The Model of Detonation Combustion in Liquid Aerosols

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1. Introduction

Regime of energy release, which provides the detonation wave self-sustaining, in aerosol systems depends not only on chemical kinetics, but in more complicated way it is determined by the preparatory physical processes of liquid atomization, evaporation of atomized mass and mixing of oxidizer with fuel vapours. It has been well established by a lot of experiments that the drop breakup behind the detonation front is a key process, because it considerably intensifies fuel transition into gas phase and the energy release, which strengthens the front. Our calculations [1] showed that generation of daughter droplets increases the total surface of liquid phase by 2-3 orders, which, together with rapid evaporation of finest droplets, leads to increasing of fuel mass transfer to gaseous phase. It is this intensification that makes it possible a self-sustained detonation regime itself. So, formation of combustible mixture must be analyzed with respect to rigorous study of each process. Such a study runs across obstacles which are caused by lack of knowledge about sizes, quantity and moments of breaking away of daughter droplets. This didn't allow to elaborate a mathematical model with ability to calculate in detail atomization kinetics and evolution of sprayed mass – its motion and evaporation with due regard to the dependence from the droplet radii r.

Thus, quantitative description of aerosol detonation can be only provided by adequate modeling and detailed calculations of a two-phase mixture formation behind detonation front. The aerosol drop atomization dictates the values of sizes and quantity of the tiny daughter droplets, as well as the moments of their breakaway. These values determine the evaporation rate and fuel-oxidizer mixture formation in gaseous phase. The closed mathematical model of liquid aerosol detonation is described in present work. We are interested in theoretical determination of the detonation regime velocity, so that two-dimensional effects are ignored (such as multi-cell structure, spinning regime). The core of the model is the description of the aerosol fuel drop atomization which yields the transient distribution of sprayed droplets by sizes. The details of mathematical model of heterogeneous detonation built on this basis and some results of calculations of mixture formation and combustion behind detonation wave are presented below.

2 Heterogeneous Flow and Phase Transformations Behind Detonation Front

We assume here a mono-dispersed aerosol with the parent fuel drop radius a_0. There are different consequences of shock front action at phases due to the differences in the phase properties. A gas phase is

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compressed; its density and temperature grow up, so that the initially stagnant gas starts moving suddenly after the shock front passage. Instead, the more inertial liquid phase is left at state of the rest with the same volumetric density ρ_{50} and temperature T_{50} as in front of the shock. These differences launch the irreversible processes of the phase relaxation: aerodynamic atomization of aerosol drops by the wake stream behind the shock and the liquid phase heating and evaporation. The former process generates the liquid component of tiny daughter droplets, while the latter supplies energy for evaporation providing quick transfer of fuel into the gaseous phase.

Thus, we have three gaseous components behind the detonation front: oxidizer of density ρ_1, fuel vapour of density ρ_2 and chemical reaction products of density ρ_3; as well, two liquid components: daughter droplets of density ρ_4 and aerosol parent drops of density ρ_5. The carrying phase density is then $\rho_c = \rho_1 + \rho_2 + \rho_3$. Due to the small difference in the thermo-mechanical properties of the gas components, we assume that they are all moving with the same velocity V_c and have the same temperature T_c.

These components are all exchanging each other with mass, momentum and energy. Kinetics of these processes must be subjected thus to comprehensive quantitative description because they form the final support to the shock front, which establishes whether or not the detonation is self-sustained.

Two-phase flow in detonation wave is considered here relative to the front (fig. 1). For a steady detonation propagating with a speed D, the flow is stationary in this coordinate frame. After the shock passage, the gas velocity is $V_c < D$, while the aerosol drop velocity is $V_5 = D$. It is convenient to consider the daughter droplet motion related to the parent drop, so that their relative velocity is w. The distance x is counted from the shock front. It is sufficient in stationary flows to consider a single "probe" drop, inasmuch as every two of such parent drops have the same history of their motion and fragmentation.

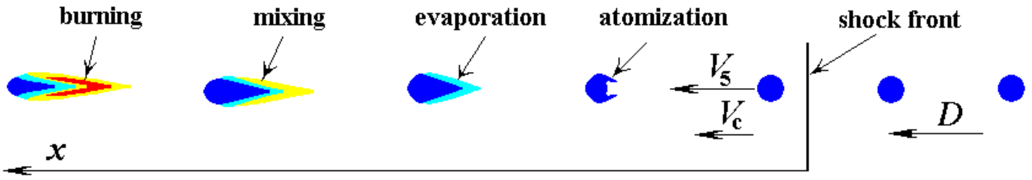

Figure 1. Schematic of inter-phase processes behind the detonation front.

Heterogeneous flow modeling is typically conducted in two levels of scaling [2]. The lower level focuses on the elementary processes of inter-phase interaction (such as droplet breakaway mechanics, aerodynamic entrainment, heating, evaporation, mixing and chemical reactions). The upper level is implemented at the whole problem scale, where the motion and mixing of the entire multi-component heterogeneous continuum is the final point in the transport process description. Consequently, the presented here model of atomization process consists of two parts: 1) breakaway droplet mechanics; and 2) the ballistics of an evaporating mist around an atomizing drop. The overall detonation model is described in Sect. 4.3.

3 The Breakaway Droplet Mechanics (Lower-Scale Modelling)

3.1. The breakaway mechanism. Description of the fuel atomization process should be based on the known underlying breakaway mechanism. Published in [1], [3]-[5] theoretical approach to the atomization process gives the opportunity to apply the simple relationships to describe the formation of a daughter droplet phase. Due to the transiency and complexity of the flow geometry around a parent drop, the issue of instability must be solved at every time-step of integration and at every elementary area of the drop surface, being built-in into a total calculation scheme of detonation combustion. The key process of a combustible mixture formation within detonation wave, – liquid fuel atomization, – is described here on the basis of the known model of a drop spraying [1], [3]-[5]. The model discussed below is based on the concept of quasi-continuous, high-frequency periodic spraying from the unstable part of the parent drop surface due to the instability of the gradient flow in conjugated gas-liquid boundary layers. An investigation of a local surface instability with due regard to changing of velocity profile across the boundary layers has revealed a new type of hydrodynamic instability for weak-viscosity liquids – "gradient instability". Mechanism of this type differs from that one of Kelvin – Helmholtz type and it is caused by sufficiently large velocity gradient inside liquid boundary layer. The theory explains the "stripping" mode of drop breakup as a quasi-continuous spraying from the unstable part, $\varphi_{\mathrm{cr}} < \varphi < \pi/2$, of drop surface ($\varphi$ is polar angle of surface area element). At some simplifications it permitted to derive differential equations of drop mass efflux and of quantity of sprayed droplets [1], [3].

3.2. Quantification of the aerosol drop atomization. In order to implement the dispersion mechanics into the calculation algorithm, we divide the unstable part of the drop surface on a system of elementary areas, $\Delta l_i = a(t)\Delta\varphi_i$, and apply the results of instability analysis to the locally plane flow at each area element. The value of the newborn droplet radius r is assumed to be proportional to the most unstable wave length λ_{m}, while the period of its breaking-off, $t_{\mathrm{b.o.}}$,– to the increment time t_{m} of e-fold growth of the unstable disturbance's amplitude at a given i^{th} area element:

$$r_i = k_{\mathrm{r}}\lambda_{\mathrm{m}i}, \quad k_{\mathrm{r}} < 0.25, \qquad\qquad t_{\mathrm{b.o.}i} = k_{\mathrm{t}} t_{\mathrm{m}i}, \quad k_{\mathrm{t}} \approx 1, \tag{1}$$

where λ_{m} and t_{m} are solved within the instability problem. The quantity of wavelengths, which are confined within i^{th} element area, is equal to $n_{\mathrm{tor}i} = \Delta l_i / \lambda_{\mathrm{m}i}$. Due to the axial symmetry of flow around the aerosol drop, this is the quantity of tori of radius $a(t)\sin\varphi_i$, which are breaking away from the spherical belt corresponding to Δl_i. By relating the volume of torus to the droplet volume, we obtain equation for quantity Δn of droplets, which are broken away from the area element by the time $t_{\mathrm{b.o.}}$, [1]:

$$\Delta n(\varphi,\tau) = B_{\mathrm{n}}\sqrt{a(\tau)(1-W(\tau))^5}\,\Psi^{-3}(\varphi)\sin^2\varphi\,\Delta\varphi\Delta\tau\,, \quad \Psi(\varphi) \equiv ((6\varphi - 4\sin 2\varphi + 0.5\sin 4\varphi)/\sin^5\varphi)^{0.5}\,, \tag{2}$$

and their radius, $r(\varphi,\tau) = B_{\mathrm{s}}\left(a(\tau)/(1-W(\tau))\right)^{0.5}\Psi(\varphi)$, $W = w/V_{\mathrm{c}}$. Ranger's [6] expression for the boundary layer thickness on a sphere, $\delta_{\mathrm{a}} = 2.2a(t)\mathrm{Re}_5^{-0.5}\Psi(\varphi)$, is used. Here $\tau = t/t_{\mathrm{ch}}$, $t_{\mathrm{ch}} = 2a_0/\beta^{1/2}V_{\mathrm{c}}$ is the characteristic time of atomization process, $B_{\mathrm{s}} = 0.51\pi\beta^{1/3}\mu^{-2/3}\mathrm{Re}_5^{-1/2}$, $B_{\mathrm{n}} = 0.15\mathrm{Re}_5^{3/2}\beta^{-7/6}\mu^{7/3}$ have a sense of scaling parameters for sizes and number of sprayed droplets, $\beta = \rho_{\mathrm{c}}^0/\rho_5^0$ and $\mu = \mu_{\mathrm{c}}/\mu_5$ are density and viscosity ratios of phases, $\mathrm{Re}_5 = 2a_0\rho_{\mathrm{c}}V_{\mathrm{c}}/\mu_{\mathrm{c}}$ – Reynolds number for a parent drop.

Due to flow variation along the parent drop surface, the sprayed droplets are distributed by sizes. In order to obtain this distribution, eq. (2) must be integrated in both φ and τ along the line $r(\varphi,0) = const$ on the (φ,τ)- plane [1]. For the case when the mass efflux rate equals to the rate of relaxational decreasing of drop – airflow relative velocity, the integration allows analytical form of the distribution function:

$$f_{\mathrm{n.s.}}(\tilde{r},\tau) = \frac{1-\exp(-A\tau)}{A\tilde{r}^2}\,\frac{B_{\mathrm{n}}\sin^3\varphi_0(\tilde{r})}{(8-2.5\tilde{r}^2\cos\varphi_0(\tilde{r}))}\,, \tag{3}$$

where $\tilde{r} = r/(a_0 B_{\mathrm{s}})$, $\varphi_0(\tilde{r})$ is an inverse with respect to $\tilde{r}(\varphi)$ function in equation of integration path:

$\tilde{r}(\varphi,0)=const$. For the conditions behind detonation waves the sprayed droplet radius lies within the range $(10^{-3}-10^{-2})a_0$. Information of sizes and derived distributions can be found in [1], [3].

4 Modelling the Combustible Mixture Dynamics (Upper-scale modeling)

4.1. Ballistics of the evaporating mist. The upper-level modeling is based on the one-dimensional point-source model of evaporating spray dynamics [5]. It describes evolution of the sprayed droplets' distribution function and reflects the spatial aerodynamics of the evaporating spray generated by the atomizing drop.

Spray polydispersity presents the largest difficulty for mathematical modeling of the spray evaporation ballistics. Polydispersity makes the daughter-droplet phase a non-homogeneous, multi-velocity medium and makes it necessary to regard the droplet size scale, r, as an independent variable for describing their velocity fields and evaporation rates. To take into account all the peculiarities of the droplet evaporation ballistics, we have introduced the transient distribution function *of daughter droplets by sizes*, $f_{\text{n.d.}}(x,r,t)$, as it exactly reflects the entire evolution of droplets in time t, in space x, and in sizes, r, resulted from the droplet acceleration and evaporation. On the parent drop current location, x, it coincides with the parent drop source distribution function: $f_{\text{n.d.}}(x,r,t)=f_{\text{n.s.}}(r,t)$ given by (3).

With regard to the large number and density of sprayed droplets, we suggest considering the daughter droplets altogether as a continuum, neglecting their collisions. Thence, the broken away droplets are considered as a multi-velocity fluid and the system of equations of the two-phase evaporating mist motion is composed below in dynamic x, r, t space.

The probe parent drop is considered as a continuous point source of daughter droplets of strength $\dot{F}_{\text{s}}(x, r, t)=\dot{f}_{\text{n.s.}}(r, t)$, which moves in axis OX direction with velocity $V_5(x, t)$. In turn, each daughter droplet is a point source of vapor of capacity $\dot{F}_{\text{v}}(y,r,t)$, which moves with velocity $w(y, r, t)$ relative to a parent drop. They altogether form the distribution of a vapor mass $m_{\text{v}}(x,t)$ within the spray. To describe the evolution of $f_{\text{n.d.}}$ in the (x, r, t)-space, we use the equation of the dispersed fuel. This equation describes the changing density of the daughter droplet distribution, $f_{\text{n.d.}}(y, r, t)$, which proceeds in space with velocity $dy/dt=w(y, r, t)$ due to droplet acceleration by gas flow, and in r-axis direction due to evaporation, which proceeds with velocity $u=dr/dt$ that is determined by evaporation law; here y is the distance of a daughter droplet to the parent drop. The equation of evolution is supplemented with equation of motion of the droplet phase continuum coupled with the equation of vapour influx in a spray volume, vaporization law accounting for the convectional enhancement in a high-speed gas flow.

4.2. Equations of spray dynamics. Thus, droplets – vapour two-phase multi-velocity flow in a wake spray of an atomizing aerosol drop is described by three dimensionless functions: $f_{\text{n.d.}}(y',\tilde{r},\tau)$, $W(y',\tilde{r},\tau)$, $M_{\text{v}}(y',\tilde{r},\tau)$, which are the solutions of *the system of differential equations of spray dynamics*

$$\begin{cases} \dfrac{\partial f_{\text{n.d.}}}{\partial \tau}+\dfrac{\partial}{\partial \tilde{r}}\left(U f_{\text{n.d.}}\right)+\dfrac{\partial}{\partial y'}\left(W f_{\text{n.d.}}\right)=0; & (4) \\ \dfrac{\partial W}{\partial \tau}+W\dfrac{\partial W}{\partial y'}=\dfrac{3}{2}\dfrac{\sqrt{\beta}\,C_{\text{dr}}}{B_{\text{s}}\tilde{r}}\dfrac{(1-W)^2}{2}; \qquad C_{\text{dr}}=24/\text{Re}+6/\text{Re}^{1/2}+0.28; & (5) \\ \dfrac{\partial M_{\text{v}}}{\partial \tau}+\dfrac{\partial M_{\text{v}}}{\partial y'}=\dot{F}_{\text{v}} f_{\text{n.d.}}\Delta\tilde{r}\,. & (6) \end{cases}$$

where $y'=y\beta^{1/2}/2a_0$, $W=w/V_c$, $U=2u/(B_s\beta^{1/2}V_c)=-\mathrm{HNu}/16\tilde{r}$, $\mathrm{H}=2\eta/\left(a_0\beta^{1/2}B_s^2V_c\right)$ is dimensionless evaporation constant, $M_v=m_v/m_0$, $\mathrm{Re}=\rho_c 2rW_{rel}/\mu_c$ is the daughter droplet's current Reynolds number, $W_{rel}=V_c-V_5+w$, $\dot{F}_v=0.1875\tilde{r}\mathrm{H}B_s^3\mathrm{Nu}$. For the reasons listed in [5], the evaporation enhancement in the high-speed flow past droplets was taken into account by using the evaporation law in Ranz–Marshall form

$$\frac{dr}{dt}=-\frac{\eta\mathrm{Nu}}{16r}, \qquad \mathrm{Nu}=2+0.6\mathrm{Re}^{1/2}\mathrm{Pr}^{1/3}, \tag{7}$$

where Nu and Pr are the Nusselt and Prandtl numbers for a daughter droplet. Two evaporation constant values $\eta=2.7\cdot10^{-6}m^2/\mathrm{sec}$ and $\eta=1.0\cdot10^{-6}m^2/\mathrm{sec}$ were used in calculations.

4.3. Equations of combustible mixture motion. When the quantitative modeling of the droplet phase – vapor mixture generation is completed, the description of a combustible mixture motion behind detonation front is feasible. The system of multi-phase motion can be written in the following general form [2]:

$$\begin{aligned}
&\frac{\partial\rho_i}{\partial t}+V_i\frac{\partial\rho_i}{\partial x}+\rho_i\frac{\partial V_i}{\partial x}=\sum_{j=1}^{5}J_{ji};\\
&\rho_i\left(\frac{\partial V_i}{\partial t}+V_i\frac{\partial V_i}{\partial x}\right)=-\alpha_i\frac{\partial p}{\partial x}+\sum_{j=1}^{5}\left[F_{ji}+J_{ji}\left(V_{ji}-V_i\right)\right];\\
&\rho_i\left(\frac{\partial\left(e_i+0.5V_i^2\right)}{\partial t}+V_i\frac{\partial\left(e_i+0.5V_i^2\right)}{\partial x}\right)=-\frac{\partial}{\partial x}(\alpha_i pV_i+q_i)-p\frac{\partial\alpha_i}{\partial t}+\sum_{j=1}^{5}\left[F_{ji}V_{ji}+Q_{ji}+J_{ji}\left(e_{ji}+\frac{p}{\rho_i^0}-e_i+\frac{V_{ji}^2-V_i^2}{2}\right)\right];
\end{aligned} \tag{8}$$

Here ρ, V, p, e, α, q are the volumetric mass density, velocity, pressure, internal energy, phase volumetric concentration, heat flux vector, correspondingly, J_{ji}, F_{ji}, Q_{ji} denote mass, impulse and energy transfer from phase "*j*" to phase "*i*" per unit volume. The proposed approach to the description of irreversible inter-phase processes behind the detonation front allows determining intensiveness (per unit time and unit volume) of mass exchange between components: burnt masses of oxidizer and fuel, m_o, m_f, ($m_o=\psi m_f$, ψ is the stoichiometric coefficient); m_{ev} – evaporated mass of daughter droplets; $m_{a.a.}$ – atomized aerosol mass. These quantities permit to find out the phase transfer rates J_{ji}, F_{ji}, Q_{ji}.

The equation set is closed by the equations of state of phases: $p=(R_1\rho_1^0+R_2\rho_2^0+R_3\rho_3^0)T_c$; $\rho_5^0=const$; where R_i are the individual gas constants, ρ_i^0 are the component true densities.

5. Regimes of Aerosol Burning Behind the Detonation Front

For a given detonation front velocity D the equation set (1)–(8) permits to calculate the detonation wave parameters $V_c, V_5, \rho_1, \rho_2, \rho_3, \rho_4, \rho_5, p, T_c, f_{n.d.}$ and in this way to determine in the one-dimensional plane approximation a flow structure behind the front of detonation wave. The value of the self-sustained regime velocity $D_{C\text{-}J}(a_0,\psi)$ is then the eigenvalues of the boundary-value problem for the combustible aerosol flow behind detonation front. They are defined as those which provide possibility of the stationary flow transition from subsonic flowfield behind the front, to the supersonic one through a sonic plane, which appears as the singular point of the system (8).

Described above mathematical model is realized for the case of stoichiometric kerosene–oxygen mixture ($\psi = 3.571$). Differential equations of dynamics of two-phase polydisperse spray (4)–(6) and monodispersed aerosol motion (8) are solved numerically with a help of Lax – Vendroff finite-difference scheme. Assumption is made that the gas components' mixing is much more rapid compared with atomization and vaporization processes, so that the mixing is instantaneous. The chemical reaction kinetics is simplified by using the Arrhenius law for the induction time: $\tau_{\text{ind}} = A\exp(E/RT_{\text{c}})$.

The flow structure inside detonation wave is determined. The intensification of evaporation by airstream is substantial, so, the fuel is presented in spray generally in the vapour phase, though the evaporation constant value influence is strong. The combustible mixture is substantially overreached, as vapor density exceeds the stoichiometric value. Besides, vapour overproduction leads to mixture overcooling.

The aerosol burning regime correlates with the flow structure. The regime is regulated by the ratio of drop atomization time t_{ch} to chemical induction time τ_{ind}, which is the governing parameter depending strongly on the shock front velocity D. When D increases, the chemical induction time drops greater than the characteristic time of physical processes, so that chemistry is "waiting" for the physics delay. Vice versa, when D drops, the chemical induction time raises greater than the characteristic time of physical processes, so that energy release is waiting for chemistry. Variation of D helps to fit the kinetics of physical versus chemical processes in such a way that the stationary self-sustained regime $D_{\text{C-J}}$ is possible.

8. Conclusions

The model is built, which is able to investigate quantitatively the internal structure of detonation combustion wave in liquid aerosol system via the detailed calculation of the main inter-phase relaxation processes: aerosol drop atomization, evaporation of the whole mass of the accelerating sprayed droplets, energy release due to chemical reaction. The model allows analyzing the feasibility of the stationary self-sustained regime of detonation in closed form, given the aerosol drop radius and aerosol properties.

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