The inversion temperature during evaporation of water solutions of ethanol and acetone into a turbulent boundary layer

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Abstract. The results of studies of heat and mass transfer during adiabatic evaporation of binary liquids of water/ethanol and water/acetone into a turbulent boundary layer of a vapor-air mixture from a flat wetted plate are presented. The dependences are obtained for the evaporation intensity of solutions of various compositions on the temperature of the air flow or the equilibrium superheated steam into which the liquids evaporate. The inversion temperature values for liquids with different concentration of the volatile component are determined. The effect of flow turbulence on the evaporation rate and inversion temperature is analyzed.

1. Introduction

The processes of heat and mass transfer during the evaporation of mixtures (solutions) of different liquids are the basis of many industrial technologies. For example, in the textile industry, the evaporation of complex solvents is an integral part of the technology of dyeing, in chemical industry, evaporation and boiling of complex solutions are observed in the processes of rectification and distillation, and in the fuel and energy complex, mixtures of liquids are used as the basis for new energy sources [1]. Biofuels based on flammable liquids from renewable raw materials (ethanol, methanol) are being developed.

For pure liquids, the laws of heat and mass transfer are presented in a number of reviews and monographs [2–4]. For liquid solutions, the analysis of heat and mass transfer processes is much more complicated. As a rule, in such systems, heat and mass transfer is non-stationary, there is an intensive change in the concentration of components in the solution, and convective movement occurs. It is known that drops of binary liquids evaporate with an uneven temperature distribution over the surface [5]. Special measures must be taken to ensure that the evaporation process is stationary in experimental studies. Stationary evaporation of water/ethanol, water/methanol, and water/acetone solutions from a porous sphere with a continuous liquid supply is studied in [6]. A formula for determining the temperature of adiabatic evaporation is proposed. In [7], heat and mass transfer during evaporation of a two-component liquid film flowing along the inner wall of a vertical cylinder is numerically studied. It is shown that the addition of methanol to benzene leads to an increase in the evaporation intensity.

The intensification of evaporation is usually one of the target functions in the development of new technological processes, which leads to a reduction in, for example, drying time, rectification and, ul-
timately, production costs. One of the obvious ways to solve this problem is to increase the temperature of the air or steam that washes the liquid. However, this is not the only way. In [8-11], it is noted that at certain temperatures of the inlet flow, evaporation into superheated water vapor becomes more intense than in dry air. This phenomenon is called inversion, and the flow temperature at which the intensity of evaporation into steam is equal to the intensity of evaporation in air is called the inversion temperature. In [12, 13], the existence of an inversion temperature during evaporation of volatile liquids (ethanol, acetone, benzene) is shown. The inversion temperature during evaporation of water solutions of ethanol and acetone into a laminar boundary layer is considered in [14].

In this paper, heat and mass transfer in a turbulent boundary layer are numerically investigated under stationary adiabatic evaporation of binary liquids of water/ethanol and water/acetone into an air flow or into a flow of superheated vapor mixture of evaporating liquids at atmospheric pressure and temperature of up to 500 °C. Data on the rate of evaporation of binary liquids into dry air and superheated vapors of equilibrium composition depending on the flow temperature are the basis for determining the inversion temperature.

2. Problem statement and solution method

The stationary flow of a three-component gas in a turbulent boundary layer on a flat plate with adiabatic evaporation of a two-component liquid over the entire range of concentrations of the light-boiling component is considered. The flow diagram and main parameters of the problem are shown in figure 1. The velocity of the inlet flow is 10 m/s and the temperature varies from 20 to 500 °C. Air properties are replaced by nitrogen properties [14]. The composition of the liquid along the length of the plate is assumed to be constant, which corresponds to the evaporation mode with constant reabsorbing and intensive mixing.

![Figure 1. The scheme of turbulent boundary layer during evaporation of water solutions on a wetted wall.](image)

The problem is solved by numerical methods based on a system of differential equations for a two-dimensional boundary layer in physical coordinates. For the flow of a multicomponent gas, the system of equations of continuity, motion, energy, and diffusion is written as follows:

\[
\frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0, \tag{1}
\]

\[
\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = \frac{\partial}{\partial y} \left( \mu + \mu_t \right) \frac{\partial u}{\partial y}, \tag{2}
\]

\[
\rho u c_p \frac{\partial T}{\partial x} + \rho v c_p \frac{\partial T}{\partial y} = \frac{\partial}{\partial y} \left( \lambda + \frac{\mu_e c_p}{Pr} \right) \frac{\partial T}{\partial y} + \sum_{i=1}^{3} c_{p(i)} \left( \rho D_{(i)}^{0} + \frac{\mu_e}{Sc} \right) \frac{\partial K_{(i)}}{\partial y}, \tag{3}
\]
\[ \rho u \frac{\partial K_i}{\partial x} + \rho v \frac{\partial K_i}{\partial y} = \frac{\partial}{\partial y} \left( \rho D_{ci}^0 + \frac{\mu_i}{S_{ci}} \frac{\partial K_i}{\partial y} \right), \quad i = 1, 2, \quad K_i = 1 - \frac{2}{\sum_{i=1}^{2} K_i}. \quad (4) \]

Secondary effects, such as the thermodiffusion and the diffusion thermoeffect were not taken into account. Turbulence was modeled using a two-parameter differential turbulence model \((q - \omega)\) [15]. The turbulent Prandtl \(P_r\) and Schmidt \(S_c\) numbers were assumed to be 0.85 and 0.8, respectively. To close the system of differential equations, boundary conditions were set at the interface of the phases and in the inlet flow. Based on the condition of adhesion of a viscous gas the longitudinal velocity component on the evaporation surface \(u_w = 0\). The transverse velocity component was expressed from the balance of flows of the substance:

\[ v_w = -\sum_{i=1}^{2} D_{w(i)}^0 \left( \frac{\partial K_i}{\partial y} \right) \left( 1 - \frac{2}{\sum_{i=1}^{2} K_{w(i)}} \right). \quad (5) \]

Adiabatic evaporation from the wetted plate occurs only due to the convective heat supply from the external gas flow. The liquid layer has a temperature equal to that of the evaporation surface, the plate is heat-insulated, and the heat fluxes due to radiation to the liquid are negligible. In this case, from the heat balance it may be inferred that:

\[ -\lambda_w \left( \frac{\partial T}{\partial y} \right)_w + \rho_v v_w r = 0, \quad (6) \]

where \( r \) is the heat of the solution vaporization, which was determined based on the heat of vaporization of the liquid components at the surface temperature by the formula:

\[ r = \sum_{i=1}^{2} \eta_{w(i)} K_{L(i)}. \quad (7) \]

It should be noted that for the studied liquids, the specific heat of dissolution does not exceed 5\% of the heat of vaporization. Taking into account the assumption that the composition of the liquid is constant, we assume that the contribution of the heat of dissolution to the balance (6) is negligible. The composition of the vapor gas mixture at the interface is determined from Dalton’s law and the equation of state of the ideal gas:

\[ K_{w(i)} = M_{w(i)}^0 P_{S(i)}^0 / \sum_{j=1}^{3} M_{w(j)} P_{S(j)}, \quad (8) \]

where \( P_{S(3)} = P_0 - P_{S(1)} - P_{S(2)} \) is the partial pressure of nitrogen above the solution. The partial pressure of the saturated vapor of each component of the binary liquid on the evaporation surface is determined by the phase equilibrium curve. For non-ideal liquid systems, the saturated vapor pressure can be represented using Raoult’s law, taking into account the liquid phase activity coefficient:

\[ P_{S(i)} = P_{w(i)}^0 X_{L(i)} \gamma_{i}^{\text{ln}}. \quad (9) \]

The method developed on the basis of the Margules equations is used to calculate the phase equilibrium in the studied solutions. The activity coefficients are presented in table 1. The analysis of various models for calculating the liquid-vapor equilibrium for the solutions under consideration is presented in [14].

| Table 1. Activity coefficients |
|------------------------------|
| water(1)/ethanol(2) by Kharin S E [16] |
| \( \ln \gamma_{i(1)} = 0.79 \left( 3 - 2X_{L(2)} \right) X_{L(2)}^2 \), \( \ln \gamma_{i(2)} = 1.58 \left( 1 - X_{L(2)} \right)^3 \) |
| water(1)/acetone (2) by Semionov I A [17] |
| \( \ln \gamma_{i(1)} = \left( 1.275 - 0.088 X_{L(i)} \right) X_{L(i)}^2 \), \( \ln \gamma_{i(2)} = \left( 1.231 + 0.088 X_{L(2)} \right) X_{L(1)}^2 \) |

The method of solving the problem is presented in more detail in [18].
3. Results and discussion

Figure 2 shows the results of calculating the local specific evaporation rate of an water ethanol solution into dry air and a superheated mixture of ethanol and water vapor, depending on the temperature of the inlet turbulent flow. The composition of the superheated vapor mixture is assumed to be equal to that of the vapor above the surface of the boiling solution of a given composition, or in other words, the equilibrium composition of the vapor. In practice, when the composition of the steam in the inlet flow differs from the equilibrium one, the vapor condensation of one of the mixture components inevitably occurs and the equilibrium composition is established. As can be seen from figure 1, at the beginning of the plate there is a non-wettable isothermal section with the length of 4 m, which at flow velocity of 10 m/s allows obtaining the flowing of the wetted part of the plate by the developed turbulent flow. The total length of the plate is 8 m. The evaporation intensity is determined at a distance of 7 m from the beginning of the plate, in the region of stabilized flow. The Reynolds number $Re_{x}$ on the wetted part of the plate, depending on the properties of the inlet flow, varies from $3.6 \times 10^5$ to $9.5 \times 10^6$. With an increase in the molar concentration of ethanol in the solution, the vaporization intensity increases, and at evaporation into superheated steam, the rate of increase in the vaporization intensity with an increase in the vapor temperature is significantly higher than when vaporized into air.

Figure 2. Local evaporation rate of ethanol water solution depending on the temperature of the inlet air flow (solid lines) or the flow of a superheated mixture of vapours of an equilibrium composition (dotted lines); vertical arrows show the inversion temperature for solutions of different compositions: $1 - X_{1} C_{2}H_{5}OH = 0.97, 2 - 0.28, 3 - 0.12, 4 - 0.04, 5 - 0.004$.

The equality of the evaporation intensity in superheated steam and dry air occurs at the inversion temperature, which depends on the composition of the solution. For an water ethanol solution $I_{inv}$ does not depend on the evaporation rate or the length of the plate. With an increase in the concentration of ethanol in the solution, the inversion temperature decreases from 480 °C (for 1% by weight of ethanol solution in water, not shown in figure 2) to 125 °C (for 99% by weight of ethanol solution in water).
Figure 3. Local evaporation rate of an water solution of acetone depending on the temperature of the inlet air flow (solid lines) or the flow of a superheated mixture of vapors of an equilibrium composition (dotted lines); vertical arrows show the inversion temperature for solutions of different compositions: 1 – \( X_{L(C,H,O)} = 0.97 \), 2 – 0.24, 3 – 0.09, 4 – 0.03, 5 – 0.003.

Table 2. Inversion temperature for evaporation of binary liquids into air and an equilibrium mixture of superheated vapors

| Mass concentration of the low-boiling component of solutions \( K_{L(3)} \) | 0.01 | 0.1 | 0.25 | 0.5 | 0.99 |
|---------------------------------------------------------------|------|-----|------|-----|------|
| water(2)/ethanol(3) | 460  | 300 | 254  | 225 | 166  |
| laminar [14]        |      |     |      |     |      |
| water(2)/ethanol(3) | 480  | 216 | 176  | 157 | 125  |
| turbulent           |      |     |      |     |      |
| water(2)/acetone(3) | 442-522 | - | 242-265 | 197-254 | 149-154 |
| laminar [14]        |      |     |      |     |      |
| water(2)/acetone(3) | 478  | 215 | 161  | 133 | 99   |
| turbulent           |      |     |      |     |      |

Figure 3 shows data on the evaporation rate of an water solution of acetone. With an increase in the concentration of acetone, the inversion temperature decreases from 478 °C (for 1 mass % of acetone solution in water, not shown in figure 3) to 99 °C (for 99 mass % of acetone solution in water). The obtained inversion temperature values for the turbulent flow regime are shown in Table 2 in comparison with the previously obtained data for the laminar flow regime [14]. For the water/acetone solution in the laminar flow regime, the specified temperature range is due to the change in the inversion temperature when the plate length changes. It may be noted that at low concentrations of light-boiling components in the solution (almost at water evaporation), the inversion temperature exceeds 450 °C in both laminar and turbulent flow regimes, which is a significant limitation for the use of superheated steam drying at atmospheric pressure. With an increase in the concentration of light-boiling components in the solution, the inversion temperature decreases. Turbulization of the inlet flow leads to a significant decrease in the inversion temperature when adding ethanol or acetone to the solution.
4. Conclusions
Studies of heat and mass transfer during adiabatic evaporation of binary solutions of water/ethanol and water/acetone into a turbulent boundary layer of a vapor-air mixture from a flat wetted plate have been carried out. The values of the inversion temperature for solutions with different concentration of the volatile component have been determined. It is shown that in a turbulent boundary layer, the dependence of the inversion temperature on the boiling point of the liquid is preserved. Previously, this conclusion was made when studying the evaporation of water into dry air and superheated steam at different pressures. In the case of evaporation of liquid solutions, the boiling point changes due to changes in the composition. An increase in the boiling point leads to an increase in the inversion temperature. The minimum value of the inversion temperature at atmospheric pressure for the solutions under consideration is 150 °C in the laminar regime, and in the turbulent regime it is 99 °C. It may be noted that under the conditions considered, the flow regime affects the inversion temperature. Turbulization of the inlet flow leads to a significant decrease in the inversion temperature when adding ethanol or acetone to water. The pressure decrease should also contribute to lowering the inversion temperature for solutions. The results obtained can be used in the development of effective technologies for the separation of mixtures (solutions) containing water, acetone, and ethanol, in absorption systems of refrigeration equipment, in evaporative cooling systems, during rectification or in drying processes.

Nomenclature

- \( c_p \) – specific mass isobaric heat capacity, J/kg·K;
- \( \delta \) – thickness of boundary layer, m;
- \( D_i^0 \) – effective diffusion coefficient, m\(^2\)/s;
- \( j_w = \rho_w v_w \) – evaporation intensity, kg/m\(^2\)s;
- \( K_{(i)} \) – mass concentration of \( i \) component;
- \( L, L_0 \) – length of the plate and length of non-wetted isothermal section, m;
- \( P \) – pressure, Pa;
- \( Pr \) – Prandtl number;
- \( q \) – heat flux, W/m\(^2\);
- \( r \) – specific heat of vaporization, J/kg;
- \( Re_i \) – Reynolds number;
- \( Sc \) – Schmidt number;
- \( t_{inv} \) – inversion temperature, °C;
- \( T \) – absolute temperature, K;
- \( u, v \) – longitudinal and transverse components of the flow velocity vector, m/s;
- \( x, y \) – longitudinal and transverse coordinate, m;
- \( X_{(i)} \) – mol concentration of \( i \) component;
- \( \gamma \) – activity coefficient;
- \( M \) – molar mass, kg/kmol;
- \( \rho \) – density, kg/m\(^3\);
- \( \mu \) – dynamic viscosity, Pa·s;
- \( \lambda \) – heat conductivity, W/m·K;
- \( \theta \) – saturation pressure of pure liquid;
- \( 0 \) – inlet flow;
- \( i, j \) – component number in the vapor mixture or in the liquid solution;
- \( L \) – liquid;
- \( S \) – saturated;
- \( t \) – turbulent;
- \( w \) – evaporation surface.

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