THE MATHEMATICAL DESCRIPTION OF PROCESS OF THE CONCENTRATION OF THE SOLUTION BY METHOD OF CONTACT-MEMBRANE DISTILLATION BASED ON TEMPERATURE-POLARIZATION

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Abstract. Insufficiency of development level of questions for the creation of mathematical models of process contact-membrane distillation (CMD) has led to the fact that their development is an urgent task, which solution is devoted work.

Keywords: distillation, contact-membrane, temperature-polarization, chemical engineering.

Introduction

In the simulation of process CMD implemented two approaches (Dytnersky, 1999). The first approach is empirical and based on the use of expressions for performance and selectivity obtained while experimental data was generalized. The disadvantage of this approach is not wide enough area of use of empirical of expressions used in the model and their not enough theoretical justification. Another approach is phenomenological and is based on approximate analytical solutions of equations of heat and mass transfer obtained under the assumption that greatly simplifies the calculations. However, sometimes, these assumptions lead to significant errors and do not allow accurately set the physicochemical basis of membrane distillation. Mathematical model of process of membrane distillation the module of flow has been created by such scientists as like Ugrozov V.V. (Ugrozov, 1994). Analyzed the influence of hydrodynamic of flow solution and distillate, size and characteristics of membrane, temperature regimes on the specific mass-flow of vapor through the membrane. Therewith, not enough attention is paid to the counting of the temperature polarization and dynamics of the process. Calculation carried out with averaging of temperatures of solution and distillate in the transverse direction of the channel for the pure solvent (water).

Method

Temperature-polarization negatively affects the performance of the process as a result of lowering the temperature of the solution and in accordance the partial pressure of vapor at the surface evaporation and its increase on surface of condensation.

The driving force of the process CMD - is the difference of partial vapor pressure of the solvent in the air above the liquid meniscus on opposite sides of the membrane pores. The partial pressure in turn depends on the temperature of the corresponding flow and component-composition of the solution. It is therefore necessary to consider as the distribution of the concentrations of the components and as the temperature field in the channels of the solution and distillate. Membrane distillation is accompanied by the heat-transfer between streams. Heat-transfer carried out in three stages: the transfer of heat from the core of solution flow to the membrane surface, transfer of heat through the membrane, heat transfer from the receiver type surface of membrane to the nucleus distillate stream. Because the thermal conductivity of the solution temperature in membranous layer is different from the temperature in the core of flow due to temperature-polarization.

Thus, for the volume elementary of the solution based on convection and in the same time heat conduction, dynamic equations are composed in the transverse of direction channels (Ladieva, 2004):

\[
\frac{\partial \theta_p}{\partial t} + U_p \frac{\partial \theta_p}{\partial x} + V_p \frac{\partial \theta_p}{\partial y} = a_p \frac{\partial^2 \theta_p}{\partial y^2},
\]

\[
\theta_p(0,t) = \theta_{p0} \quad \theta_p(x,0) = \theta_{p\partial},
\]
where $\theta_p$ – solution temperature, K; $U_p$, $V_p$ – solution in accordance with the speed of the longitudinal and transverse directions, m/s; $a_p$ – coefficient of thermal diffusivity of solution, m$^2$/s.

Given the transfer of heat through the membrane, boundary conditions on the surface of the membrane from the hot side of solution can be written:

$$-\lambda_p \frac{\partial \theta_p}{\partial y}_{y=-l_p} = \alpha_p \left[ \theta_p - \theta_i \right],$$

(2)

where $\alpha_p$ – coefficient of heat transfer from the hot solution to the membrane surface, W/(m$^2$ K); $\lambda_p$ – coefficient of thermal conductivity of solution, W/(m K); $\theta_i$ – surface temperature of the membrane from the side of solution, K; $l_p$ – height channel of solution, m.

By analogy with equation (1) subject to the distillation temperature distribution along the channel and on channel height membrane made dynamic equations:

$$\frac{\partial \theta_d}{\partial t} + U_d \frac{\partial \theta_d}{\partial x} + V_d \frac{\partial \theta_d}{\partial y} = a_d \frac{\partial^2 \theta_d}{\partial y^2},$$

(3)

$$\theta_d(0,t) = \theta_{d0}, \quad \theta_d(x,0) = \theta_{d,0},$$

(4)

with boundary conditions

$$-\lambda_d \frac{\partial \theta_d}{\partial y}_{y=-l_d+\delta} = \alpha_d \left[ \theta_2 - \theta_d \right],$$

(5)

where $\theta_d$ – temperature of distillate K; $\theta_2$ – surface temperature of the membrane from the side of distillate, K; $U_d$, $V_d$ – solution in accordance with the speed of the longitudinal and transverse directions, m/s; $a_d$ – coefficient of thermal diffusivity of solution, m$^2$/s; $\delta$ – thickness of the membrane, m.

Provided that the external walls of the channels of solvent and distillation heat-insulated for tight adiabatic limit, the boundary conditions at the membrane surface:

$$\frac{\partial \theta_d}{\partial y}_{y=0}, \quad \frac{\partial \theta_d}{\partial y}_{y=-l_d+\delta+\delta} = 0,$$

(6)

where $l_d$ – height channel of distillate, m.

Process of membrane distillation is accompanied by phase transitions and determined heat-transfer and mass transfer in membrane systems. Heat transfer through the membrane in two ways: heat-conduction through the polymer-structure and vapor in the pores of the membrane (Ladieva, 2004), the integral mass flow of solvent vapors. Thus, for the total heat flux through the membrane can be written:

$$\alpha_p \left( \theta_p - \theta_i \right) = -\lambda_M \frac{\partial \theta_M}{\partial y}_{y=-l_p} + J_r \left( \bar{\theta} \right),$$

(7)

$$-\lambda_M \frac{\partial \theta_M}{\partial y}_{y=-l_p+\delta} + J_r \left( \bar{\theta} \right) = \alpha_d \left( \theta_2 - \theta_d \right),$$

(8)

where $\lambda_M$ – effective coefficient of thermal conductivity of the membrane, W/(mK); $\theta_M$ – membrane temperature, K; $\bar{\theta}$ - average temperature of the membrane, K; $r$ – latent heat of vaporization, J/kg; $J_n$ – local vapor mass flow per unit area, kg/(m$^2$·s·Pa).

The system of equations describing the heat-mass exchange in the channels of the solvent and distillation complemented by the equation of Navier-Stokes and continuity:

$$\frac{\partial U_i}{\partial t} + U_i \frac{\partial U_i}{\partial x} + V_i \frac{\partial U_i}{\partial y} = -\frac{1}{\rho_i} \frac{\partial p_i}{\partial x} + \nu_i \frac{\partial^2 U_i}{\partial y^2},$$

$$\frac{\partial (\rho_i U_i)}{\partial x} + \frac{\partial (\rho_i V_i)}{\partial y} = 0,$$

(9)

with boundary conditions
\[ \frac{\partial U_p}{\partial y} \bigg|_{y=0} = 0, \quad \frac{\partial U_d}{\partial y} \bigg|_{y=\delta} = 0, \]

where \( \rho_p, \nu_p -\) density and kinematic viscosity of the solution and distillate \( \text{kg/m}^3 \text{cSt} \). Effective coefficient thermal conductivity of the membrane is determined by:

\[ \lambda_{ij} = \varepsilon \lambda_{ij} + (1 - \varepsilon) \lambda_{st}, \quad (9) \]

where \( \lambda_{st} -\) coefficient thermal conductivity of vapor and compositional structure of the membrane, respectively, \( \text{W/(m K)} \); \( \varepsilon -\) coefficient of porosity of the membrane.

In describing the diffusive transport of vapor capillary porous environments use equations describing molecular, knudson-diffusion and transitional flow regime. The decisive parameter of the regime of flow - is correlation average of the mean free path of the molecules and the pore diameter. The flow of vapor through the membrane is proportional to the differential pressure of the solvent vapor at opposite surfaces of the membrane. In addition, the permeability of the membrane depends on temperature, pressure, composition of vapor and structure of the membrane. Pressure gradient is also dependent on temperature and medium composition on the surface and in the volume of flow. Therefore, the calculation of transmembrane of flux can be realized only at the joint solution of the equations of heat-mass method of successive approximations.

To calculate the local mass flow of steam were used correlation in the case of transfer of vapor in the pores of the membrane by the way of molecular diffusion (Ugrozov, 1994):

\[ J_i = \frac{\dot{I}}{\delta R \theta} \ln \left( \frac{p_d - \delta_2(\theta)}{p_p - \delta_1(\theta)} \right), \quad (10) \]

where \( M_o -\) molecular weight of water vapor, \( \text{kg / kmol} \); \( D_{mn} -\) effective coefficient of mutual diffusion of vapor in air, \( \text{m}^2/\text{s} \); \( p_o, p_d -\) total pressure vapor in the warm and cold sides of the membrane, \( \text{Pa} \); \( p_1, p_2 -\) partial vapor pressure of the solvent (water-vapor) in warm and cold sides of the membrane, \( \text{Pa} \); \( R -\) universal gas constant, \( \text{J/(kmol K)} \); \( \theta_m -\) temperature membrane, \( \text{K} \).

The equations that take into distribution the temperature of solution and distillate in the longitudinal and transverse directions of the cell membrane module (1), (3) with boundary conditions on the surface of the membrane from the side of the hot solution (2) and from the side of the cold distillate (4), supplemented by the continuity equation (8) based on the total heat transfer across the membrane (6), (7) is a mathematical model of the process of contact membrane distillation.

The system of equations, resolved by the numerical-stratified method. The procedure for calculating the equation is as follows:

1. Velocity distribution on the input section and a first approximation \( \frac{\partial p}{\partial x} \) are given.

2. The distribution of temperature solvent and distillation on the input section specified.

   To determine the surface-temperature \( \theta_1 \) i \( \theta_2 \) was using a system (6) - (7), that is, resolved using the method of Hooke-Jeeves. Posed the following approximation \( \frac{\partial P}{\partial x} \), taking into account the pressure loss due to friction in the channels of the membrane. From the Navier-Stokes equations define longitudinal velocity component \( U \) in the next layer. Calculated local flow of steam from the formula (10).

3. From the boundary conditions for the system (8) was transverse velocity component \( V \), then equation (8) were solved with respect to the longitudinal velocity component of \( U \).

4. System of equations was resolved (1) and (3) with the appropriate boundary conditions and the temperature distribution was \( \theta_s, \theta_t \) on the next layer.

Algorithm of calculating was continued until we have got the temperature of the solution and the distillate at the outlet of the membrane module.

For the numerical solution of equations (1) - (10), using an explicit scheme of numerical integration. Equation approximated by the following scheme of difference.

As a result of solution of equations (1) - (10) obtained numerical values change of the temperature field in the channels of the solution, distillate, on the surface of the membrane, the length and height of the
membrane module. We obtained the temperature distribution in the transverse direction of the membrane at different distances from the entrance. Reducing the temperature of the solution from the core of flow to the surface of the membrane is explained by the temperature-polarization and is in few degrees.

Temperature distributions of solution in the core of flow and on membrane surface are shown in Fig. 1. The temperature of solution in the core of flow along the membrane channel falls at 1.5 °C. For industrial-membrane type modules change in temperature of the solution along the channel is more significant.

The adequacy of the mathematical model is tested by comparing the results of computational experiment and experimental studies on laboratory installation of membrane module for the distillation of standard solution. Comparison of distribution of temperature of solution in the core of flow in the continuous-direction and the experimental data showed that the mathematical model has a maximum relative error of 6 - 15%. Duration of transition of process, which is calculated using a mathematical model is 8 - 15 s, and obtained in a laboratory setting - 15 s when the input temperature of the solution in the range of 60 - 80 °C and a flow rate of 0.1 m/s.

The difference in the duration of the transient characteristic recorded on the experimental setup and calculated using a mathematical model (1) - (10) is due to unaccounted heat accumulation in the membrane cell design (wall of module, the base web). The difference between values the temperature of the solution at the output of the module in the experiment and calculations can be explained by errors in the adopted dependencies to determine the flow of the steam and heat through the membrane.

![Fig. 1. Temperature distribution solution in the longitudinal direction of the channel](image)

**Conclusion**

Thus, it is essential, in order to control the process - to take accounting of the distribution temperature of solution in the continuous direction of the channel.

**References**

