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Optimization and control algorithm for calculating separating membranes pore shapes

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ABSTRACT

This work was aimed at researching and developing a computer model, as well as an optimization and control algorithm for calculating pore shapes for separating membranes in separation processes. Two types of flow fluid rates through separation membranes with various pores configurations were considered. Here, the first type of pores had the form of a tortuous channel with sharp narrowing endings, which, in turn, could be assumed as "zero" wall thickness holes. The second type of pores had conical narrowing at the ends, which is closer to the real shape of the pores. As a result of the analysis of the performed calculations and models, data were obtained on the effect of the thickness of the selective layer on the performance of the membrane. In computer calculations, it was determined that the optimal volumetric porosity should be limited to 0.15, which affects the mechanical strength of the membrane. Calculations were also carried out on the Chemcad software product, which resulted in graphs of the optimal permeability of various liquids, depending on the differ curvature and pore volume of the separation membranes.

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1. INTRODUCTION

The existing ideas about the structure of porous adsorption layers are based on the possibility of describing pores as formations having certain geometric shapes and sizes. According to this type, the classification of porous membrane systems is usually based on the likening of real systems to artificial schemes built on models with a structure organized according to certain rules. The most common model is with different types of stuffing balls or other bodies of the same size. On the basis of such a model, a model of capillaries of various shapes and lengths, as well as a model of pores as conditional channels between contacting balls, was built.

The model of an adsorption layer in the form of a layer of packed spheres began to develop in our work [1], as well as, for example, in the thesis of Alsheri [2], which touches on the engineering aspects of membrane technology and covers the modeling, simulation, and optimization of membranes as a single process or as separate operation in a hybrid system. Various parametric analyzes have shown that only the parameters of membrane selectivity and transmembrane pressure coefficient determine the ability of a membrane to perform a particular separation task. Moreover, both the membrane selectivity and the pressure ratio have been

found to have a minimum value, which is determined only by the composition of the feedstock, the purity of the product, and the recovery factor. These results were used to develop simple and accurate empirical correlations to predict reachability behavior in real membranes, which showed good agreement with experimental and simulation results for various applications. Using these schemes, they describe the flow of liquids through real porous media, as well as adsorption processes in such media.

For example, a model of a filtration layer is used in the form of a system of correctly packed spherical bodies. However, as has been repeatedly noted [3]-[5] a system of correctly packed balls, referring to an artificially constructed type of porous medium, determines the features inherent in this particular type and does not describe hydrodynamic and mass transfer processes in real packings of even identical balls [1], [5], [6].

The design of the membrane filter can be widely vary depending on the application, in terms of both the internal structure of the pores (microscale design) and how the membrane is unfolded (macroplan). Although design improvements can be achieved through trial and error. Mistakes, prototyping, and testing can be costly, and the process can be difficult or impossible to systematize. In the study by Sun [5], an effect was considered where the microstructure of the membrane affects the filtration efficiency; in particular, the influence of different pore sizes along the depth of the filter membrane.

Due to the fact that the studies carried out so far did not affect fractional separation processes, our research was directed mainly to determining the pore size of the separated membranes in order to optimize the separation process. As a result of the study, on the basis of the developed mathematical models, an algorithm for optimizing the calculation of the shape of the pores of separating membranes and controlling separation processes was developed [5]. However, with a wide variety of types of porous systems that one has to deal with, it is difficult to indicate a single sign of their classification and belonging to a particular type of systems [1], [6]. This study is of value to developers of membrane seals that take into account the pore dimension, since so far not much work has been done on modeling the effect of pore shape on the membrane hydraulic resistance and its permeability [6], [7].

2. METHOD

As a result of membrane processes, the solution is forced through the membrane, which allows the molecules of the solvent to pass through, but retains the molecules or ions of the solute, thereby separating the molecules by size. A distinctive feature of this method is the simplicity of the installation design, the possibility of carrying out the process at a low or even room temperature, efficiency in combination with known separation methods-rectification, adsorption, and extraction.

To determine the pressure, drop of a membrane pore over an internal section of width L, we consider the flow rates of liquids (gases) through membranes with different pore configurations. For example, let's take a pore in the form of a tortuous channel that has sharp narrowings at the ends (let's take these narrowings as holes with zero wall thickness [1], [4], [6], [7]), then the pressure drop will be calculated using the Hagen-Poiseuille as shown in (1):

$$\Delta P_1 = \frac{8q\mu LU}{R^2} \quad (1)$$

where ΔP_1 is the pressure drop, U-flow velocity within a pore, R – pore radius, μ - medium dynamic viscosity coefficient, q- tortuosity coefficient (Figure 1).

Let us determine the tortuosity coefficient by the formula (here l is the average pore length):

$$q = \frac{l}{L} (2)$$

further, the pressure drops across the hole in the “zero” thickness baffle will be calculated by (3).

$$\Delta P_2 = \frac{3\alpha\mu\pi R^2 U}{r^3} \quad (3)$$

Here r is the hole radius at the pore outlet to the membrane surface, α is the coefficient takeт into account the asymmetric location of the hole pore outlet relative to its axis. The Figure 1 shows the radius of the opening of the pore exit to the surface of the membrane determined earlier. It is noteworthy that in the first approximation, the difference in the pressure value in the entire pore will be equivalent to the measurement of all pressure differences at the end constrictions of the cylindrical part [1], [6], [7]:

$$\Delta P = \Delta P_1 + \Delta P_2^i + \Delta P_2^e \quad (4)$$

ΔP_2^i where is the drop on the inner edge; ΔP_2^e - difference on the outer edge.

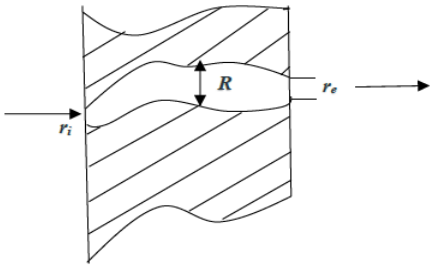

Figure 1. The radius of the opening of the pore exits to the membrane surface

Considering that N is the number of pores per unit area of the membrane surface, it is possible to calculate the coefficient of the free section of the membrane or the surface porosity.

$$p = \pi r^2 N \tag{5}$$

The volumetric porosity of a membrane ε with given configurations is related to the surface porosity by (6).

$$\varepsilon = pq \tag{6}$$

Next, the pressure differences at the edge of the membrane are obtained a shown in (7).

$$\Delta P_2 = \frac{3\alpha\mu\pi\varepsilon U}{pr} \tag{7}$$

$$\Delta P_2 = \frac{3\alpha\mu\pi q U}{r} \tag{8}$$

Further, it can be derived the relationship between the fluid flow filtered by the Q membrane with area F, with its geometric characteristics [1], [7]:

$$\Delta P = \frac{\mu q^2 Q}{\varepsilon F}\left[\frac{8L}{R^2} + 3\pi\left(\frac{\alpha_i}{r_i} + \frac{\alpha_e}{r_e}\right)\right] \tag{9}$$

Now let the pore have conical narrowings at the ends, which is closer to the real shape of the pores, which can be obtained in practice [5]-[8].

If we assume that the cylindrical part of the length L passes into narrowings of a conical shape with a length l_k at the ends, which in turn end with holes of radius r, in this case the pressure difference ΔP_k in the conical section of the pore, taken into account by small taper angles γ, is expressed by the following relationship [1], [6]-[10]:

$$\Delta P_k = \frac{8q\mu Q R^2 l_k}{3r^4 \varepsilon F}(z + z^2 + z^3) \tag{10}$$

where,

$$z = 1 - \frac{\gamma l_r}{R} \tag{11}$$

the formula for the final pressure drops across an asymmetric membrane, which we can lead to an increase in pressure drop in internal and conical sections.

$$\Delta P = \frac{8q\mu Q}{\varepsilon F}\left[\frac{Lq}{R^2} + \frac{R^2}{3}\left(\frac{l_{ki}}{r_i^4}(z_i + z_i^2 + z_i^3) + \frac{l_{ke}}{r_e^4}(z_e + z_e^2 + z_e^3)\right)\right] \tag{12}$$

If the pore is of an asymmetric configuration, then the narrowing occurs only on one side of the membrane.

$$\Delta P = \frac{8q\mu Q}{\varepsilon F}\left[\frac{Lq}{R^2} + \frac{R^2}{3}\left(\frac{l_{ki}}{r_i^4}(z_i + z_i^2 + z_i^3)\right) + \frac{3\pi q \alpha_e}{r_e}\right] \quad (13)$$

In work of the Vorotyntsev *et al*. [11], experiments are presented where glass capillaries are the objects of the model. Here, geometric characteristics such as the lengths of the cylindrical and conical parts, pore diameters, etc., are correlated with the characteristics of the track membranes. Zero wall thickness or a sharp cone configuration was learned by gluing a metal diaphragm with a hole in the form of a circle with a diameter of 1.0 mm to the end of a cylindrical capillary [1], [6], [7]. The diaphragm thickness was found to be significantly less than the diametrical hole and was 200 μm.

The pressure drop P = 353 Pa was decisive when measuring the volumetric flow rate of semi-synthetic engine oil. The relevant calculated meanings show that the errors in determining the time and amount of the leaked liquid introduced an error of less than 1% into the final result. The coefficient of dynamic viscosity of the oil was taken equal to 0.293 Pa*s (measured at 18.5 °C). Under these conditions, the liquid flow corresponded to Reynolds numbers of the order of 0,001 – 0,01.

As a result of calculations, the ratios of flow rates for various capillaries, calculated separately from the fixed and predicted values, correspond the most. The inconsistencies are related to some extent to errors in the calculation of the pressure difference and viscosity. From all this it follows that the experimental data and theoretical data for capillaries 5 and 6 correspond to 0.107:0.091=1.17 and 0.101:0.088=1.15.

For capillaries 4 and 5, which have a large value of measurement and diameter (1.15) of the channel in cross section, the ratio is equivalent to the calculated calculation: experimental - 21.5 and calculated 23.5. Here, the permeability measured per unit mass is 4 times higher for the capillary number 4. The transitional shape of the cylindrical shape from cylindrical to conical, the performance increases. Even as a result of significant simplifications, the experimental data with capsule 2 are obtained with data calculations. These results allow us to conclude that the above method is quite adequate and can be used to optimize the shape of pores in membranes [1], [6], [7], [12]-[14].

Using the derived relationships, we calculate the specific productivity of membranes with different pore configurations. Within the same configuration, we will vary the ratio between *R* and *r*, as well as between *L* and *l*. Our task will be to find such a combination of membrane parameters for which the volumetric flow rate for a given fixed *r* will be maximum.

We will calculate the specific productivity of the membrane, related to a single porosity. In this case, the results of calculations can be presented in a two-dimensional coordinate system, namely, in the form of a function $Q_m/\varepsilon\ (R)$ [1] for varying values of the parameters *l* and *r* and a fixed *L* [15]-[17]. Futher provides a description of the optimization algorithm and software designed to implement this algorithm and the methodology for calculating the effective pore size of membranes. The calculation of optimization algorithm is presented in a schematic form in Figure 2. An approximate quantitative description of the known parameters and the presence of random and systematic errors can affect the accuracy of the initial data [1], [6]. Considering the remarks made, the algorithm for finding the effective molecular diffusion coefficient and the optimal pore shape, we can observe the entire process indicated in the Figure 2.

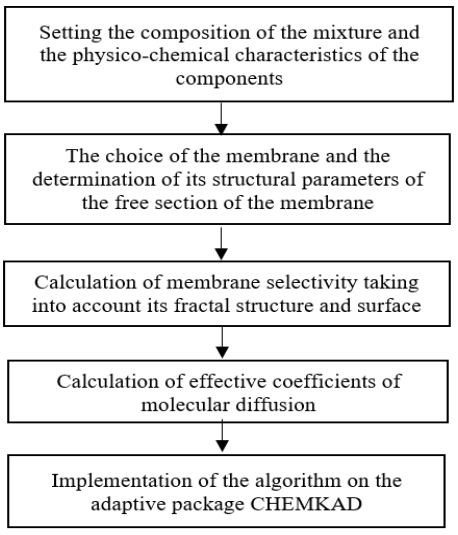

Figure 2. Optimization flowchart for control the effective pore size of membranes

3. RESULTS AND DISCUSSION

Based on the analysis of the obtained calculations of the thickness of the selective layer of membranes, the main aspects can be distinguished. The performance of the membrane increases by a maximum of 4 times, in the case of the tendency of the thickness of the selective layer to zero. Further, the specific productivity of the membrane reaches a maximum with an increase in the inner radius of pores, referred to the unit of porosity [1], [6], [7]. In addition, the position of the maximum specific productivity of the membrane depends on the thickness of the selective layer. In this case, if the thickness of the selective membrane layer is 3 μm, then the change in characteristics is insignificant. Consequently, the performance of the membrane with a selective layer thickness of 1 μm will increase due to the fact that the optimal ratio of the pores of the selective membrane layer and the inner radius in the selective membrane layer is in the range from 3 to 3.5 [1], [6], [7], [17]-[19].

Since the strength of the membrane in a mechanical sense has its own allowable limits, in computer calculations it was assumed that the volumetric porosity should be limited to a value of 0.15. The selection of the final optimal parameters is carried out only experimentally. This follows from the fact that track membranes having a base in the form of a film are strong enough with a porosity coefficient not exceeding the range from 0.15 to 0.25.

Along with this, the optimization procedure should take into account the dependence of the membrane strength not only on the bulk porosity, but also on the film thickness and pore density [1], [6], [7], [18]. Membranes with a lower pore density have better mechanical characteristics, even if the compared membranes have the same volumetric porosity, but the pore density is different from the other [1], [6], [7], [20], [21]. To view the calculation results obtained using the CHEMCAD application program package, the program provides several options: some calculation results are presented in the on-screen menus of the devices, where the initial data for calculations are entered. Below are graphs of the permeability of various nitrogen compounds through the membrane surface, taking into account the enthalpy and size of the simulated membrane pores (Figure 3, Figure 4, and Figure 5).

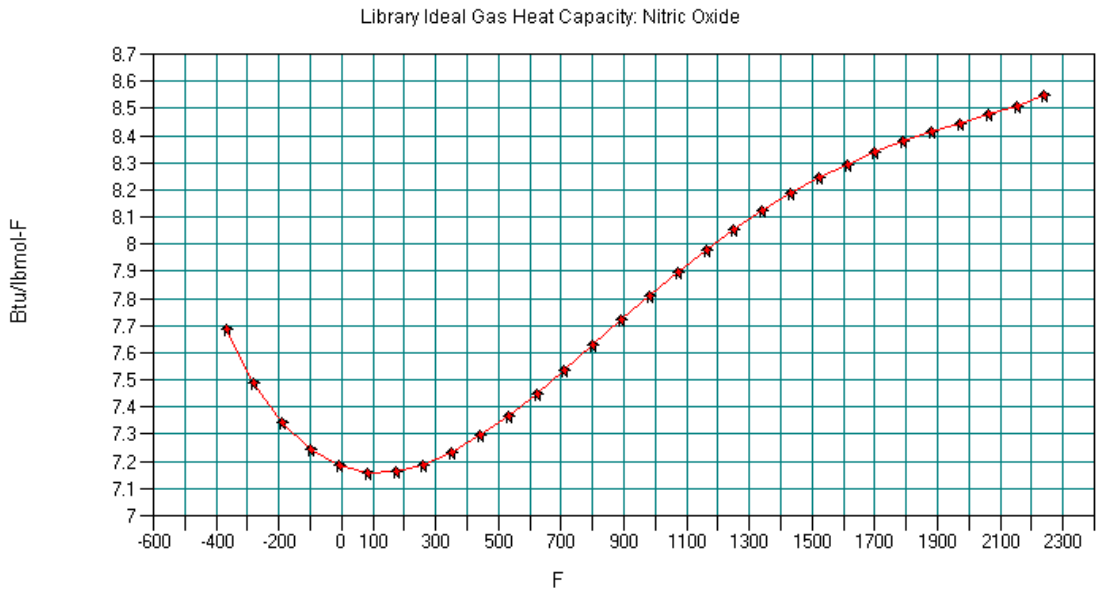

Figure 3. The permeability of nitric oxide through the membrane surface, taking into account the enthalpy and size of the simulated membrane pores

All the obtained results are substantiated and reliable, since the existing properties and characteristics of the physical nature and thermodynamic mechanisms of transport processes in membrane systems were taken into account in the study and construction of the learned models [1], [22]-[24]. The results of a system analysis of separation processes in polymeric membranes and selected control parameters, as well as models that take into account both energy and mass transfer characteristics of membrane systems determine the scientific novelty [1], [25], [26].

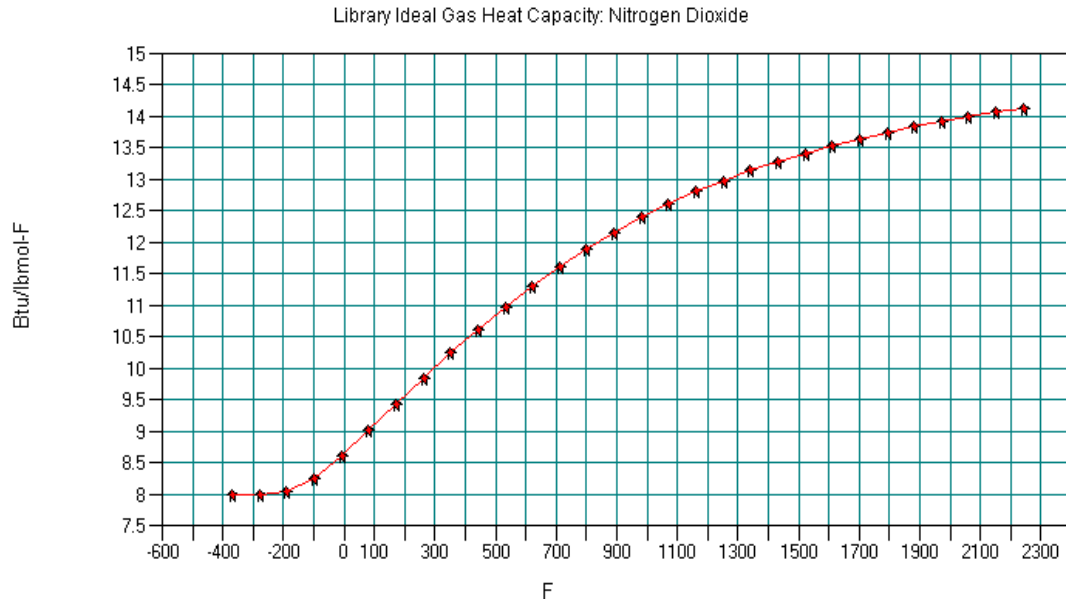

Figure 4. The permeability of nitrogen dioxide through the membrane surface, taking into account the enthalpy and size of the simulated membrane pores

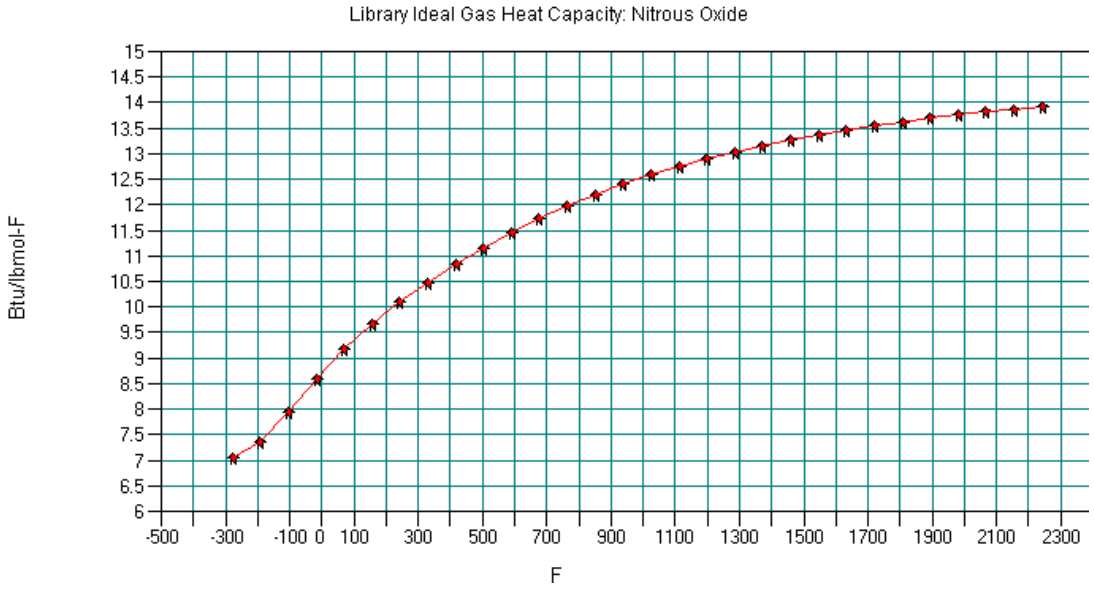

Figure 5. The permeability of nitrouc oxide through the membrane surface, taking into account the enthalpy and size of the simulated membrane pores

4. CONCLUSION

We have received approximate calculations of models, which are very important for obtaining the optimal characteristics of membranes in the development of their production technology. In particular, following the correctness of our assumptions, computer simulation and an optimization calculation algorithm for the shapes of membrane pores led us to obtain the specific productivity of membranes with given thin separation layers. Also, we concluded that if the thickness of the selective membrane layer is reduced, then the final performance of the membrane is consequently increased. This was precisely the initial task of finding the optimal membrane layer in separation processes.

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