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# Microexplosion model of hydrocarbon−water composite droplets: an accurate solution

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The paper presents an analytical solution to the problem of temperature dynamics inside a composite spherical droplet consisting of a water microdroplet located in the center of a liquid hydrocarbon droplet around which hot gas flows. To the hydrocarbon−water boundary the coupling conditions are imposed, while for the outer boundary the condition of heat exchange with hot gas is defined. The unsteady temperature of the composite droplet is represented by the eigenfunctions expansion of the Sturm−Liouville problem. The results of calculations via the obtained analytical formula agree satisfactorily with experimental data.

**Keywords:** composite hydrocarbon fuel, eigenfunctions and eigenvalues of the Sturm−Liouville problem, coupling conditions, spherical Bessel functions.

Water−organic fuel emulsions are promising in view of reducing pollutant releases and increasing the efficiency of organic fuel droplets dispersion due to boiling up of water microdroplets located inside hydrocarbon droplets. Composite fuels are studied both experimentally and theoretically [1–6].

A number of papers [7–9] have proposed a simple mathematical model and approximate solution to the problem of temperature dynamics within a composite fuel droplet. In those works, a droplet is represented as a spherical volume of heavy hydrocarbon (diesel fuel), in the center of which there is a water microdroplet. In solving the problem, the fluid convective motion inside a non-isothermal droplet is assumed to be negligible. This simplification is valid for high-viscosity diesel fuel droplets less than a few millimeters in diameter.

The method for solving the model problem proposed in [7] is unreasonably cumbersome and hardly reproducible. In the framework of modern methods of mathematical physics, this problem is solved by conventional expansion of the Sturm−Liouville problem in terms of eigenfunctions. Besides, the solution method [7] exhibits a number of fundamental inaccuracies. First, the problem is defined with a first-kind boundary condition instead of a third-kind one which is consistent with the experimental conditions. Second, the given description of the temperature distribution in the hydrocarbon is incorrect. The Bessel equations have two independent solutions: a first-order Bessel function having a finite value at zero, and a second-order one with logarithmic divergence at zero. Temperature distribution in hydrocarbon should include spherical Bessel functions of both the first and second order. Third, the correct solution of the problem provides an analytical formula in the form of a series in eigenfunctions, which does not require numerical

integration over time. The temperature may be obtained from the solution formula for any moment and any point of the droplet.

The goal of this paper was to present a brief summary of the conventional method for finding an analytical solution based on expansion in a system of orthogonal eigenfunctions.

Fig. 3, $b$ presents a schematic illustration to the problem. Having the initial temperature, a spherical liquid-hydrocarbon droplet ($Oil$) and water microdroplet ($Water$) located in its center get into the hot gas flow having temperature $\Theta_G$. Due to heating, surface temperature of the water microdroplet reaches boiling point $\Theta_{Wboil}$ during time $t_{boil}$. Fig. 1, $b$ demonstrates an example of the temperature distribution within a composite droplet calculated via the analytical solution described below.

Under the experimental conditions with which the calculations are being compared, the contribution of radiative heat transfer is significantly lower than that of convective heat transfer and, thus, is neglected in calculations. The equation for the composite droplet temperature and formula for the initial temperature distribution are

$$\rho c \frac{\partial \Theta}{\partial t} = \lambda \Delta \Theta, \quad \Theta\Big|_{t=0} = \Theta_0. \tag{1}$$

Here $\rho$, $c$, $\lambda$ are the composite droplet density, heat capacity and thermal conductivity coefficient. Let us designate the water and hydrocarbon droplet temperatures as

$$\Theta(r, t) = \begin{cases} \Theta_W(r, t), & r < R_W, \\ \Theta_O(r, t), & R_W < r < R_O, \end{cases}$$

where $R_W$, $R_O$ are the radii of the water droplet and hydrocarbon droplet surface; thermophysical properties of

hydrocarbon and water are different

$$\rho, c, \lambda = \begin{cases} \rho_W, c_W, \lambda_W, & r < R_W, \\ \rho_O, c_O, \lambda_O, & R_W < r < R_O. \end{cases}$$

At the media interface, the coupling conditions are satisfied (the temperature and heat flow continuity):

$$\Theta_W|_{r=R_W} = \Theta_O|_{r=R_W}, \quad -\lambda_W \frac{\partial \Theta_W}{\partial r}\Big|_{r=R_W} = -\lambda_0 \frac{\partial \Theta_O}{\partial r}\Big|_{r=R_W}. \quad (2)$$

To the droplet surface, the boundary condition of convective heat exchange according to the Newton's hypothesis is imposed. The calculations imply that the heat transferred to the drop is spent on its heating and evaporation of liquid from the droplet surface:

$$-\lambda_O \frac{\partial \Theta_O}{\partial r}\Big|_{r=R_O} = \alpha_O \left( \Theta_O|_{r \in R_O} - \Theta_G \right) - \rho_O \Delta H_O \frac{dR_O}{dt}. \quad (3)$$

Here $\alpha_O$ is the heat exchange coefficient in case the hot gas flows around the evaporating droplet [10]; $\Delta H_O$ is the evaporation enthalpy.

The symmetry boundary condition is imposed on the droplet center:

$$\frac{\partial \Theta_W}{\partial r}\Big|_{r=0} = 0. \quad (4)$$

During heating the composite droplets to the water boiling point, evaporation changes the hydrocarbon droplet volume only slightly, and hereinafter the droplet radius is assumed to be constant, namely $dR_O/dt = 0$ [9].

Equation (1), coupling conditions (2), boundary condition (3) exclusive of variations in the droplet volume, and symmetry condition (4) shall be reduced to a dimensionless form. Dimensionless temperatures of water and hydrocarbon are $\Theta_W^* = (\Theta_W - \Theta_G)/\Theta_G$, $\Theta_O^* = (\Theta_O - \Theta_G)/\Theta_G$. Dimensionless coordinate is $r^* = r/R_O$. Dimensionless time is defined as $t^* = \kappa_O t/R_O^2$ ($\kappa_O = \lambda_O/(\rho_O c_O)$ is the hydrocarbon thermal conductivity coefficient). Hereinafter, dimensionless variables are marked with asterisks.

Let us try to find the problem (1)–(4) dimensionless solution in the form of a series in terms of zero-order spherical Bessel functions. The temperature distribution in hydrocarbon includes spherical Bessel functions of the first and second order, while that in the water microdroplet includes first-order spherical Bessel functions automatically meeting symmetry condition (4). The Sturm–Liouville problem for calculating eigenfunctions and eigenvalues of the Laplace operator with a discontinuous transfer coefficient is set up. Based on the coupling conditions, the eigenfunction functional form shall be defined.

Boundary condition (3) provides a characteristic equation whose numerical solution gives the eigenvalues. Fig. 2, $a$ demonstrates the shape of function $\Psi_O(\omega^*)$ whose roots $\omega_n^*$ are the eigenvalues. Breaks of the problem eigenfunctions at the media interface (Fig. 2, $b$) are caused by the difference in thermophysical properties of water and hydrocarbon.
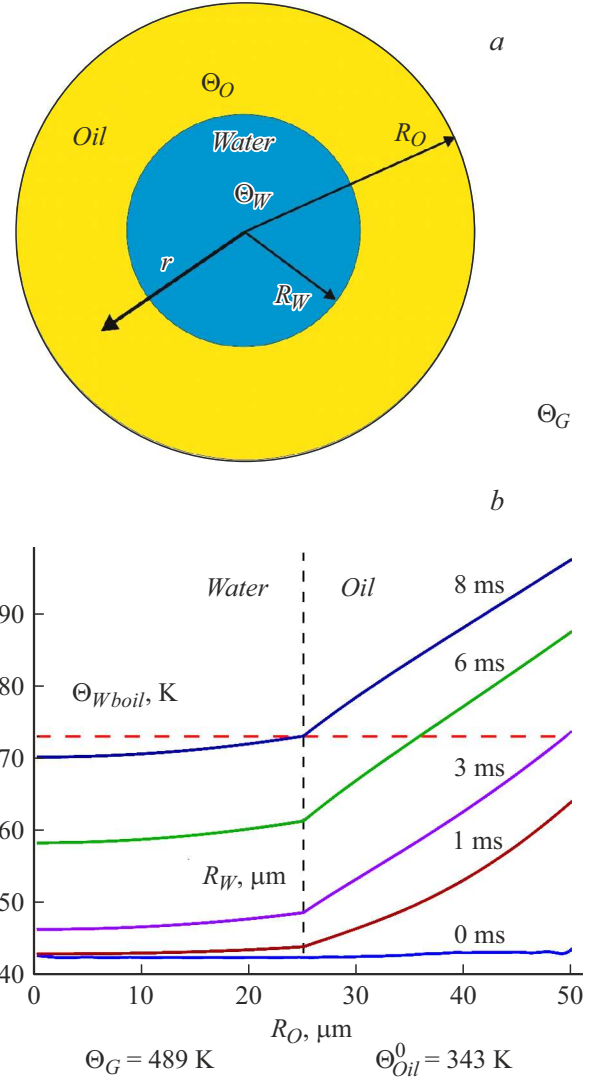


**Figure 1.** The problem schematic diagram ($a$) and an example of the composite droplet temperature dynamics ($b$).

Fig. 1, $b$ demonstrates the dimensionless temperature dynamics in the composite droplet. The calculations were performed via the analytical formula

$$\Theta^*(r^*, t^*) = \sum_{n=1}^{\infty} A_n \exp(-\omega_n^{*2} t^*) X_n^*(r^*), \quad (5)$$

where $A_n$ are the expansion coefficients determined based on the initial temperature distribution,

$$A_n = \frac{1}{\| X_n^* \|^2} \int_0^1 \rho^* c^* \Theta_0^*(r^*) X_n^*(r^*) r^{*2} dr^*,$$

$$\| X_n^* \|^2 = \int_0^1 \rho^* c^* X_n^{*2}(r^*) r^{*2} dr^*.$$

Here $c^*$, $\rho^*$ are the discontinuous heat capacity and density of the composite droplet, $\| X_n^* \|$ is the eigenfunction norm.
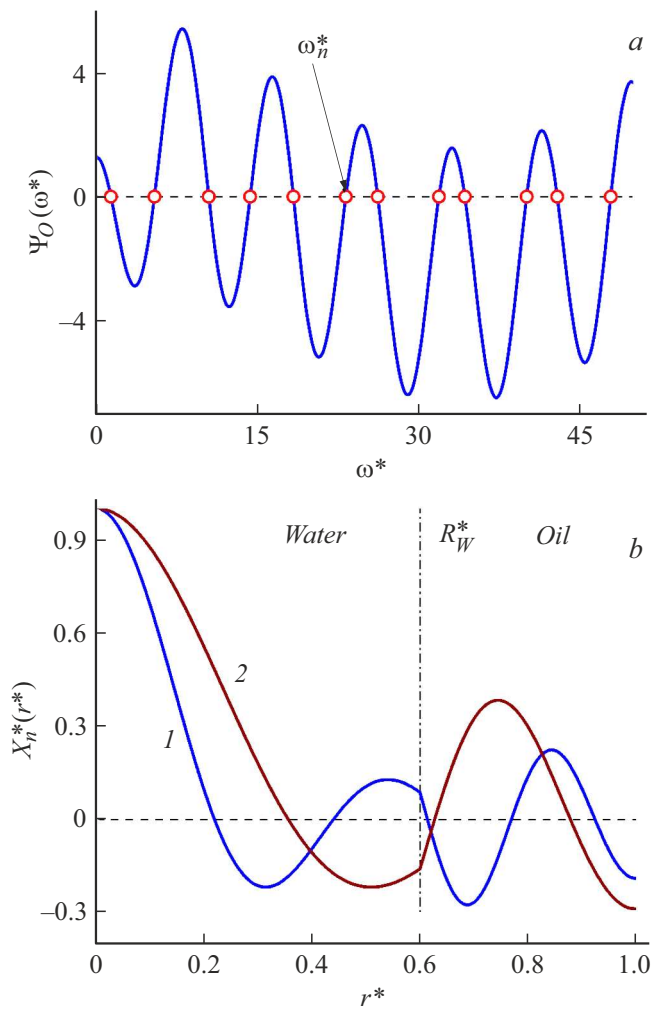
**Figure 2.** *a* — illustration to the characteristic equation solution. The points represent eigenvalues $\omega_n^*$; the volume fraction of water is $\chi_W = 22\%$. *b* — Sturm−Liouville problem eigenfunctions $X_n^*(r^*)$ of different orders: $n = 7$ (*1*) and $5$ (*2*).

In calculation, the hydrocarbon droplet diameter shall be preset, while the water microdroplet diameter shall be determined based on the volume concentration specified in the experiments. Temperature of the hot gas flowing around the droplet, gas velocity, and initial temperature of the composite drop shall be preset. Via the analytical formula in dimensionless coordinates, the moment when the temperature of the water microdroplet surface reaches the boiling point shall be determined. This time is assumed to be the microexplosion delay time.

In calculations, the first 31 terms of expansion in eigenfunctions (5) are taken into account. Increasing the number of terms in the series does not significantly affect the calculation results.

In experiments [7–9,11], the time necessary to heat the composite droplet to the initial boiling point is recorded; this time is regarded as the microexplosion delay time.

Fig. 3 shows the calculations obtained via analytical formula (5) of the time necessary for heating the water microdroplet surface to the boiling temperature. As the model hydrocarbon, N-dodecane (n-dodecane $C_{12}H_{26}$) was chosen [7]. Fig. 3, *a* demonstrates the effect of initial temperature of the composite droplets $50 < d_O < 200\,\mu m$ in diameter on the time of heating till the microexplosion. As the droplet size increases, the share of radiative heat transfer enlarges, which reduces the microexplosion delay time. Since the boundary condition allowing for the radiative heat transfer is nonlinear, a closed analytical solution can hardly be obtained in this case. Therefore, the
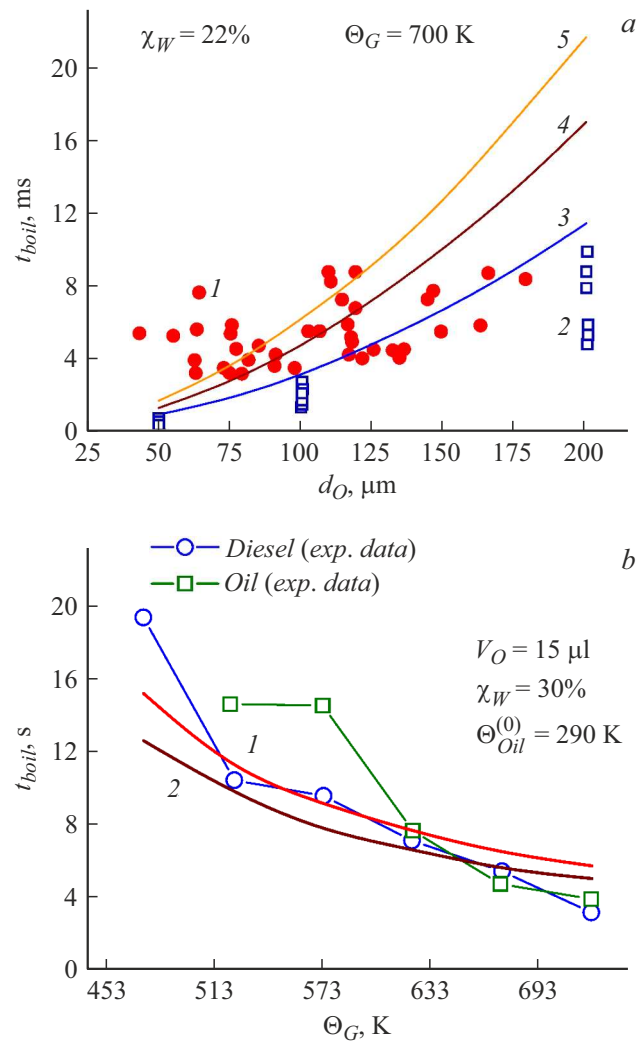


**Figure 3.** Comparison of calculations of the composite-fuel droplet heating time with experimental data. *a* — the effect of the initial temperature of composite droplets $50 < d_O < 200\,\mu m$ in diameter on the time of heating to the microexplosion. Points *1* — experimental data [7,8], points *2* — calculations via the model given in [7]. Lines are the results of calculations via (5) at droplet temperatures $\Theta_{Oil}^0 = 363$ (*3*), $353$ (*4*) and $343$ K (*5*). *b* — time $t_{boil}$ for droplets $d_O = 3\,mm$ in diameter versus gas temperature $\Theta_G$. Points represent the experimental data [11], lines are the calculations via formula (5) at flowing gas velocities $U_G = 1$ (*1*) and $2\,m/s$ (*2*).

radiative heat transfer is ignored in deriving the analytical solution. Notice that this approximation is used in the referred publications.

Fig. 3, $a$ clearly shows that calculations via the model given in [7] are significantly lower than experimental data. Fig. 3, $b$ shows the effect of gas temperature on the time of heating droplets $d_O = 3\,\mathrm{mm}$ in diameter (volume $V_O \approx 15\,\mu\mathrm{l}$) by the hot gas flow. In the experiments [11], the gas velocity was $U_G = 2\,\mathrm{m/s}$.

During the experiment, the droplets were suspended on specially twisted wires and retained an almost spherical shape. The n-dodecane boiling point exceeds $200°\mathrm{C}$. The calculations show that, during the microexplosion time delay, the hydrocarbon surface temperature was no less than $50°\mathrm{C}$ below the boiling point. The heavy-hydrocarbon saturated vapor pressure at the droplet surface temperature is low, and evaporation-induced mass loss from the surface during the experiment may be neglected. This conclusion has been also confirmed by the estimates presented in almost all the referred papers. Weak internal convective motion of the highly viscous fluid is detectable only in large droplets greater than $3\,\mathrm{mm}$ in size [11]. Internal convective heat transfer of viscous n-dodecane was neglected in calculations.

Thus, the paper presents an analytical solution to the problem of heating a droplet of hydrocarbon−water composite fuel. Comparing the calculations with experimental data, we can conclude that, contrary to the calculations obtained by the model presented in [7], the correct solution of the problem ensures satisfactory agreement with experiment and does not need additional empirical modifications [8,9].

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## Conflict of interests

The authors declare that they have no conflict of interests.

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