shifted continuously owing to bubble dynamics and microdroplets evaporation.

To describe the thermodynamic parameters of the mixture inside the bubble, a modification of the model of chemical kinetic [2] is performed. This modification allows us to take into account the

significant change of molar mass of the gas, adiabatic index, heat release of the chemical reaction and possible soot formation inside the bubble owing to the recombination and dissociation processes and liquid evaporation. The behavior of the soot was approximated by the one of graphite.

It is assumed, that partial pressure and total volume of the soot are negligibly small. Soot particles are in mechanical and thermal equilibrium with the gas. The following assumption was also used: carbon atoms, which lack of oxygen atoms for forming CO, immediately transform into soot.

The following parameters of the model need to be experimentally defined: M_L, D_0, t_{inj} and the induction period t_i of chemical reaction. These parameters were optimised from experimental results described in the literature as well as those obtained in [2,3].

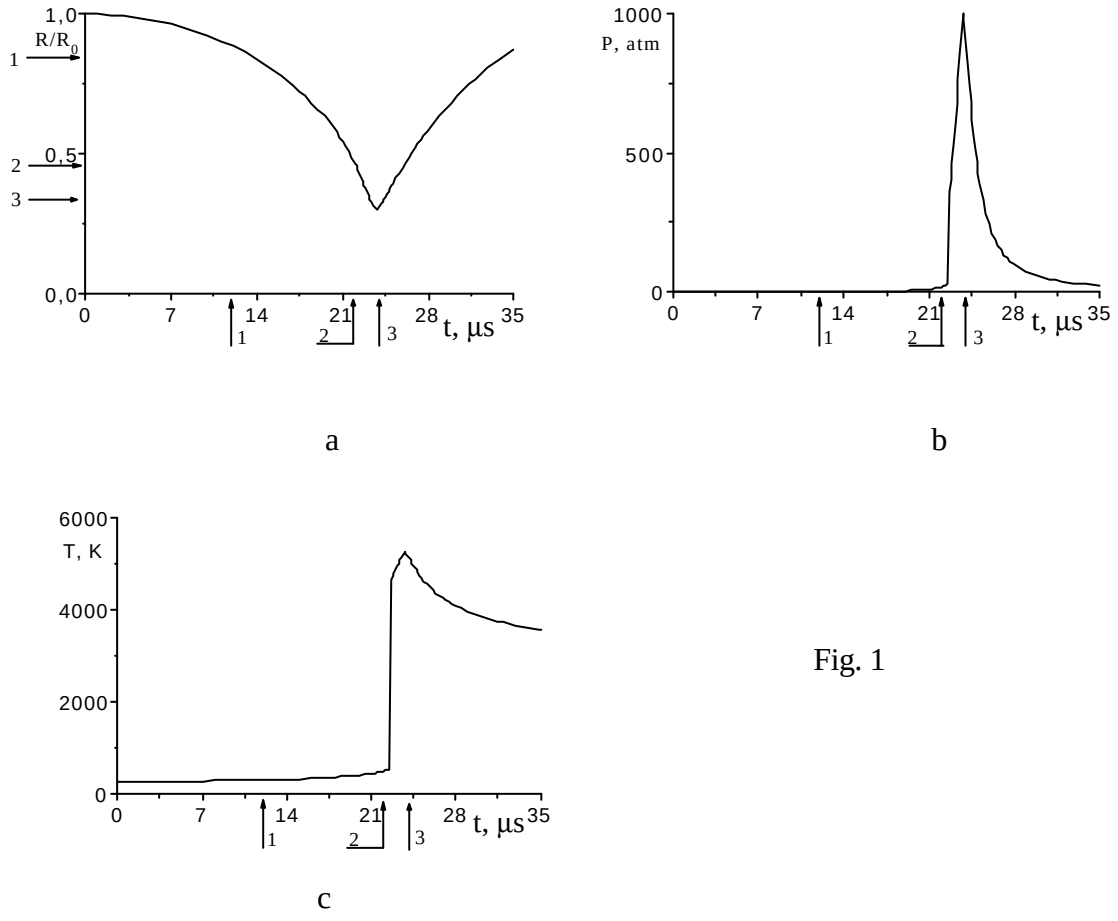

Fig. 1

The bubble dynamics and ignition of the system O_2 (gas) – cyclohexane (liquid) is calculated according to the proposed model. Fig. 1 presents the comparison between calculated parameters of the first bubble pulsation and experimental results (t is the time after the start of compression, T is

the gas temperature, R is the bubble radius; index *"0"* corresponds to the initial stage). Parameters of calculation: P_0 = 1 atm, T_0 = 290 K, R_0 = 1.85 mm, D_0 = 1 μm, M_L = 0.05 M_0, where M_0 is initial mass of the gas inside the bubble. The shock wave pressure P_{shock} is constant and equal to 40 atm. The jump of gas parameters is the result of instantaneous bubble ignition. The arrows on the t-axis show the experimentally observed characteristic points in time of the bubble dynamics and ignition. The first arrow points to the start of cumulative jet formation. The second corresponds to the point of bubble ignition. The third shows the point of maximal bubble compression t_{min}. The arrows on the R-axis (Fig. 1a) show the corresponding experimentally measured bubble radius. There is a satisfactory correlation between calculated and experimental values of t_i, t_{min}, and minimal bubble radius. Fig. 1b allows to estimate the parameters of the shock wave, which is emitted by a single bubble owing to collapse and ignition.

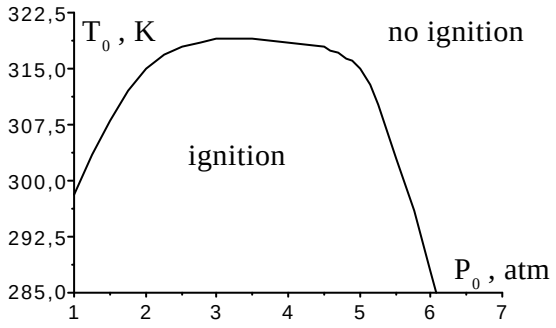

Fig. 2

Fig. 2 presents the calculated explosion limits of the bubble at different initial temperatures and pressures, P_{shock} = 120 atm, M_L = 0. It was assumed, that there is not bubble ignition, if the time of the first bubble pulsation is less than the induction period of chemical reaction.

Fig. 3 presents the calculated parameters of bubble dynamics of the first pulsation in the case of soot formation. The parameters of the calculation are: P_0 = 1 atm, T_0 = 290 K, R_0 = 1.6 mm, D_0 = 1 μm, M_L = 0.05 M_0 , t_{inj}= 11.0 μs, P_{shock} = 120 atm, α is the mass fraction of soot in the gas-soot mixture, m is the mass of microdroplets. The soot formation starts at the moment 11.6 μs, when about 70 % of injected mass is evaporated, and ended at the point in time of total microdroplets evaporation at the expansion stage of the first bubble pulsation. It can be seen (Fig. 3c,d), that the thermodynamic parameters of the mixture: the molar mass of the gas m and the adiabatic index g

change essentially owing to recombination and dissociation processes and change of the fuel-oxidiser ratio in gas phase.

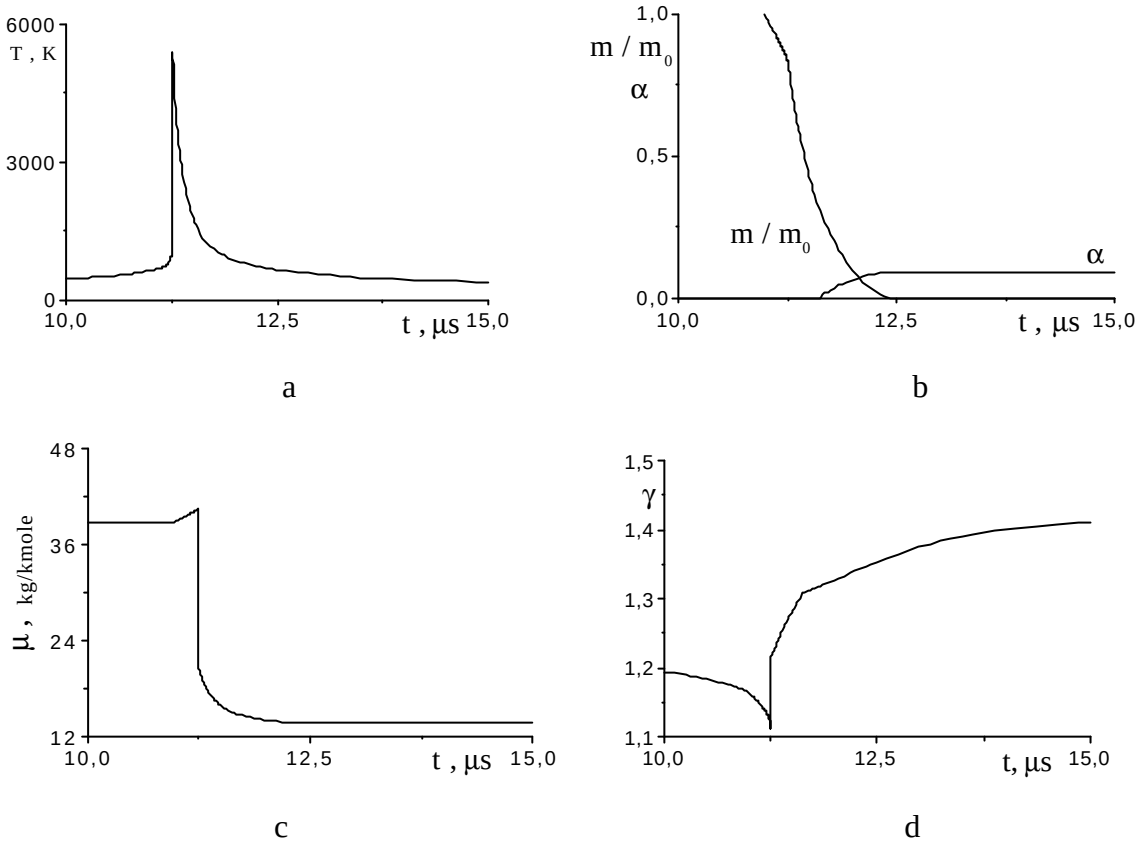

Fig. 3

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References

1. Yu.A. Nikolaev, P.A. Fomin. Approximate equation of kinetics in heterogeneous systems of gas-condensed-phase type. *Combustion, Explosion and Shock Waves*, 1983, 19, 6, pp. 737-745.

2. K. Mitropetros, H. Hieronymus, J. Steinbach, B. Plewinsky. Shock induced ignitions of oxygen bubbles in cyclohexane under normal conditions. *Archivum Combustionis* (accepted for publication in 2003).

3. K. Mitropetros, H. Hieronymus, J. Steinbach, B. Plewinsky. First oscillation shock induced oxygen bubble dynamics and ignition inside a cluster of a monodispersed bubbly organic liquid. Submitted to 19th ICDERS, Japan, 2003.