Spray injection and ignition in a heated chamber modeling

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Abstract: - Computer simulation of liquid fuel jet injection into heated atmosphere of combustion chamber, mixture formation, ignition and combustion need adequate modeling of evaporation, which is extremely important for the curved surfaces in the presence of strong heat and mass diffusion fluxes. Combustion of most widely spread hydrocarbon fuels takes place in a gas-phase regime. Thus, evaporation of fuel from the surface of droplets turns to be one of the limiting factors of the process as well. The problems of fuel droplets atomization, evaporation being the key factors for heterogeneous mixtures reacting mixtures, the nonequilibrium effects in droplets atomization and phase transitions will be taken into account in describing thermal and mechanical interaction of droplets with streaming flows. In the present lecture processes of nonequilibrium evaporation of small droplets will be discussed. It will be demonstrated, that accounting for nonequilibrium effects in evaporation for many types of widely used liquids is crucial for droplets diameters less than 100 microns, while the surface tension effects essentially manifest only for droplets below 0.1 micron. Investigating the behavior of individual droplets in a heated air flow allowed to distinguish two scenarios for droplet heating and evaporation. Small droplets undergo successively heating, then cooling due to heat losses for evaporation, and then rapid heating till the end of their life time. Larger droplets could directly be heated up to a critical temperature and then evaporate rapidly. Atomization of droplets interferes the heating and evaporation scenario.

Key-Words: - Combustion, ignition, phase transition, heat flux, evaporation, non-equilibrium, diffusion, mathematical simulation

1 Introduction

Investigations of acute problems of heat and mass exchange accompanied by phase transitions need adequate modeling of evaporation, which is extremely important for small droplets and sprays [1-4]. Combustion of hydrocarbon fuels takes place mostly in a gas-phase regime. Thus, evaporation of fuel from the surface of droplets turns to be one of the limiting factors of the process [5-7].

Evaporation under terrestrial conditions is strongly influenced by gravity induced thermoconvective flows. Those effects mask the influence of non-equilibrium processes in phase transitions making the proper understanding of the phenomenon very difficult in the ground-based experiments. Besides, non-equilibrium effects have a stronger manifestation under low gravity conditions for interfaces of high curvature.

The aim of the present study is to develop a mathematical model for the non-equilibrium evaporation and to determine the applicability limits for the existing quasi-equilibrium models. The problem will be solved taking evaporation of small droplets as an example.

Mathematical models for individual droplets evaporation incorporated in polydispersed mixtures modeling, are usually based on the assumptions of the equilibrium character of phase transitions.⁵ Comparison of theoretical and experimental data shows that this assumption being undoubtedly valid for large droplets and flat surfaces, brings to essential errors for small droplets [4, 10, 11].

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Fig. 1. Schematic picture of diffusion flame surrounding fuel droplet in the atmosphere of an oxidant.

The aim of the present study is to develop a mathematical model for the non-equilibrium evaporation of droplets and to determine the applicability limits for the existing quasi-equilibrium models.

2 Mathematical model

We regard an axis-symmetrical problem in the coordinate system with the center coinciding with the center of a droplet, the zone $x > x_W$ occupied by a gas mixture, the zone $0 < x < x_W$ - by liquid, $x = x_W$ being the phase interface.

The system of equations for the gas mixture above the interface ($x > x_w$) has the form:

$$\frac{\partial \rho}{\partial t} + \frac{1}{x^k} \frac{\partial \rho v x^k}{\partial x} = 0, \qquad (1)$$

$$\frac{\partial \rho Y_i}{\partial t} + \frac{1}{x^k} \frac{\partial \rho Y_i v x^k}{\partial x} = \frac{1}{x^k} \frac{\partial}{\partial x} x^k \rho D_i \frac{\partial Y_i}{\partial x},$$

 $i = 1, \dots N$
(2)

$$\frac{\partial \rho h}{\partial t} + \frac{1}{x^k} \frac{\partial \rho v h x^k}{\partial x} = \frac{1}{x^k} \frac{\partial}{\partial x} x^k \lambda \frac{\partial T}{\partial x} +$$
(3)

$$+\frac{1}{x^{k}}\frac{\partial}{\partial x}\left(x^{k}\rho T\sum_{i=1}^{N}D_{i}c_{pi}\frac{\partial Y_{i}}{\partial x}\right)$$
(5)

$$p = \rho \frac{R}{m} T = \rho RT \sum_{i=1}^{N} \frac{Y_i}{m_i} = const , \quad (4)$$

The system of equations for multi-component fluid $(0 < x < x_w)$ looks as follows:

$$\frac{\partial \hat{\rho}}{\partial t} + \frac{1}{x^k} \frac{\partial \hat{\rho} v x^k}{\partial x} = 0, \qquad (5)$$

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$$\frac{\partial \hat{\rho} Y_i}{\partial t} + \frac{1}{x^k} \frac{\partial \hat{\rho} Y_i v x^k}{\partial x} = \frac{1}{x^k} \frac{\partial}{\partial x} x^k \hat{\rho} D_i \frac{\partial Y_i}{\partial x}, \quad (6)$$

$$i = 1, \dots N$$

$$\frac{\partial \hat{\rho} \hat{h}}{\partial t} + \frac{1}{x^{k}} \frac{\partial \hat{\rho} v \hat{h} x^{k}}{\partial x} = \frac{1}{x^{k}} \frac{\partial}{\partial x} x^{k} \lambda \frac{\partial T}{\partial x}, \qquad (7)$$

where ρ is density of the mixture; v - velocity; Y_i mass concentration of the *i*-th component; m_i - its molar mass; D_i - diffusion coefficient; λ - heat conductivity; T - temperature; $h = c_p T = \sum_{i=1}^{N} c_{pi} Y_i T$

- specific enthalpy of the mixture; c_{pi} - specific heat capacity of the component at constant pressure; k=0,1,2 correspond to the cases of plane, cylindrical and spherical symmetry respectively. The specific volume for fluid mixture $1/\hat{\rho} = \sum_{i=1}^{N} Y_i / \rho_i + L\Delta V_x$, and the specific enthalpy is $\hat{h} = \sum_{i=1}^{N} h_i Y_i + L\Delta h_x$, where $L\Delta V_x$, $L\Delta h_x$ are specific extra volume and extra enthalpy for the solution.

The boundary conditions at phase interface $x = x_W$ are:

$$(\rho v)_g = (\rho v)_l = \dot{m} , \qquad (8)$$

$$(\rho v Y_i)_g - (\rho D_i \frac{\partial Y_i}{\partial x})_g = (\rho v Y_i)_l - (\rho D_i \frac{\partial Y_i}{\partial x})_l = \dot{m}_i$$
$$\sum_{i=1}^N h_{Li} \dot{m}_i = \left(\lambda \frac{\partial T}{\partial x}\right)_g + \left(\lambda \frac{\partial T}{\partial x}\right)_l + \dot{m} L \Delta h_x,$$

where subscripts g,l denote the values of parameters in gas and liquid phases respectively; h_{Li} is the specific enthalpy of phase transition. The modified Hertz-Knudsen equation for non-equilibrium evaporation will serve as an additional boundary condition:

$$p_i = p_e X_i = p_i^*(T_W) - \frac{1}{\delta_i} \sqrt{\frac{2\pi RT}{m_i}} \dot{m}_i,$$
 (9)

where X_i is the molar concentration of the *i*-th component; p_i is the partial pressure of the *i*-th component above the interface; δ_i is the accommodation coefficient; $p_i^*(T_W)$ is the equilibrium vapor pressure for the *i*-th component at a temperature T_W , which could be determined from the Clausius-Clapeyron equation or its simplified solutions:

$$\frac{p_0}{p_i^*} = \exp\frac{h_{Li}m_i}{R} \left(\frac{1}{T_W} - \frac{1}{T_0}\right).$$
 (10)

The boundary conditions at infinity $(x \rightarrow \infty)$ are the following:

$$T = T_e, Y_i = Y_{ie}, i = 1,...N$$
 (11)

The boundary conditions in the center $(x \rightarrow 0)$ are:

$$\frac{\partial T}{\partial x} = 0, \frac{\partial Y_i}{\partial x} = 0, i = 1, \dots N .$$
(12)

To solve the system (1)-(7) along with the boundary conditions (11)-(12) one needs to pose initial distributions for temperature and concentrations, which would not contradict the boundary conditions.

The sensitivity of results on non-equilibrium evaporation to variation of droplets radii and other parameters [11] brought us to the necessity to search for a universal dimensionless parameter, which could characterize the deviation of the evaporation process from an equilibrium one. To obtain an analytical solution we regard the simplified problem of a steadystate evaporation of a single droplet under nonequilibrium conditions.

3 Steady-state solution for nonequilibrium evaporation

Regard the steady-state problem of nonequilibrium evaporation of uni-component uniformly heated liquid droplet of a constant radius. The governing system of equations takes the form:

• $x > x_W$

$$\frac{d}{dx}(\rho v x^2) = 0, \qquad (13)$$

$$\frac{d}{dx}(\rho Y_i v x^2) = \frac{d}{dx}(x^2 \rho D_i \frac{dY_i}{dx}), \quad (14)$$

$$\frac{d}{dx}(\rho v h x^2) = \frac{d}{dx}(x^2 \lambda \frac{\partial T}{\partial x}) +$$
(15)

$$+\frac{d}{dx}\left(x^{2}\rho T\sum_{i=1}^{N}D_{i}c_{pi}\frac{dY_{i}}{dx}\right)$$

$$p = \rho \frac{R}{m}T = \rho RT \sum_{i=1}^{N} \frac{Y_i}{m_i} = const , \quad (16)$$

• $0 < x < x_W$

$$Y_{Nl} = 1, Y_{il} = 0, i = 1, \dots, N - 1, T = T_{W}$$
(17)

• $x = x_W$

$$(\rho v)_g = (\rho v)_l = \dot{m}, \qquad (18)$$

$$\dot{m}Y_{ig} = (\rho D_i \frac{dY_i}{dx})_g, \qquad (19)$$

$$\dot{m}(Y_{Ng}-1) = (\rho D_N \frac{dY_N}{dx})_g,$$
 (20)

$$h_L \dot{m} = \left(\lambda \frac{dT}{dx}\right)_g,\tag{21}$$

$$p_e X_i = p_i^*(T_W) - \Delta p_i , \qquad (22)$$

where $\Delta p_i = \frac{1}{\delta_i} \sqrt{\frac{2\pi RT}{m_i}} \dot{m}_i$ for the non-equilibrium

model of phase transitions, and $\Delta p_i = 0$ - for an equilibrium one. The boundary conditions at infinity $(x \rightarrow \infty)$ take the form:

$$T = T_e, Y_i = Y_{ie}, i = 1, ..., N.$$
 (23)

As it follows from the equation (13) and the boundary condition (18) the following integral is valid within the gas phase:

$$\rho v = \dot{m} \frac{x_W^2}{x}.$$
 (24)

The equation (15) could be converted into the following form

$$\frac{d}{dx}(\rho vhx^{2}) = \frac{d}{dx}\left(x^{2}\frac{\lambda}{c_{p}}\frac{\partial T}{\partial x}\right) + \frac{d}{dx}\left(x^{2}\lambda T\sum_{i=1}^{N}(Le_{i}-1)\frac{dY_{i}}{dx}\right),$$
(25)

which shows that for gases $(Le_i = \rho D_i c_{pi} / \lambda \approx 1)$ the last term in the right hand side of the equation could be neglected.

On introducing the following dimensionless variables

$$z = \frac{x}{x_w}, \chi_h = \frac{h}{h_e}, \chi_L = \frac{h_L}{h_e}, \chi_i = Y_i, Pe = \frac{mx_w}{\rho D}$$

the system of equations (14), (15) takes the form:

$$\frac{d\chi_j}{dz} = \frac{d}{dz} \frac{z^2}{Pe} \frac{d\chi_j}{dz}, i = 1, \dots, N, h. \quad (26)$$

The boundary conditions for z=1 are

$$\chi_{iW} = \frac{1}{Pe} \frac{d\chi_{ig}}{dz} \bigg|_{W}, \quad \chi_{NW} - 1 = \frac{1}{Pe} \frac{d\chi_{Ng}}{dz} \bigg|_{W}, \quad (27)$$

$$\chi_L = \left(\frac{1}{Pe}\frac{d\chi_h}{dz}\right)_W,\tag{28}$$

$$X_N = X_N^* - \varsigma_N, \qquad (29)$$

where
$$\zeta_N = \frac{\Delta p_N}{p_e} = Pe \cdot I_N \cdot \sqrt{\frac{c_{pe}m_e}{c_{pN}m_N}} \chi_{hW},$$

$$I_N = \frac{D_{eN}}{\delta_N x_W} \sqrt{\frac{2\pi}{R_e T_e}}.$$
(30)

Due to our derivations the deviation of the process from the equilibrium one could be characterized by a dimensionless parameter I_N .

The boundary conditions at infinity $(z \rightarrow \infty)$ are:

Introducing a new variable

$$\xi(z) = \int_{z}^{+\infty} \frac{Pe}{z^2} dz \Longrightarrow \frac{d}{dz} = -\frac{Pe}{z^2} \frac{d}{d\xi}, \quad (32)$$

which varies in the range $(\xi_W, 0)$

$$\frac{z \Rightarrow \xi}{(1,+\infty) \Rightarrow (\xi_W,0)}, \quad \xi_W = \int_1^{+\infty} \frac{Pe}{z^2} dz,$$

one could transform the equation (26) as follows

$$\frac{d\chi_j}{d\xi} = -\frac{d^2\chi_j}{d\xi^2}.$$
 (33)

The solution of (33) is the following:

$$\chi_j = A_j + B_j e^{-\xi}, j = 1, ..., N, h$$
, (34)

where A_j, B_j can be determined from the boundary conditions.

$$Y_{jW} = Y_{je}e^{-\xi_{W}}, j = 1,..., N - 1;$$

$$Y_{NW} = 1 - (1 - Y_{Ne})e^{-\xi_{W}};$$

$$\chi_{hW} = 1 + \chi_{L}(1 - e^{\xi_{W}}).$$
(35)

Substituting (35) into the boundary condition (29) one obtains the equation determining the dimensionless evaporation rate ξ_W or the Peclet number *Pe*:

$$Y_{NW} \frac{m_{W}}{m_{N}} = X_{N}^{*}(\chi_{hW}) - Pe \cdot I_{N} \cdot \sqrt{\Gamma_{eW} \frac{m_{W}}{m_{N}} \chi_{hW}};$$

$$m_{W} = \left(\sum_{i=1}^{N} \frac{Y_{iW}}{m_{i}}\right)^{-1}; \Gamma_{eW} = \frac{\gamma_{e}(\gamma_{W} - 1)}{\gamma_{W}(\gamma_{e} - 1)}; \gamma = \frac{c_{p}}{c_{v}};$$
 (36)

$$X_{N}^{*} = \frac{p_{0}}{p_{e}} \exp\left[\chi_{L} \frac{m_{W}}{m_{N}} \frac{\gamma_{W}}{(\gamma_{W} - 1)} \left(\frac{1}{\chi_{h0}} - \frac{1}{\chi_{hW}}\right)\right].$$

The last expression for the phase equilibrium function could be also substituted by the data from the tables on the thermophysical properties of substances [13].

The solutions (34) providing flow parameters distribution around evaporating droplet then take the form:

$$Y_{i} = Y_{ie}e^{-\xi};$$

$$Y_{N} = 1 - (1 - Y_{Ne})e^{-\xi};$$

$$\chi_{h} = 1 - \chi_{L}e^{\xi_{W}}(1 - e^{-\xi});$$

where ξ_W could be obtained from solution (35), (36). To determine the $\xi(z)$ function analytically one could assume that $\rho D = const / \rho$, which could be a good approximation for constant pressure problems [6]. Then the equalities are valid

$$\frac{\rho D}{\rho_e D_e} = \frac{\rho_e}{\rho} = \frac{h}{h_e} \frac{Rc_{pe}}{c_p R_e} = \chi_h \frac{\gamma - 1}{\gamma} \frac{\gamma_e}{\gamma_e - 1},$$

which neglecting the γ variation in space provide the following formula

$$\frac{\rho D}{\rho_e D_e} = \chi_h \,. \tag{37}$$

Formula (37) allows to express Peclet number in the following way

$$Pe = \frac{\dot{m}x_W}{\rho D} = \frac{\dot{m}x_W}{\rho_e D_e} \frac{\rho_e D_e}{\rho D} = \frac{Pe_e}{\chi_h},$$

which being substituted into (32) provides an equation:

$$\frac{d\xi}{dz} = -\frac{Pe_e}{\chi_h z^2}, \quad \xi(1) = \xi_W. \quad (38)$$

Substituting the solution $\chi_h(\xi)$ and integrating the equation (38) one obtains analytical formula providing the link between *z* and ξ :

$$z = \frac{Pe_e}{\xi + \chi_L e^{\xi_W} (1 - \xi - e^{-\xi})},$$

$$Pe_e = (1 - \chi_L e^{\xi_W}) \xi_W + \chi_L (e^{\xi_W} - 1) =$$

$$= \xi_W - \chi_L \xi_W^2 / 2 - O(\xi_W^3).$$

The set of equations (35), (36) allows to determine the unknown Peclet number in non-equilibrium phase transitions as a function of the following parameters:

$$\frac{m_i}{m_N}, \chi_L, \frac{p_0}{p_e}, Y_{ie}, \Gamma_{eW}, X_N^*(\chi_{hW}), \quad I_N.$$

The first six of them characterize the media and the boundary conditions. The seventh parameter I_N characterizes the deviation of the system from the equilibrium state. The value I_N is zero for the case of equilibrium, and it grows remaining positive($I_N > 0$) with the increase of the deviation from the equilibrium.

4 The role of non-equilibrium effects

To investigate the influence of non-equilibrium effects in phase transitions Peclet numbers for droplets evaporation were determined for different values of I_N parameter (Fig.1). The values of the other governing parameters were assumed to be the following

$$\frac{m_i}{m_N} = 4.75; \ \chi_L = 0.54; \ \frac{p_0}{p_e} = 1; \ Y_{Ne} = 0.1,$$
$$\Gamma_{eW} = 1, \ \chi_{h0} = 0.9$$

The Fig. 1 gives the plots of Peclet numbers, obtained within the frames of non-equilibrium (Pe_{ne}) and quasi-equilibrium (Pe_{eq}) models. The

value of $|\delta Pe|$ is also plotted in Fig. 2 to characterize the relative deviation of Peclet number from its equilibrium value ($\delta Pe = (Pe_{ne} - Pe_{eq})/Pe_{eq}$). The Peclet number for non-equilibrium evaporation could be determined by the formula

$$\frac{Pe}{Pe_{eq}} = \Psi_S(I_N, \frac{m_i}{m_N}, \chi_L, \frac{p_0}{p_e}, Y_{ie}, \Gamma_{eW}, X_N^*(\chi_{hW})), (39)$$

wherein the value of the Ψ_s – *factor* as a function of I_N parameter for the chosen values of other governing parameters is shown in Fig. 2a. The equilibrium Peclet number as obtained from the quasi-steady solution has the following form:

$$Pe_{eq} = \log_e \left(1 + \frac{c_{pe}T_e - c_{pW}T_W}{h_L} \right). \quad (40)$$

The results of comparison of non-equilibrium and quasi-equilibrium Peclet numbers for droplet evaporation show that the rate of evaporation strongly depends on the value of the parameter I_N . On increasing I_N Peclet number decreases rapidly as compared with the equilibrium evaporation; the deviations of the evaporation rates from those predicted by the equilibrium model turn to be larger and larger. For $I_N <1$ the divergence of equilibrium and non-equilibrium solutions $|\delta Pe|$ does not exceed 4%, for $I_N = 10$ the deviations increases up to 25%, for $I_N > 100$ the deviation surpasses an order of magnitude. Thus in order to have adequate estimates for small droplets evaporation rate one needs to use the nonequilibrium model for $I_N > 1$.

To have adequate data for small droplets $(I_N > 1)$ evaporation rates it is necessary to use the non-equilibrium model.



Fig. 2a. Peclet number variation versus I_N parameter for equilibrium and non-equilibrium evaporation.



Fig. 2b. Droplet dimensionless radius variation versus time for different initial values of I_{Ne} parameter characterizing deviation of the system from the equilibrium.

To obtain an analytical formula for dimensionless evaporation rate ξ_W let us assume that it is a small value $\xi_0 \ll 1$, which means that (Pe $\ll 1$). Then for the two component mixture (N = 2 - evaporating component, i = 1 - inert component) one obtains the following formula:

$$\xi_{W} = \frac{E - \frac{Y_{2e}}{Y_{2e} + \frac{m_{2}}{m_{1}}(1 - Y_{2e})}}{\frac{m_{2e}}{m_{1}}(1 - Y_{2e})^{2} + \frac{m_{2e}}{R}(c_{p1} + \Delta c_{p}Y_{2e})\chi_{L2}^{-2} \cdot E + I_{N}\sqrt{\frac{c_{pe}R_{2}}{(c_{p1} + \Delta c_{p}Y_{2e})R_{e}}}}$$

where

$$E = \exp\left[\frac{h_{L2}m_2}{R}\left(\frac{1}{T_0} - \frac{\left(c_{p1} + \Delta c_p Y_{2e}\right)}{c_{pe}T_e}\right)\right] = \\ \exp\left[\frac{\chi_{L2}m_2}{R}\left(\frac{c_{p0}}{\chi_0} - \left(c_{p1} + \Delta c_p Y_{2e}\right)\right)\right]$$

The last formula can be essentially simplified on assuming the absence of fluid vapor at infinity $Y_{2e} = 0$:

$$\xi_{0} = \frac{\frac{m_{2}}{m_{1}} \frac{\chi_{L2}m_{2}}{R} \left(\frac{c_{p0}}{\chi_{0}} - c_{p1}\right)}{1 + c_{p1}\chi_{L2}^{3} \frac{m_{2}}{m_{1}} \left(\frac{m_{2}}{R}\right)^{2} \left(\frac{c_{p0}}{\chi_{0}} - c_{p1}\right) + I_{N} \frac{m_{2}}{m_{1}} \sqrt{\frac{c_{pe}R_{2}}{c_{p1}R_{e}}}$$

The above formulas testify that the increase of parameter I_N brings to a decrease of dimensionless evaporation rate.

The results of theoretical and numerical analysis show that in order to have adequate data for

evaporation rates of small droplets ($I_N > 1$)it is necessary to use the non-equilibrium model.

5 Quasi-steady solution for a single droplet evaporation

Investigations of unsteady-state droplet evaporation show that for small droplets flow parameters in gas phase reach their quasi-steady values very quickly. Thus the quasi-steady approximation regarding droplet evaporation could be used, which means that its radius decreases in time much slower than gas flow parameters come to a steady state. Thus it is assumed, that the rate of droplet evaporation for each time moment could be determined based on the obtained steady non-equilibrium solution. Then the decrease of the droplet radius can be determined by the following formula:

$$\frac{dx_W}{dt} = -\frac{\dot{m}}{\rho_{Nl}}.$$
(41)

On introducing dimensionless variables

$$r = \frac{x_W}{x_{W0}}, \quad \tau = \frac{t}{t_0}, \quad t_0 = \frac{\rho_{Nl} x_{W0}^2}{2\rho_e D_e P e_{eq}} \quad (42)$$

equation (41) takes the form $\frac{1}{2}$

$$\frac{dr}{d\tau} = -\frac{mt_0}{\rho_{Nl}x_{W0}} = -\frac{Pe}{r}\frac{\rho_e D_e t_0}{\rho_{NL}x_{W0}^2},\qquad(43)$$

where x_{W0} is the initial radius, t_0 is the characteristic time for droplet evaporation under equilibrium conditions.

Fig. 2b presents the comparison of $r(\tau)$ functions (trajectories) obtained for different initial values of *I* parameter ($I_e = \frac{D_e}{\delta_N x_{W0}} \sqrt{\frac{2\pi}{R_e T_e}}$)

characterizing initial deviation of the system from an equilibrium state. Increasing the initial deviation from the equilibrium brings to a decrease of the slope of the curve and increases the actual time for droplet evaporation.

6 Droplet evaporation in a streaming flow

Droplets in quiescent gas could be observed only in microgravity and investigation of their evaporation is performed to obtain material and kinetic data. Under normal gravity condition on evaporating in a heated atmosphere droplet generates a cooler environment due to energy consumption for evaporation. Thus thermo-convective induced flows are possible. The effect of thermal convection is essential as long as Mar number is larger then unity Mar = $t_{evap}/t_{conv} > 1$. This number for evaporating droplet could be evaluated as Mar = $t_{evap}/t_{conv} = \frac{\sqrt{gr_0^3}h_L}{Dc_{pe}(T_e - T_W)}$. For small

droplets Mar number could be less then unity, and thermal convection is no longer essential. Another case is streaming flows, which are characterized by presence of velocity difference between gas and droplet.

The momentum equation for a single droplet motion in the gas flow has the following form

$$m\frac{d\vec{u}}{dt} = m\vec{g} - \phi \cdot \nabla p + \vec{f}_d, \quad \frac{d\vec{r}}{dt} = \vec{u}, \quad (44)$$

where the drag force could be expressed as follows:

$$\vec{f}_{d} = \frac{C_{d}}{2} \rho_{g} \frac{\pi d^{2}}{4} (\vec{v} - \vec{u}) |\vec{v} - \vec{u}|, \qquad (45)$$

the drag coefficient being the function of Reynolds number [5]

$$C_d = \left(\frac{24}{\text{Re}} + \frac{4,4}{\sqrt{\text{Re}}} + 0,42\right)\beta \cdot K, \qquad (46)$$

$$\operatorname{Re} = \frac{\rho |\vec{v} - \vec{u}| d}{\mu}, \qquad (47)$$

$$\beta = \sqrt{\frac{\rho}{\rho_s} \left(2 - \frac{\rho}{\rho_s}\right)}, \quad K = \left(\frac{T}{T_s}\right)^{4/5}, \text{ where}$$

$$\underline{\rho_s} = \begin{cases} \left(1 + \frac{\gamma - 1}{2}M^2\right)^{-\gamma}, & M < 1; \end{cases}$$

(

$$\overset{\frown}{\rho} = \left[\frac{(\gamma+1)M^2}{(\gamma-1)M^2+2} \left(1 + \frac{\gamma-1}{2} \cdot \frac{(\gamma-1)M^2+2}{2\gamma M^2 - (\gamma-1)} \right)^{1/(\gamma-1)}, M \ge 1.$$

(48)

Gravity induced streaming flows could exist for rather long time, while in the absence of gravity the characteristic time for the streaming flow being essential is the function of droplet initial diameter and relative gas velocity. It could be estimated by the following formula

$$\tau = \frac{v_0}{a_0}$$
, where $a_0 = \frac{f_d(t=0)}{m_0}$. (49)

The energy equation for a droplet has the following form

$$m\frac{de}{dt} = q + Q_s$$
, where $e = c_{vs}T_s + h_f^0$. (50)

The energy of phase transitions could be determined by the formula:

$$Q_s = \frac{dm}{dt} h_L, \qquad (51)$$

where h_L is the latent heat of evaporation. Heat flux to a single droplet from the surrounding gas flow is determined as follows [5]

$$q = \begin{cases} \pi d\lambda \cdot \operatorname{Nu} \cdot (T - T_s), & \operatorname{Re} < 1000; \\ \pi d^2 \rho |\vec{v} - \vec{u}| \cdot \operatorname{St} \cdot (H_r - H_w), & \operatorname{Re} \ge 1000. \end{cases}$$
(52)

where

Nu = 2+0,16 · Re^{2/3} · Pr^{1/3}, St =
$$\frac{C_d}{2}$$
 Pr^{-2/3}, (53)

On reaching by the droplet temperature the boiling value the evaporation rate is determined by a simple formula

$$\frac{dm}{dt} = -\frac{q}{h_L}, \quad T = T_b.$$
(54)

Else the non-equilibrium evaporation model is used to determine the evaporation rate

$$\dot{m} = \pi d \cdot \rho D \cdot \operatorname{Nu} \cdot \log\left(\frac{1 - Y_e}{1 - Y_w}\right),$$
 (55)

$$Y_{w} = \frac{W_{N}P_{0}}{Wp} \exp\left[\frac{H_{b}}{R}\left(\frac{1}{T_{b}(P_{0})} - \frac{1}{T_{s}}\right)\right] - \dot{m}\frac{\sqrt{2\pi RT_{s}}}{\pi\delta_{e}pd^{2}}.(56)$$

The dynamic interaction of liquid droplets with the gaseous flow could bring to instability of the interface and atomization of droplets. The criterion for liquid droplets instability is that of the critical Weber number [17]: $\mathbf{We} = \frac{\rho v_{rel}^2 d}{\sigma}$, where σ is the surface tension at the interface, v_{rel} is relative velocity of a droplet

wersus 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 approximate formula [16, 18] determining mean diameters of droplets d_a originating in breakups of initial droplets (diameter d).

$$d_{a} = \begin{cases} d = \left(\frac{6\alpha_{2}}{\pi n}\right)^{\frac{1}{3}}, \ \mathbf{We} < \mathbf{We}_{*}; \\ \frac{d\mathbf{We}_{*}}{\mathbf{We}}, \ \mathbf{We}_{*} \le \mathbf{We} \le \mathbf{We}_{**}; \\ d_{*}, \ \mathbf{We} > \mathbf{We}_{**}; \end{cases}$$
(57)

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:

$$\mathbf{W}\mathbf{e}_{*} = 12(1 + \mathbf{L}\mathbf{p}^{-0.8}), \ \mathbf{W}\mathbf{e}_{**} = 350,$$
 (58)

where the Laplace number $Lp = \frac{d\rho_c \sigma}{\mu_c^2}$, 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 by a droplet elastic energy spent for the breakup. The assumption, that the breakup energy was spent for the formation of new free surface [19] makes it possible to evaluate the number *N* and the mean diameter d_* of the formed droplets:

$$N = \left(1 + \frac{E_*}{\sigma \pi d^2}\right)^3; \ d_* = \frac{d}{1 + \frac{E_*}{\sigma \pi d^2}}.$$
 (59)

The breakup energy could be 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:

$$E_* = A_{drag} - \sum_{i=1}^{N_*} \frac{m_i v_{i*}^2}{2} .$$
 (60)

Assuming that the initial droplet is split into N_* equal droplets ($N_* = \frac{d^3}{d_*^3}$) 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:

$$A_{drag} = \frac{1}{8} N_* \rho C_d v_{rel}^2 \pi d_*^2 d_*;$$

$$d_* = \frac{d}{1 + \frac{1}{4} \left(\frac{1}{2} C_d \rho v_{rel}^2 - \frac{1}{3} \rho_c v_*^2\right) \frac{d}{\sigma}}.$$
 (61)

The mean velocity of the cloud expansion v_* could be evaluated based on the condition of matching the two formulas for d_* at $We = We_{**}$. The reason to perform that matching is that both formulas for breakup regimes were obtained from experiments, thus, indirectly the expansion of the cloud of droplets after the breakup should have been taken into account. On the other hand, the dependence of characteristic droplets diameters on the Weber number should be continuous. Then, finally one obtains

$$d_* = \frac{d\mathbf{W}\mathbf{e}_*}{\frac{1}{8}C_d(\mathbf{W}\mathbf{e} - \mathbf{W}\mathbf{e}_{**})\mathbf{W}\mathbf{e}_* + \mathbf{W}\mathbf{e}_{**}}.$$
 (62)

In modeling droplets breakup in a gas flow the inertia of the process should be taken into account.

Fragmentation does not take place instantaneously: it needs time for small droplets to separate from the initial one, i. e. it needs a definite time for the liquid bridges between the droplets to be established, elongated and broken [40]. The first order estimate of the breakup time gives the following formula:

$$t_* = \frac{d}{v_{rel}} \frac{\mathbf{W} \mathbf{e}_*}{\mathbf{W} \mathbf{e}} \left(1 + \frac{3}{8} C_d \frac{\rho}{\rho_c} \left(1 - \frac{4}{C_d \mathbf{W} \mathbf{e}_*} \right) \right). \quad (63)$$

The problem of droplet interaction with the streaming gas flow was investigated taking into account mechanical drag, atomization of droplets, nonequilibrium heat and mass transfer. A series of model problems was regarded, in which gas flow and droplet initially had different relative velocities and temperatures, and then relaxation took place. Those model problems are similar to that encountered in shock wave initiation of detonation in combustible dispersed fuel-air mixtures. The two-phase flow becomes strongly non-equilibrium behind the shock wave, because due to mechanical inertia droplets keep their speed practically constant and gas accelerates on passing the shock wave. Besides, due to thermal inertia, temperature inside droplets practically does not change, while gas temperature increases instantaneously behind the shock wave. Due to that reason gas temperature in all the numerical experiments was assumed to be higher than the boiling temperature for liquid droplets.

The thermophysical properties for gas and droplets were assumed similar for all numerical experiments: ambient pressure p = 1,013 bar, temperature T = 1000 K, gaseous phase – air, liquid – n-decane (C₁₀H₂₂). Initial droplet temperature was assumed to be T = 300 K.



Fig. 3. Velocity relaxation versus time for droplets of different diameters. $V_0 = 50m/s$, taking into account atomization.



Fig. 4. Mean droplet temperature variation versus time for droplets of different initial diameters. $V_0 = 50m/s$

The relaxation processes for droplets of different diameters were regarded. Numbered lines on the successive figures correspond to the following initial diameters of droplets (curves $1(1\mu m)$, $2(5\mu m)$, $3(10\mu m)$, $4(50\mu m)$, $5(100\mu m)$, $6(500\mu m)$, $7(1000\mu m)$).

Figs. 3-6 illustrate parameters of droplets variation in the process of mechanical and thermal relaxation for the set of numerical experiments assuming initial velocity difference to be equal to 50 m/s. Fig. 3 illustrates velocity relaxation. It is seen that on decreasing initial droplet radius the relaxation process turns to be faster. The decrease of the relaxation time is monotonous. Some curves begin lower than 50 m/s because the relaxation process is too fast for small droplets, and the time scale on the x-axis is logarithmic beginning from a definite small value.



Fig. 5. Droplet diameter variation versus time. $V_0 = 50m/s$

Fig. 4 illustrates droplet temperature variation versus time for droplets of different initial diameters.

The dynamics of droplet heating is the following. For small droplets (curves $1(1\mu m)$, $2(5\mu m)$, $3(10\mu m)$, $4(50\mu m)$) in the very beginning the temperature increases due to external heating. On rapid decrease of droplet relative velocity evaporation in the stream of gas brings to a decrease of temperature. Then on decreasing droplet radius heat fluxes growth brings to an increase of temperature until the droplet disappears. The first

increase of temperature is higher for larger droplets, which relative velocity decreases much slower than for small droplets (curves $5(100 \ \mu m)$), $6(500 \ \mu m)$, $7(1000 \ \mu m)$). Large droplets follow different scenario: The first increase of their temperature goes as high as up to the critical value. Then evaporation takes place at a critical temperature very rapidly. Arrows with numbers in Fig. 4 and 6 indicate the end of droplet life time. That is the reason for a larger droplet (curves 5, 6, 7 in Figs. 4 and 6) to have a shorter life time.

Fig. 5 illustrates droplet diameter variation due to evaporation. It is seen from the figure that evaporation time increases with the increase of initial droplet diameter, but the increase does not take place monotonously: the increase of life time (curves 1, 2, 3, 4) changes for a decrease (curves 4, 5) and then comes back to an increase (curves 5, 6, 7). That testifies the effect of manifestation of different mechanisms depending on the characteristic size of droplets. The first rapid decrease of droplet radius (curves 6, 7 in Fig. 5) is due to atomization of large droplets. The breakup of large droplets (Fig. 5) brings to the conditions that behavior of droplets of initial diameter 500 microns and 1000 microns looks absolutely similar after some time necessary for atomization to proceed.

Fig.6 presents the results for droplet temperature variation versus normalized time t/τ (49), i.e. in the relative time scale characterizing each droplet. As it is seen from the figure all maxima and minima of temperature correspond to nearly the same normalized time moments independently on initial droplet radius. The difference between the two scenarios for droplet behavior in the stream of heated air could be clearly distinguished from this figure.



Fig. 6. Mean droplet temperature variation versus normalized time for droplets of different diameters. $V_0 = 50m/s$, taking into account atomization.



Fig. 7. Velocity relaxation versus time for droplets of different diameters. $V_0 = 100m/s$, taking into account atomization.

Figs. 7 - 9 present the results of similar numerical experiments, but for higher initial relative velocity: $V_0 = 100m/s$. Two different scenario for droplet behavior could be distinguished as well. But for the higher relative velocity smaller droplets already reach critical temperature during the first temperature increase (Fig. 9). Thus curve 4 belongs already to the second group of curves, which corresponds to the second scenario of droplet heating and evaporation. Fragmentation is more essential for higher relative velocity: curves 4, 5, 6, 7 converge in time due to equalizing of droplet radii in fragmentation (Fig. 9).



Fig. 8. Droplet diameter variation versus time for droplets of different diameters. $V_0 = 100m/s$, taking into account atomization.



Fig. 9. Mean droplet temperature variation versus time for droplets of different diameters. $V_0 = 100m/s$, taking into account atomization.



Fig. 10. Droplet diameter variation versus time for droplets of different initial diameters. $V_0 = 50m/s$, atomization not taken into account.

Atomization of droplets changes droplet lifetime and evaporation scenario for large droplets. Figs. 10-11 illustrate droplet diameter variation for droplets of different initial size in interaction with streaming flow not accounting for atomization. Comparison with Figs. 5 and 8 representing results with account of atomization clearly demonstrates the effect.



Fig. 11. Droplet diameter variation versus time for droplets of different diameters. $V_0 = 100m/s$, atomization not taken into account.

7 Droplet cloud combustion modeling.

To investigate the cloud slowing down, heating of particles and surrounding atmosphere, atomization of droplets and shock wave formation due to the transformation of the kinetic energy of the cloud into thermal and kinetic energy of the surrounding gas it is necessary to apply the models for multiphase media accounting for the two-way coupling effects for fragments and gas, thermochemical and mechanical destruction of fragments.

Mathematical models for the non-equilibrium polydispersed mixture flows and breakup of pressurized vessels in non-uniform internal loading are described in details in the papers [19, 20].

The cloud of small droplets injected into the chamber slows down very rapidly due to the drag forces. The deceleration for fragments is proportional to $1/r_0$ and grows up with the decrease of a characteristic size r_0 . The velocity variation versus distance could be estimated by formula:

$$v_{rel} = v_{rel}^0 \exp(-\frac{3}{8}C_d \frac{\rho}{\rho_c} \frac{x}{r_0})$$
(60)

It is seen from (60) that on decreasing droplet size the slowing down distance also decreases. Since droplet cloud incorporates a variety of droplets having different size and speed its evolution could bring to a peculiar non-uniform pattern of droplets distribution within the combustion chamber.

On slowing down the cloud its kinetic energy is converted into the internal energy of the surrounding gas. Droplets are being heated and evaporate. Thus mixture formation takes place.

Numerical modeling of jet injection into a gas-filled cylindrical containment from the wall along the axis was performed based on the developed mathematical models [16, 19]. A cylindrical containment of 0.1 m radius and 0.2 m height was regarded. A cloud of small droplets, characterized by the average diameter 0.3 mm and stochastic deviations 0.05 mm was injected from left bottom along the axis. The fragments initial temperature was 400 K with stochastic deviations \pm 10 K; maximal velocity in the axial direction was assumed to be 20 m/s, average velocity 15 m/s with stochastic deviations 5 m/s both in axial and radial directions. The average density of liquid was assumed as $\rho_c = 1000 \text{ kg/m}^3$, viscosity and surface tension in the liquid 10⁻³ Ns and 10⁻² N/m respectively. The gas pressure inside the containment was varied from 0.01 MPa up to 1.5

MPa, initial temperature $T_0 = 700$ K, molar mass 0.028 kg/mol.



Fig. 12. Model particles location for droplet cloud injection into the chamber with low gas pressure $p_0 = 0.01$ MPa (0.1 atm).



Fig. 13. Successive stage for droplet cloud injection into the chamber with low gas pressure $p_0 = 0.01$ MPa (0.1 atm).



Fig. 14. Model particles location for droplet cloud injection into the chamber with high gas pressure $p_0 = 1$ MPa (10 atm).



Fig. 15. Successive stage for droplet cloud injection into the chamber with high gas pressure $p_0 = 1$ MPa (10 atm).



Fig. 16. Final stage for droplet cloud injection into the chamber with high gas pressure $p_0 = 1$ MPa (10 atm).

Figs. 12 and 13 show the model particles location for the two successive times. The initial pressure of gas inside the containment was rather low: $p_0 = 0.01$ MPa (0.1 atm). The size of circles showing model particles is much larger than their real size, but directly proportional to it. The intensity of color reflects particles temperature.

Figs. 14, 15 and 16 illustrate the model particles locations for the case of a relatively high gas pressure inside the containment ($p_0 = 1$ MPa (10 atm)). The aerodynamic drag is much more essential for the present case. On entering the containment fragmentation of liquid droplets due to their interaction with the atmosphere brings to a formation of very fine droplets in the front part of the cloud (Fig. 14). The droplets, representing smaller fragments, are illustrated by dots in Fig. 14. Nevertheless, the major mass of the cloud is represented by those dots, and only a smaller number of low velocity particles keep its initial size.

The small droplets slow down very rapidly and loose their kinetic energy much faster then the large ones. thus the large fragments, that had initially much lower velocity, come to overtake the small ones (Figs. 15, 16).

Numerical investigations of detonation initiation in dispersed hydrocarbon fuel - air mixtures after mild ignition via DDT and by shock waves of different intensities were performed. The vessel was 0.5 m long and 0.05m diameter. The aerosol occupied the cylindrical coaxial zone beginning from 0.1 m along the axis its diameter being equal to 0.015 m. 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, initial temperature 300 K. The number of model particles used in calculations was 20000. Validation of numerical scheme was performed based on comparing the obtained results of numerical simulations for the detonation wave velocities in dispersed mixtures with available experimental data [16]. To simulate hydrocarbons the following parameters were taken: $\rho = 850 \text{ kg/m}^3$; $\Delta H =$ 43 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 100 μ m, minimal diameter – 10 μ m, maximal $-200 \mu m$. The droplets size distribution function was assumed to be a triangular one. The initial droplets density was varied from 5 to 20 kg/m^3 .

The results of simulations show that for different fuel concentration and intensity of shock wave initiation different scenarios of the process are possible. There could be formed a combustion wave lagging behind attenuating shock. There could be onset of detonation, or galloping detonation in the dispersed layer. For high average density of fuel droplets within the layer combustion does not take place inside layer, where pressure is maximal, however high speed detonation type process onset on the periphery is observed supported by the piston effect due to induced vapor combustion in the zones within the concentration limits.





Fig. 17. Hydrocarbon concentration for successive times of shock wave propagation in dispersed mixture (a, b - initial fuel density 5 kg/m³; c, d - initial fuel density 20 kg/m³).



Fig. 18. Temperature maps (K) for successive stages of shock wave propagation in dispersed mixture (a, b - initial fuel density 5 kg/m^3 ; c, d - initial fuel density 20 kg/m^3).

Thus the results illustrate the fact, that increase of droplet concentration above definite value inhibits the onset of detonation in dispersed mixtures and gives birth to a detonation mode typical for nonpremixed systems.

Conclusions

It was demonstrated that non-equilibrium models more adequately describe final stages of droplet evaporation. Those models are free from the common drawbacks of all quasi-equilibrium models, because non-equilibrium approach allows to avoid non-physical growth of the evaporation rate on decreasing droplet radius.

Accounting for non-equilibrium effects produces an influence on the integral characteristics

of droplet evaporation process. The lifetime for single evaporating droplet could be several times longer under non-equilibrium conditions as compared with equilibrium ones.

Investigating the behavior of individual droplets in a heated air flow allowed distinguish two scenarios for droplet heating and evaporation. Small droplets undergo successively heating, then cooling due to heat losses for evaporation, and then rapid heating till the end of their life time. Larger droplets could directly be heated up to a critical temperature and then evaporate rapidly. Atomization affects droplet life time.

Investigation of poly-dispersed multi-velocity droplet cloud injection into the heated atmosphere of a combustion chamber showed that flow scenario essentially depends on gas state (pressure and temperature) inside the chamber. The fastest droplets undergo fragmentation and slow down rapidly, while the slowest droplets remain big and overtake small ones. This droplet size separation effect manifests stronger for the case of higher gas density inside the chamber.

Increase of droplet concentration above definite value inhibits the onset of detonation in dispersed mixtures and gives birth to a detonation mode typical for non-premixed systems.

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