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RESEARCH ARTICLE

Modeling of membrane separation of liquid mixture in Aspen HYSYS

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Abstract

Objectives. To develop and subsequently verify the calculation block of the mass transfer process in the pervaporation membrane module based on a HybSi[®] ceramic membrane using experimental data as a basis for the verification process.

Methods. The task was implemented using a mathematical simulation within the Aspen HYSYS application package, which is designed for modeling chemical engineering processes. The differential equations of the mathematical model were represented as a system of difference equations, which were then solved numerically with an adaptive area step. The membrane pervaporation module of area S during its modeling is divided into n intervals, based on ensuring within the i th interval the condition that the temperature change ΔT is less than 1°C. A model was constructed to simulate the performance of the membrane module under isothermal and adiabatic operating conditions.

Results. The mathematical model of the pervaporation process employed in the developed computational membrane pervaporation module considers variations in the concentration and temperature of the feedstock flux along the surface of the HybSi[®] membrane. The performance of the software module was evaluated by comparing the calculated results with the available experimental data for the dehydration of ethanol and isopropanol. The results demonstrated a high degree of agreement for three isotherms (60, 70, and 80°C) and two variations of pressure on the permeate side (5 and 20 mm Hg). Modeling of the operation of the membrane module with the area of 1 m² in adiabatic mode showed that the processes of alcohol dehydration on HybSi[®] membranes are accompanied by significant thermal effects associated with heat consumption to provide evaporation through the membrane due to large transmembrane fluxes.

Conclusions. The comparative analysis of the results of modeling the HybSi[®] membrane module in isothermal and adiabatic modes of operation demonstrated that the calculation of the membrane module without consideration of thermal effects results in significant errors. These include an overestimation of the permeate flow rate by up to 50% and an underestimation of the water concentration in the retentate by up to 1.3–1.8 times. It can be reasonably deduced that the omission of thermal effects in design calculations will result in a considerable underestimation of the requisite membrane module surface area.

Keywords

modeling, pervaporation, HybSi[®] membrane, Aspen HYSYS, alcohol dehydration

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НАУЧНАЯ СТАТЬЯ

Моделирование процесса мембранного разделения жидкой смеси в среде Aspen HYSYS

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Аннотация

Цели. Разработка и последующая верификация на основе экспериментальных данных расчетного блока процесса массопереноса в первапорационном мембранном модуле на основе керамической мембраны HybSi®.

Методы. Задача решалась при помощи математического моделирования в прикладном пакете Aspen HYSYS, предназначенном для моделирования химико-технологических процессов. Дифференциальные уравнения математической модели были представлены в виде системы разностных уравнений, которая решалась численным способом с адаптивным шагом по площади. Мембранный первапорационный модуль площадью S в ходе его моделирования разбивается на n интервалов, исходя из обеспечения внутри i -го интервала условия, чтобы изменение температуры ΔT было меньше 1°C . Работоспособность программного модуля проверялась на основе сравнения результатов расчета с имеющимися экспериментальными данными по обезвоживанию этанола и изопропанола. Моделирование работы разработанного мембранного модуля проводилось в изотермических и адиабатических режимах.

Результаты. Используемая в разработанном расчетном первапорационном мембранном модуле математическая модель процесса первапорации учитывает изменение концентрации и температуры потока сырья вдоль поверхности мембраны HybSi®. Показано хорошее согласование для трех изотерм (60 , 70 и 80°C) и двух вариантов давления со стороны пермеата (5 и 20 мм рт. ст.). Моделирование мембранного модуля площадью 1 м^2 в адиабатическом режиме работы показало, что процессы обезвоживания спиртов на мембранах HybSi® сопровождаются значительными тепловыми эффектами, связанными с расходом тепла на испарение через мембрану ввиду больших трансмембранных потоков для данной мембраны.

Выводы. Сравнительный анализ результатов моделирования мембранного модуля HybSi® в изотермическом и адиабатическом режимах работы показал, что расчет мембранного модуля без учета тепловых эффектов приводит к существенным ошибкам: в определении расхода пермеата — до 50% , в определении концентрации воды в ретанте до 1.3 – 1.8 раз. Поэтому выполнение проектных расчетов без учета тепловых эффектов будет приводить к существенному занижению требуемой поверхности мембранного модуля.

Ключевые слова

моделирование, первапорация, мембрана HybSi®, Aspen HYSYS, обезвоживание спирта

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INTRODUCTION

The separation processes of multicomponent liquid mixtures represent a fundamental aspect of chemical technology. The most energy-intensive processes are those involved in the separation of azeotropic mixtures, including extractive and azeotropic distillation, extraction, etc. [1]. In order to enhance the efficiency of liquid mixture separation processes, a range of measures are currently being explored. These encompass the thermal integration of technological

process flows and the modification of the agents employed in the separation process itself [2, 3]. In this instance, an alternative to the aforementioned processes may be the separation of liquid mixtures by the pervaporation method, which represents a promising avenue of development within the field of membrane technologies. Initially, pervaporation was regarded as a potential technology for the dewatering of alcohols. The world's first industrial scale pervaporation plant was constructed for the purpose of ethanol dehydration at a pulp and paper mill in Germany [4]. Depending on

the membrane used, pervaporation can be a successful approach for solving complex separation processes, including dehydration of organic solvents [5–7], extraction of organic compounds from aqueous solutions [8], separation of organic mixtures [9, 10], removal of sulfur components [11], and water desalination [12]. Currently, membranes made of organic (polymer), inorganic (ceramic, zeolite) and hybrid (combined organic and inorganic) materials are used in the processes of pervaporation [13].

The topic of membrane technology in production, encompassing its development, design, and implementation, has recently been the subject of growing interest. Mathematical modeling of chemical technology processes constitutes a principal instrument for the investigation, conceptualization, and optimization of industrial procedures. In practice, universal modeling programs (UMP) for mathematical modeling of chemical technological processes and systems are used to solve these problems. The products of *Aspen Technologies*, *Chemstations*, and *Invensys Systems* are most widely used for modeling membrane separation processes [14]. Unfortunately, the libraries of the UMP calculation modules, including Aspen HYSYS (*Aspen Technologies*, USA), which was used in this work, do not have a built-in module for modeling pervaporation processes. However, the open architecture of Aspen HYSYS offers the advantage of enabling the creation of bespoke thermodynamic and kinetic models, as well as models of equipment units, through the utilization of the integrated programming language. This presents the opportunity to develop a calculation module for the pervaporation process in Aspen HYSYS. The inclusion of the calculation module of the pervaporation in the UMP allows users to design both individual membrane installations themselves and technological systems that include these installations.

When modeling the separation of liquid mixtures according to the pervaporation method using UMP, issues of solvent dehydration are mainly considered: ethanol when feeding the initial mixture in liquid form [15–17] (on an industrial PERVAP 2210 membrane and a silicon dioxide-based membrane) and when feeding the initial mixture in a vapor phase state [18] (membrane with a selective layer of polyvinyltrimethylsilane); isopropanol (on an industrial PERVAP 2210 membrane) [19]; isobutanol (on industrial membranes PERVAP 4060 and 1510) [17, 20]; acetic acid (on a membrane based on silicon dioxide) [16].

Due to their being among the first polymer composite membranes made available for commercial use, PERVAP membranes are the most represented in research. When describing the process of pervaporation on polymer membranes, the dissolution–diffusion

model, originally proposed by R. Reitenbach [21], is used. Later, due to problems in describing the process of pervaporation of water–alcohol mixtures with a high-water content in the initial mixture, it was improved [22]. This model has proven itself well in the calculation of organophilic and hydrophilic pervaporation processes on polymer composite membranes [20, 23]. The separation properties of polymer membranes strongly depend on their structural materials and manufacturing methods used, as well as membrane thickness and operating conditions, such as temperature and partial pressure differences above the membrane. This leads to the need to determine the parameters of the transmembrane flow model from experimental data for each membrane [24].

In the present work, the HybSi® ceramic pervaporation membrane [25–27], another commercially available membrane designed to solve the problems of alcohol dehydration, was considered. A HybSi® membrane represents a three-layer composite membrane in which a selective layer of an organo-inorganic hybrid material with an inorganic silicon dioxide base is applied to a supporting layer of amorphous silicon dioxide, which is located in turn on the inner surface of ceramic porous tubes made of α -Al₂O₃.

Mathematical model of the membrane pervaporation module

As a basis for the model of the membrane module, a three-parameter mathematical model of the stationary process of pervaporation separation of a water–alcohol binary mixture on a HybSi® membrane was used [27]:

$$\beta(x_A^F - x_A^B) + jx_A^B = P_A^m \frac{(p_A^B - p_A^P)}{\delta_m} \varepsilon_a, \quad (1)$$

$$\beta(x_A^B - x_A^F) + j(1 - x_A^B) = P_B^m \frac{(p_B^B - p_B^P)}{\delta_m} \varepsilon_a, \quad (2)$$

$$x_A^P = \frac{\beta(x_A^F - x_A^B) + jx_A^B}{j}, \quad (3)$$

where j is the total molar flux of the two components through the membrane, mol/(m²·s); x_A and x_B are the molar fractions of component A (water) and B (alcohol), respectively; the upper indices F , B , P correspond to the concentrations of the components in the initial mixture, at the boundary with the membrane and in the permeate, respectively; δ_m is the thickness of the selective layer of the HybSi® material, $\delta_m = 200$ nm; β is the mass transfer coefficient, mol/(m²·s); p_A^B and p_A^P are the partial pressures of component A at the boundary with the membrane in solution and in

permeate, respectively, Pa; P_A^m and P_B^m are the permeability coefficients for component A and B , respectively, mol/(m·s·Pa); ε_a is the share of active pores of the selective membrane layer:

$$\varepsilon_a = \frac{1}{1 + Cx_B k_B}, \quad (4)$$

where C is the molar density of the mixture, mol/m³; k is the dimensionless coefficient:

$$k_B = 8.078 \cdot 10^{-9} \exp\left(-\frac{5446.374}{T}\right).$$

The permeability coefficients P_A^m and P_B^m for the components were determined by the following expression:

$$P^m = \frac{(C_1 T + C_2) \delta_m}{M(p^V - p)}, \quad (5)$$

where T is the temperature, °C, M is the molecular weight of the component; p^V is the saturated vapor pressure of the component, Pa; p is the pressure from the permeate, Pa; C_1 and C_2 are the coefficients of linear approximation of the flow of the pure component through the membrane (see Table).

Table. Linear approximation coefficients for the flow of matter [27]

Substance	C_1	C_2
Water	0.2775	-10.2183
Ethanol	0.004	-0.16
Isopropanol	0.000915	-0.05315

The partial pressure of the component from the initial mixture was determined by the formula $p_A^B = p_A^V \gamma_A^B x_A^B$, where p_A^V is the saturated vapor pressure of component A ; γ_A^B is the activity coefficient of component A in the liquid phase. The Non-Random Two Liquid model was used in the calculations. The partial pressure in the permeate was determined by the formula $p_A^P = p \cdot x_A^P$.

A feature of the pervaporation process is the presence of a phase transition of components from a liquid state to a vaporous one, for which energy, i.e., the heat of vaporization, is required. In [27], an isothermal pervaporation regime was provided during experiments to determine the characteristics of the membrane at a constant driving force of the process. In

practice, the process occurs under adiabatic conditions within the membrane module, the energy required for permeate formation being derived from the feed stream. Consequently, the temperature of the retentate will decline throughout this process. In accordance with the dissolution–diffusion model [28], a decline in temperature can influence the rate of permeate sorption on the membrane and diffusion capacity of permeate within the membrane, as well as the driving force of pervaporation. Consequently, the overall selectivity and permeate flow will change significantly with a drop in temperature, which may not be observed in other membrane processes occurring without a phase transition. Therefore, the applied membrane area in the module should be limited to a size that provides an acceptable temperature drop. If the temperature drops below 50°C, the pervaporation process is usually stopped [17].

In most cases, during the pervaporation process, the evaporation heat is supplied only from the initial mixture, so the temperature gradient develops mainly in the direction of the flow of the initial mixture. In this case, the thermal balance for the membrane module will be written as follows [29]:

$$FC_p^F \Delta T = -P \Delta H, \quad (6)$$

where F and P are the molar flow rates of the initial mixture and permeate; C_p^F is the heat capacity of the initial mixture; ΔH is the heat of permeate vaporization; ΔT is the temperature drop between the input and output streams of the module. From the Eq. (6) The temperature drop in the membrane module can be determined:

$$\Delta T = -\frac{P \Delta H}{F C_p^F}. \quad (7)$$

To describe the flow structure inside the HybSi[®] membrane module, consisting of cylindrical tubes inside which the raw material flow must move at a linear velocity of at least 2 m/s [26, 27], an ideal displacement model was used:

$$\frac{dF}{dz} = -\frac{j(T) dS}{dz}, \quad (8)$$

$$\frac{dT}{dz} = -\frac{j(T) \Delta H}{F C_p^F} \frac{dS}{dz}. \quad (9)$$

The system of Eqs. (8) and (9) can be used calculate the process of pervaporation in a membrane module with an area of S taking into account the model of substance transfer through the membrane (1)–(3).

Since there are no built-in mathematical functions in HYSYS, the system of differential Eqs. (8) and (9) was presented as a system of difference equations

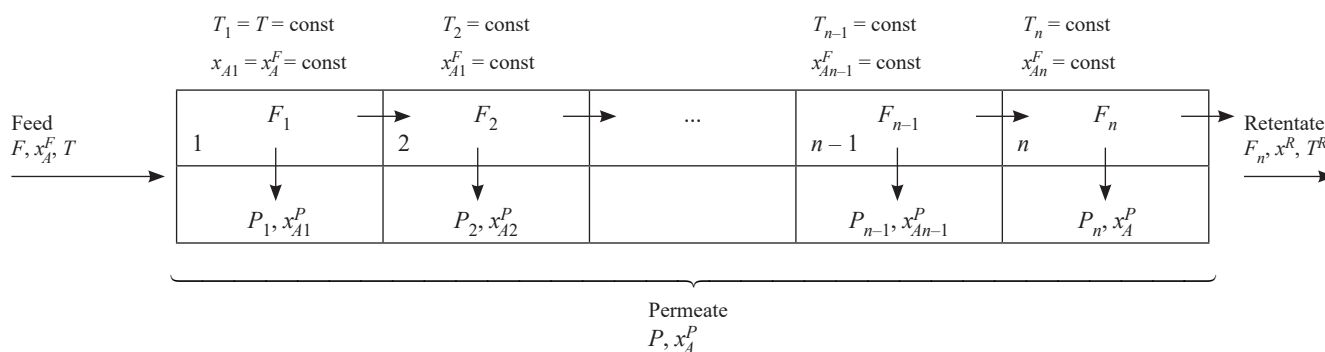


Fig. 1. Schematic of membrane module modeling

to be solved numerically with an adaptive area step. The process conditions should be close to isothermal $\Delta T \leq 1^\circ\text{C}$; therefore, the magnitude of the temperature change was checked at each step. If this condition was not met, the area step was reduced until the process became isothermal. In the task, an assumption was made about the constancy of the composition and temperature of the raw materials at each step. Thus, the membrane pervaporation module with an area of S was divided into n intervals. Figure 1 shows a schematic of the membrane module modeling.

The amount of permeate passed through the membrane at the i th step was determined as follows:

$$P_i = \left(\sum_{l=1}^k J_l \right) \Delta S_i, \quad (10)$$

where ΔS_i is the area step; J_l is the flow of the l th component; k is the number of components passing through the membrane. The feed stream F_n determined at the last step will be retentate R coming out of the membrane module.

Creating a custom membrane pervaporation module in Aspen HYSYS

The equations of the mathematical model (8), (9) and their corresponding solution methods for the pervaporation process were refined for direct use in HYSYS without the need for external special programming.

The program code of the membrane module is implemented using the built-in editor MacroLanguageEditor and includes three main routines:

- 1) Initialize(), which defines the view of the window of the technological object;
- 2) Execute(), which includes the equations of the mathematical model and calling methods for calculating the properties of a mixture of components;
- 3) StatusQuery(), which generates messages about the status of program code execution.

The developed pervaporation process module is universal to the input mixture of components. The selection of the key components of permeate and retentate is carried out by the user based on their ID in the list of components of the mixture. The calculation of vapor–liquid equilibrium, physicochemical and thermodynamic properties of mixtures of substances is performed in real time based on the user-selected package of properties in HYSYS. The pervaporation module has a unique identifier in HYSYS that allows it to be accessed from third-party applications. An enlarged algorithm for calculating the pervaporation module, objects and their main properties are shown in Fig. 2.

Container.Feeds1 defines the module's input stream object (.Item(1)), its properties, and access methods. Container.Products1 contains a set of permeate and retentate output streams (.Item(0), .Item(1)). The initial data of the process is defined in the form of user variables through a graphical interface, the current values of internal variables are displayed as a spreadsheet.SpreadsheetOp using an .Operations object.

The parameters of the components that make up the mixture are accessed by the component name "CompName" in the form:

ActiveCase.Flowsheet.FluidPackage.Components.
Item("CompName").

The parameters of the selected thermodynamic package are accessed through the property. PropertyPackage of the FluidPackage object:

ActiveCase.Flowsheet.FluidPackage.PropertyPackage.

After the membrane module added by the user in the project is adjusted to the conditions of the pervaporation process, the calculation is carried out. As a result of the solution, permeate and retentate streams are transferred from the developed module to the HYSYS environment in the required HYSYS package format, which can be sent further along the separation process scheme.

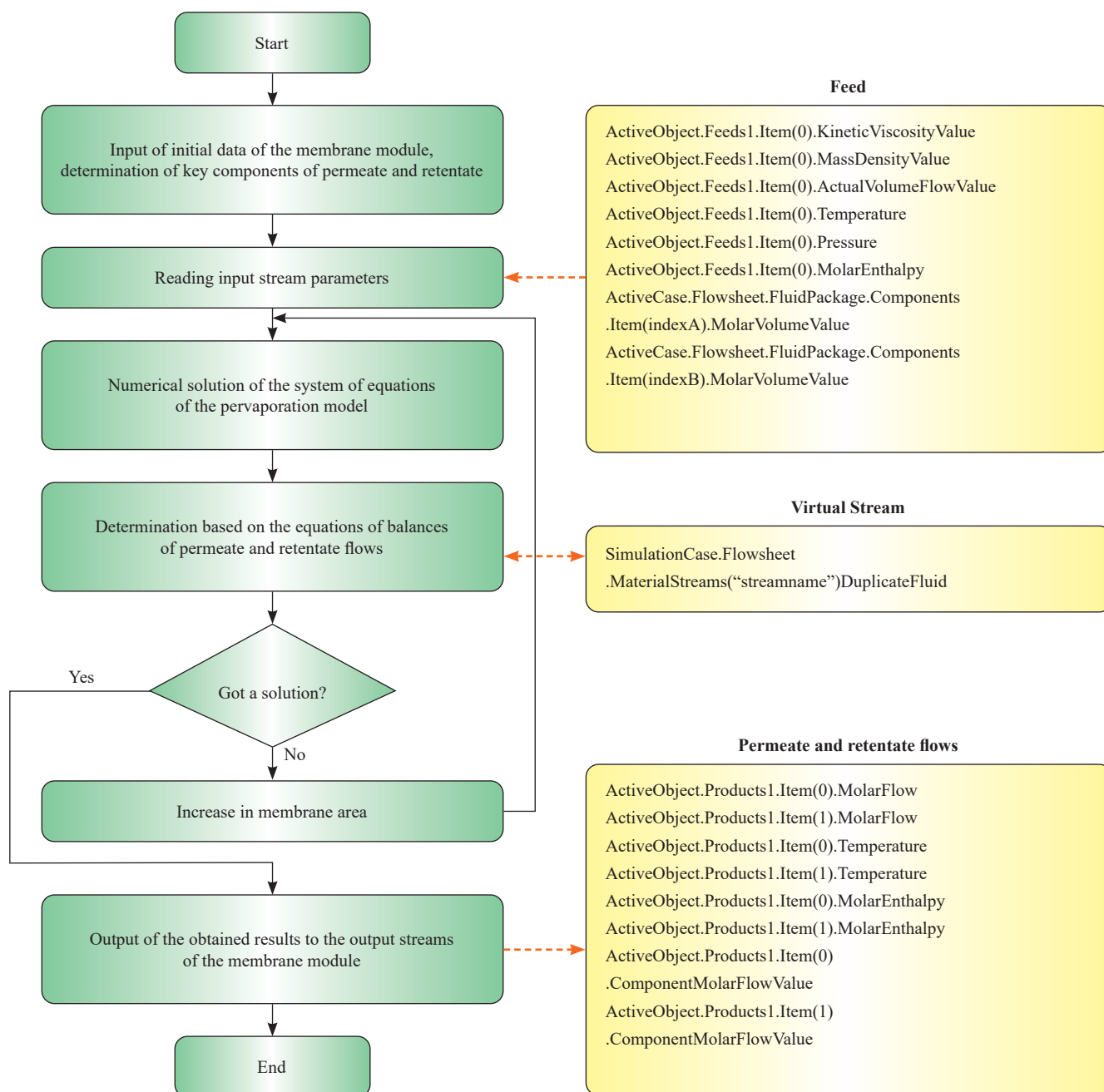


Fig. 2. Enlarged algorithm for calculating the membrane module

Comparison of calculation results in Aspen HYSYS with experimental data

The adequacy of the developed module was tested for binary water–alcohol mixtures. Figures 3 and 4 show a comparison of the calculation results of the pervaporation process for a mixture of ethanol–water and isopropanol–water at a permeate pressure of 5 and 20 mm Hg with experimental data presented in [27].

As can be seen from the results presented of modeling the operation of the membrane module in isothermal mode, the data obtained are in good agreement with the experimental data for 3 isotherms at different permeate pressures, representing a test of the operability of the module and the correct use of the HYSYS data structure in it.

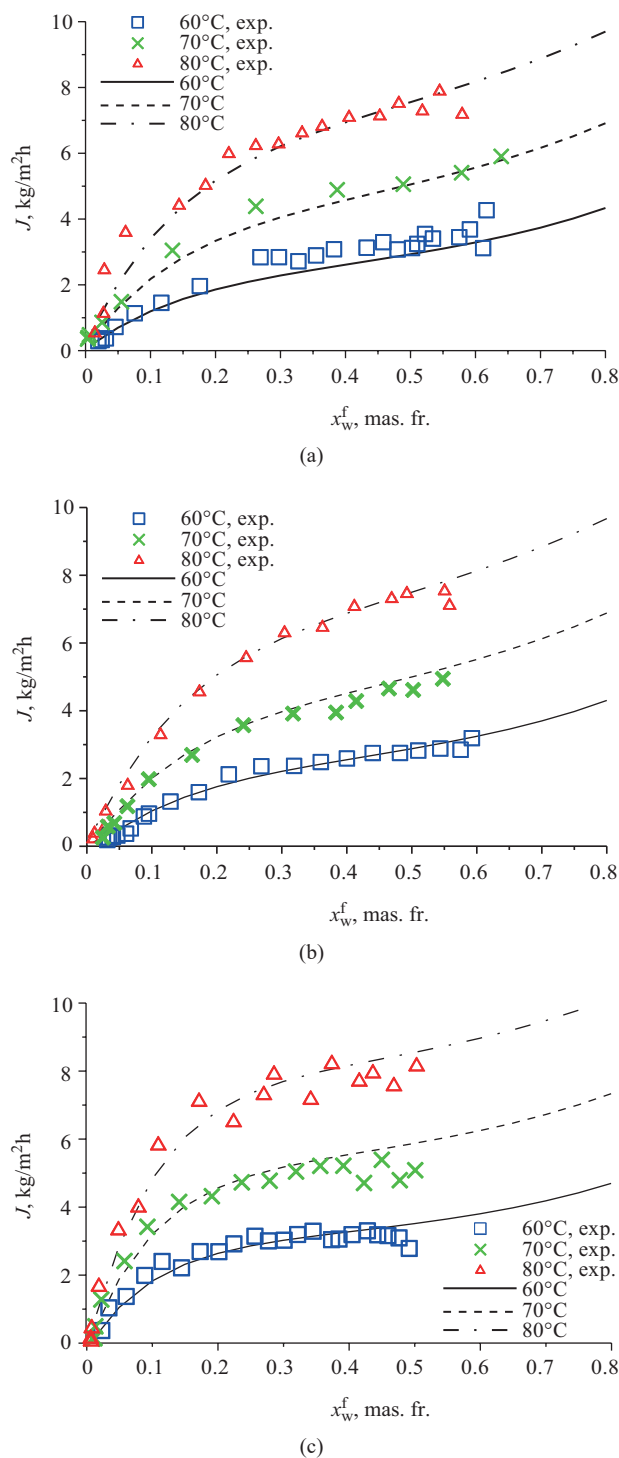


Fig. 3. Total permeate flow J through the HybSi[®] membrane depending on the concentration of water in the feed x_w^f :
(a) ethanol–water, 5 mm Hg;
(b) ethanol–water, 20 mm Hg;
(c) isopropanol–water, 20 mm Hg.
Geometric shapes are experimental data [27]

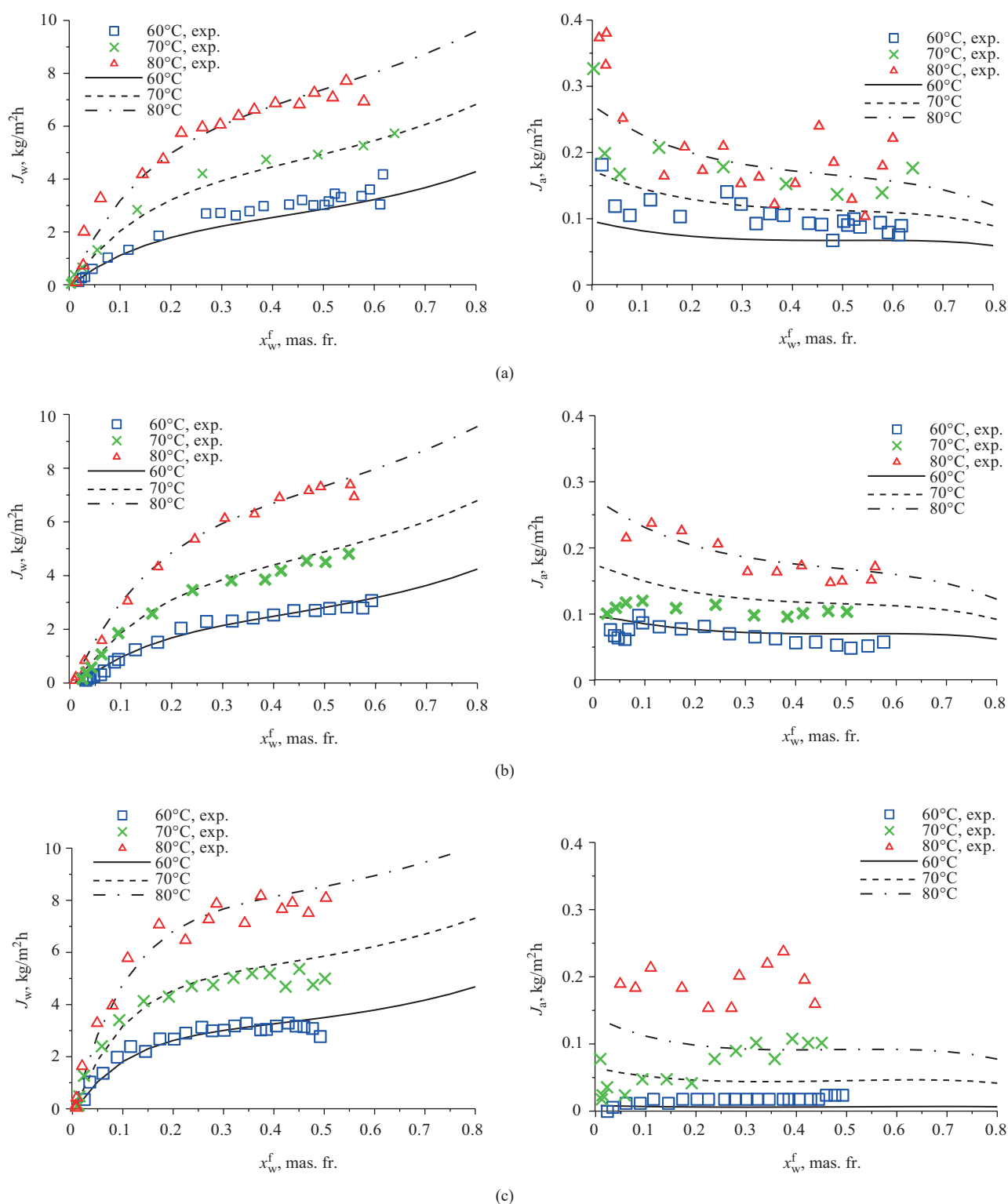


Fig. 4. Flow of individual components through the HybSi[®] membrane depending on the concentration of water in the feed x_w^f . The left graphs show the flow of water J_w , the right graphs show the flow of alcohol J_a :
(a) ethanol–water, 5 mm Hg;
(b) ethanol–water, 20 mm Hg;
(c) isopropanol–water, 20 mm Hg.
Geometric shapes are experimental data [27]

SIMULATION RESULTS AND DISCUSSION

The next stage of the research was to calculate the membrane module in adiabatic mode. Figure 5 depicts a comparative analysis of the dehydration process of ethanol and isopropanol. In the first case (Fig. 5a), the simulation results are presented depending on the water content in the initial mixture on a membrane module with an area of 1 m^2 . In the second case (Fig. 5b), the results of modeling the separation of a mixture of alcohols with an initial water content of 15 wt % as a function of the membrane module area are obtained. In both cases the simulation was carried out with a permeate side pressure of 20 mm Hg and a capacity of 100 kg/h for the initial mix.

If taking the value of the temperature difference between the inlet and outlet of the membrane module to be equal to 5°C , an isothermal operating mode can be assumed to be approximately maintained. Then, as can be seen from Fig. 5a, when isopropanol is dehydrated on a module of equal area, the area of isothermal operation for the concentration of water in the initial mixture will be smaller. At an inlet temperature of 60°C , these are mixtures of isopropanol and ethanol having an initial water content of no more than 4.75 and 10.4 wt %, respectively. Similarly, the water content in these mixtures at 70°C will be 2.95 and 5.23 wt %; at 80°C , 2.1 and 3.3 wt %, respectively. In addition, the temperature

change at the outlet of the module for isopropanol is characterized by a greater drop than for ethanol. This behavior is fully correlated with the values of the total fluxes for these alcohols (see Fig. 3): for an isopropanol mixture, the total flux is greater than for an ethanol mixture all other things being equal.

As can be seen from Fig. 5b, when dehydrating isopropanol with a water content of 15 wt % in the feedstock, the size of the module in which conditions are maintained close to the isothermal regime is smaller compared to ethanol. Ethanol at 80°C requires ~ 1.6 times the membrane area than isopropanol. When the temperature drops to 60°C , the area difference increases to ~ 1.8 times. From this point of view, when modeling the operation of the pervaporation module on a HybSi[®] membrane, it is advisable not to be guided by the same size of membrane modules, but rather by the constant temperature of the retentate at the outlet of the module, which, as shown by the example of commercial polymer membranes, is more advantageous [30]. In this case, an additional amount of heat must be added to the retentate flow after each module to increase the driving force of the process.

Figure 6 shows the results of modeling the process of first stage dehydration of ethanol and isopropanol with an initial water content of 15 wt % in the initial mixture on membrane modules with different surface areas. The simulation of the membrane module operation

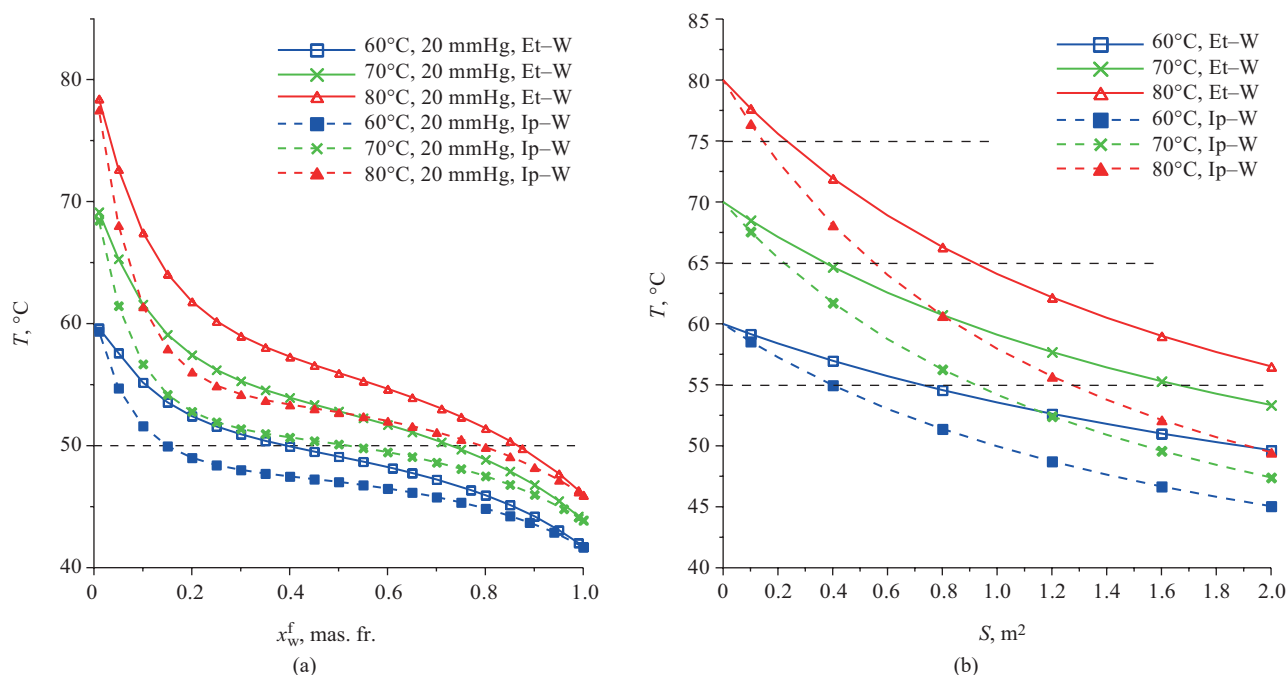


Fig. 5. Retentate temperature T at the outlet of the HybSi[®] membrane module for a mixture of ethanol–water (Et–W) and isopropanol–water (Ip–W) depending on the composition x_w^f and area S :
(a) $S = 1 \text{ m}^2$;
(b) mixture with a water content of 15 wt %

was carried out in adiabatic mode and without taking into account thermal effects (in isothermal mode), at a pressure on the permeate side of 20 mm Hg. Figure 6 shows the values of the total permeate flow and the concentration of water in the retentate at the outlet of a single membrane module as a function of its surface area.

As can be seen from Fig. 6, the discrepancy between the total permeate flow for ethanol in isothermal and adiabatic modes of operation will be 20.9% at 60°C and 30.1% at 80°C for a module with an area of 1 m².

For modules with a larger area (2 m²), the discrepancy will already be at 34.7 and 44.3% for 60 and 80°C, respectively. For isopropanol, with a module area of 1 m², the total flow discrepancy will be 30.6% at 60°C and 38.0% at 80°C, and with a module area of 2 m², the discrepancy will already be 46.8 and 51.8% at 60 and 80°C, respectively. A similar pattern is observed for the water concentration in the retentate: in the isothermal mode, where it decreases significantly, the discrepancy between concentrations can reach 1.3–1.8 times compared to the adiabatic mode.

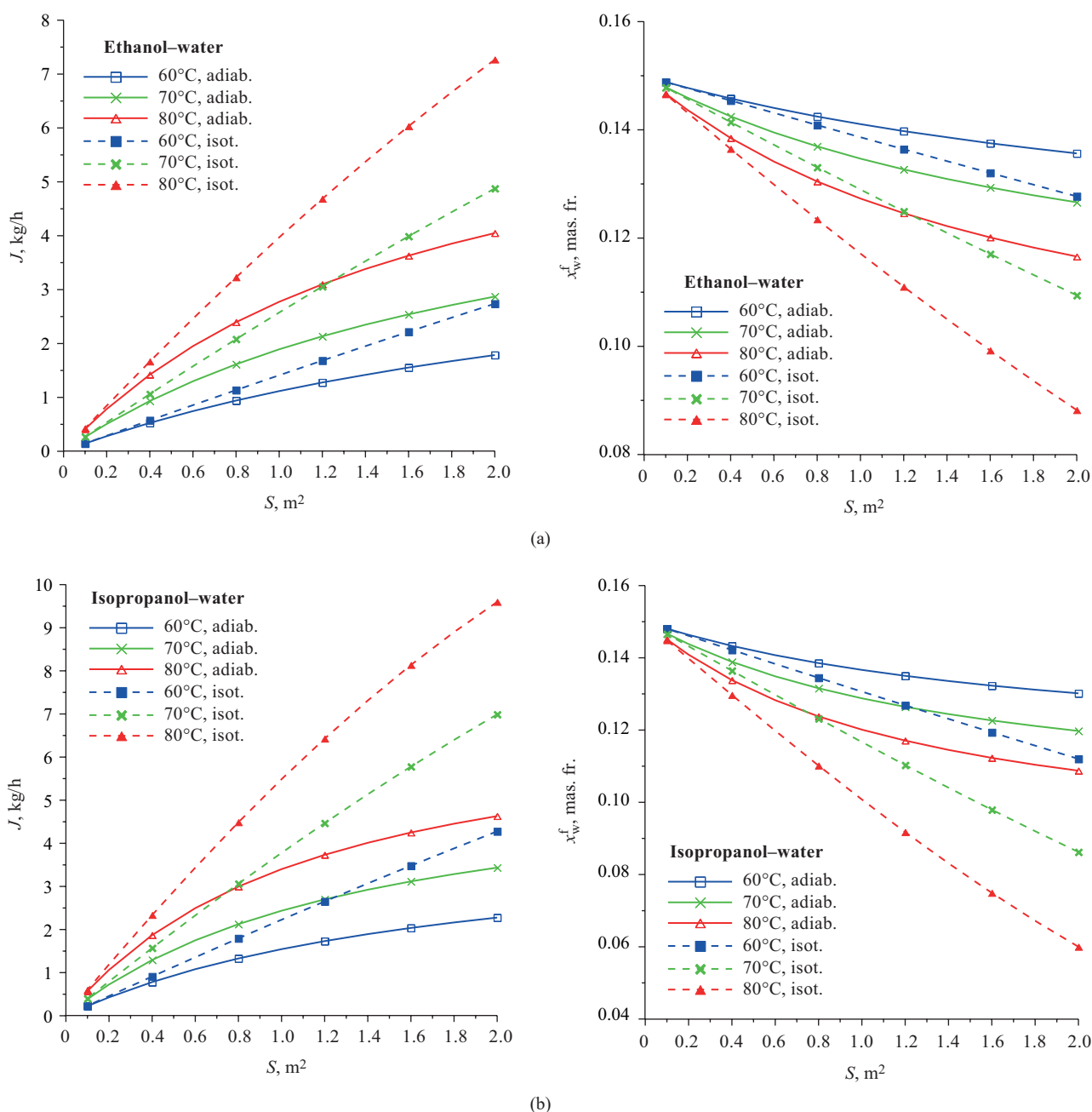


Fig. 6. Total permeate flow J and water concentration in the retentate x_w^r in isothermal and adiabatic modes of operation:
 (a) ethanol–water, the water content is 15 wt %;
 (b) isopropanol–water, the water content is 15 wt %

As can be seen from the results presented (Figs. 5 and 6), the processes of alcohol dehydration on HybSi® membranes are accompanied by significant thermal effects. In order to avoid errors in determining the required surface area of membrane modules, these effects must be taken into account in the development and design of membrane modules. In addition, the error in determining the required surface area of the membrane module is not constant, but increases with the temperature of the raw materials supplied.

If we compare the flow rates through HybSi® membranes with commercial PERVAP 2210 polymer membranes [31], the permeate flow at a water content of 5 wt % is several times higher for ceramic membranes under the same process conditions. This suggests that a smaller total surface area of HybSi® membrane modules is required to perform the alcohol dehydration process.

CONCLUSIONS

In order to calculate the process of pervaporation on a HybSi® ceramic membrane, an algorithm was developed along with a software module in the Aspen HYSYS UMP. A three-parameter mathematical model of initial separation (1)–(3) was used as the basis for the development of the module. This model was supplemented with the heat balance Eq. (6) to determine the temperature change of the raw material stream (7) passing through the module. Comparison of the simulation results with experimental data for dehydration of ethanol and isopropanol at different feed temperatures and permeate pressures confirmed the reliability of the developed membrane pervaporation module (Figs. 3 and 4).

The research results showed that the processes of alcohol dehydration on HybSi® membranes are accompanied by significant thermal effects (Fig. 5) due to large transmembrane currents (Fig. 3). Calculating

the module in isothermal mode without taking thermal effects into account can lead to significant errors. When determining the permeate consumption, these errors, which increase with increasing feed temperature, can be up to 50%; when determining the water concentration in the retentate, they can be 1.3–1.8 times (Fig. 6). When performing design calculations, this will result in a significant underestimation of the required surface area of the membrane module.

The calculation module of the pervaporation process developed in the work can be considered as a tool for use in Aspen HYSYS UMP for modeling the processes of alcohol dehydration both as a separate module and for modeling various schemes of dehydration processes.

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Authors' contributions

A.V. Malygin—development of the idea and algorithm for creating a calculation module of the pervaporation process, analysis and interpretation of the results obtained, and writing the text of the article.

I.I. Emel'yanov—development of algorithms of numerical methods for the calculation module of the pervaporation process at Aspen HYSYS, analysis and interpretation of the results obtained.

R.V. Semin—writing the program code of the membrane module, debugging and testing it.

A.R. Fazlyev—graphical preparation of experimental data, consulting.

N.N. Ziyatdinov—management and scientific consulting, analysis of research materials.

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