ISSN 1392-1207. MECHANIKA. Vol. 30, No. 4, 2024: 324–332

Numerical Modelling of Phase Transformations of Water Droplets for Efficient Heat Recovery from Biofuel Flue Gas

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https://doi.org/10.5755/j02.mech.35992

Nomenclature

B_M – Spalding mass transfer parameter; B_T – Spalding heat transfer parameter; D – diffusivity, m^2/s; g_v – vapour flux to droplet surface, kg/s; m_v – vapour flux density, kg/(m^{2}s); Nu – Nusselt number; r – radial coordinate, m; R –radius of a droplet, m; Sh – Sherwood number; t – temperature, °C; q – heat flux density, W/m^2; X_v – vapour volume fraction in air; Y_v – vapour mass fraction in air; ρ – density, kg/m^3; τ – time, s;.

Subscripts: *co* – condensation; *c* – convection; *dp* – dew point; *ee* – equilibrium evaporation; *f* – phase change; *g* – gas; *l* – liquid; *m* – mass average; *r* – radiation; *s* – saturated; *v* – vapour; *vg* – vapour-gas mixture; 0 – initial state

1. Introduction

The injection of liquid fuels and water into a gas flow is used for energy and industrial applications. Liquid fuels in dispersed form are the most common in fuel combustion, while water droplets have a wide range of applications. Water spraying applications for air conditioning [1], high-temperature gas flow cooling and fire front suppression [2] are already traditional technologies. A new application field for dispersed water has been discovered in modern energy with the reduction of fossil fuel use and the shift towards renewable energy production [3]. Water is sprayed to humidify the supplied combustion air, reduce the temperature in the furnace and prevent slagging, clean the combustion products of pollutants, and recover the heat of phase transformations from the removed humid flue gases [4-6].

The droplet phase transformation processes define the efficiency of liquid injection technologies. In liquid fuel combustion, it is important that the droplets would evaporate as quickly as possible. In the case of water injection into humid flue gas, droplet condensation phase transformation is also relevant. The condensation droplet mode is not desirable when injecting water to humidify the supply air, to regulate the combustion process in the furnace to reduce the concentration of toxogens in the flue gases, or to cool it. However, the heat of phase transformations can only be recovered from the removed flue gases by condensing the water vapour from them. Therefore, a good understanding of the full phase transformation mode cycle behaviour of injected water droplets is essential for the development of an efficient and environmentally friendly biofuel combustion technology. The start of the droplet phase transformations is identified when the injection time of water is ($\tau = 0$) and the end of the droplet evaporation is ($\tau = \tau_f$). The period $\tau \equiv 0 \rightarrow \tau_f$ defines the duration of the phase transformations of the water droplets injected in the biofuel flue gas flow. It includes the condensation $\tau \equiv 0 \rightarrow \tau_{co}$, the transitional evaporation $\tau \equiv \tau_{co} \rightarrow \tau_{ee}$ and the equilibrium $\tau \equiv \tau_{ee} \rightarrow \tau_f$ phase transformation modes. The condensation mode of the droplets is achieved by the injection of water at a temperature below the dew-point t_{dp} temperature. In the transient evaporation mode, the droplets are heated to the t_{ee} temperature, which is characteristic of the equilibrium evaporation. During equilibrium evaporation, all the heat provided for the droplets evaporates the water.

In the phase transformation regimes of droplets, there is an intense interaction of complex transfer processes [7] that are defined by different factors. The droplets slipping in the flue gas flow increase the convective heating and induce a forced circulation of the liquid within them [8]. The Stefan hydrodynamic flow, that accompanies the phase transformations, weakens the convective heating of the droplets but accelerates their evaporation [9]. In semi-transparent water, the radiation flux is absorbed by the water together affecting the heating of the droplets and forming a non-stationary temperature field gradient [10]. The combination of these factors determines the thermal and energetic state of water droplets and the dynamics of phase transformations. In biofuel combustion technology, water injection into the flue gas flow of the furnace and in the condensing economiser can be considered as traditional case. The injection of water into the flue gas flow prior to the condensing economiser is a viable option to cool the flue gas to near dew point temperature and to ensure efficient heat recovery of the phase transformations. For each water injection case, the boundary conditions for droplet heat and mass transfer are different. Therefore, the influence of the factors defining the interactions between the transfer processes also varies. This must be taken into account when selecting water injection modes to ensure efficient combustion of biofuels. Numerical modelling of the phase transformations of the droplets in the case of compound convective-radiative heating is time-consuming due to the need to evaluate the spectral absorption of the radiation in semi-liquid water [10, 11].

Water is semi-transparent liquid; therefore, droplets partially reflect, transmit and absorb the falling light beam. These optical effects are defined by the complex index of refraction, which is significantly changing in the infrared spectrum [11, 12]. The complex heat transfer in water droplets is defined by the local radiation flux, which regularities has an impact for droplet thermal state variation in the whole phase change regimes. In semi-transparent spherical droplet, the local radiation flux is described by the spectral radiation model [10] based on optical geometry theory, where optical effects on the droplet surface are defined according to [13] recommendations. The impact of radiation is already confirmed in the complex transfer processes interaction [7], however, the impact of water dispersity in the flue gases temperature range relevant for biofuel combustion technologies is still not evaluated.

This work aims to investigate the influence of radiation on the droplet's phase transformations in a biofuel flue gas flow at different temperatures, to assess the limits of the applicability of a simplified model of convective heating, to summarize numerically the phase transformations of water injected in the exhausted flue gas before the condensing economizer, and to determine the influence of the droplet dispersity and the influence of the temperatures of the flue gas and water.

2. Two phase flow numerical calculation methodology

Assumptions: 1. Water is injected into a cleaned biofuel flue gas, which is defined as a $X_v \equiv 0.1 \rightarrow 0.4$ humid airflow. 2. Convective heating of the droplets is defined by the Re_0 number. 3. In the case of composite heating, the spectral radiation flux impact on the droplets is defined by the radiation from the water vapour and the soot-coated walls and is close to the blackbody radiation. 4. The ratio of injected water and air flows is relatively small, so the droplet/droplets phase transformations do not affect the air flow parameters.

The variation of the droplet mass and vapour flux in the phase transformation regime is described by the evaporation dynamics equation:

$$\frac{\partial\left(\frac{4}{3}\pi\rho_l R^3\right)}{\partial\tau} = -\frac{g_v}{4\pi R^2}. \tag{1}$$

The vapour flux in the condensation mode of the droplet is assumed to be negative, while in the evaporation mode it is assumed to be positive and is described by a modified Fick's law [8]:

$$g_v = 2\pi R\rho_{vg}D_{vg}\left[2\,ln\left(1+B_M\right)+\frac{B_M\left(Sh-2\right)}{\left(1+B_M\right)^{0.7}}\right]; \tag{2a}$$

$$B_M = \frac{Y_{v,R}-Y_{v,g}}{1-Y_{v,R}}. \tag{2b}$$

In the steam flow Eq. (2a), the influence of the Stefan hydrodynamic flow is taken into account by the Spolding mass transfer B_M parameter described by expression (2b).

The heat flux of the phase transformations is defined by the steam flux:

$$q_f = \frac{g_v}{4\pi R^2}\bigg| L. \tag{3}$$

The convective heating of a droplet is defined by the modified Newton's law of heat release [8, 10]:

$$q_{c,g} = \lambda_{vg}\frac{t_g-t_R}{2R}\left[2\frac{ln\left(1+B_T\right)}{B_T}+\frac{Nu-2}{\left(1+B_T\right)^{0.7}}\right]; \tag{4a}$$

$$B_T = c_{p,vg}\frac{t_g-t_R}{L_l}\left(1-\frac{q_{c.l}}{q_{c,g}}\right). \tag{4b}$$

In the convective heat flux Eq.(4a), the influence of the Stefan hydrodynamic flow is taken into account by the Spolding mass transfer BM parameter described in expression (4b) [10].

The convective heat transfer inside the droplet is defined by a modified Fourier's law of heat conduction:

$$q_{c,l} = -k_{c,l}\lambda_l\frac{\partial T\left(r,\tau\right)}{\partial r}\bigg|_{r=R}. \tag{5}$$

The temperature gradient of the convective heat flux inside the droplet in Eq. (5) is described according to the methodology of [10] for compound radiative-conduction heating, and the influence of water circulation is taken into account by the effective thermal conductivity $k_{c,l}$ parameter [8]. The radiation absorbed in a semi-transparent droplet by the local flux $q_r(r)$ is defined by a spectral model based on the geometrical optics theory [10], in which the complex water refractive index is chosen according to the data [12]. In the case of convective heating, $q_r(r)=0$.

The thermal state of a droplet in the phase transformation regimes is defined by its mass-averaged temperature:

$$t_{l,m} = \int_0^R \rho_l c_{p,l} t_l r^3 dr \Big/ \int_0^R \rho_l c_{p,l} r^3 dr. \tag{6}$$

The variation of the thermal state of a droplet is related to the dynamics of its energy state in phase transformation regimes:

$$t_R\left(\tau\right) \leftrightarrow q_{c,g}\left(\tau\right)+q_{c,l}\left(\tau\right)-q_f\left(\tau\right)=0. \tag{7}$$

The heat flux balance Eq. (7) is specified by expressions (2-4) and solved numerically by an iterative $it=1\rightarrow IT$ cycle as a function of the droplet surface temperature $t_R(\tau)$, according to the methodology in [7]. The iterative cycle is performed at the extracted control moments of time τ_i. The final IT iteration of each cycle defines the average droplet surface temperature $t_{R,i,it}$=IT that fulfil the requirement:

$$t_{R,i,IT} \rightarrow \left|1-\frac{q_{c,g,i,IT}}{q_{c,l,i,IT}-q_{f,i,IT}}\right|\times 100\,\% \le 0.05\,\%. \tag{8}$$

The droplet diameter $2R_{i,\,it}$ is adjusted after each iteration by numerically solving Eq. (1).

3. Results and discussion

The phase transformations of injected water droplets in a humid air flow are numerically simulated in two stages. The first one defines the influence of radiation on the heating and evaporation of water droplets in a humid air flow at different temperatures and assesses the possibility of applying the convective "c" heat exchanger model to define the phase transformations of the droplets. In a second step, the regularity of the droplet phase transformations for water injection into the removed flue gas before a condensing economiser was numerically investigated under typical boundary conditions.

3.1. Influence of radiation on the heating and phase transformation of water droplets in a humid gas flow

The heat and mass transfer of water droplets was numerically simulated for X_v=0.3 humidity and t_g=150°C→1000°C temperature convective "c" and combined convective-radiative "cr" heating cases. The convective heating of the droplets is defined by the initial Reynolds number Re_0=50 with air velocity of 10 m/s. In the case of compound heating, the temperature of the radiation source is equated to the air temperature.

The air temperature t_g influences the convective heat transfer and the radiation source temperature t_{sour}≡t_g influences the external radiation. Therefore, the variation of the thermal state of water droplets (Figs. 1, a and 2) and the dynamics of phase transformations (Fig. 1, b) depend on their heating process and the temperature of the gas flow. In

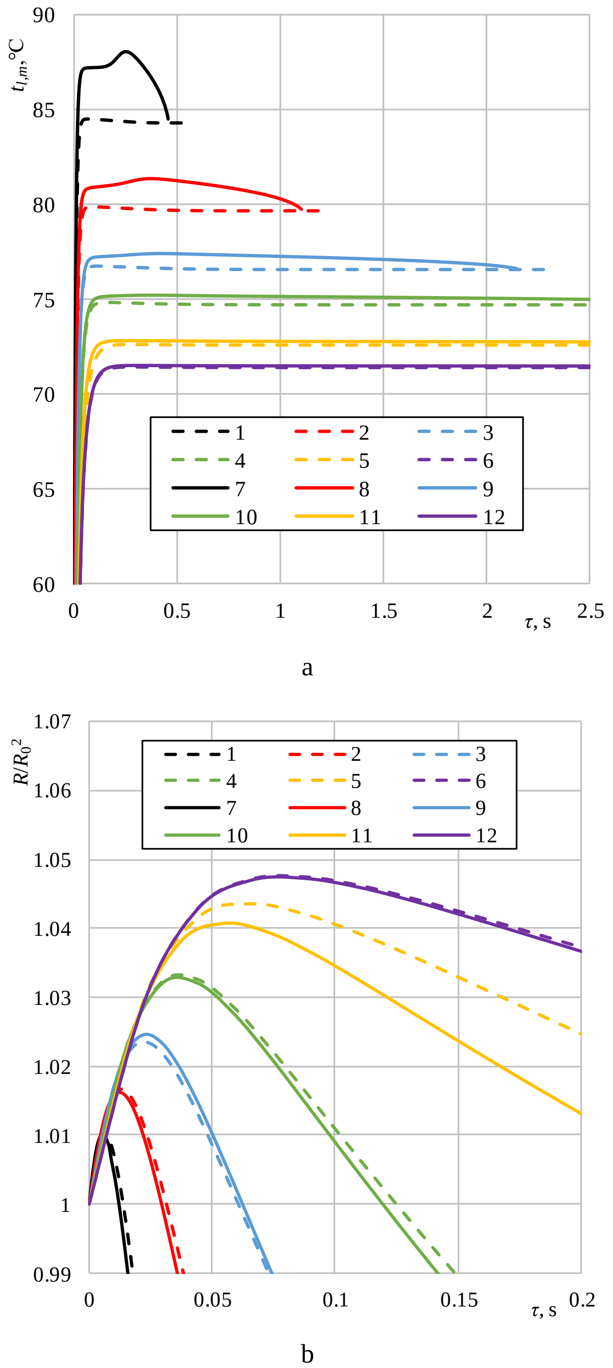


Fig. 1 Time history of water droplet temperature (a) and dimensionless surface area (b) in the case of convective ”c” (1-6 dotted lines) and complex ”cr” heating (7-12 solid lines) cases; t_g, °C: (1, 7) 1000, (2, 8) 600, (3, 9) 400, (4, 10) 300, (5, 11) 200, (6, 12) 100; X_v=0.3; Re_0=50; w_g=10 m/s; $t_{l,0}$=40°C

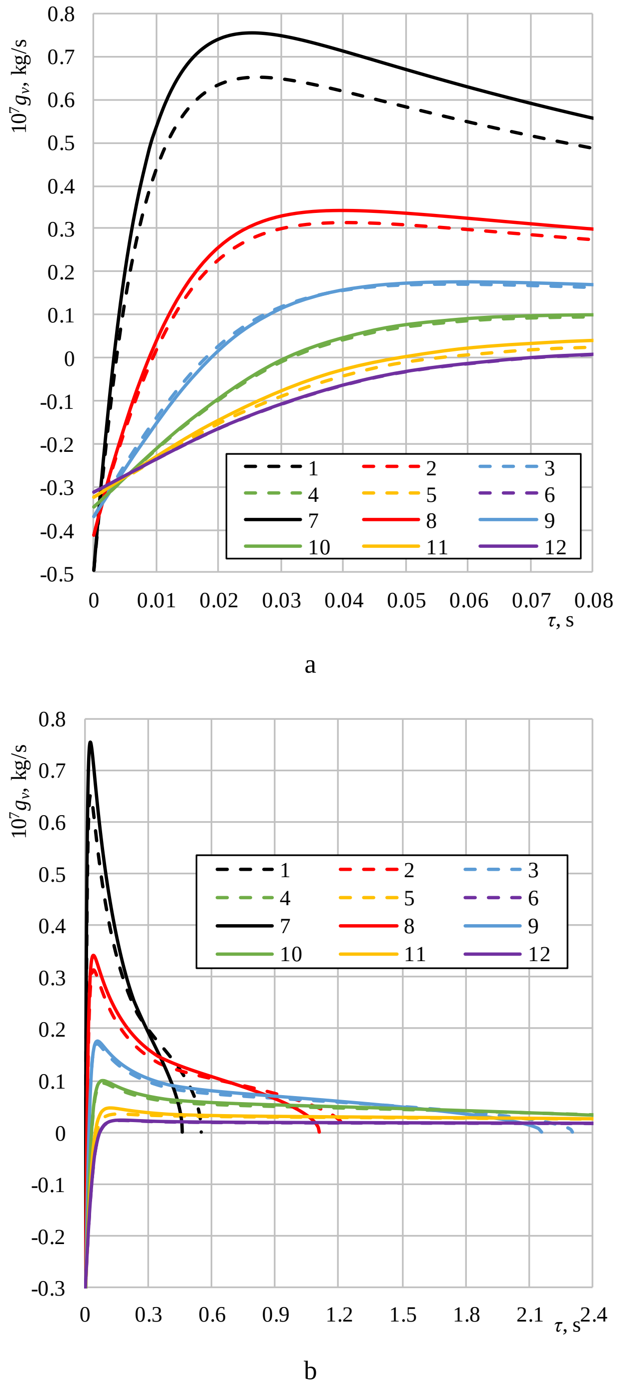


Fig. 2 Time history of vapor dynamics in condensation regime (a) and in phase change regimes cycle (b); marking as in Fig. 1

the phase transformation regimes, the temperature of the droplets varies in a specific way. In the simulated case, the temperature of the injected water of t_l=40°C is below the dew point temperature of t_{dp} = 69.4°C, so in the condensation regime the droplet surface warms up to t_{dp}. The influence of the heating process on the duration of τ_{co} in the condensation mode is not significant, while the influence of the air temperature is relevant (e.g. $\tau_{co,\text{“c“}}$=0.0036 s and $\tau_{co,\text{“cr“}}$=0.0032 s, when t_g=1000°C, and $\tau_{co,\text{“c“}}$=0.049 s and $\tau_{co,\text{“cr“}}$=0.043 s, at t_g=200°C).

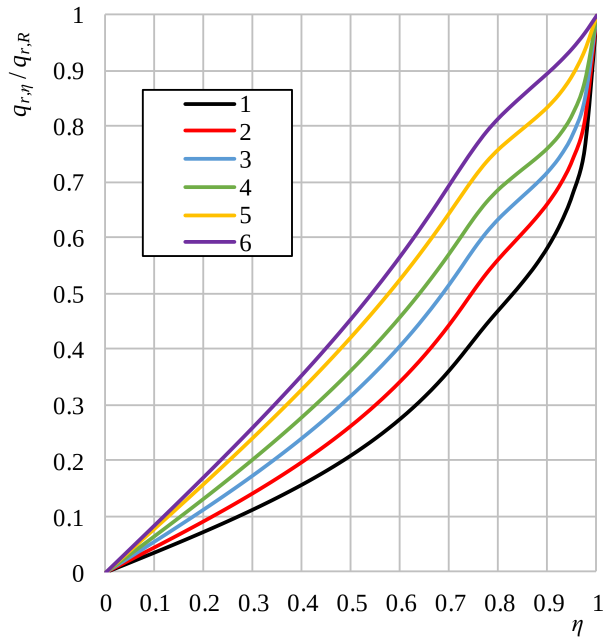
In the transit evaporation mode, the droplets heats to a thermal state characteristic to equilibrium evaporation, which is defined qualitatively by the heating process, air temperature and humidity (Fig. 1, a). In transit evaporation, the droplets warm up to the temperature $t_{l,m,ee}$, which is higher in the case of compound heating (Fig. 1, a). When the air flow temperature decreases, the difference between the temperatures $t_{l,\,m,ee}$,"cr" and $t_{l,m,ee}$ "c" decreases rapidly (e.g. $t_{l,m,ee,\text{“c“}}$=84.5°C and $t_{l,m,ee,\text{“cr“}}$=88.1°C, at t_g=1000°C, and $t_{l,m,ee,\text{“c“}}$=72.6°C and $t_{l,m,ee,\text{“cr“}}$=72.8°C, and t_g=200°C)). Therefore, it can be concluded that the radiation impact for the droplets thermal state is not significant for water injection into the flue gas flow at temperature range t_g=150°C→200°C in a condensing economiser.

In the condensation mode, droplets grow when condensate enters and the warming water expands. In the initial phase of transient evaporation, droplets grow until evaporation begins to compensate water expansion process (Fig. 1, b). At this point droplet volume is the largest, interestingly, in the simulated cases, the effect of radiation on droplet growth is the most significant at the 200°C temperature flue gas (Fig. 1, b curves 5, 11). This is explained by the fact that among the factors that have an impact on radiation, the spectral source temperature is important and influences the duration of the condensation regime (Fig. 2) and the distribution of absorbed local flux inside the droplet (Fig. 3). The duration of the condensation mode τ_{co} is indicated by the zero-point value of the vapour flux when the phase transformation mode regime changes from condensation to evaporation (Fig. 2, a).

Semi-transparent water partially reflects and absorbs the light falling on a droplet surface. These processes are defined by the spectral complex refractive index, which for water material varies non-linearly in the wave spectrum [12] and is also dependent on the water temperature [13].

The intensity of the spectral radiation described by Planck's law is variating and has a temperature-dependent maximum. In addition, the light beam falling on the droplet is partially reflected by the inner surface of the droplet, and fully reflected when the falling angle exceeds the Brewster angle [14]. The combination of these factors defines the absorbed radiation flux integral and determines its different distribution inside the droplet. The local radiation flux depends on the droplet size and source temperature (Fig. 3). When a high temperature source is radiating, the water droplets are more transparent in the infrared spectrum, so it could be observed that local variation of the radiant flux is close to linear (Fig. 3, a)

In the case of a relatively low-temperature source, the radiation absorption is very intense inside large droplets (Fig. 3, b curves 1, 2), while in the smaller droplets, even extremes and inflection points can form in the curve of the $q_r(\eta)$ function (Fig. 3). The extremum and inflection points in the plots of the local radiative flux $q_r(\eta)$ functions are due to the reflection of light waves on the inner surface of the droplet. The discussed factors determine the thermal state variation of water droplets in the phase transformation regimes and influence the dynamics of the phase transformations. In smaller droplets, radiation absorption is not so bright [10, 11], therefore the absorbed radiative flux decreases rapidly in the final stage of the droplet evaporation (curve 1 in Fig. 4, b), and its effect on the individual droplet is suffocating in all modelled cases (Fig. 5).



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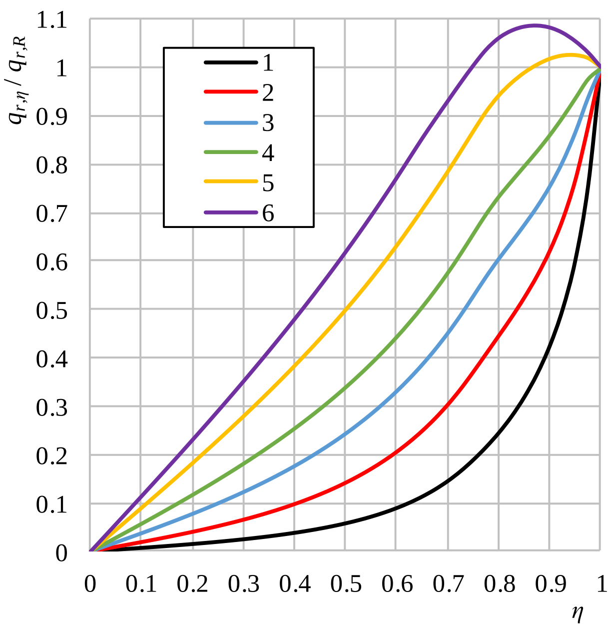
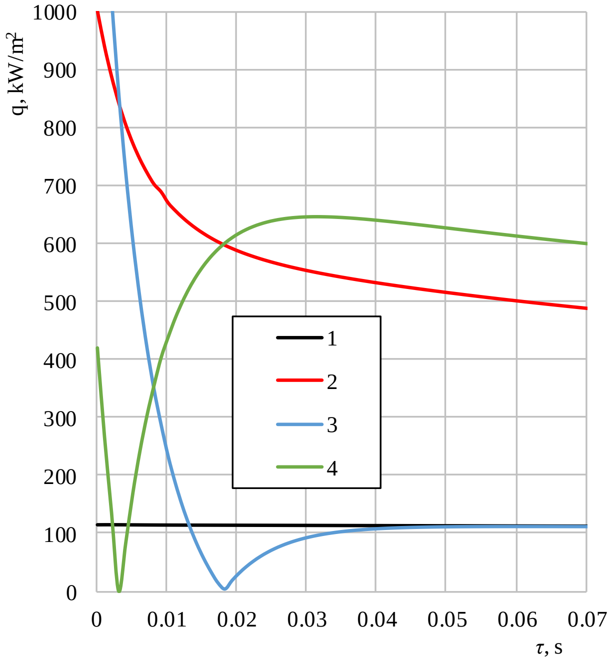


b

Fig. 3 Variation of dimensionless local radiation flux in water droplet during phase changes in high 1000°C (a) and relatively low 200°C (b) temperatures air flow, when t_{sour}=t_g. 2R, μm: (1) 300, (2) 230, (3) 150, (4) 100, (5) 40, (6) 20

In the transient regime, the heat fluxes q_f of the phase transformations and $q_{c,l}$ of the convective transfer inside droplet undergoes a pronounced transformation in the case



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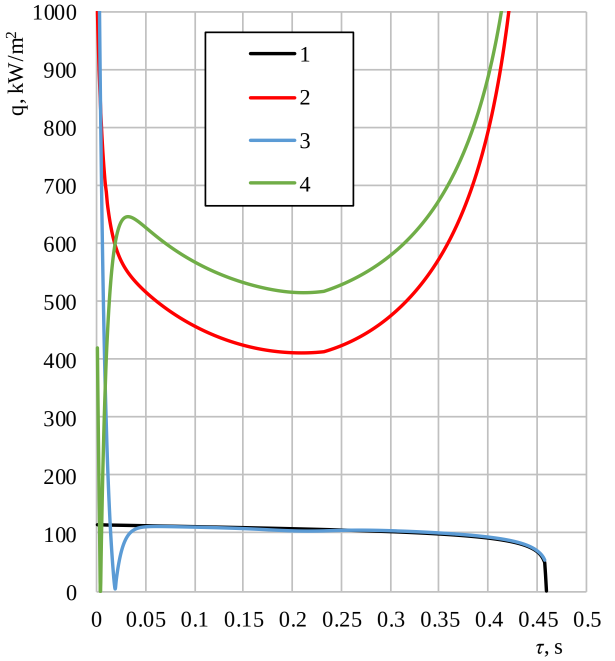


b

Fig. 4 Time history of heat fluxes in transient regime (a) and in phase change regimes cycle (b) in the droplet complex heating cases in 1000°C air flow. q: (1) q_r, (2) $q_{c,g}$, (3) $q_{c,l}$, (4) q_f

of compound "c" heating (Fig. 4). The phase transformation heat flux decreases to zero in the condensation regime and increases in the transient evaporation regime to the sum of the heat fluxes $q_f = q_{c,g} + q_{r,l}$ for the droplet (Fig. 4, a curve 4). The convective heat flux inside droplet $q_{c,l}$ decreases to zero during the transient evaporation regime $\tau\equiv 0\rightarrow\tau_r$ and then increases to the radiation flux absorbed by the droplet $q_{r,l}$ (Fig. 4, a curve 3). The time τ_r is clearly defined by the change of the temperature gradient inside the droplet from positive to negative when the gradient becomes zero (Fig. 6). The effect of radiation on the droplet phase transformation cycle was pronounced in all simulated cases (Fig. 7).

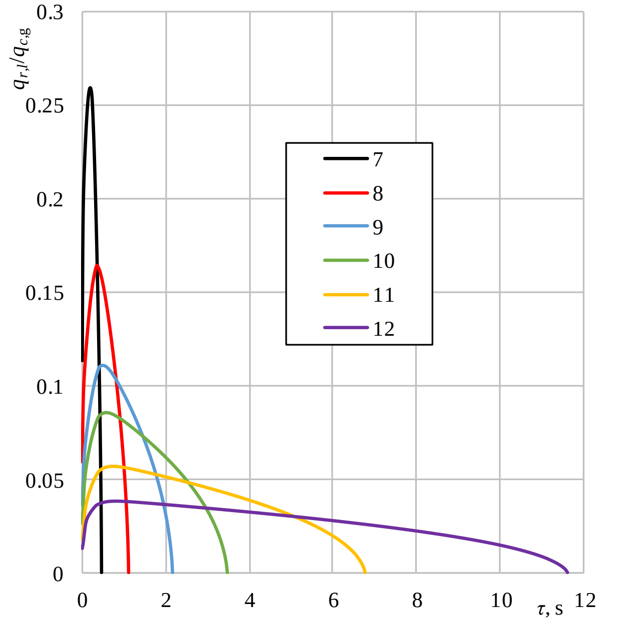


Fig. 5 Time history of flux's $q_{r,l}/q_{c,g}$ ratio; marking as in Fig. 1

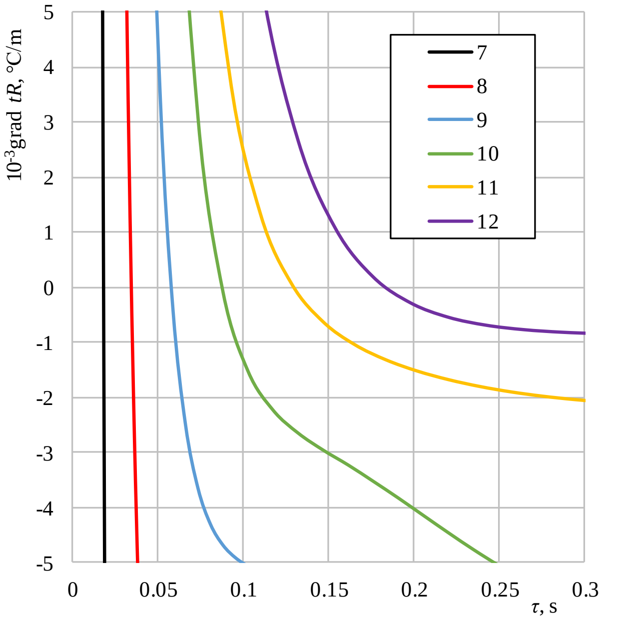
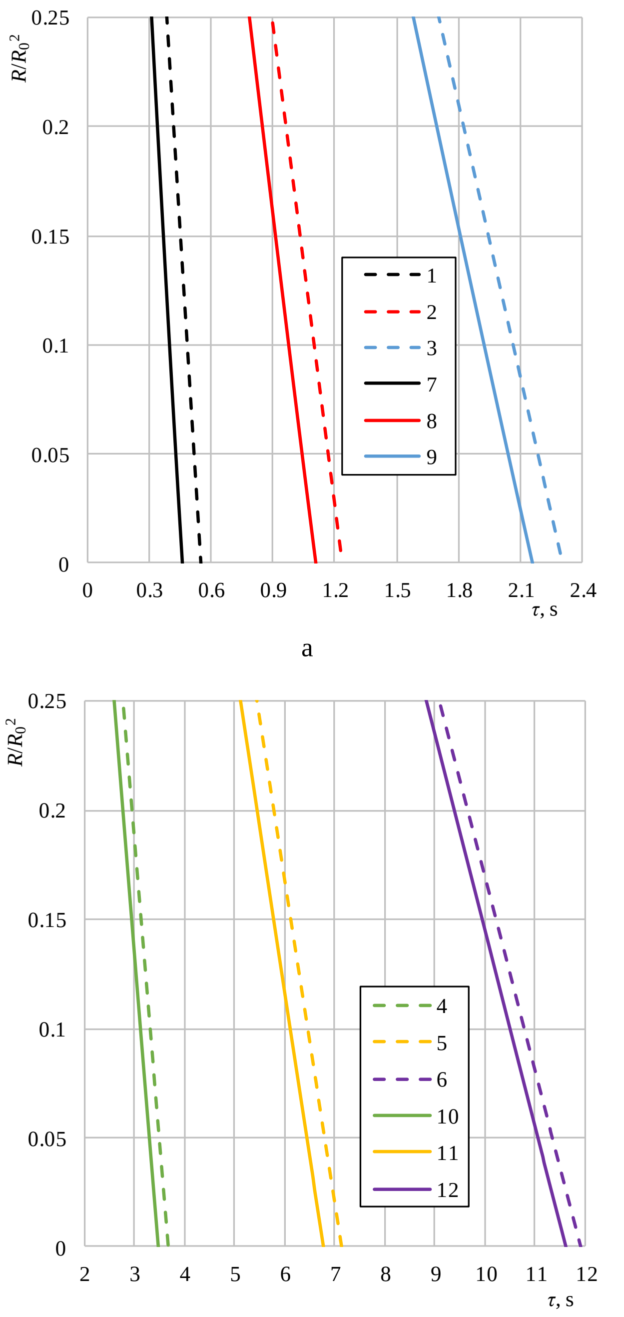


Fig. 6 Time history of droplet temperature gradient variation in transient phase change regime; marking as in Fig. 1

The droplet evaporation time is longer for convective heating in both high-temperature (Fig. 7, a) and relatively low-temperature (Fig. 7, b) surroundings (e.g., $\tau_{f,\text{“c”}}$ = 0.55 s; $\tau_{f,\text{“cr”}}$=0.46s, at t_g=1000°C, and $\tau_{f,\text{“c”}}$=7.13 s and $\tau_{f,\text{“cr”}}$=6.77, at t_g=200°C). Therefore, the influence of radiation must be taken into account when modelling the phase transformations of water droplets in the flue gas before the condensing economiser.

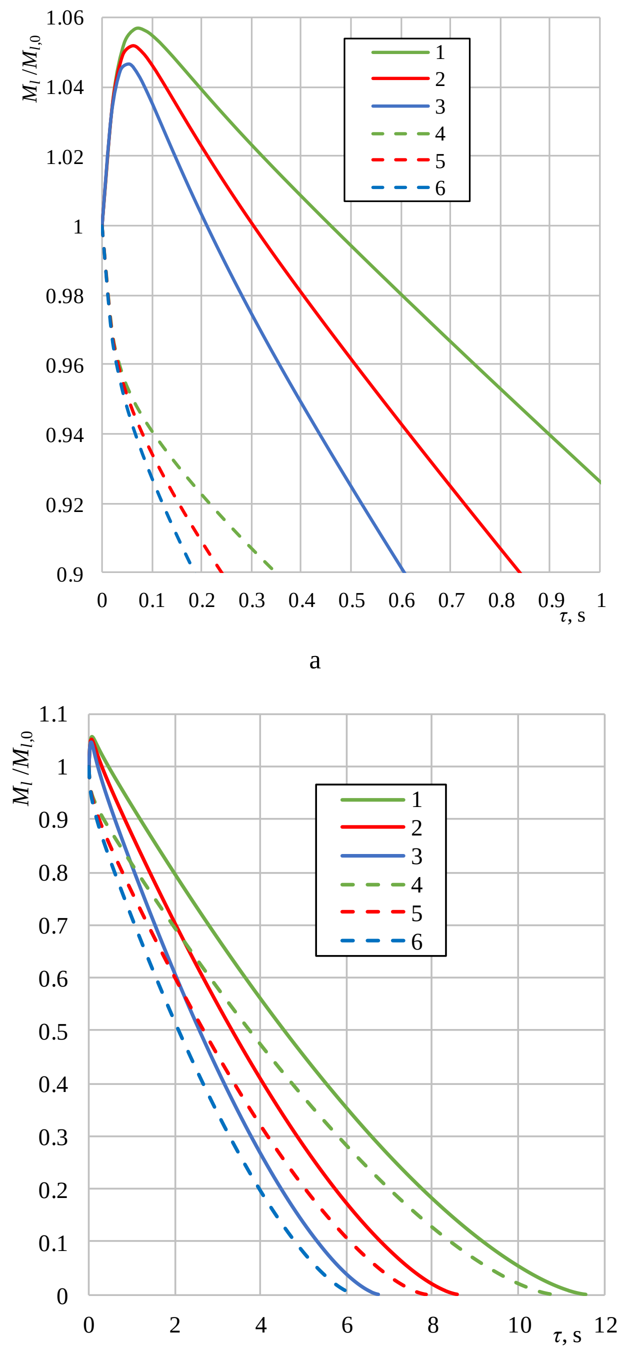
3.2. Influence of water temperature and spray dispersion on the phase transformation of droplets in flue gas before a condensing economiser

In biofuel combustion, the flue gas flow is traditionally injected with pollutant-cleaned condensate at a temperature of 40°C for various technological purposes, which



b

Fig. 7 Time history of water droplet dimensional area ratio in (a) high t_g, °C: (1, 7) 1000, (2, 8) 600, (3, 9) 400, and (b) relatively low t_g, °C: (4, 10) 300, (5, 11) 200, (6, 12) 100 temperature air flow in the final stage of evaporation



b

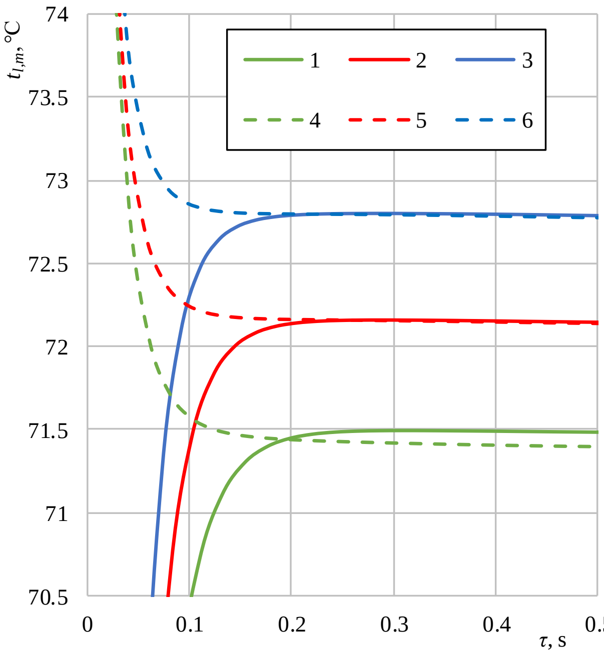
Fig. 8 Influence of water temperature towards droplet mass variation in transient regime (a) and in phase change regimes cycle (b), t_l,°C: (1-3) 40, (4-6) 80; t_g,°C: (1, 4) 150, (2, 5) 175, (3, 6) 200; X_v=0.3; Re_0=50; w_g=10 m/s

is collected from a condensing economiser, where the heat of the phase transformations of the water-steam is recovered from the removed humid flue gas.

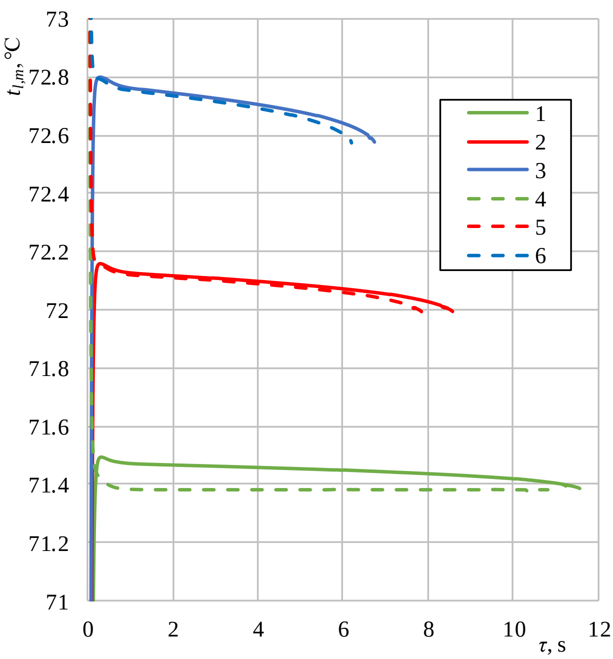
Water droplets injected into the removed flow upstream of the condensing economiser at 40°C can increase by 4-5% during the initial phase transformation phase (Fig. 1, b). This is not desirable because the aim of water injection is to effectively cool the flue gas to near dew point temperature. For this purpose, it is important that droplets would evaporate intensively. Numerical simulations have confirmed that the evaporation rate of the droplets increases with the injection of additional heated water (Fig. 8, b). The temperature of the removed upstream of the condensing economiser ranges from 150°C to 200°C. The mass of water droplets injected at 40°C increases by 4-6 percent in the condensing mode (Fig. 8, a – curves 1-3).

It is important to warm the water above the dew point temperature before injection and to avoid condensation phase transformations. The droplet mass of injected water at 80°C is reduced by 6-8 percent in the initial phase transformation stage (curves 4-6 in Fig. 8, a), as the droplets start to evaporate right away. When water injected at 40°C is heated to 80°C, 300 micrometre diameter droplets at 150°C, 175°C and 200°C evaporate 0.73 s, 0.74 s and 0.54 s faster, respectively, in the flue gas flow (Fig. 8, b). This is influenced by the fundamental change of the thermal state of the droplets (Fig. 9). At 40°C, the water droplets in the flue gas before the condensing economiser warm up in the phase transition regime (Fig. 9a curves 1-3), while at 80°C the water droplets cool down (Fig. 9, a – curves 4-6). The heat flux is proportional to the enthalpy change of the cooling droplets and additionally evaporates water, this increases the evaporation intensity (Fig. 10, 4-6 curves). The intensity of vapour condensation on the surface of water droplets at 40°C in the initial state is close to the evaporation intensity of water droplets at 80°C (Fig. 10).

The heat and mass transfer simulation results for the initial droplets 40°C and 80°C temperatures in a 175°C



a



b

Fig. 9 The influence of water temperature to variation of droplet thermal state in transient regime (a) and in phase change regimes cycle (b); marking as in Fig. 8

flue gas flow confirmed that dispersion of the water spray has a significant influence on the droplets phase transformations (Fig. 11). The water temperature and droplet size factors induce qualitative changes in the phase transformation dynamics in the transient regime (Fig. 11, a) and define quantitative changes in the phase transformation mode cycle (Fig. 11, b).

The diameter of injected water droplets into the flue gas before the condensing economiser at 40°C increases by about two percent in the transient regime (curves 1-4 in Fig. 11, a), and decreases by one and three percent at 80°C (curves 5-8 in Fig. 11, a).

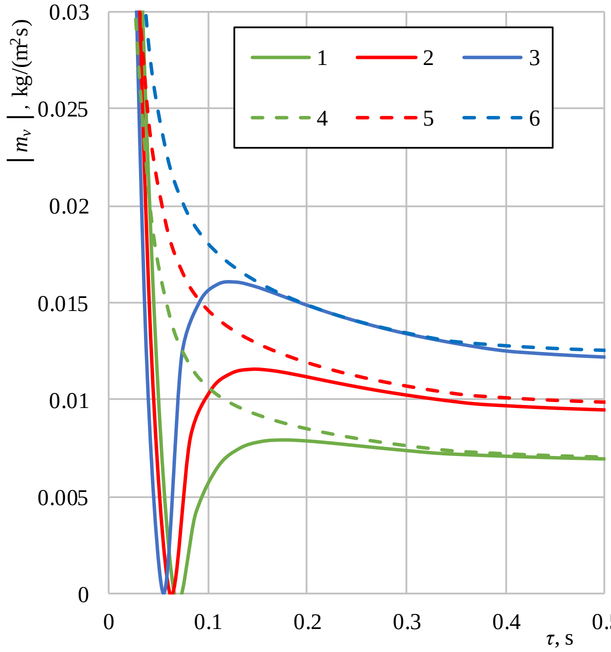
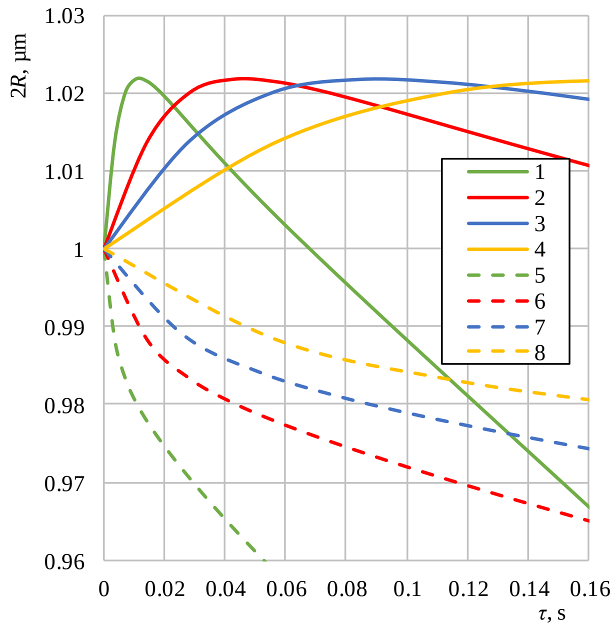
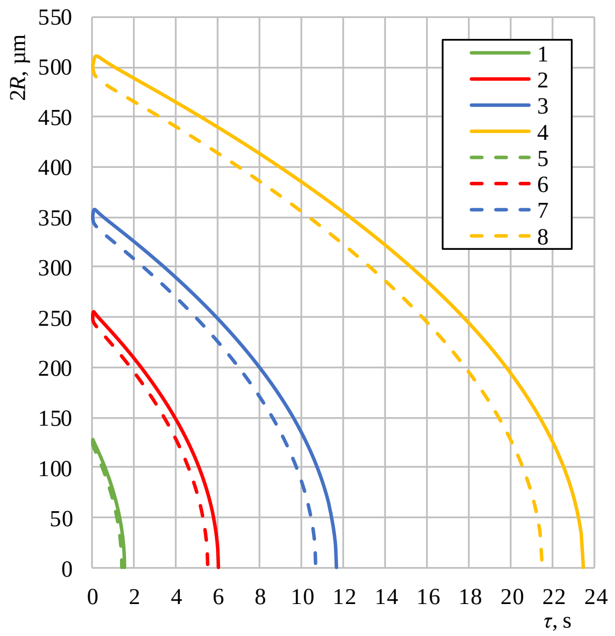


Fig. 10 Influence of water temperature to vapour flux density; marking as in Fig. 8



a

Fig. 11 Influence of water temperature and droplet size to diameter variation in transient regime (a) and in phase change regimes cycle (b); t_l, °C: (1-4) 40, (5-8) 80; R_0, µm: (1, 5) 125, (2, 6) 250, (3, 7) 350, (4, 8) 500; t_g=175°C; X_v=0.3; Re_0=50; w_g=10 m/s



b

Fig. 11 Continuation

Water droplets at 40°C evaporate in 1.53; 6.02; 11.66; and 23.47 seconds when diameters are 125µm; 250 µm; 350 µm; and 500 µm, respectively (curves 1-4 in Fig. 11, b), and for water droplets with the same size but having initial temperature 80°C evaporation times are 1.4; 5.51; 10.67 and 21.51 seconds when diameters are 125 µm; 250 µm; 350 µm; and 500 µm, respectively (curves 5-8 in Fig. 11, b).

4. Conclusions

The results of the water droplet phase change numerical modelling in flue gas flow confirmed the following:

1. The phase transformation of droplets in a humid flue gas flow is determined by the temperature of the flue gas and water, droplets dispersivity and their heating regime.
2. In the flue gas temperatures range of 150°C→200°C for water injection before a condensing economiser, the influence of radiation on the thermal state of the quantitatively injected water droplets is not significant, but it induces qualitative changes in the temperature field and leads to the formation of a negative gradient temperature field inside the droplets.
3. In the phase transformation cycle of the droplets the effect of the radiation flux absorption in semi-transparent water was significant in all simulated cases. Therefore, it is necessary to use droplet composite radiative convective heating models for all simulation processes of water injection in biofuel combustion technology.
4. For efficient cooling and humidification of the flue gas, the water heated above the dew point temperature must be injected before the condensing economiser, by splitting the water into fine droplets.

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NUMERICAL MODELLING OF PHASE TRANSFORMATIONS OF WATER DROPLETS FOR EFFICIENT HEAT RECOVERY FROM BIOFUEL FLUE GAS

S u m m a r y

The phase transformations of water droplets in the humid air flow for water injection into the flue gas in biofuel combustion technology under typical boundary conditions have been simulated. The numerical study was performed in two stages. The first one defines the influence of radiation on the thermal state of the water droplets and on the cycle of phase transformation modes. It is shown that the influence of radiation in a flue gas flow of 150℃→200℃ temperature on the thermal state of quantitatively injected water droplets is not significant, but it induces qualitative changes in the temperature field and influences phase transformations cycle of the droplets. In the second step, the cycling of the droplet phase transformation modes for water injection into the exhaust flue gas prior to a condensing economiser under typical boundary conditions was numerically investigated. It was justified that for efficient cooling and humidification of the flue gas before the condensing economiser it is necessary to inject water heated above the dew-point temperature by dispersing it into fine droplets.

Keywords: water droplets, phase change, complex heating, condensation, transient and equilibrium evaporation.

Received January 9, 2024
Accepted August 19, 2024