

# NUMERICAL SIMULATION OF WATER AND WATER EMULSION DROPLETS EVAPORATION IN FLAMES WITH DIFFERENT TEMPERATURES

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**Key words:** Water Droplet, Evaporation, High-Temperature Gas Environment.

**Abstract.** The models of heat and mass transfer and phase transition for “water droplet – flame” system have been developed using non-stationary nonlinear partial differential equations. The system of differential equations was solved by the finite-difference method. The locally one-dimensional method was used to solve the difference analogous of differential equations. One-dimensional differential equations were solved using an implicit four-point difference scheme. Nonlinear equations were solved by the iteration method. The evaporation rates of water droplets (with sizes from 0.05 mm to 5 mm) in the flame zone (at the temperatures from 500 K to 1200 K) were determined. Theoretical analysis established essentially nonlinear (close to exponential) form of dependence of the water droplet evaporation rate on the temperature of the external gas area and the temperature of a droplet surface. In particular, the water droplet evaporation rate varies from 0.25 to 0.29 kg/(m<sup>2</sup>s), when the temperature of external gas area is about 1100 K. On the other hand, the water droplet evaporation rate does not exceed 0.01 kg/(m<sup>2</sup>s) when the temperature of external gas area is about 350 K. Besides, it has been found out that droplets warm up at different rates depending on their initial temperature and velocity. As a result, the integral characteristics of droplet evaporation can increase substantially, when droplets move through the external gas area at the same temperature. We performed a similar investigation of droplet streams with droplet concentration 0.001–0.005 m<sup>3</sup> in 1 m<sup>3</sup> of gas area (typical parameters for modern spray extinguishing systems).

## 1 INTRODUCTION

The study of sprayed water phase transitions during the motion in high-temperature gas environment has been getting more and more attention in recent years [1, 2]. The results of these studies have a large number of practical applications. For example, they can be used in the technologies of polydisperse extinguishing, two-phase gas-vapor coolant formation with the specified parameters, wastewater combustion neutralization, and others [3-5]. Currently, new optical methods have emerged, that enable visualization and video recording of heat and mass transfer fast processes during the evaporation of fine liquid flow in high-temperature gases. Thus, it became possible to develop experimental methods for studying these processes. However, it is still of topical interest to develop numerical models for calculating

the parameters of the system “sprayed liquid – high-temperature gas environment” taking into account the experimental characteristics of liquid spray motion and evaporation (the deformation and entrainment of droplets, the evaporation rate, etc.).

The aim of this work is to develop the numerical model of heat and mass transfer of water droplets during their motion in high-temperature gas environment.

### 1 PROBLEM STATEMENT

In formulating the problem, it was considered that a water droplet moved (in free fall) in high-temperature gas environment (Figure 1). Under the conditions of phase transition, water vapor was blown into the near-wall part of the droplet and mixed with combustion products. It was believed that mass transfer was implemented by diffusion and convection mechanisms in the external environment. It was assumed that droplet size decreased under the conditions of intensive evaporation. After some time, the droplet evaporated completely. In formulating the problem of heat and mass transfer, a cylindrical droplet (elongated in the direction of its motion) was examined (Figure 1). It was considered that gas environment was binary (“combustion products – water vapor”). It was also assumed that the thermal characteristics of reacting substances do not depend on the temperature.

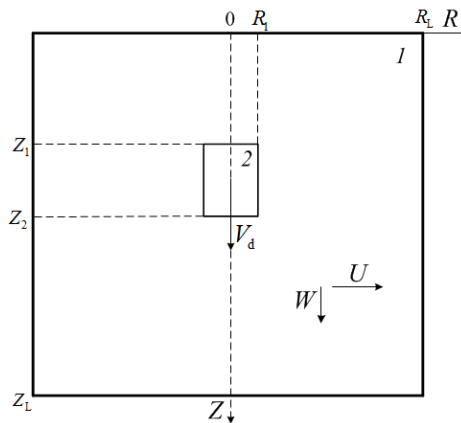


Figure 1: A diagram of the solution area of the problem of heat and mass transfer: 1 – high-temperature gas mixture, 2 – water droplet

### 1 MATHEMATICAL MODEL AND SOLUTION METHODS

The system of non-stationary nonlinear partial differential equations is derived from the physical model that has been formulated taking into account convective flows in a mixture of combustion products and water vapor. The system is as follows ( $0 < \tau < \tau_d$ ) [6]:

$$0 < R < R_L, 0 < Z < Z_1, Z_2 < Z < Z_L; R_1 < R < R_L, Z_1 < Z < Z_2$$

Poisson’s equation:

$$\frac{\partial^2 \Psi}{\partial R^2} - \frac{1}{R} \frac{\partial \Psi}{\partial R} + \frac{\partial^2 \Psi}{\partial Z^2} = -R\Omega \tag{1}$$

vorticity equation:

$$\frac{1}{\text{Sh}} \frac{\partial \Omega}{\partial \tau} + U \frac{\partial \Omega}{\partial R} + V \frac{\partial \Omega}{\partial Z} - U \frac{\Omega}{R} = \frac{1}{\text{Re}_1} \left[ \frac{\partial^2 \Omega}{\partial R^2} + \frac{1}{R} \frac{\partial \Omega}{\partial R} + \frac{\partial^2 \Omega}{\partial Z^2} - \frac{\Omega}{R^2} \right] + \frac{\partial \Theta_1}{\partial R} \quad (2)$$

energy equation for the mixture of water vapor and combustion products:

$$\frac{1}{\text{Sh}} \frac{\partial \Theta_1}{\partial \tau} + U \frac{\partial \Theta_1}{\partial R} + V \frac{\partial \Theta_1}{\partial Z} = \frac{1}{\text{Re}_1 \text{Pr}_1} \left[ \frac{\partial^2 \Theta_1}{\partial R^2} + \frac{1}{R} \frac{\partial \Theta_1}{\partial R} + \frac{\partial^2 \Theta_1}{\partial Z^2} \right] \quad (3)$$

water vapor diffusion equation:

$$\frac{1}{\text{Sh}} \frac{\partial \gamma_w}{\partial \tau} + U \frac{\partial \gamma_w}{\partial R} + V \frac{\partial \gamma_w}{\partial Z} = \frac{1}{\text{Re}_1 \text{Sc}_1} \left[ \frac{\partial^2 \gamma_w}{\partial R^2} + \frac{1}{R} \frac{\partial \gamma_w}{\partial R} + \frac{\partial^2 \gamma_w}{\partial Z^2} \right] \quad (4)$$

balance equation:

$$\gamma_w + \gamma_f = 1 \quad (5)$$

$$0 < R < R_1, Z_1 < Z < Z_2$$

heat equation for the droplet:

$$\frac{1}{\text{Fo}_2} \frac{\partial \Theta_2}{\partial \tau} = \frac{\partial^2 \Theta_2}{\partial R^2} + \frac{1}{R} \frac{\partial \Theta_2}{\partial R} + \frac{\partial^2 \Theta_2}{\partial Z^2} \quad (6)$$

$$\text{Sh} = \frac{v_m t_m}{z_m}, \quad \text{Re}_1 = \frac{V_m z_m}{v_1}, \quad \text{Pr}_1 = \frac{v_1 \rho_1 C_1}{\lambda_1}, \quad \text{Sc}_1 = \frac{v_1}{D_1}, \quad \text{Fo}_2 = \frac{\lambda_2 t_m}{\rho_2 C_2 z_m^2}.$$

Initial ( $\tau=0$ ) conditions (Figure 1):  $\Theta=\Theta_0$  at  $0 < R < R_1, Z_1 < Z < Z_2$ ;  $\Theta=\Theta_f, \gamma_f=1, \gamma_w=0, \Psi=0, \Omega=0$  at  $0 < R < R_L, 0 < Z < Z_1, Z_2 < Z < Z_L; R_1 < R < R_L, Z_1 < Z < Z_2$ .

Boundary ( $0 < \tau < \tau_d$ ) conditions (Figure 1): at the interface “liquid – gas” ( $R=R_1, Z_1 < Z < Z_2; Z=Z_1, Z=Z_2, 0 < R < R_1$ ) – IV type of boundary conditions was assumed for energy equations taken into account vaporization, II type of boundary conditions was specified for energy equations taken into account water vapor blowing; at the external borders ( $R=0, R=R_L, 0 < Z < Z_L; Z=0, Z=Z_L, 0 < R < R_L$ ) – the condition of zero gradients of the respective functions was assumed for all equations.

Boundary conditions were specified to emphasize the effect of water vapor blowing on the conditions of heat transfer on all droplet faces for energy equations:

$$R=R_1, Z_1 < Z < Z_2: \frac{\partial \Theta_2}{\partial R} = \frac{\lambda_1}{\lambda_2} \frac{\partial \Theta_1}{\partial R} - Q_e W_e \frac{z_m}{\Delta T \lambda_2} - \rho_3 C_3 v_e (\Theta_{3s} - \Theta_{2s}) \frac{z_m}{\lambda_2},$$

$$Z=Z_1, Z=Z_2, 0 < R < R_1, \frac{\partial \Theta_2}{\partial Z} = \frac{\lambda_1}{\lambda_2} \frac{\partial \Theta_1}{\partial Z} - Q_e W_e \frac{z_m}{\Delta T \lambda_2} - \rho_3 C_3 v_e (\Theta_{3s} - \Theta_{2s}) \frac{z_m}{\lambda_2}.$$

The motion equation of the droplet under the conditions of vaporization taking into account the forces of resistance and gravity:

$$\frac{dv_d}{dt} = \frac{3\rho_3}{4\rho_2 2r_d} c_\chi |v_d - v_e| (v_d - v_e) + g,$$

where  $v_d(0) = v_0$ .

The following equation was used for the drag coefficient in numerical simulation taking into account the nonsphericity of the droplet, its unsteady motion [7], evaporation on the body surface [8] and movement (of convection flows) inside the droplet:

$$c_\chi = 24.3 k_g \frac{1}{B+1} \frac{1 + \frac{2\mu_2}{3\mu_3}}{1 + \frac{\mu_2}{\mu_3}} (A+1)^{1.2 \pm 0.03} \text{Re}^{-0.635}.$$

The geometric factor  $k_g$  characterizes the form deviation from spherical (for cylindrical disks  $k_g = 1.64$ ). The ratio  $1/(B+1)$  is a coefficient that describes the effect of droplet evaporation on resistance force ( $B = C_2(T_{3s} - T_{2s}) / (Q_e + q_v / W_e)$ ) [8]. The ratio  $[1 + (2\mu_2/3\mu_3)] / [1 + (\mu_2/\mu_3)]$  is the coefficient taking into account possible convective flows inside the droplet. The ratio  $(A+1)^{1.2 \pm 0.03}$  characterizes the accelerated body motion ( $A$  – dimensionless complex, which describes the relative acceleration ( $A = \frac{d}{v_d^2} (\frac{dv_d}{dt})$ ) [7].

The following expression was used to determine the mass evaporation rate:

$$W_e = \frac{\beta}{1 - k_\beta \beta} \frac{(P^n - P)}{\sqrt{2\pi R_t T_e / M}},$$

where  $k_\beta$  – dimensionless coefficient ( $k_\beta \approx 0.4$ ).

The layer thickness of the evaporating droplet was determined by the formula  $l_e = \frac{W_e t}{\rho_2}$ .

The following scale variables were used to convert the equations into the dimensionless form: characteristic average droplet size ( $z_m = 1$  mm); time scale ( $t_m = 1$  s); temperature scale ( $T_m = 1000$  K); rate scale ( $v_m = 1$  m/s).

Where:  $\tau$  – dimensionless time;  $\tau_d$  – dimensionless time of droplet existence;  $\Psi$  – dimensionless equivalent of the current function;  $\Omega$  – dimensionless equivalent of vorticity;  $\Theta$  – dimensionless temperature;  $U, V$  – dimensionless velocity components of water vapor and combustion products in the direction of the axis  $R$  and  $Z$  respectively;  $\gamma_f$  – dimensionless concentration of combustion products;  $\gamma_w$  – dimensionless water vapor concentration;  $\lambda$  –

thermal conductivity,  $W/(m \cdot K)$ ;  $Q_e$  – thermal effect of liquid evaporation,  $J/kg$ ;  $W_e$  – evaporation rate,  $kg/(m^2 \cdot s)$ ;  $\Delta T$  – temperature difference ( $\Delta T = T_m - T_0$ );  $C$  – specific heat capacity,  $J/(kg \cdot K)$ ;  $v_d$  – droplet velocity,  $m/s$ ;  $v_e$  – linear velocity of vapor outflow from the droplet surface,  $m/s$ ;  $c_\chi$  – dimensionless drag coefficient;  $g$  – acceleration of gravity,  $m/s^2$ ;  $\beta$  – dimensionless evaporation coefficient;  $P$  – water vapor pressure near the boundary of evaporation,  $N/m^2$ ;  $P^n$  – saturated water vapor pressure,  $N/m^2$ ;  $R_t$  – universal gas constant,  $J/(mol \cdot K)$ ;  $T_e$  – droplet surface temperature,  $K$ ;  $M$  – molar mass,  $kg/kmol$ ; indexes: 0 – initial state, 1 – high-temperature gases, 2 – water droplet, 3 – water vapor, d – droplet, e – evaporation, f – fuel, m – scale, s – surface, v – vapor, w – water.

The system of non-stationary partial differential equations (1)–(6) was solved by the finite difference method [9]. The difference analogues of differential equations were solved by the local one-dimensional method [9]. One-dimensional differential equations were solved by the sweep method using an implicit four-point difference scheme [9]. Nonlinear equations were solved by the iteration method. Irregular dimensionless steps in time ( $10^{-8} \div 10^{-6}$ ) and in coordinate grid ( $10^{-4} \div 10^{-2}$ ) were used to increase the accuracy when solving the system of non-stationary differential equations (1)–(6). The method for assessing the reliability of the results of numerical studies was performed, based on the verification of applied difference scheme conservativeness, similar to [6].

Numerical studies were carried out at the following parameters [10, 11]: initial temperatures of liquid droplets  $\Theta_0 = 0.3$  and gas  $\Theta_f = 0.3 \div 1.1$ ; thermal effect of evaporation  $Q_e = 2.26$  MJ/kg; droplet sizes  $R_d = 0.25$ ,  $Z_d = 1$  and solution area  $R_L = 10$ ,  $Z_L = 1000$ ; initial droplet velocity  $V_0 = 0.5$ ; water molar mass  $M = 18$  kg/kmol.

### 3 RESULTS AND DISCUSSION

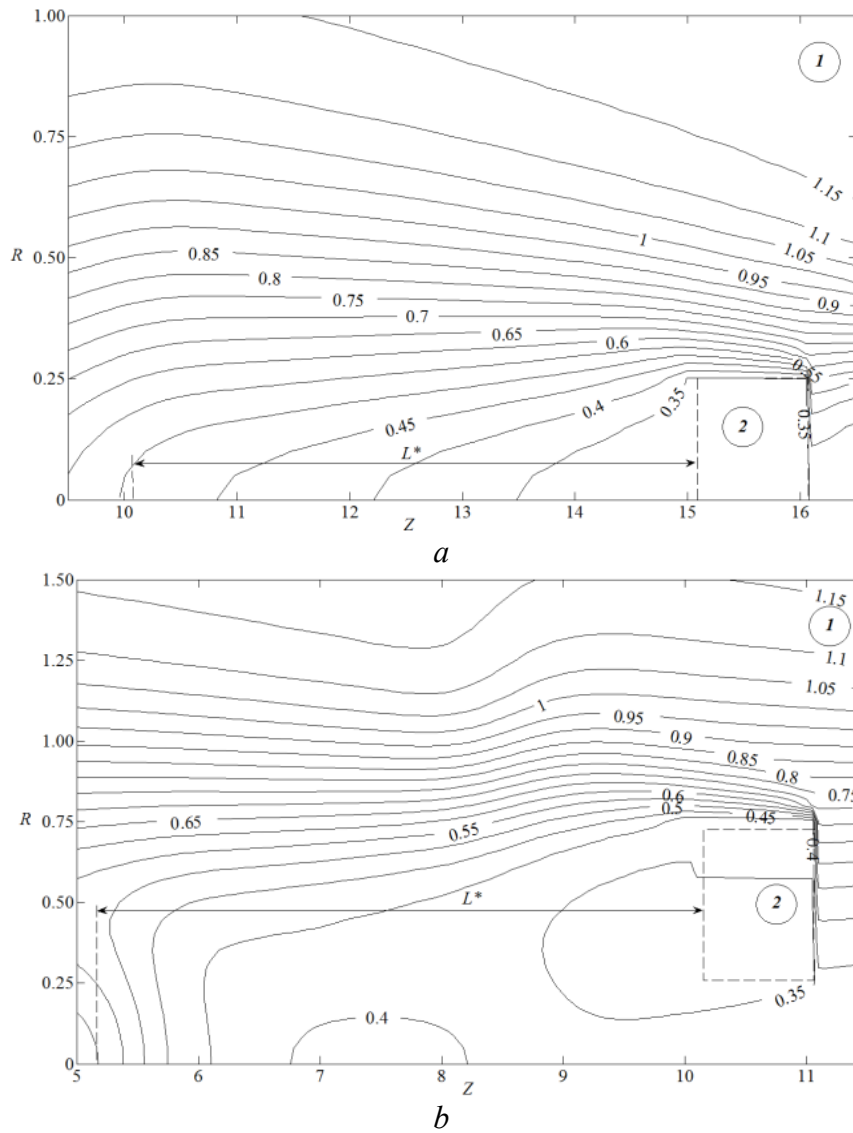
Table 1 shows the dependence of the mass rate of water droplet evaporation on the temperature of gas environment. Data in the table was obtained as a result of the calculations using the developed model of heat and mass transfer. The essentially nonlinear nature of the relation  $W_e = f(\Theta_f)$  was established from the results of theoretical research.

**Table 1:** The dependence of the mass rate of water droplet evaporation on the temperature of gas environment

$\Theta_f$	0.3	0.5	0.7	0.9	1.1	0.3
$W_e, kg/(m^2 \cdot s)$	0.005	0.0116	0.065	0.155	0.214	0.005

The values have been obtained that correspond to the mass rate of droplet evaporation during the motion through high-temperature gases. These values correlate well with the results of previous experiments [12]: the evaporation rate was  $W_e = 0.006$   $kg/(m^2 \cdot s)$  at the temperature of fuel combustion products  $T_f = 300$  K, and  $T_f = 1100$  K,  $W_e = 0.270$   $kg/(m^2 \cdot s)$ .

Figure 2 shows the isotherms at  $\tau = 0.02$  (correspond to the beginning of the motion) for two schemes considering the mutual disposition of droplets. In the case of two (Figure 2a), and five (Figure 2b) droplets moving consecutively, the parameter  $L_n$  varied from 0.01 to 5.



**Figure 2:** Isotherms ( $\Theta$ ) for the system with two droplets moving consecutively at  $\tau=0.02$ ,  $R_d=0.25$ ,  $Z_d=1$ ,  $L_n=1$  (a) and five droplets at  $\tau=0.02$ ,  $R_d=0.25$ ,  $Z_d=1$ ,  $L_n=2$  (b): 1 – high-temperature gas environment, 2 – water droplet

Figure 2 demonstrates a decrease of the gas temperature in the vicinity of droplets. It can be seen that the temperature in the droplet track varies considerably. This is primarily due to the evaporation of droplets. The trajectory of each droplet also plays a decisive role. The temperature in the track changes slightly (relative to the initial droplet temperature) in contrast to that in a small neighborhood of the line corresponding to the trajectory when varying  $L_n$  in a wide range.

Satisfactory compliance with the results of theoretical studies and the data obtained in the experiments allow us to conclude on the adequacy of the developed model of heat and mass transfer during the motion and evaporation of droplets and droplet liquid flow in high-temperature gas environment.

The research results have been obtained using established numerical model; they can be used to develop new and improve existing technologies, providing the implementation of phase transitions in the system “liquid spray – high-temperature gas environment”.

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