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MODELOWANIE MATEMATYCZNE PROCESU DESTYLACJI Z ZASTOSOWANIEM MEMBRANY PRÓŻNIOWEJ

Streszczenie: Opracowano model matematyczny opisujący transfer masy i energii w procesie destylacji etanolu z zastosowaniem membrany próżniowej. Wyznaczono wartości podstawowych parametrów procesu. Na podstawie opracowanego modelu wyznaczono charakterystyki statyczne oraz dynamiczne procesu odpowiadające kolejnym trybom działania modułu z membraną. Aby określić charakterystyki dynamiczne dopasowano model dynamiczny uwzględniając przestrzenie stanów.

Słowa kluczowe: model matematyczny, membrana, rozrzedzenie, koncentracja/stężenie, linearyzacja, przestrzeń stanów

MATHEMATICAL MODELING OF THE PROCESS OF VACUUM MEMBRANE DISTILLATION

Summary: A mathematical model was developed to describe the transfer of mass and energy in the process of ethanol section by means of vacuum membrane distillation. Are the basic parameter values of the process. According to the developed model, static and dynamic characteristics of the process corresponding to the operation mode of the membrane module are constructed. For dynamic characteristics, the dynamics model is adjusted to the state space.

Keywords: mathematical model, membrane, rarefaction, concentration, linearization, space of states.

1. Introduction

At present, the world's energy balance is formed mainly on the basis of three non-renewable hydrocarbon energy sources - natural gas, oil and coal.

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The problem of natural resources has led to an intensive study of renewable energy, in particular bioenergy.

One of the renewable energy sources is biofuel - bioethanol.

Bioethanol is ethanol obtained from the fermentation of sugar in biomass materials such as corn grain and other agricultural waste. It is used in its pure form, but more often as an additive to gasoline in internal combustion engines in a ratio of 10% ethanol, 90% gasoline. Brazil and the United States have achieved the greatest success in bioethanol production.

To increase the concentration of alcohol in the final product, vacuum membrane distillation is introduced using a mathematical model which is given below. There are two membrane processes: membrane distillation and pervaporation. The main difference between these processes is the types of membranes used. In membrane distillation, a porous membrane is used, in pervaporation it is non-porous. The porous membrane provides more than 100 times faster separation of ethanol and solution compared to non-porous ones. This is why membrane distillation is being introduced in the industry. The membrane is a semi-permeable barrier that prevents direct contact between the two phases. The stream flowing through the membrane is called permeate or filtrate. The advantage of the process is: the possibility of continuous removal of ethanol at the stage of production of fuel alcohol, which prevents the inhibition of fermentation by the product and thereby increase production; increase of alcohol concentration by 8.8 times compared to raw materials; economy - the initial solution should not be brought to the boiling point; simple structure of the object - the object is a regular vessel divided into two by a molecular lattice; linear parameter dependence - process conditions are easy to predict, since they have a direct proportional relationship [1].

2. Mathematical model approach

There are currently few models of the vacuum membrane distillation process, but Soni, Abildskov, Jonsson, and Gani (2008) have proposed a model that includes 62 equations and 57 parameters, making it a high complexity model.

There are also mathematical models of contact membrane distillation. One of them is a mathematical model of the process of contact membrane distillation L. Ladieva, A. Zhulinsky This model takes into account the possibility of dynamic control of the process, which is not present in most models of this process.

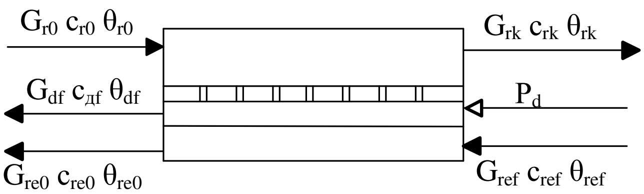

Figure 1. The design scheme of the membrane module

In Fig. 1 shows a design of a distillation scheme, which dehydrates ethanol to a predetermined concentration. This object has the following options:
F – membrane area, m^2; c_1 – the concentration of ethanol in solution, mol/m^3; c_2 – the concentration of ethanol that has passed through the membrane, mol/m^3; G_{r0} – input raw material consumption, kg/s; c_0 – concentration of ethanol in raw materials, mol/m^3; I – ethanol stream passing through the membrane, $kg/(m^2s)$; α – relative volatility of the mixture Wt/(mK); G_{rf} – outlet solution flow rate, kg/s; θ_{r0} – solution temperature at the inlet, °K; c_{r0} – heat capacity of the solution at the inlet, J/kg*°K; κ_1 – coefficient of heat transfer from solution to wall, $Wt/(m^2°K)$; F – area of heat exchange, m^2; θ_{rf} – outlet solution temperature, °K; θ_{df} – the outlet distillate temperature, °K; β – coefficient of mass recovery of water and ethanol [1] $kg/(m^{2*}s*Pa)$; ξ_1 – coefficient of partial pressure of raw material vapors; ξ_2 – coefficient of partial pressure of ethanol vapor; r – specific heat of vaporization, J/kg; P_d – pressure on the distillate side, Pa; κ_2 – coefficient of heat transfer from the wall to the refrigerant, $Wt/(m^2°K)$; θ_{ref} – outlet refrigerant temperature, °K; θ_{re0} – refrigerant inlet temperature, °K; c_{re} – heat capacity of the refrigerant, J/kg*°K; G_{re0}– inlet refrigerant consumption, kg/s; G_{ref}– inlet refrigerant consumption, kg/s.

When creating a mathematical model, the following assumptions were made:
1. the membrane is perfect, is hydrophobic with the same pore radius and intact selective layer;
2. the effect of temperature and concentration polarization is not taken into account;
3. unaccounted for change in temperature and concentration along the channels of the membrane module;
4. The capacity of the membrane was not considered, given its insignificant thickness compared to the height of the channels of the solution and the distillate.

In the mathematical modeling of the vacuum distillation process the following equations were obtained:

$$G_{r0}c_{r0}\theta_{r0} - k_1F_1(\theta_{rf} - \theta_{df}) - \beta(\xi_1\theta_{rf} - \xi_2\theta_{df})Fr - G_{rf}c_{rf}\theta_{rf} = = V_r\rho_r c_r \frac{d\Delta\theta_{rf}}{dt} \quad (1)$$

$$k_1F_1 * (\theta_{rf} - \theta_{df}) + \beta(\xi_1\theta_{rf} - \Delta P_d)Fr - k_2F_2(\theta_{df} - \theta_{ref}) = = V_d\rho_d c_d \frac{d\Delta\theta_{ref}}{dt} \quad (2)$$

$$G_{re0}(c_{re0}\theta_{re0} - c_{ref}\theta_{ref}) + k_2F_2(\theta_{df} - \theta_{ref}) = V_{re}\rho_{re}c_{re}\frac{d\Delta\theta_{ref}}{dt} \quad (3)$$

$$G_{r0}c_{r0} - \beta F_1(\xi_1\theta_{rf} - \xi_2\theta_{df})C_2 - G_{rf}C_1 = m_r\frac{d\Delta c_1}{dt} \quad (4)$$

Equation 1 considers the thermal balance of the process of evaporation of ethanol from the raw material. The thermal energy of the raw material due to the dilution in the pores of the membrane leads to the active evaporation of ethanol and its subsequent passage through the membrane. The output yields raw materials with less ethanol content and lower temperature.

Equation 2 deals with the thermal balance of the ethanol condensation process on the permeate side. Passing through the membrane under the action of partial pressure in the pores of the membrane, ethanol condenses, because on the other side of the membrane is provided a lower temperature by means of the refrigerant supplied to the membrane.

Equation 3 examines the thermal balance of heat transfer from the ethanol condensation process to the refrigerant. Ethanol is cooled by condensation and removed from the unit as well as a heated refrigerant.

Equation 4 deals with the balance of concentrations of the input and the final product - permeate, taking into account temperature and pressure differences.

Below are the values of the basic process parameters are in Tab. 1.

Table 1. The values of the basic parameters of the process

Name	Marking	Numeric value	Dimension
Inlet solution temperature	Θ_{r0}	338	°K
Outlet solution temperature	θ_{rf}	333	°K
Inlet refrigerant temperature	Θ_{re0}	293	°K
Outlet refrigerant temperature	Θ_{ref}	303	°K
Raw material consumption	G_{r0}	0,006	kg/c
Heat capacity of raw materials	c_r	3897	J/(kg*°K)
Heat capacity of the refrigerant	c_{re}	4200	J/(kg*°K)
Heat transfer coefficient	κ_1	69,869	Wt/(m²*°K)
Heat transfer coefficient	κ_2	7,112	Wt/(m²*°K)
The surface area of heat transfer	F	$4{,}5*10^{-3}$	m^2

3. The main static characteristics of the model

- « Consumption of solution – solution temperature ».

$$\theta_{rf}(G_{r0}) = \frac{\theta_{df} * \left(k_1 F_1 + \beta F \xi_2 \theta_{rf} r\right) - c_{r0}\theta_{r0}G_{r0}}{\beta F r \xi_1 + k_1 F + G_{rf} c_{rf}}$$

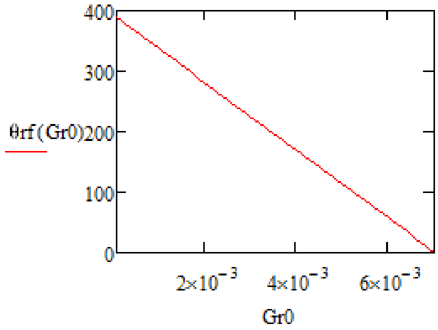

Figure 2. Static characteristic of the channel Gr0 - θrf

- «Distillate channel pressure – the distillate temperature»

$$\theta_{df}\left(\mathrm{P}_{df}\right) = \frac{\theta_{rf} * (k_1 F_1 + \beta F r \xi_1) + \mathrm{P}_{df}\beta F - \theta_{ref} k_2 F_2}{k_1 F + k_2 F_2}$$

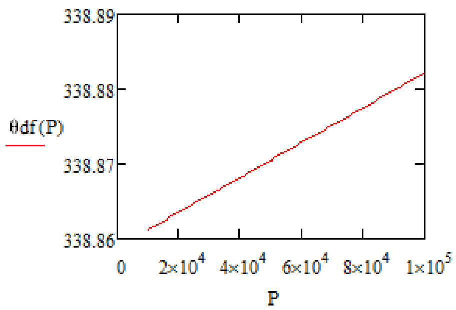

Figure 3. Static channel characteristic P – θ_{df}

- «Consumption of refrigerant – refrigerant temperature»

$$\theta_{ref}(G_{re0}) = \frac{G_{re0} c_{re0} \theta_{re0} + k_2 F_2 \theta_{ref}}{G_{re0} c_{re0} - k_2 F_2}$$

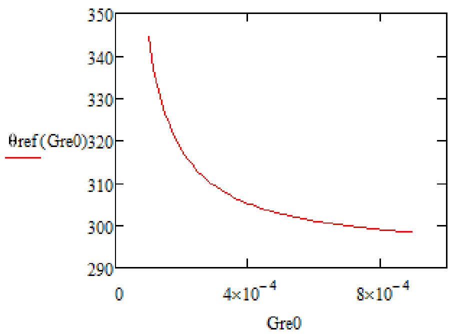

Figure 4. Static channel characteristic G_{re0} – θ_{ref}

- «Distillate channel pressure – ethanol concentration»

$$C_1(P_{df}) = \frac{G_{r0}c_{r0} - \xi_1 F_1 C_2 \frac{\theta_{df} * (-k_1F_1 - k_2F_2) - P_{df}\beta Fr + \theta_{ref}k_2F_2}{k_1F_1 + \xi_1\beta Fr} - \xi_2\theta_{df}F_1C_2}{G_{rf}}$$

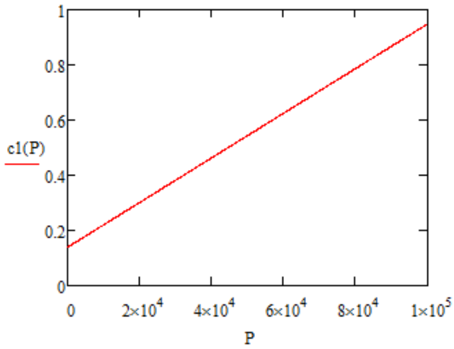

Figure 5. Static channel characteristic P – c_1

4. The main dynamic characteristics of the model.

To obtain dynamic characteristics, we will linearize the equations

$$\Delta G_{r0}c_{r0}\theta_{r0} - k_1F_1(\Delta\theta_{rf} - \Delta\theta_{df}) - \beta(\xi_1\Delta\theta_{rf} - \xi_2\Delta\theta_{df})Fr - -G_{rf}c_{rf}\Delta\theta_{rf} = V_r\rho_r c_r\frac{d\Delta\theta_{rf}}{dt}$$

$$k_1F_1(\Delta\theta_{rf} - \Delta\theta_{df}) + \beta(\xi_1\Delta\theta_{rf} - \Delta P_{df})Fr - k_2F_2(\Delta\theta_{df} - \Delta\theta_{ref}) = = V_d\rho_d c_d\frac{d\Delta\theta_{df}}{dt}$$

$$\Delta G_{re0}(c_{re0}\theta_{re0} - c_{ref}\Delta\theta_{ref}) + k_2F_2(\Delta\theta_{df} - \Delta\theta_{ref}) = V_{re}\rho_{re}c_{re}\frac{d\Delta\theta_{ref}}{dt}$$

$$G_{r0}c_{r0} - \beta F_1(\xi_1\Delta\theta_{rf} - \xi_2\Delta\theta_{df})C_2 - G_{rf}C_1 = m_r\frac{d\Delta c_1}{dt}$$

We perform algebraic transformations for a convenient look:

$$\Delta\theta_{rf}(-\beta F\xi_1 r - k_1F_1 - G_{rf}c_{rf}) + \Delta\theta_{df}(k_1F_1 - \beta F\xi_2 r) + \Delta G_{r0}c_{r0}\theta_{r0} = = V_r\rho_r c_r\frac{d\Delta\theta_{rf}}{dt}$$

$$\Delta\theta_{rf}(\beta F\xi_1 r + k_1F_1) + \Delta\theta_{df}(-k_1F_1 - k_2F_2) - \Delta\theta_{ref}k_2F_2 - \Delta P_{df}\beta Fr = = V_d\rho_d c_d\frac{d\theta\Delta_{df}}{dt}$$

$$\Delta G_{re0}c_{re0}\theta_{re0} - \Delta\theta_{ref}(G_{re0}c_{rfe} - k_2F_2) + k_2F_2\Delta\theta_{df} = V_{re}\rho_{re}c_{re}\frac{d\Delta\theta_{ref}}{dt}$$

$$G_{r0}c_{r0} - \Delta\theta_{rf}\beta\xi_1F_1C_2 + \beta\xi_2F_1C_2\Delta\theta_{df} - G_{rf}\Delta C_1 = m_r\frac{d\Delta C_1}{dt}$$

To construct the dynamic characteristics, we present the dynamics equation in the state space. General view of an object in the state space:

$$\frac{dX}{dt} = AX + BU$$

In which matrices A and B look like themselves:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

$$B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ 0 \end{bmatrix}$$

Each element of the matrix A and B are respectively equal:

$a_{11} = \frac{-\beta F\xi_1 r - k_1F_1 - G_{rf}c_{rf}}{V_r\rho_r c_r}$; $a_{12} = \frac{k_1F_1 - \beta F\xi_2 r}{V_r\rho_r c_r}$; $a_{13} = 0$; $a_{14} = 0$;

$a_{21} = \beta F\xi_1 r + k_1F_1\ \frac{\beta F\xi_1 r + k_1F_1}{V_d\rho_d c_d}$; $a_{22} = \frac{-k_1F_1 - k_2F_2}{V_d\rho_d c_d}$; $a_{23} = \frac{k_2F_2}{V_d\rho_d c_d}$; $a_{24} = 0$;

$a_{31} = 0$; $a_{32} = \frac{k_2F_2}{V_{re}\rho_{re}c_{re}}$; $a_{33} = \frac{G_{re0}c_{ref} - k_2F_2}{V_{re}\rho_{re}c_{re}}$; $a_{34} = 0$;

$a_{41} = \frac{\beta\xi_1F_1C_2}{m_r}$; $a_{42} = \frac{\beta\xi_2F_1C_2}{m_r}$; $a_{43} = 0$; $a_{44} = \frac{G_{rf}}{m_r}$;

$$b_1 = \frac{c_{p0}\theta_{p0}}{V_r\rho_r c_r};$$

$$b_2 = \frac{\beta Fr}{V_d\rho_d c_d};$$

$$b_3 = \frac{c_{\text{хл}0}\theta_{\text{хл}0}}{V_{re}\rho_{re}c_{re}};$$

$$b_4 = 0;$$

The following dynamic process characteristics are obtained using Matlab software:

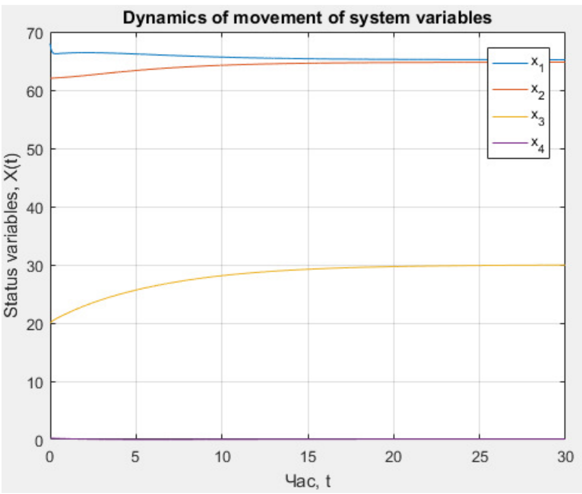

Figure 6. Transient characterization of the process by channels $G_{r0} - \theta_{rf}$, $P - \theta_{df}$, $G_{re0} - \theta ref$

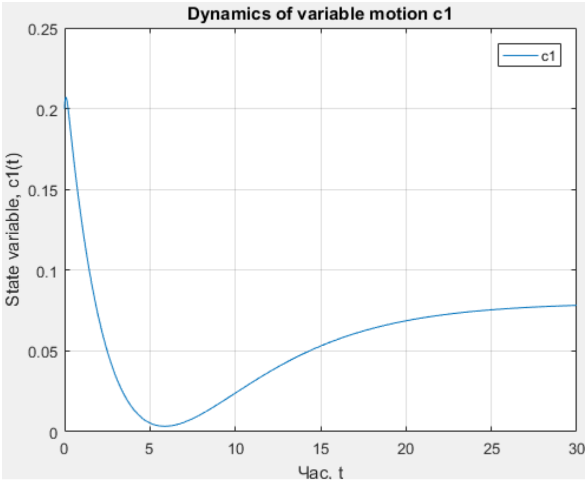

Figure 7. Transient characterization of the process by channel $P – c_1$

5. Conclusions

As the process is new, it is difficult to find research and a mathematical model of the vacuum membrane distillation process now. That is why research and implementation of this process is promising and important, because the process is noted for its productivity, quality, simplicity and speed of the process.

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