Mathematical Model of Contact Cooling and Purification of the Dispersed Phase of Gases in Packed Scrubbers

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Abstract—The work contains a numerical solution of the scientific and technical problem of the determination of the efficiency of packed scrubbers during condensation cooling and purification of the dispersed phase of gases in the process of a stationary film liquid flow through regular and chaotic contact devices. A system of differential equations with partial derivatives of the conjugate transfer of heat, the mass of water vapor, and the dispersed phase in the packing layer is written. The heat and mass transfer and the transfer of dispersed particles between the gas and liquid phases are taken into account with volume source terms of the interfacial transfer, averaged over the local volume of the layer. Expressions are given to determine the source parameters. The results of the numerical solution of the system of equations in terms of the temperature and moisture content fields and comparison with known experimental data are presented. The dependence of the efficiency of gas purification from a finely dispersed phase on the gas velocity is shown. Comparative characteristics of packings, as well as scientific and technical solutions for the modernization of scrubbers introduced in the industry, are given.

Keywords: gas cooling, gas cleaning, packing, scrubber, mathematical model, apparatus modernization **DOI:** 10.1134/S0040579522020105

INTRODUCTION

Interfacial heat and mass transfer in apparatuses with chaotic and regular contact devices (packings) in countercurrent film mode is widely used for the absorption, rectification, and cooling or heating of gases and liquids. Moreover, the cooling of flue and process gases is often accompanied by purification of the dispersed phase.

The development of mathematical models of such combined processes is relevant for energy and chemical technology in various industries [1–4].

Packed devices for interfacial heat and mass transfer are most often calculated with the ideal phase displacement model (the method of the number and height of transfer units) or the diffusion model of the flow structure, as well as numerical methods with various software systems [5–8]. However, these models and software systems do not always allow calculations of new types of contact devices that have no analogs, especially with process intensifiers.

The gas phase for cooling and cleaning is fed into the lower part of the scrubber under the section with packing. The liquid phase (usually water) enters the upper part of the column through special sprinklers and is evenly distributed over the packing. The process of countercurrent film of liquid and gas is organized. The gas velocity for the counterflow is calculated based on the design features of the packing and the irrigation density; under normal conditions, they are in the range of $0.5-2.0$ m/s, and the irrigation density is $10-50$ m³/m² or sometimes higher for special designs of contact devices. The regime and design parameters of the scrubber are found in the modeling of processes that depend on the technical and technological requirements for the design or modernization of the column.

The purpose of this work is the numerical solution of a system of equations for the conjugate heat and mass moisture transfer, as well as equations for the turbulent transfer of fine particles in a scrubber with chaotic and regular packings and the comparative characteristics of contact devices.

MATHEMATICAL MODEL

An approach used in the modeling of transport phenomena in two-phase media of packed columns, a two-fluid model, is based on the compilation of a macroscopic balance with averaging of the local single-phase equations of conservation of momentum, mass and energy, and conjugation conditions at the boundary. With this approach, differential equations are written for each phase separately, but, since the macroscopic fields in the phases are not independent of each other, the equations use local interphase

source terms in the elementary volume that take into account the transfer of substances between the phases.

It is known that the turbulent regime of gas motion in an irregular (chaotic) packing begins at Reynolds numbers Re_e of more than 15–40. In a regular packing with intensifiers (notches, protrusions, corrugations, etc.), it begins at more than 500, where the Reynolds number is calculated from the average actual gas velocity in the packing and the equivalent packing diameter. The movement of a falling liquid film over the surface of packed bodies most often occurs at a Reynolds number less than 2000, i.e., the flow regime is laminar wave.

In the formulation of the conjugate transfer equations considered below, the conjugate transfer equations are written in cylindrical coordinates for the entire packed column with fictitious phase velocities related to the entire cross section of a column with volumetric local sources of heat transfer, moisture mass, and a finely dispersed phase on the right side.

The volumetric sources with a uniform distribution of phases are averaged over the entire volume of the layer; with a nonuniform distribution for local areas the real hydrodynamic situation and the driving forces of the transfer processes are taken into account.

This approach has been successfully used to model transport phenomena in film cooling towers [9], packed distillation and absorption columns [10], aerosol gas separators [11], and other apparatuses [12, 13].

For a scrubber with regular or chaotic packings, the system of equations for the conjugate heat and mass transfer, as well as the dispersed phase in the cylindrical coordinate system of the column, is given below.

The equation of convective heat transfer in the liquid phase is

$$
u_{\text{liq}}(r)\rho_{\text{liq}}c_{\text{p,liq}}\frac{\partial T_{\text{liq}}}{\partial z} = \frac{\lambda_{\text{liq}}}{r}\frac{\partial}{\partial r}\left[r\frac{\partial T_{\text{liq}}}{\partial r}\right] + \frac{q dF}{dV}.
$$
 (1)

In the gas phase,

$$
W_{\rm gas}(r)\rho_{\rm gas}\frac{\partial I}{\partial z} = \frac{1}{r}\frac{\partial}{\partial r}\bigg[r\lambda_{\rm t, gas}\frac{\partial T_{\rm gas}}{\partial r}\bigg] - \frac{q dF}{dV},
$$

\n
$$
I = f(T_{\rm gas}, x).
$$
 (2)

The moisture transfer equation in the gas phase is

$$
W_{\rm gas}(r)\frac{\partial x}{\partial z} = \frac{1}{r}\frac{\partial}{\partial r}\bigg[rD_{\rm t, gas}\frac{\partial x}{\partial r}\bigg] + \frac{j_x dF}{\rho_{\rm gas} dV}.\tag{3}
$$

The transfer equation for a finely dispersed phase is

$$
W_{\rm gas}(r)\frac{\partial C}{\partial z} = \frac{1}{r}\frac{\partial}{\partial r}\bigg[rD_{\rm t.d}\frac{\partial C}{\partial r}\bigg] - \frac{j_c dF}{dV},\tag{4}
$$

where dF/dV is the specific surface of phase contact in the local volume of the layer, m^2/m^3 ; at $z = 0$, it is the gas inlet and liquid outlet in the lower part of the column.

In equations (1)–(4), the velocities $u_{liq}(r)$ and $W_{\rm gas}(r)$ are a function of the radial coordinate.

In the compilation of the mathematical model, the following assumptions were made:

— the main heat and mass transfer and separation of the dispersed phase (more than 90%) occur in the packed zone in the film mode;

— the main resistance to heat and mass transfer is concentrated in the gas phase (more than 99%);

— the phase motion is stationary and stabilized;

— the regime of gas movement in the packing layer is turbulent;

— the disruption and entrainment of liquid droplets from the surface of the flowing film is insignificant;

— the column walls are thermally insulated from the environment.

The velocity profile of the liquid phase depends on the number of irrigation points and, with the use of good distributors, can be taken in the upper section of the layer $u_{\text{liq}}(r) = u_{\text{liq,in}}$ to be uniform. However, when the liquid flows down the packing, the liquid phase is gradually redistributed towards the column wall, especially in a chaotic packing. It is known that a significant redistribution of liquid to the wall occurs when $H > 4D_{\text{out}}$. Since the value in gas cooling scrubbers is the packing in the case of $H > 4D_{\text{out}}$ is located in sections with phase redistributors. Thus, the fluid velocity profile can be assumed to be uniform. $H < 4D_{\text{out}}$, the packing in the case of $H > 4D_{\text{out}}$

The gas-velocity profile significantly depends on the conditions of entry into the apparatus and the hydraulic resistance of the packing along the cross section. Experimental studies show a complex relationship $W_{\rm gas}(r)$ for various packings [14, 15]. As a first approximation, one can take $W_{\rm gas}(r) = W_{\rm av}$, and then it can be refined according to experimental data or from the numerical solution of the system of equations of gas motion.

The heat transfer during the condensation cooling of gas $(x > x^*)$ occurs due to phase contact (convective and molecular transport mechanisms), as well as the condensation of moisture from gases onto the surface of a falling film of water (or another liquid), which can lead to cooling below the dew point [16].

The heat balance at an evaporation coefficient close to unity is written as

$$
Q = Gc_{p,\text{gas}}(T_{\text{in,gas}} - T_{\text{out,gas}})
$$

+
$$
G(I_{\text{in}}x_{\text{in}} - I_{\text{out}}x_{\text{out}}) - G(x_{\text{in}} - x_{\text{out}})c_{p,\text{liq}}T_{\text{liq,out}}.
$$
 (5)

Also, the flow of heat transferred from the gas to the liquid phase can be represented with the equations of heat and mass transfer in countercurrent.

The heat flow during gas cooling by liquid during countercurrent movement of phases in the column is

$$
Q = KF\Delta T + I_{\text{vap}}\rho_{\text{gas}}F\beta_{\text{gas}}\Delta x.
$$
 (6)

When cooling a gas with a liquid, almost all heat transfer resistance is concentrated in the gas phase; the heat transfer coefficient is then assumed to be equal to the heat transfer coefficient $K = \alpha_{\text{gas}}$.

When the Lewis analogy in the gas phase and the known expressions for enthalpy related to gas temperature and moisture content are applied, expression (6) is presented in the form [17]

$$
Q = \beta_x F \Delta I_{\text{av}}.\tag{7}
$$

Then, the heat-flux density in the gas phase can be expressed with the mass-transfer coefficient, which is related to the difference in moisture content and the driving force of heat transfer in the form of an enthalpy difference;

$$
q = \beta_x (I - I_b). \tag{8}
$$

The water-vapor mass flux density is

$$
j_x = \beta_{\rm gas} \rho_{\rm gas} (x - x^*). \tag{9}
$$

The local mass flow of particle deposition to the interfacial surface of the film is

$$
j_c = u_t(C - C_b). \tag{10}
$$

The mass transfer coefficient in the gas phase can be calculated from expression [18]:

$$
Sh_{\rm gas} = 0.175 \, \text{Re}_{\rm e}^{0.75} (\xi/2)^{0.25} \text{Sc}_{\rm gas}^{0.33},\tag{11}
$$

and the coefficient of turbulent diffusion in the core of the gas phase flow in chaotic and regular packings with intensifiers according to the formula [18] is

$$
D_{\rm t, gas} = 3.87 v_{\rm gas} \sqrt{\xi \rm Re_e}.
$$
 (12)

In equation (2), it is taken as $\lambda_{t, gas} \approx \rho_{gas} c_{p, gas} D_{t, gas}$.

The coefficient of turbulent diffusion of particles in the core of the gas flow [19] is

$$
D_{\rm td} = \frac{D_{\rm t,gas}}{1 + \omega_{\rm E} \tau_{\rm p}}.\tag{13}
$$

Numerous experimental studies by various authors of the turbulent migration of aerosol particles have shown that the rate of particle settling on the channel walls in the turbulent mode of gas motion is several orders of magnitude higher than the rate of diffusion settling of the same particles from a laminar flow. Moreover, in the turbulent regime, the deposition efficiency increases with increasing gas velocity. This characterizes the inertial nature of the particle transfer phenomenon. This form of deposition was called the turbulent-inertial mechanism of aerosol deposition [19, 20].

Turbulent migration is a form of transverse motion of particles in a shear turbulent flow. This form, which was discovered by Fortier, Fletcher, and independently by Mednikov, is of fundamental importance in aerosol mechanics [19].

In a theoretical analysis of all forms of motion of aerosol particles in a turbulent flow, the following assumptions are usually made [19].

1. The particle diameter is small as compared to the scale of the pulsating vortices carrying them.

2. The particle flow occurs at low Reynolds numbers.

3. The particles have a shape that is almost spherical. The polydispersity of aerosol particles is considered fractionally.

4. In addition:

(a) the particles do not hamper the movement of each other in the course of mutual displacements;

(b) do not collide and do not coagulate with each other;

(c) do not have a noticeable effect on the turbulent characteristics of the medium.

The values of particle concentrations under the above conditions, according to the experimental data of Rossetka and Pfefer, are taken to be \leq 200 g/m³, i.e., approximately ≤ 0.17 kg/kg (for air at atmospheric pressure).

5. The electrostatic and other forces of a nonhydrodynamic nature are insignificant.

6. The separation of the precipitated dispersed phase and water drops from the surface of the liquid film is insignificant.

A number of empirical and semi-empirical dependences are known for the calculation of the reduced (dimensionless) velocity of turbulent particle settling

 $\frac{u_t}{t} = \frac{u_t}{t}$, which is related to the particle velocity relax-∗ $u_t^+ = \frac{u_t}{u}$ *u*

ation time [19]:

$$
\tau_{\rm r} = \frac{d_{\rm par}^2 \rho_{\rm par}}{18 \rho_{\rm gas} v_{\rm gas}}.
$$
 (14)

The calculations use the dimensionless relaxation time:

$$
\tau^+ = \frac{\tau_r u_*^2}{v_{\text{gas}}},\tag{15}
$$

where $u_* = \sqrt{\tau_b / \rho_{gas}}$ is the dynamic speed, m/s and τ_b is the shear stress at the interface between the gas phases and the liquid film, Pa.

To calculate u_t^+ , the Uzhov and Mednikov expressions are more often used in mathematical models. They generalize a large amount of experimental data for tubes [19]:

at
$$
\mu_r^2 \tau^+ \le 16.6
$$

\n
$$
u_t^+ = 7.25 \times 10^{-4} \left(\frac{\tau^+}{1 + \omega_E \tau_r} \right)^2,
$$
\n(16)

Fig. 1. Dependence of flue gas temperature on the irrigation coefficient for a packing made of ceramic rings with dimensions of $35 \times 35 \times 4$ mm at an initial gas temperature of $T_{gi} = 250-280$ °C and water $T_{li} = 12$ °C. The packing height is 1000 mm. The solid line is the calculated values, and the circle shows the experimental values. (*1*), area of calculated values; (*2*) averaged calculation.

$$
at \mu_r^2 \tau^+ > 16.6
$$

$$
u_t^+ = 0.2, \t(17)
$$

where the dimensionless parameter $\mu_r = 1/(1 + \omega_E \tau_r)^{0.5}$; $\omega_{\rm E} = u_* \big/ (0.05 d_{\rm e})$ is the frequency of energy-intensive pulsations, s^{-1} .

It follows from the above expressions that the velocity of the turbulent particle migration $u_t = u_t^+ u_*$ significantly depends on the value of the dynamic speed u_* or the shear stress at the interface $\tau_{st} = u_*^2 \rho_{gas}$.

The average value of the dynamic speed on the surface of chaotic packings ($Re_e > 40$), as well as regular ones with intensifiers ($Re_e > 500$), is calculated with expression [18] $u_* = 1.55 W_{gas} (\xi/Re_e)^{0.25}$.

The boundary conditions for the system of equations (1) – (3) are as follows:

at $z = H$ (water inlet and gas outlet):

$$
u_{\text{liq}}(r) = u_{\text{liq,in}}(r); \quad T_{\text{liq}} = T_{\text{liq,in}};
$$

$$
\frac{\partial I}{\partial z} = 0; \quad \frac{\partial x}{\partial z} = 0;
$$

at $z = 0$ (water outlet and gas inlet):

$$
W_{gas}(r) = W_{gas,in}(r); \quad I = I_{in};
$$

$$
\frac{\partial T_{liq}}{\partial z} = 0; \quad x = x_{in}.
$$

at $r = 0$ (on the column wall):

$$
\frac{\partial x}{\partial r} = 0; \quad \frac{\partial T_{\text{liq}}}{\partial r} = 0; \quad \frac{\partial I}{\partial r} = 0.
$$

In Figs. 1 and 2, the gas temperature profile and the moisture content profile obtained from the numerical solution of the system of equations (1) – (3) with a uniform distribution of gas and liquid and experimental data are presented to check the adequacy of the math-

Fig. 2. Dependence of the moisture content of the exhaust gases on the irrigation coefficient. Designations are the same as in Fig. 1.

ematical model [16]. The solution involved a wellknown expression that relates the enthalpy *I*, moisture content *X*, gas temperature T_{gas} and the specific heat capacities of dry gas $c_{p, dry}$ and the heat capacity of steam $c_{p, \text{van}}$: $I = (c_{p, \text{div}} + c_{p, \text{van}} x) T_{\text{gas}} + R_{\text{li}} x$. As a result of the numerical solution of (1) – (3) , satisfactory agreement with experiment was obtained for the Rashigapri rings $W_{\text{gas}} = 0.4$ to 1.9 m/s and irrigation density $U_{\text{well}} = 3 - 55 \text{ m}^3/\text{m}^2 \text{ h}.$ $c_{p,\text{vap}}$: $I = (c_{p,\text{dry}} + c_{p,\text{vap}} x) T_{\text{gas}} + R_{\text{liq}} x.$

THERMAL AND SEPARATION EFFICIENCY

With a known profile of the gas temperature along the layer height and its value at the outlet, it is possible to determine the thermal efficiency of gas cooling.

Let us write the thermal efficiency of the process in the gas phase in the form

$$
E_{\rm gas} = \frac{T_{\rm in, gas} - T_{\rm out, gas}}{T_{\rm in, gas} - T_{\rm in, liq}}.
$$
 (18)

The thermal efficiency is also written as the ratio of the enthalpy difference:

$$
E_{\rm gas} = \frac{I_{\rm in} - I_{\rm out}}{I_{\rm in} - I_{\rm out}^*}.
$$
 (19)

The values of E_{gas} in (18) and (19) are written based on the actually achieved indicators of gas cooling relative to the maximum possible.

The thermal efficiency of water heating is

$$
E_{\text{liq}} = \frac{T_{\text{out,liq}} - T_{\text{in,liq}}}{T_{\text{in,gas}} - T_{\text{in,liq}}}.
$$
 (20)

Fig. 3. Dependence of the thermal efficiency in the gas phase on the gas velocity in the column: (*1*) 45-m Inzhekhim 2012 packing; (*2*) 60-mm packing; irrigation water density, $q_{\text{liq}} = 25 \text{ m}^3/\text{m}^2$ h. The packing layer height is $H = 2.0$ m. Flue gas cooling.

The moisture condensation efficiency is

$$
E_{\rm gas} = \frac{x_{\rm in} - x_{\rm out}}{x_{\rm in} - x_{\rm out}^*}.
$$
 (21)

The separation efficiency of the dispersed phase is

$$
\eta = \frac{C_{\text{in}} - C_{\text{out}}}{C_{\text{in}}}.
$$
\n(22)

The final temperatures $T_{\text{out,gas}}$, $T_{\text{out,liq}}$, the moisture content x_{out} , and the concentration of the dispersed phase C_{out} is found from the solution of the system of equations (1) – (4) .

Figure 3 shows the results of calculations of the thermal efficiency E_{gas} (18) in flue gas cooling $(T_{\text{in,gas}} = 150^{\circ}\text{C})$ with water $(T_{\text{in,liq}} = 15^{\circ}\text{C})$ in a scrubber with a chaotic metal packing Inzhekhim 2012 with a height of $H = 2.0$ m and a nominal element size of 45 mm $(a_v = 166 \text{ m}^2/\text{m}^3)$ and 60 mm $(a_v = 70 \text{ m}^2/\text{m}^3)$. The 45-mm packing at a gas speed of $W_{\rm gas} = 3\,$ m/s and an irrigation density of $25 \text{ m}^3/\text{m}^2$ h is close to the beginning of the suspension of the liquid phase. Therefore, the use of a larger packing of 60 mm is recommended in this mode.

Figure 4 shows the results of calculations of the separation efficiency (22) for particles with $d_{\text{par}} = 5 \text{ }\mu\text{m}$ and a density of $\rho_{\text{par}} = 3000 \text{ kg/m}^3$ from flue gases in the layer $H = 2.0$ m for 45 and 60-mm packings. The calculations show a significant increase in separation efficiency at $W_{\text{gas}} > 2.5 \text{ m/s}$, which, as noted above, characterizes the inertial-turbulent mechanism of particle transfer.

Fig. 4. Dependence of the separation efficiency of the dispersed phase $d_{\text{par}} = 5 \mu \text{m}$ on the speed of the gas. (*1*) 45-mm Inzhekhim 2012 packing; (*2*) 60-mm packing; irrigation density, $q_{\text{liq}} = 25 \text{ m}^3/\text{m}^2 \text{ h}.$

COMPARATIVE CHARACTERISTICS OF CONTACT DEVICES

Based on the application of the presented mathematical model, numerical studies were carried out and comparative characteristics of various types of metal regular and irregular packings [15, 21] were obtained for a given thermal efficiency $E_{\text{gas}} = 0.8$ and identical temperature and hydrodynamic conditions.

1. Raschig rings, 25 mm: $a_v = 220 \text{ m}^2/\text{m}^3$; $\epsilon_{\text{free}} = 0.92$.

2. Raschig rings, 50 mm: $a_v = 110 \text{ m}^2/\text{m}^3$; $\epsilon_{\text{free}} = 0.95$.

3. Mobius rings, 40 mm: $a_v = 190 \text{ m}^2/\text{m}^3$; $\epsilon_{\text{free}} = 0.88$.

4. Inzhekhim 2012 packing, 24 mm: $a_v = 166 \text{ m}^2/\text{m}^3$; $\varepsilon_{\text{free}} = 0.96$.

5. Inzhekhim 2012 packing, 45 mm: $a_v = 100 \text{ m}^2/\text{m}^3$; $\varepsilon_{\text{free}} = 0.97$.

6. Inzhekhim segment-regular roll: $a_v = 380 \text{ m}^2/\text{m}^3$; $\varepsilon_{\text{free}} = 0.94$.

7. Rolled corrugated with a rough surface: $a_v = 280 \text{ m}^2/\text{m}^3$; $\varepsilon_{\text{free}} = 0.95$.

The histogram in Fig. 5 shows the calculated data on the packing height necessary to achieve thermal efficiency in the gas phase $E_{\text{gas}} = 0.8$ at an irrigation density of 15 m^3/m^2 h and an average gas velocity of

Fig. 5. Required packing bed height and pressure drop at $E_G = 0.8$. Chaotic packings: (*1*) Raschig rings, 25 mm; (*2*) Raschig rings, 50 mm; (*3*) Mobius rings, 40 mm; (*4*) Inzhekhim 2012 packing, 24 mm; (*5*) Inzhekhim 2012 packing, 45 mm. Regular packings: (*6*) segment-regular; (*7*) rolled corrugated.

given.

It follows from the results that packings with values of 3, 4, and 6 provide the specified efficiency at a layer height $H = 0.35-0.4$ m and a pressure drop from 50 to 170 Pa, i.e., with small scrubber dimensions and energy characteristics.

Thus, a mathematical model of conjugate heat and mass transfer in a packed bed was obtained in this work. Its numerical solution makes it possible to predict the efficiency of the cooling and purification of gas and the heating of water (or other liquids) depending on the operating and design characteristics of the film scrubber.

Based on the presented mathematical model for the calculation of gas cooling and purification, technical solutions were developed for the modernization of three scrubber columns for pyrogas cooling with water at gas separation units in ethylene production. The largest scrubber has a diameter of 3.2 m, a pyrogas consumption of $G = 80 - 120$ t/h, and a cooling-water consumption of 200 t/h in the upper part and up to 800 t/h in the lower part. In addition, there is wet cleansing of pyrogas from particles of coke and resins after pyrolysis furnaces. As a result of the replacement of obsolete contact devices in the upper part of the column with a random packing $(H = 2.0 \text{ m})$ and in the lower part with a regular corrugated packing $(H=4.0 \text{ m})$, Inzhekhim [21] increased the productivity of the scrubber and reduced the outlet pyrogas temperature to regulatory values. Therefore, the adequacy of the mathematical model is confirmed by data from the industrial operation of scrubbers after their modernization.

 $W_{\text{gas}} = 1.5 \text{ m/s}$. The pressure drop values are also tance in heat engineering, heat-power engineering and chemical technology. The theoretical or, rather, numerical simulation of conjugate heat and mass transfer is associated with the solution of a system of differential equations with partial derivatives. When a falling liquid film interacts with a gas flow under the conditions of a known distribution of the interfacial surface in space (vertical channels, plane-parallel contact devices, etc.), differential equations for heat and mass transfer are written for each phase separately with boundary conditions on the interface of the fourth kind. However, when a liquid film flows down randomly located contact elements, it is not possible to set the boundary conditions on the interfacial surface. In such cases, volume interfacial sources of momentum, energy, and mass are used; they are a simplified form of the multivelocity continuum model. Volume sources are recorded for local areas for the nonuniform distribution of phases and for the entire working volume of the device in the case of a conditionally uniform distribution.

> A distinctive feature of the mathematical model in this article is the ability to calculate the source parameters (coefficients of the heat and mass transfer and turbulent particle migration) and the average coefficient of turbulent exchange, both in local areas and for the entire packed bed with the experimentally obtained coefficient of hydraulic resistance (pressure drop). This significantly reduces the time and material costs in the modeling of the developed gas-liquid contact devices.

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CONCLUSIONS

The solution of the problems of conjugated heat and mass transfer is of theoretical and applied impor-

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