Bubble detonation model based on the interphase heat and mass exchange

Pavel A. Fomin, Sergey P. Taratuta

Lavrentyev Institute of Hydrodynamics Siberian Division of the Russian Academy of Sciences Novosibirsk, 630090, RUSSIA taratuta@hydro.nsc.ru

Abstract

A model of detonation in the two-phase heterogeneous mixture of gas bubbles and a liquid is proposed. The model is built with regard to the compressibility and viscosity of liquid, interphase heat and mass exchange, the presence of induction period of chemical reaction and chemical equilibrium shift.

Detonation of bubble media is accompanied by processes of heat and mass exchange intensified by instability of bubble surface, cumulative jets, forming microdrops and their further vaporizing. Naturally, the above processes sufficiently influence on process of chemical reaction in gas phase in a bubble. Moreover, in the system, where fuel and oxidizer are in different phases, forming detonation wave is impossible without intensive interphase heat- and mass exchange leading to forming chemically reacting mixture.

Real heat and mass exchange processes are substituted for an instant (at a moment after the onset of compression) injection of liquid microdroplets with diameter D_o and total mass **M** into a gas and for their subsequent evaporation. A similar method of assumption as to the instant evaporation of microdroplets is used in [1] in solving problems on dynamics of a solitary bubble in liquid. Notice that the interphase heat and mass exchange caused by mechanical agitation of phases (the production and evaporation of microdroplets) greatly surpasses diffusion and heat conductivity processes which are commonly taken into account in problems of the wave dynamics of steam-gas systems.

The bubble dynamics has been described according to the generally accepted practice. In this case it is suggested, that the bubble does not lose its sphericity.

The gas is ideal. All chemical reactions proceed in gas. A steam-gas mixture state is assumed to correspond to a gas which is chemically non-reacting until the moment of elapsed induction period and thereafter it becomes chemically equilibrium. The chemical equilibrium is shifted as a bubble radius changes and liquid transforms into gas. Condensing was not considered. Microdrops evapourize not instantaneously. At every step of integrating a continuous evapourizing of microdrops was simulated by instant evapourizing a mass of liquid, which value is determined from the well known equation of liquid drop burning in gas.

Thermodynamic parameters of the mixture are calculated by the high-precision kinetic model [2, 3] without using the inert gas adiabate traditionally in such kind of problems. This allows pioneering in an adequate consideration of wide change range of molecular mass, adiabatic index, heat capacities and heat effect of chemical reaction as the result of recombination and dissociation processes and change of the fuel-oxidizer ratio in gas phase. For instance, for initial cryogenic mixture H₂ (gas) - O₂ (liquid), a gas molecular mass can vary by an order. This model is applicable for hydrogen-oxygen systems of arbitrary chemical contents (including ones with inert components).

The moment of gas ignition t_* is determined by the conventional condition:

$$1 = \int_{0}^{t_{*}} dt / \tau_{l}$$

where τ_i is the induction period of a homogeneous gas mixture with constant parameters. Up to the end of the induction period, the gas is chemically non-reacting:

$$\mu = \mu_o \left(1 + M_L / M_0 \right) / (1 + M_L \mu_o / M_o \mu_L),$$

where μ and μ_0 are the current and initial molar masses of gas, μ_L is the molar mass of liquid, M_o is the initial mass of gas in the bubble, M_L is the mass of liquid, evaporated into bubble. It is evident, that if $M_L = 0$, then $\mu = \mu_0$. If microdroplets are totally evaporated, $M_L = \mathbf{M}$. After the moment of gas ignition we use the following equation of chemical equilibrium:

$$\rho (1 - \mu/\mu_{\text{max}})^2 \exp(E/\Re T) / (\mu/\mu_{\text{min}} - 1) = A T^{\frac{3}{4}} (1 - \exp(-\Theta/T))^{\frac{3}{2}} / 4K_+,$$

where A, K_+ are the rate constants of dissociation and recombination of the generalized reaction products, T, μ are the temperature and molar mass of gas, μ_a , μ_{\min} , μ_{\max} are the molar masses of gas in the atomic, most dissociated, and most recombined states, Θ is the effective excitation temperature of the vibrational degrees of freedom of the molecules, \Re is the universal gas constant, E is the mean dissociation energy of the reaction products.

The jump of gas parameters at the moment of end of induction period was calculated from the energy reservation law and equations of state and chemical equilibrium. Bubble radius and gas density at the jump moment are constants.

The parameters of μ_a , μ_{min} , μ_{max} are the functions of M_0 , M_L and initial chemical compositions of gas and liquid. For example, for mixture H₂ (gas) - O₂ (liquid):

if $M_{\rm L}/\mu_{\rm O2} \le M_0/2\mu_{\rm H2}$ then $\mu_{\rm max} = \mu_{\rm H2} (1 + M_L/M_{\rm o})$,

if $M_{\rm L} / \mu_{\rm O2} > M_0 / 2 \mu_{\rm H2}$ then $\mu_{\rm max} = (M_0 + M_L) / (M_L / \mu_{\rm O2} + M_o / 2 \mu_{\rm H2}).$

In both cases: $\mu_a = \mu_{min} = (M_o + M_L) / (M_L / \mu_{O2} + M_o / 2\mu_{H2}).$

Here μ_{02} , μ_{H2} are the molar masses of hydrogen and oxygen. Specific internal energy U of the gas is described according to:

$$U = \left[(3(\mu/\mu_a + 1)/4 + 3(\mu/\mu_a - 1) \Theta/2T (\exp(\Theta/T) - 1) \right] \Re T/2\mu + E(1/\mu - 1/\mu_{\min}).$$

These formulas eliminates the need for traditional artificial assumptions regarding the heat release, molecular mass of the gas and adiabatic process :

 $U = \Re T/(\gamma - 1)\mu$, $\gamma = \text{const}$, $\mu = \text{const}$, Q = const.

Here Q is the heat release of chemical reaction, γ is the adiabatic index of the gas.

Moreover, instead of the commonly used formula $P/\rho^{\gamma} = \text{const}$ we supposed the special algorithm. For example, in absence of heat- and mass exchange, we use the equation:

 $\mathrm{d}T/\mathrm{d}\rho = -\left(U_{\mathrm{u}}\,\mu_{\mathrm{o}} - \Re T/\rho\mu\right)/\left(U_{\mathrm{T}} + U_{\mathrm{u}}\,\mu_{\mathrm{T}}\right),$

here U_{μ} , μ_{ρ} , U_{T} , μ_{T} are the derivatives with respect to indexes.

The obtained non-stationary equations were integrated in the Lagrange coordinates by the explicit numerical scheme with artificial viscosity. At the left-hand boundary of the tube containing this mixture, a constant pressure sufficient for the excitation of the detonation is maintained. Calculated according to the proposed model, are the detonation parameters in systems *I* [explosive gas bubbles $(2H_2+O_2)$ - liquid (water and glycerin mixture)] and *II* [explosive bubbles (H_2) - liquid oxidizer (O_2)] at initial pressure 1 atm and initial temperatures 293 K and 87 K respectively. The calculations for wave initiation and for the case when the wave reaches a stationary regime are presented.

Calculation demonstrated weak dependence of wave parameters on initial size of bubbles. It is obtained, that the moment of droplets injection at the stage of bubble compression doesn't influence on the wave parameters. In this connection, it was supposed that droplets injection takes place at first pulsation when the bubble radius reduces in 3 times. Diameter and total mass of microdroplets variation was accomplished.

The structure of stationary detonation wave in system *II* is represented on Fig. 1a; k = 2%, $\mathbf{M} = 6 M_0$, $D_0 = 5 \mu m$. The wave propagates from left to right; *x* is the distance from left boundary, *m* is the microdroplet mass (initial mass is m_0), β is the dimensionless bubble radius. Picture scale does not allow to show a parameter leap at a moment of induction period end. It should be noted, that gas molar mass sufficiently increases (from 2 to 14 g/mole, i.e. approximately by an order) of takes place. Analogous calculation of wave structure for mixture *I* is presented on Fig. 1b; k = 1%, $\mathbf{M} = M_0$, $D_0 = 5 \mu m$. It is seen, that structures of detonation waves in mixtures *I* and *II* are similar. Note, that change of molar mass of gas in mixture *I* is less, than in mixture *II*.

Unexpected result was obtained: **M** increasing led to rise of wave velocity u_0 in system *I*. In system *II* detonation wave velocity increases monotonously with **M** growth. Wave pressure *P* passes through maximum at $\mathbf{M} = 8 M_0$, where M_0 is the initial mass of gas in a bubble (Fig. 2, initial volume fraction of gas in the mixture k = 2%. Note, that at $M / M_0 < 1$, $D_0 = 1 \mu m$ and $M / M_0 < 0.5$, $D_0 = 5 \mu m$ self-sustained wave is not formed.). This maximum corresponds to stoichiometry mixture between fuel and oxidizer in gas. In system *I* detonation velocity is practically constant for droplets diameter under 20 μm and monotonously decreases with diameter growth over this value. In system *II* detonation velocity decreases and wave pressure increases with growth of initial droplets diameter (Fig. 2).

The dependence of velocity and pressure of detonation wave on gas volume fraction was obtained. The calculation results for system II at $\mathbf{M} = 4 M_0$ are represented on Fig. 3. It was shown, that in systems I and II detonation velocity monotonously decrease with k growth. Calculation results for system I are in good agreement with experiment. Experimental data for system II are absent.

The model of bubble detonation suggested here is the development of model [4] and is the first model, where intensive interphase heat- and mass transfer is taken into account. This, in particularly, allows pioneering in simulation of detonation in systems, where fuel and oxidizer are in the separate phases (for example, system *II*).



It was shown in [4] that wave propagation at supersonic velocity (relative to the frozen sound velocity) is possible in system I with large initial pressures in the mixture. In the presented work, for the first time, supersonic

detonation wave velocity is obtained in system *II* as well. The structure of the wave in sub- and supersonic conditions is significantly different. In the first case, there is smooth pressure variation in the compression wave; in the second, there is a pressure discontinuity at the leading shock front of the wave.

For mixture *I* the dependence of detonation velocity on initial composition of gas is constructed. The results of calculations are presented on Fig. 4. The initial contents of gas is $H_2 + \lambda O_2$, M = 0. It is seen, that magnitude u_0 weakly depends on gas composition and has a little maximum at stiochiometric ratio between fuel and oxidizer. ($\lambda = 0.5$).



Analyzed here, is the dependence of detonation velocity on liquid viscosity in systems of *I* and *II* types. It was obtained, that at changing liquid viscosity in system *II* from real value to zero, detonation wave velocity practically does not vary. As a rule, in experimental investigations increase of liquid viscosity in systems of *I* type is realized by increasing share of glycerin in water. Thus, in the presented calculations corresponding to system *I*, changing share of glycerin in water was considered using corresponding changing values of density and viscosity of liquid, sound velocity in it and constants in the equation of state. The obtained results prove, that at increasing glycerin share, detonation velocity remains practically constant. This contradicts to known experimental results, according to which wave velocity increases at rising concentration of glycerin in water.

References

- Fomin P.A., Kedrinskii V.K. and Taratuta S.P., "Dynamics of single bubble in a liquid with chemical reactions and interphasic heat- and mass- exchange", 27th International Symposium on Combustion. Abstracts of Work-in-Progress Papers., p.185 (1998)
- [2] Nikolaev Yu.A. and Fomin P.A., "Approximate equation of kinetics in heterogeneous systems of gascondensed-phase type", Combustion, Explosion and Shock Waves, Vol. 19, N 6, pp.737-745 (1983) (translated from Russian by Plenum Publ. Corp.).
- [3] Fomin P.A. and Trotsyuk A.V., "An approximate calculation of the isentrope of a gas in chemical equilibrium", Combustion, Explosion and Shock Waves, Vol. 31, N 4, pp. 455-457 (1995) (translated from Russian by Plenum Publ. Corp.).
- [4] Trotsyuk A.V. and Fomin P.A., "Model of bubble detonation", Combustion, Explosion and Shock Waves, Vol. 28, N 4, pp. 439-445 (1992) (translated from Russian by Plenum Publ. Corp.).