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Modelling of water droplets heat and mass transfer in the course of phase transitions. I: Phase transitions cycle peculiarities and iterative scheme of numerical research control and optimization

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Abstract. The peculiarities of the widely applied in practice sprayed water droplets phase transition cycle are discussed in this article. Theoretical fundamentals of droplets heat and mass transfer modelling by combined analytical-numerical method and numerical simulation peculiarities are outlined. Water droplet phase transitions were modelled on the energy flow balance condition basis. The control mechanism of iterative scheme used to determine the droplet surface temperature was highlighted. The optimal finite number of members in the infinite integral equation set for droplet temperature field and its gradient parameter calculation was defined by the numerical experiment.

Keywords: water droplets, heat and mass transfer, Fourier time scale, phase transition cycle, numerical modelling, optimization and control.

1 Introduction

Water in the form of droplets is widely observed in natural phenomena and applied in technologies. Dispersed in the gas liquid has developed contact surface which ensures intensive heat and mass transfer between the liquid and gaseous phases. Therefore, water injection is a powerful tool to suppress the fire front, to regulate the thermal state in the gas scrubbers, turbochargers, steam superheaters and flame of burners or to protect the surface from the intense heat flux by biphasic flow curtains, to utilize the latent heat of flue gas by condensing economizer, to improve operation of various other widely adaptable devices in thermal technologies.

The definition of heat exchange and mass transfer intensity between dispersed water and gaseous surrounding is directly related with research of the droplet thermal state and phase transitions on it's surface. This *droplet* problem can already be considered as a classic [2], but its versatility in thermal technology aspect and very broad variety of transfer processes in droplets and their surrounding still provides researcher's attention [12].

In today's *droplet* problem research phase, the widely used theoretical studies of transfer processes are based on analytical and numerical analysis of fundamental equations the control of which is based on the results of the experimental studies. *Droplet* problem has significant components of *external* and *internal* tasks. Intensity of heat exchange between the droplet and its surrounding as well as the phase transitions speed on droplet surface are defined by solutions of *external* task.

Whereas these parameters are essential to define the vapour flow pervasive from evaporating droplet (which is very important parameter for determining the efficiency of the thermal technologies), therefore *external* task traditionally is considered to be the main. Evaluation problem of Stefan's hydrodynamic flow influence on heat exchange and the phase transitions intensity raises by solving it. Its solution has old traditions [2], in which a droplet of convective heat exchange and evaporation tasks are successfully solved by models based on the similarity theory [1, 10, 11, 14]. It is promising to simulate the evaporation process by using vapour flux density algebraic solutions that were obtained analytically [4, 13]. Holistically *droplet external* task can be considered as unambiguously described if droplet surface temperature temporal function is known $T_R(\tau)$ and the parameters of droplets surrounding are determined [8].

The essential role of the function $T_R(\tau)$ for the liquid droplet phase transition sequence in droplet life cycle, which begins at the moment $\tau = 0$ when the liquid is sprayed of and ends at the moment τ_f of vaporized droplet extinction, should be taken into account. When the temperature of sprayed water is lower when the dew point temperature of surrounding air, the life cycle of water droplets $0 \div \tau_f$ can be splitted into condensing τ_{co}, unsteady $\tau_{ue} = \tau_{uf} - \tau_{co}$ and equilibrium evaporation phase $\tau_{ee} = \tau_f - \tau_{uf}$ transition regimes

$$0 \div \tau_{co} \div \tau_{uf} \div \tau_f. \tag{1}$$

The driving force in the condensation phase transition regime can be reflected by difference between water vapour partial pressure in droplet surrounding gas and near the droplet surface $\Delta p_v = p_{v,\infty} - p_{v,R} = p_{v,\infty} - p_s(T_R)$. During the condensation regime, the droplet surface warms to the dew point temperature. Unsteady evaporation phase transition regime starts when the droplet surface heats up to dew point temperature. During it the droplet temperature increases until it reaches the temperature of equilibrium evaporation $T_{ee}(\tau = \tau_{ee})$. At this temperature, condition $q^+_\Sigma \to q^+_{ee}$ is satisfied. The warming droplet thermal state is approaching asymptotically to the state defined by temperature T_{ee} so unsteady evaporation regime duration $\tau_{ue} = \tau_{uf} - \tau_{co}$ can be defined conditionally agreed on the terms which define the beginning of equilibrium evaporation regime [7]. However, uncertainty of τ_{ue} does not cause confusion in cycle (1) modelling, because intensity of the transfer processes at the end of droplet unsteady evaporation regime and at the beginning of the equilibrium evaporation regime are close to each other [6]. Duration of the equilibrium evaporation regime $\tau_{ee} = \tau_f - \tau_{uf}$ is defined by the moment of droplet disappearance $R(\tau \to \tau_f) \to 0$, and the peculiarities of the function $T_R(\tau = \tau_{uf} \div \tau_f)$ are affected by the droplet heating method [5].

Therefore, the definition of the droplet surface function $T_R(\tau)$ is the key for *droplet* problem solve. It is impossible to define droplet surface temperature in the unsteady phase regime only according to solutions of *droplet external* task. This requires a complex analysis for transfer processes inside the droplet and its surrounding. The surface temperature of the droplet can be defined by the energy flux balance condition on the droplet surface, which requires the matching of the energy flux that approach surface (both from the liquid and droplet surroundings) with energy flux that leak from it (both to the liquid in the droplet and the surroundings). Assuming that the droplet is a spherical semitransparent body with assumed inner and outer surfaces and its inner surface is defined by the radius R^- and the outer by R^+ ($|R^+| = |R^-| = R$). The symmetrical heat exchange energy flux balance condition, in the assumptions frame of quasi stationary transfer processes, can be described by the formal expression

$$\overrightarrow{q}_{\Sigma}^{+}\big(R^{+},\tau\big) + \overrightarrow{q}_{\Sigma}^{-}\big(R^{-},\tau\big) + \overrightarrow{q}_{f}^{+}\big(R^{+},\tau\big) = 0. \tag{2}$$

On the whole, expression (2) is a transcendental equation, because it requires a known related *external* and *internal droplet* problem solution. In order to concretize expression (2), it is necessary to solve the following problems [6]: the first problem is related with the description of the intensity of droplet phase transitions m_v^+ and the intensity of convective heating q_c^+, considering the influence of Stefan's hydrodynamic flow; the second is related to the evaluation of spectral radiation absorption in semitransparent liquid and the optical effects on the surface of the droplet, while calculating the integral intensity of the radiation flux q_r; the third problem is caused by the need to calculate the unsteady temperature field gradient in the droplet $\mathrm{grad}T_{r=R}$ in the conditions of combined heat exchange processes in the droplet. These problems are related. In general, the heat fluxes in expression (2) are described by the system of nonlinear integro-differential equations. Its solution can be defined by iterative methods.

In the articles cycle, it is expected to reveal the regularities of interaction of water droplet combined heat and mass transfer processes and to highlight the effect of droplet heat exchange conditions impact. The aim of this work is to reveal the essence of combined analytical-numerical research methods used in modelling of the *droplet* problem and to highlight the control and optimization aspects of the iterative numerical scheme.

2 Methodology of *droplet* problem solving

The methodology is based on the droplet surface temperature iterative calculations by equation (2). Equation (2) is concretized by expressing it in a form of integro-differential equations system that is further transformed to a system of algebraic and integral equations. Such system is solved numerically. Temporal functions of droplet surface temperature and other heat and mass transfer parameters $P(\tau)$ are defined. The combined analytical and numerical *droplet* problem method basics are developed in works [5, 11]. The main advantage of this method is to ensure the stability of numerical schemes in the integral type expression (2) and easily controlled convergence.

There are two development trends of combined analytical and numerical methods used in solving the *droplet* problem. They are separated by the researcher's relationship with the methodology of calculating the droplet surface temperature function $T_R(\tau)$.

In the first trend, the idea of droplet surface temperature calculation using iterative methods is developed [5]. Despite the susceptibility of machine computing time, the iterative method allows to seek numerical results that are close to analytical.

In the second case, the idea of replacing droplet surface temperature to effective temperature T_{ef} is developed [11]. The latter is described by empirical expressions in algebraic form by known parameters of the droplet and its surroundings. Afterwards, numerical research schemes that are not very susceptible to computation time are formed. They are easily adapted in complex numerical modelling schemes of dispersed liquid combustion processes in thermal equipment. However, *droplet* models that are based on temperature T_{ef} allow to approximate calculations of $\approx P(\tau)$ functions, which reliability is evaluated by comparative analysis by experiment or, in the first case, with defined $P(\tau)$ functions.

This article continues the direction of research of *droplet internal* task developed in article [5]. Phase transition flux is considered to be positive in liquid evaporation regime. The heat flux vectors on the surface of the droplet are defined by the temperature difference $\Delta T_{R^+} = T_g - T_R$ and droplet temperature gradient $\mathrm{grad}T_{r=R^-}$. The energy balance condition (2) is rewritten as follows:

$$(q_r^+ - q_r^-) + \frac{\lambda_{vg}\mathrm{Nu}_f}{2R}(T_g - T_R) - m_v^+ L - k_c^- \lambda_l \frac{\partial T_r}{\partial r}\bigg|_{r=R^-} = 0. \tag{3}$$

The first member of expression (3) reflects the radiation flux on the surface of the droplet, defined by model [16]. It is granted by the thermal emission in the part of the spectrum where the light absorption coefficient χ_ω is very high ($\chi_\omega > 10^6\ \mathrm{m}^{-1}$). Assuming that $q_r^+ - q_r^- \cong 0$, seems that radiation flux does not effect on the function $T_R(\tau)$, but radiative energy that is absorbed inside the droplet change temperature field inside it.

External convective heat flux is evaluated by using Nuselt number for solid particle. Influence of Stefan's hydrodynamic flow is evaluated by using corrective function f_{B_T} based on Spalding transfer parameter B_T [15]. Depending on droplet movement conditions classical function $f_{B_T} = \ln(1 + B_T)/B_T$ or empirical correlation $f_{B_T} = (1 + B_T)^{-0.7}$ can be applied. Combined them model of Abramzon and Sirignano [1] was applied at present paper.

Heat flux on the surface of the droplet caused by phase transition is defined by the analytical water vapor flux density m_v^+ model [4]

$$\begin{aligned} q_f^+ &= m_v^+ L \\ &= L\frac{D_{vg}\mu_v}{T_{vg,R}R_\mu R}\left[p_{v,R} - p_{v,\infty} + \frac{\mu_v}{\mu_g}\left(p\ln\frac{p - p_{v,\infty}}{p - p_{v,R}} - p_{v,R} + p_{v,\infty}\right)\right], \end{aligned} \tag{4}$$

where D_{vg} – mass diffusivity; L – latent heat of evaporation; μ_v, μ_g – molecular mass of water vapour and surrounding gas; R_μ – universal gas constant; R – droplet radius; p, $p_{v,R}$, $p_{v,\infty}$ – pressure of surrounding, vapour on the droplet surface and far from it, respectively. The main problem in expression (3) is the definition of droplet unsteady temperature field gradient. The main case of heat exchange in the droplet is defined by a system of the following equations: the integro-differential energy equation as well as

Navier–Stocks differential equations. In the case of convective heat transfer, this system is not solved analytically and its numerical solution is complicated. Therefore, alternative solutions are searched for. In the *droplet* problem, these solutions are complex analytical and numerical research methods. Often, they are based on by the model of radiative-conductive heat spread in the droplet. A possible effect of liquid circulation on the heat spread in the droplet is evaluated by the effective heat conductivity coefficient $\lambda_{ef} = \lambda_l \cdot k_c^-$. The convection corrective coefficient k_c^- is, in turn, described by the empirical dependence from the Peclet number for the liquid $k_c^- = f_c(\mathrm{Pe}_l)$ [1].

The non-stationary temperature field in a droplet heated by conduction and radiation that is described by the energy equation

$$\rho_l c_{p,l} \frac{\partial T}{\partial \tau} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \lambda_l \frac{\partial T}{\partial r} \right) + F_{q_r}, \tag{5}$$

where ρ_l, $c_{p,l}$, λ_l – liquid density, mass specific heat and thermal conductivity. Source function in expression (5) takes into account the effect of semitransparent liquid absorbing radiation heat on the thermal state of the droplet. The expression of function F_{q_r} depends on the model of radiation flux. Usually, models q_r are based on theories of geometrical optics or electromagnetic waves. In the first case, the density of local radiation flux in the droplet is described, while in the second case, the description of heat flux in the volume of the droplet is deemed satisfactory [16]. The local radiative flux in the droplet described by integro-differential equation:

$$q_r = 2\pi \int\limits_0^\infty \int\limits_0^\pi I_\omega \sin\varphi \cos\varphi \, \mathrm{d}\varphi \, \mathrm{d}\omega, \qquad \frac{\mathrm{d}I_\omega}{\mathrm{d}s} = \chi_\omega \big(n_\omega^2 I_{\omega 0} - I_\omega \big), \tag{6}$$

where φ – characteristic angle of thermal radiation in sphere (rad); ω – wave number; I_ω, $I_{\omega 0}$ – intensity of radiation of a grey and a black body; n_ω – spectral index of refraction; s – freely selected direction. The system of equations (5), (6) can be solved only by numerical iterative method. Numerical scheme for $q_r(r)$ calculation was established according to equation (6) integral solution [9]. When forming the iterative numerical solution scheme of the *droplet problem*, the local radiative flux $q_{r,i,j,it}$ in droplet at iteration it is defined by the temperature field $T_{r,i,j,it-1}$ calculated in the previous iteration $it - 1$. Here i – index of time in a numerical scheme, j – index of radial coordinate, it – index of iteration. Radiative flux source function

$$F_{q_r} = -\frac{1}{r^2} \frac{\partial}{\partial r} \big(r^2 q_r \big). \tag{7}$$

is considered to by defined.

Initial conditions for system (5), (7) are $R(\tau = 0) = R_0$, $T(r, \tau = 0) = T_0$. Boundary condition is formulated by unknown function of droplet surface temperature $T_R(\tau)$:

$$T(r = R, \tau) = T_R(\tau). \tag{8}$$

Assuming thermal diffusivity $\lambda/(c_p\rho) = a = a_1^2$ and $\partial\lambda_l(r)/\partial r \approx 0$, and by using variable $\Theta = r(T - T_R)$ system (5), (7), (8) is easily reformed to Dirichlet carryover task with a defined source function [4]

$$\frac{\partial\Theta}{\partial\tau} = a_1^2\frac{\partial^2\Theta}{\partial r^2} + F_{sor}, \tag{9}$$

where $F_{sor} = -(1/c_{\rho,l}\rho_l r)(\partial(r^2 q_r)/\partial r) - r(\mathrm{d}T_R/\mathrm{d}\tau)$. Then, the unsteady temperature field of the droplet is defined by the infinite series of integral equations

$$T(r,\tau) = T_R(\tau) + \frac{2}{r}\sum_{n=1}^{\infty}\sin\frac{n\pi r}{R}\int\limits_0^{\tau} f_n \exp\left[-a\left(\frac{n\pi}{R}\right)^2(\tau - \tau_*)\right]\mathrm{d}\tau_*, \tag{10}$$

in which, the function of member f_n of the infinite sum evaluates the rate of heating and intensity of radiation absorption within the droplet [5]:

$$f_n = (-1)^n\frac{R}{n\pi}\frac{\mathrm{d}T_R}{\mathrm{d}\tau} + \frac{1}{Rc_{p,l}\rho_l}\int\limits_0^{R} q_r\left(\frac{n\pi r}{R}\cos\frac{n\pi r}{R} - \sin\frac{n\pi r}{R}\right)\mathrm{d}r. \tag{11}$$

Differentiating expression (10) and using the condition $r = R$, an integral equation for calculating the temperature field gradient in expression (3) is formed:

$$\left.\frac{T(r,\tau)}{\partial r}\right|_{r=R^-} = \frac{2\pi}{R^2}\sum_{n=1}^{\infty}(-1)^n n\int\limits_0^{\tau} f_n \exp\left[-a\left(\frac{n\pi}{R}\right)^2(\tau - \tau_*)\right]\mathrm{d}\tau_*. \tag{12}$$

The rate at which the mass of the droplet changes is determined by the changing water vapour flux during phase transitions:

$$\frac{\mathrm{d}M_l}{\mathrm{d}\tau} = -4\pi R^2 m_v^+. \tag{13}$$

Volume of the droplet is changing also because of thermal expansion.

System (3), (4), (8), (10)–(13) is finally defined by using for the droplet Nu number description that is known from empirical equations [1] for hard particles. For the droplet being heated by conduction (k heat transfer) $\mathrm{Nu}_f = 2f_{B_T}$. In the case of complex heat transfer by radiation and conduction ($k + r$ heat transfer), the system needs to be supplemented by the local radiation flux for the droplet model [5, 9].

System (3), (4), (8), (10)–(13) is solved numerically. During phase transitions the droplet diameter changes. Therefore, the complex heat transfer carryover is conveniently analyzed in coordinates $\overline{\mathrm{Fo}}$ and $\eta = r/R$, ensuring the unit duration of the phase transition mode that's under observation as well as a constant unit radius $\eta = (r = R)/R = 1$ of the droplet within selected regime. Non-dimensional droplet phase transition interval is defined by a modified Fourier number

$$\overline{\mathrm{Fo}} = \frac{\mathrm{Fo}}{\mathrm{Fo}_{fv,k}}. \tag{14}$$

The time grid of the numerical scheme is graded based on the modified Fourier number coordinate, changing i from 1 to $I-1$:

$$\overline{\mathrm{Fo}} = \frac{i-1}{I-1}, \quad \text{when} \sum_{i=2}^{I} (\overline{\mathrm{Fo}}_i - \overline{\mathrm{Fo}}_{i-1}) = 1. \tag{15}$$

The Fourier number $\mathrm{Fo} = (a_{et}/R_0^2)\tau$ is calculated in respect of standard liquid – water at 278 K temperature [6]. The Fourier number is calculated in respect of standard liquid $\mathrm{Fo} = (a_{et}/R_0^2)\tau$. As the normalizing number $\mathrm{Fo}_{fv,k}$ can be used any Fourier number evaluated in the droplet life cycle characteristic moments.

In the non-dimensional unit radius of the droplet $\eta = 0 \div 1$, the integer J of spherically symmetrical cuts is adopted and the numerical scheme radial coordinate grid is graded by changing j from $j = 1$ to $j = J-1$:

$$\eta_j = \frac{j-1}{J-1}, \quad \text{when} \sum_{j=2}^{J} (\eta_j - \eta_{j-1}) = 1. \tag{16}$$

When calculating the non-stationary temperature field and its gradient by expressions (10) and (12), it is necessary to decide on the number N, which is the number of assessable finite members in the infinity integral equation series.

Then, the integrals in expressions (10)–(12) can be changed to finite integral sums:

$$R \sum_{j=2}^{J} q_r^j \int\limits_{\eta_{j-1}}^{\eta_j} \bigl(n\pi\eta\cos(n\pi\eta) - \sin(n\pi\eta)\bigr)\,\mathrm{d}\eta, \tag{17}$$

$$\frac{R_0^2}{a_{et}} \sum_{i=2}^{I} f_n^i \int\limits_{\mathrm{Fo}_{i-1}}^{\mathrm{Fo}_i} \exp\left[-(n\pi)^2 \frac{a}{a_{et}} \frac{R_0^2}{R^2} (\mathrm{Fo} - \mathrm{Fo}_*)\right] \mathrm{dFo}_*. \tag{18}$$

Integrals in sums of expressions (17), (18) are easily solved analytically, when

$$q_r^j = \frac{q_{r,j-1} + q_{r,j}}{2}, \qquad f_n^i = \frac{f_{n,i-1} + f_{n,i}}{2}. \tag{19}$$

For each $\overline{\mathrm{Fo}}_{i>1}$ moment in time, the iterative it cycle is executed in order to define the surface temperature $T_{R,i,it}$ of the droplet. In order to do that, expression (3) is minimized. Method of steepest descent is applied. It is considered that $T_{R,i} = T_{R,i,it=IT}$ and the iterative cycle ends, when in the iteration $it = IT$ the calculated approaching and receding heat flux on the surface of the droplet meet the condition

$$\left[1 - \frac{\overline{q}^{-}_{\Sigma,it} + \overline{q}^{+}{}_{f,it}}{\overline{q}^{+}{}_{\Sigma,it}}\right] \cdot 100\% < \delta_{acc}. \tag{20}$$

In this condition, (20) heat flux that spreads towards the droplet surface is considered to be positive. In each iterative cycle, the droplet parameters in Fourier $P(\mathrm{Fo}_i)$ and in real time $P(\tau_i)$ scales are calculated. To ensure the stability of the numerical scheme, in the iterative it cycle, the diameter of the droplet is not changed: $2R_{i,it} = 2R_{i-1}$. The change of droplet dimension $\Delta R_i = R_i - R_{i-1}$ is calculated by expression (13), when the temperature $T_{R,i}$ is already defined in the iterative cycle. A new iterative cycle begins after making the step $\Delta\overline{\mathrm{Fo}}_i$. The numerical experiment ends when planed iterative cycles are completed, the cycle $it_{i=1}$ or, when the radius of the vaporizing droplet becomes $R_i < 5 \cdot 10^{-6}$ m. Geometrical optics theory is not valid for smaller droplets and it is necessary to evaluate the influence of the Knudsen layer for their heat exchange and phase transitions. In the *droplet* model, under discussion the influence of the Knudsen layer is not assessed.

The reliability of the numerical scheme depends on the quality of its grid. It is very important to properly choose the dimensionless coordinates. When calculating the non-stationary temperature field and its gradient by expressions (10) and (12), it is necessary to decide on the number N, which is the number of assessable members in the infinity integral equation series. Thus before η and $\overline{\mathrm{Fo}}$ grid optimisation the optimal number of infinite sum members N_{op} should be defined. The numerical scheme control system and defined optimal number of infinite sum members $N = N_{op}$ are presented in this paper. These results allow further optimization of the numerical scheme.

3 Control of numerical schemes and definition of N_{op}

For the control mechanism of the numerical scheme and defining the optimal number of members in the infinite sum, water droplet unsteady phase transition cycle in the heat exchange k and $k+r$ cases was analysed. Heating by conduction was modelled following presumption that $q_{r,j} = 0$ and $\mathrm{Nu} = 2$. Physical properties of vapour gas mixture were selected depending on the temperature which satisfies the $1/3$ rule: $T = T_R + (T_g - T_R)/3$. In the case of combined heating by conduction and radiation, an assumption of absolutely black external radiation source of the droplet surrounding temperature was used. The local radiation flux inside the droplet was calculated according to the methodology [5]. Optical effects on droplet surface and complex refraction index peculiarities in radiation spectrum [3] were taken into account.

Unsteady phase transitions of water droplet with initial diameter of $150 \cdot 10^{-6}$ m and temperature $T_0 = 290$ K sprayed in the dry ($\overline{p}_{v,\infty} = p_{v,\infty}/p = 0$) and wet ($\overline{p}_{v,\infty} = 0.25$) air with parameters (pressure 0.1 MPa and temperature 1000 K) were modelled. Values of parameters $J = 81$ and $I = 41$ were assumed in the numerical scheme grid, when $\mathrm{Fo}_{uf,k} = 0.7$. Considering the thermal radiation, the spectrum range quantified by wave numbers $\omega = 1/l_b$ from $\omega_1 = 10^4$ m^{-1} to $\omega_2 = 1.25 \cdot 10^6$ m^{-1} was selected. The linear grid of the radiation flux calculation scheme $\sum_{m=1}^{M-1}(\omega_{m+1} - \omega_m) = \omega_2 - \omega_1$ ensures heightened attention on short-wave area. In this area, the spectral radiation is intensive and sufficient changes in water optical properties occur [3]. The details of radiation flux calculations will be revealed more in depth in further article of this cycle.

The physical properties of water and air, that are necessary for modelling are defined by linearly interpolating already known array of experimental data of properties. The saturated water vapor pressure and temperature function $p_s(T)$, in the interval of droplet surface temperature change $0 \div 95\,^{\circ}\mathrm{C}$ is defined by an accurate Gerry empirical correlation. Coefficient of water vapor diffusion in the air is defined by known empirical expressions:

$$D = \begin{cases} 5.385 \cdot 10^{-10} \cdot T^{1.88}, & T < 400\ \mathrm{K}; \\ 1.732 \cdot 10^{-9} \cdot T^{1.685}, & T > 400\ \mathrm{K}. \end{cases} \tag{21}$$

In thermal parameter calculation schemes, the number of assessed members of the infinite sum is changed freely.

3.1 Control of numerical iterative scheme

During the iterative calculations, the functional formed on expression (3) basis is minimized by the method of steepest descent in respect to the droplet temperature $T_{R,i,it}$. This temperature is freely chosen by a specialized sub-program from the temperature interval defined by primary conditions. For each $T_{R,i,it}$ value, heat fuxs on the surface of the droplet that match each one, are calculated and their compliance to condition (20) are tested.

During the numerical experiment, the process of each iterative cycle $it = 1 \div IT$ is controlled (Fig. 1). When iterations are nearing the temperature $T_{R,i,it=IT}$ (Fig. 1a) that meets the balance condition, the heat flux imbalance δ decreases (Fig. 1b). Practically, the condition $\delta = 0$ cannot be ensured, because δ approaches to zero when $T_{i,J,it} - T_{i,J} \to 0$. This would require to assess temperature changes of around 10^{-4} what is not reasonable in the physical sense (Fig. 1a). In the iterative cycles, the balance of heat flux on the surface condition $|\delta_{acc}| = 0.02\%$ was satisfied. The droplet heat and mass exchange

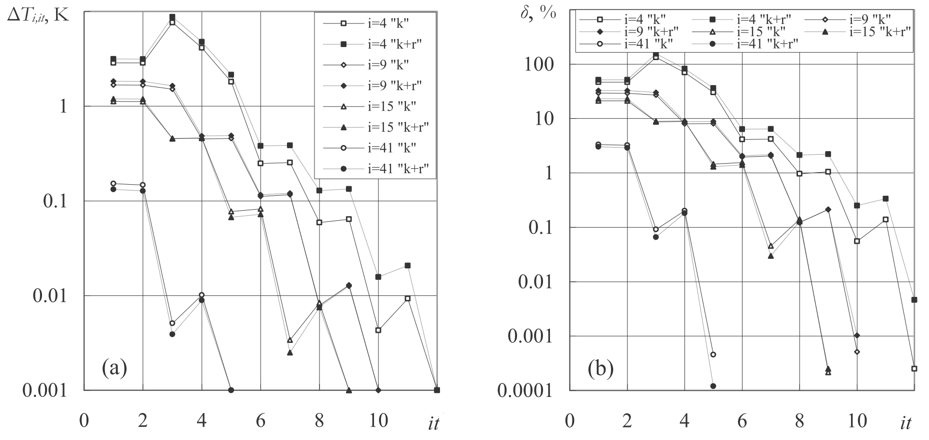

Figure 1. Control of iterative cycle of droplet surface temperature $T_{R,i}$ defining: (a) deviation of surface temperature; (b) imbalance of heat flux. $T_{R,i,k}$: (4) 302.424 K, (9) 312.421 K, (41) 332.686 K; $T_{R,i,k+r}$: (4) 303.397 K, (9) 314.399 K, (41) 335 K; $\Delta T_{i,it} = 0.001 + |T_{i,J,it} - T_{i,J,IT}|$; $\overline{p} = 0$; $N = 151$.

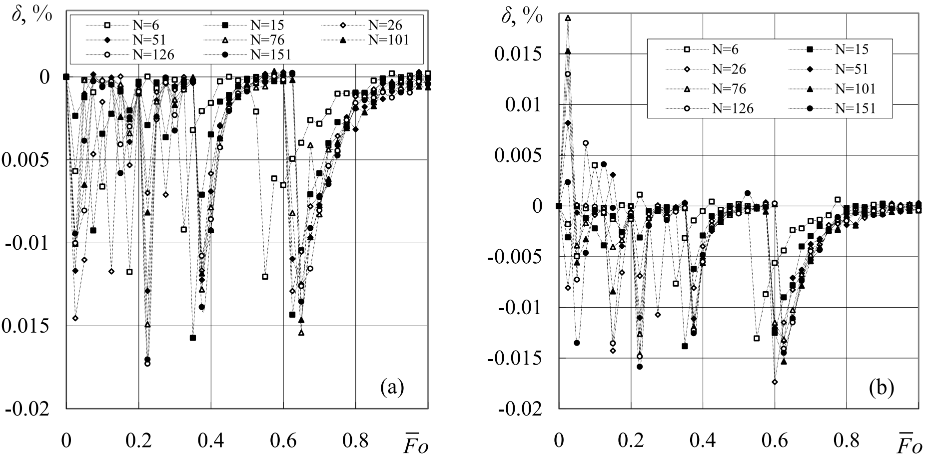

Figure 2. Imbalance of heat flux on the droplet surface at iteration $it = IT$, when temperature $T_{R,i}$ is defined: (a) conductive heating; (b) combined heating.

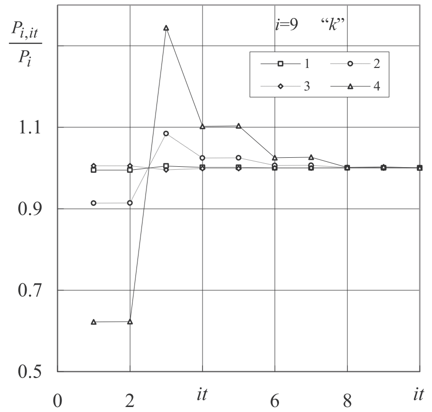

Figure 3. The droplet heat and mass parameters P change during the iterative cycle. P meaning: (1) T_R, (2) m_v^+, (3) q_k^+, (4) q_k^-; $T_{R,i} = 312.421$ K; $m_{v,i}^+ = 0.04702$ kg/(m^{2}s); $q_{k,i}^+ = 373.943$ kW/m^2; $q_{k,i}^- = 261.511$ kW/m^2; $N = 151$.

parameters sensitivity to change of assumed in the iterative cycle $T_{R,it}$ is quite different (Fig. 3). However, an imbalance of heat flux approaching and receding from the surface of the droplet lower than $\pm 0.02\%$ was ensured independently from the chosen number of members N of the infinite sum (Fig. 2).

3.2 The optimal number of evaluated members in the infinite sum

In order to define the optimal number N_{op} of assessable members of the infinite sum, an in-depth analysis of droplet heat and mass transfer thermal parameters $P_T(\mathrm{Fo}, N)$ function has been accomplished. It is justified that N_{op} worth to associate with the al-

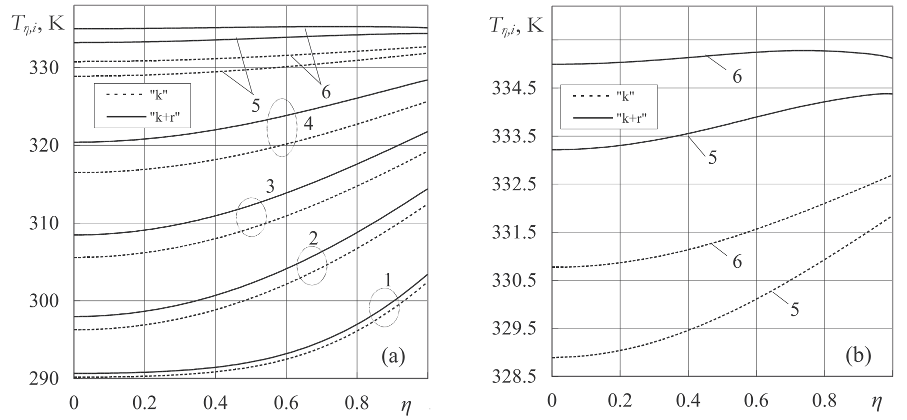

Figure 4. Droplet warming method influence on its thermal state: (a) in non-stationary evaporation phase; (b) in its final stage. $\overline{\text{Fo}}$: (1) 0.075, (2) 0.2, (3) 0.325, (4) 0.5, (5) 0.875, (6) 1.

lowed error of the numerical experiment. For that, a graph of the droplet non-stationary temperature field function $T(\eta, \text{Fo})$ was formed for different N values was used.

By the additional numerical experiment was justified that the effect of function f_n calculated with (11) to infinite sums in expressions (10) and (12) is insignificant when $n > 150$. Therefore, for function $T(\eta, \text{Fo}, N)$ comparative analysis, the supporting functions consider to be $T(\eta, \text{Fo}, N = 151)$, were used. The influence of the heating method on supporting functions is obvious (Fig. 4).

For comparative analysis the time moments $\overline{\text{Fo}}_{i=9} = 0.2$ and $\overline{\text{Fo}}_{i=41} = 1$ were chosen (Figs. 6–8). The first moment in time $\overline{\text{Fo}}_{i=9} = 0.2$ represents the primary intensive droplet warming stage (Fig. 6a). Absorbed heat flux cause only quantitative changes in droplet thermal state (Fig. 4a), but temperature field type doesn't change qualitatively: minimal temperature occur in the center of the droplet $T_{min} = T_C$ and maximal on the surface $T_{max} = T_R$. Therefore in the initial heating stage gradient of temperature field is positive.

The other chosen moment in time $\overline{\text{Fo}}_{i=41} = 1$ represents the final modeled phase transition regime stage (Fig. 4b). In this stage, the droplet's thermal condition depends on the method of droplet heating. In the case of conductive heating (k heat transfer case), temperature field gradient in the droplet consider to be positive when the droplet's thermal state consistently approaches to closely isothermal (Fig. 4b).

In the case of complex heating ($k + r$ heat transfer), the radiation flux absorbed by the droplet qualitatively affects the droplet's thermal state in the final non-stationary evaporation stage and a negative temperature field gradient is formed within the droplet (Fig. 4). That forms premises for the radiation flux that is absorbed by the droplet to act in the liquid evaporation process [8].

When researching the effect of the number of assessable members in the infinite sum on functions $T_{i,k}(\eta)$ and $T_{i,k+r}(\eta)$, the number of members N was gradually increased from 5 to 151. Selected number N has a significant impact on droplet thermal state during modelled phase transitions. When N is closer to chosen for supporting functions value

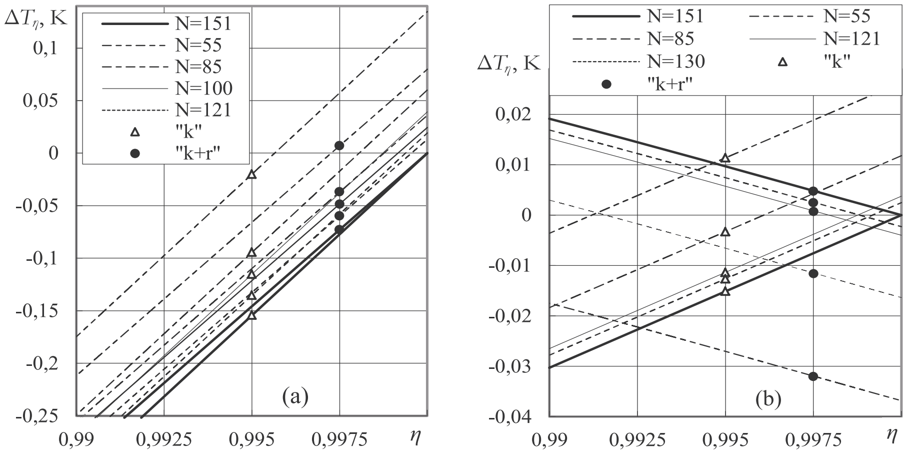

Figure 5. Deviation of function $T(\eta, \overline{\text{Fo}}, N)$ versus $T(\eta, \overline{\text{Fo}}, N = 151)$ in the outer layers of the droplet. Heating moment: (a) $\overline{\text{Fo}} = 0.2$; (b) $\overline{\text{Fo}} = 1$. $\Delta T_\eta = T(\eta, N) - T(\eta, N = 151)$.

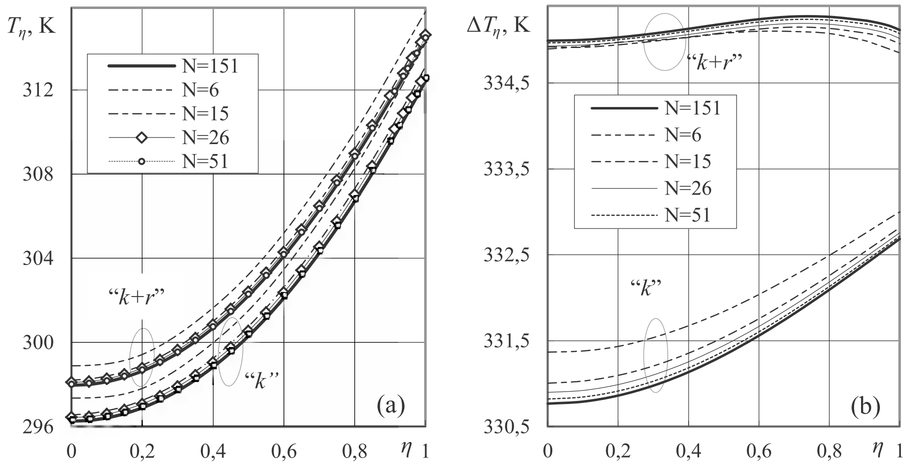

Figure 6. Influence of chosen number of evaluated members N in infinite sum on calculated droplet thermal parameters, when $N < 52$: (a) $\overline{\text{Fo}} = 0.2$; $T_{\eta,k}(\eta = 1, N = 151) = 312.421$ K; $T_{\eta,k+r}(\eta = 1, N = 151) = 314.39$ K; (b) $\overline{\text{Fo}} = 1$; $T_{\eta,k}(\eta = 1, N = 151) = 332.686$ K; $T_{\eta,k+r}(\eta = 1, N = 151) = 335.117$ K.

$N = 151$ temperature field graph became closer to $T(\eta, \overline{\text{Fo}}, N = 151)$. Deviation of functions $T(\eta, \overline{\text{Fo}}, N)$ versus $T(\eta, \overline{\text{Fo}}, N = 151)$ is evaluated by difference $\Delta T_{\overline{\text{Fo}},N}(\eta) = T(\eta, \overline{\text{Fo}}, N) - T(\eta, \overline{\text{Fo}}, N = 151)$. This difference inside the droplet depends on heating duration and type (Fig. 5).

In the primary warming phase, a smaller number of assessable members N of the infinite sum determine a higher calculated droplet temperature for model k and $k+r$ cases

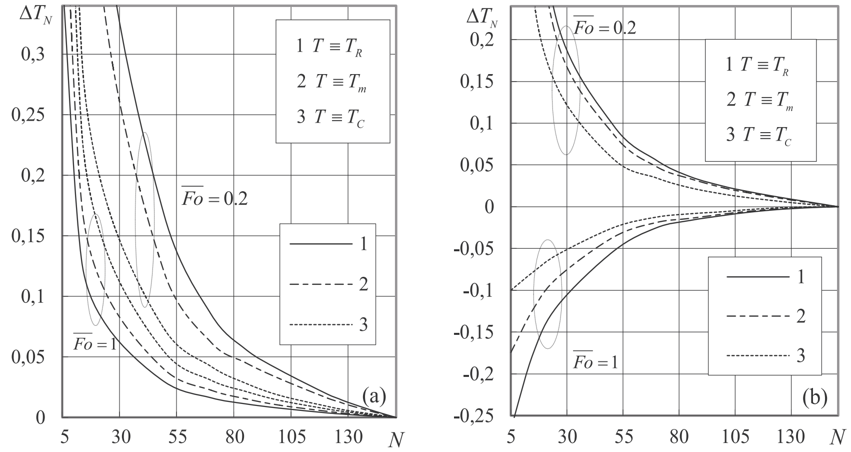

Figure 7. Influence of N on calculated characteristic temperatures: (a) conductive heating k; (b) combined $k + r$ heating.

(Fig. 6). In the final k warming phase stage, a smaller number of assessable members N of the infinite sum also determine a higher calculated temperature, however, in the case of $k + r$ heating, we already notice a lower calculated droplet temperature (Fig. 6b).

Analysis of distribution of functions $\Delta T^{k}_{\overline{\mathrm{Fo}},N}(\eta)$ and $\Delta T^{k+r}_{\overline{\mathrm{Fo}},N}(\eta)$ in graphs has shown that the choice of N_{op} is associated with the strictness of requirements that are posed for the solving of *droplet* problem. The primary, engineering and strict scientific cases of the *droplet* problem solutions evaluations were distinguished.

In the model of *droplet* problem under development, the essential role is played by the droplet surface temperature T_R, because it is determines phase transition regime and most mass of the droplet is accumulated in the surface layers of the droplet. Detailed analyses of N influence on temperature field were provided (Fig. 5). Looking for optimal N it is reasonable to evaluate its influence on other characteristic temperatures too (Fig. 7).

For the first evaluation stage results of modelling with $N < 55$ were analysed. Case with $N_{op} = 51$ was assessed as acceptable, because its ensured les then 0.15 K deviation in initial stage of evaporation and less then $|\pm 0.05|$ K deviation in final stage of $T_{R,N}$, $T_{C,N}$ and $T_{m,N}$ from $T_{R,N=151}$, $T_{C,N=151}$ and $T_{m,N=151}$. The accuracy of surface temperature calculation allows the assertion that number $N_{op} = 51$ will ensure that condition (20) will be met in five percent reliability in the first evaluation stage (Fig. 1).

Range of $55 < N < 105$ for engineering evaluation was selected. Case with $N_{op} = 101$ was assessed as acceptable, because its ensured les then 0.04 K deviation in initial stage of evaporation and less then $|\pm 0.02|$ K deviation in final stage (Fig. 7). Value $N_{op} = 100$ will ensure condition (20) to be met in half percent reliability in the engineering evaluation of the *droplet* problem.

Half percent reliability is acceptable in scientific analysis too. When tenths of percent reliability of (20) condition is requested, the changes of droplet surface temperature less than 10^{-2} K should be taken into account (Fig. 1). Number $N_{op} = 121$ was selected (Fig. 7). The gradient of non-stationary temperature field in the evaporating droplet is

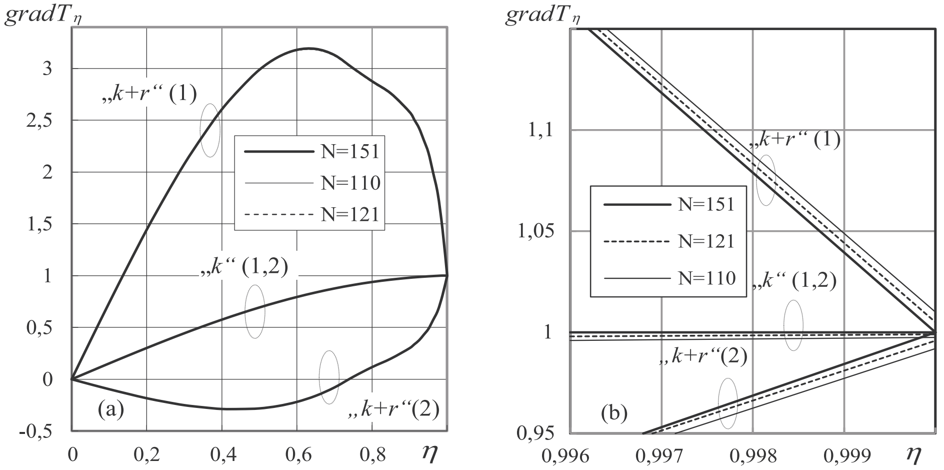

Figure 8. Influence of N on calculated temperature gradient: (a) inside the droplet, (b) in the surface layers of the droplet. (1) $\overline{\mathrm{Fo}} = 0.2$; (2) $\overline{\mathrm{Fo}} = 1$. $\mathrm{grad}\overline{T}_\eta = \mathrm{grad}T(\eta, N)/\mathrm{grad}T(\eta = 1, N = 151)$. $\mathrm{grad}T_k(\eta = 1, N = 151)$, K/m: (1) 412142.1, (2) 41457.2; $\mathrm{grad}T_{k+r}(\eta = 1, N = 151)$, K/m: (1) 386942.2, (2) -28314.7.

calculated with high precision (Fig. 8). This gradient is essential for determining the heat transfer by conduction. By the peculiarities of $\mathrm{grad}T_\eta$ is it possible to justify the moment of transition from non-stationary evaporation to balanced evaporation stage: in the case of k, heat transfer $\mathrm{grad}T_{r=R,k}(\mathrm{Fo} \to \mathrm{Fo}_e) \to 0$, while in the case of complex heating, it must ensure the output of radiation, which was absorbed by the droplet, by conduction to the surface of the droplet

$$\mathrm{grad}T_{r=R,k+r}(\mathrm{Fo} \to \mathrm{Fo}_e) \cdot \lambda_l \to q_r^-(\mathrm{Fo} \to \mathrm{Fo}_e). \tag{22}$$

Among the many parameters that influence the droplet heat and mass transfer, the exclusive role belongs to the droplet surrounding gas temperature T_g and vapour concentration $\overline{p}_{v,\infty}$ there. The temperature difference $T_g - T_R$ is unimportant characteristic of the environmental impact on a droplet, which determines the rate of droplet heating and evaporation intensity. When the partial vapour pressure in the droplet surround gas is $\overline{p}_{v,\infty} > 0$ condensing phase transitions regime is possible on the surface of the droplet and droplet is heated up to a higher temperature in unsteady evaporation regime compared to $\overline{p}_{v,\infty} = 0$ case (Fig. 9).

The droplet thermal state change can be defined by temporal functions $T_R(\tau)$, $T_C(\tau)$ and $T_m(\tau)$. According to the function $T_R(\tau)$ can be unambiguously defined phase transition regime: condensing when $T_R(\tau) < T_{dp}$, unsteady evaporation when $T_{dp} < T_R(\tau) < T_{ee}$, and equilibrium evaporation when $T_R(\tau) = T_{ee}$. Temperature difference between the droplet surface and its centre $|T_R - T_C|$ reflects the thermal conditions in which opportunity of spontaneous fluid circulation inside the droplet can be defined. Thermal state of non-isothermal droplet can be integrally evaluated by the mass average temperature $T_m = \int_0^R \rho_{l,r} T_r r^3 \,\mathrm{d}r / \int_0^R \rho_{l,r} r^3 \,\mathrm{d}r$.

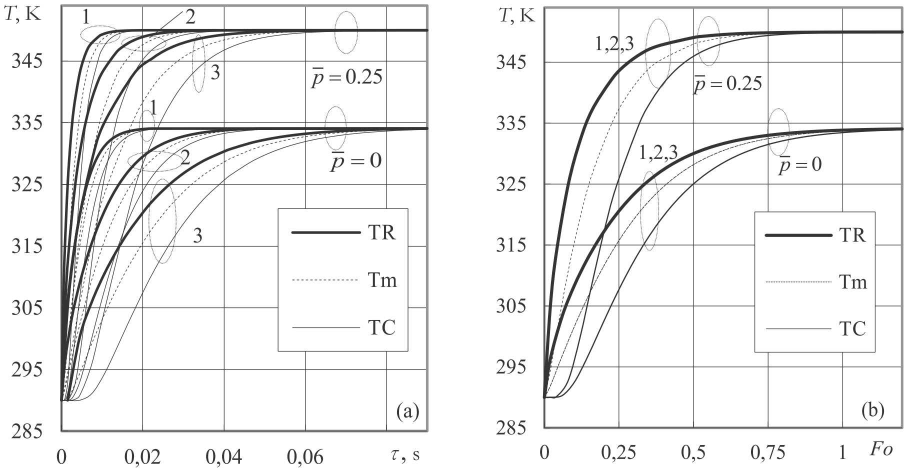

Figure 9. Influence of air humidity on droplet heating: (a) in real time, (b) in Fourier number scale. The case of conductive heating. $T_g = 1000$ K, $T_0 = 290$ K, $N = 121$, $J = 81$, $I = 61$, $R_0 \cdot 10^6$ m: (1) 50, (2) 70, (3) 100.

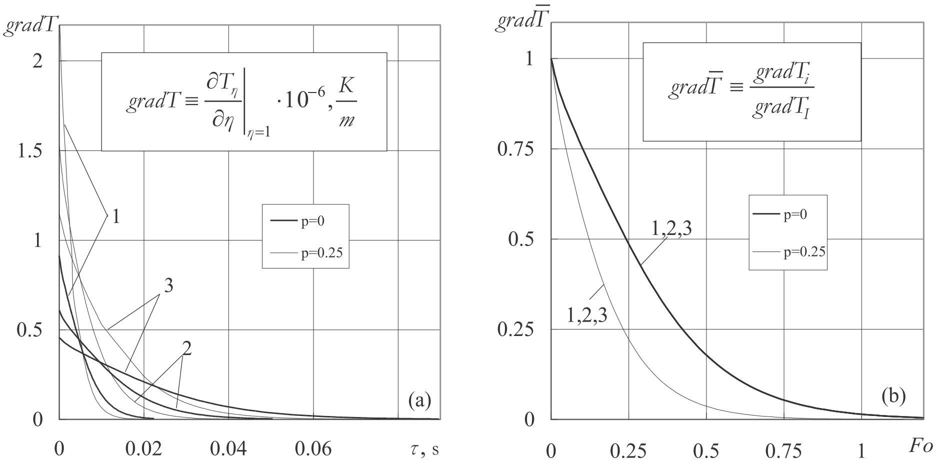

Figure 10. Influence of air humidity on the non-stationary temperature field gradient of the droplet: (a) in real time, (b) in Fourier number scale. The case of conductive heating. $T_g = 1000$ K, $T_0 = 290$ K, $N = 121$, $J = 81$, $I = 61$, $R_0 \cdot 10^6$ m: (1) 50, (2) 70, (3) 100.

In thermal technologies, droplet flows of different dispersivity are met. In the general case, the function $T(r, \tau)$ for droplets in these flows is determined by numerical experiments, taking into account their size within the whole diameter spectrum.

In the case of k heat transfer, the extent of the experiments can be reduced by calculating phase transfers of a freely chosen one diameter droplet. In order to do that, the real time and droplet dimension function $T_k(r, \tau)$ must be transformed into a universal time and universal droplet dimension coordinates $T_k(\eta, \mathrm{Fo})$. Functions $T_{R,k}(\mathrm{Fo})$, $T_{C,k}(\mathrm{Fo})$

and $T_{m,k}(\mathrm{Fo})$ are insensibil to droplet dispersivity (Fig. 9b), in the case defined by parameters T_g, $\overline{p}_{v,\infty}$ and $T_{l,0}$.

By analogy, insensitive to droplet dispersivity, gradient functions of temperature field within the droplet (Fig. 10) can be formed, using the dimensionless function $\mathrm{grad}\overline{T}_R(\mathrm{Fo}) = \mathrm{grad}T_R(\mathrm{Fo})/\mathrm{grad}T_{R,0}$ (Fig. 10b). Here, it is necessary to discuss the conception of the primary gradient $\mathrm{grad}T_{R,0}$. In strict assessment, the isothermal primary regime gradient within the droplet is zero. In this case as the primary gradient is taken $\mathrm{grad}T_{R,0} = (q^+_{\Sigma,0} + q^+_{co})/\lambda_{l,0}$ which is calculated at the primary moment of interaction between the droplet and surrounding.

When the parameters T_g, $\overline{p}_{v,\infty}$ and $T_{l,0}$ are defined, functions that are independent from droplet dispersivity $\overline{P}_k(\mathrm{Fo}) = P_k(\mathrm{Fo})/P_0$ can be formed by the results of modelling heat and mass transfer of a droplet with a freely chosen size. These functions can be used to evaluate influence of more complicated heating than k heat transfer case for droplet phase transition processes.

4 Conclusion

In this article, the droplet heat and mass transfer model is provided, which allows to define numerically variation of the droplet's thermal state and phase transitions in the whole droplet life cycle, from liquid spraying to full evaporation. The peculiarities of forming the numerical scheme grid are discussed. The control mechanism, based on the condition of energy flow balance on droplet surface, is highlight.

Non-stationary phase transitions of water droplets in the air, in conduction and complex heating cases have been modelled.

The optimal for the primary, engineering and strict scientific cases of the *droplet problem* solutions number of a finite number of members in the infinite integral equations for droplet temperature field and its gradient parameters calculations was defined by the numerical experiment ($N_{op} = 51, 101$ and 121 accordingly). These results allow further *droplet* problem numerical scheme optimization.

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