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MATHEMATICAL SIMULATION OF NANOFILTRATION PROCESS: STATE OF ART REVIEW

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Abstract. A review of publications devoted to the mathematical simulation of the nanofiltration process was carried out, the advantages, limitations, and areas of application of various modeling approaches were determined. It was found that the most effective approaches are based on the extended Nernst–Planck equation, Donnan equilibrium, as well as methods of computational fluid dynamics and molecular dynamics. The use of software for solving nanofiltration simulation problems was considered.

Keywords: membrane; nanofiltration; mathematical model; optimization; software.

1. Introduction

In chemical technology, the mixture separation including water treatment processes plays an extremely important role[1–4]. In recent decades the application of nanofiltration process is significantly increasing. This is the relatively new pressure-driven membrane process for the separation of liquid systems, which is able to replace reverse osmosis in many applications due to lower energy consumption and higher productivity. This process is widely used in many branches of industry, in particular in the treatment of textile effluents, the separation of pharmaceutical products from fermentation media, the treatment of whey in the dairy industry, and the removal of metals from wastewater. Moreover, NF is a promising technology for the removal of inorganic contaminants and natural organic matter from surface waters, the purification of drinking water, *etc*.[5].

The mathematical simulation of the processes has important value for understanding the process mechanism and choosing the optimal or most advantageous condition of the membrane equipment performance. However, at the present time, the generally accepted understanding of the mechanism of the nanofiltration process does not exist, and there are several competing approaches. Therefore, the attempt to systematize and generalize the approaches to the mathematical simulation of the pressure-driven membrane processes, including nanofiltration, was made in the previous publication[6], where the articles published from 2000 to 2010 were considered. This work is the continuation of this research and reviews the approaches to the mathematical simulation of the NF process, similar to the review[7] that was made for the reverse osmosis process.

During the considered period, NF occupied the second place by the scope of publications after reverse osmosis among the pressure driven membrane processes[7]. The distributions of publications by years are represented in Fig. 1. It can be seen that, despite some decrease in the number of publications in 2014 and 2017, a clear trend of increasing the number of publications from the beginning to the end of the decade is observed. This demonstrates the growing relevance of the topic under consideration.

Since no systematic generalizations of the state of the art in modeling nuclear power processes have been found, a review such as this one seems reasonable.

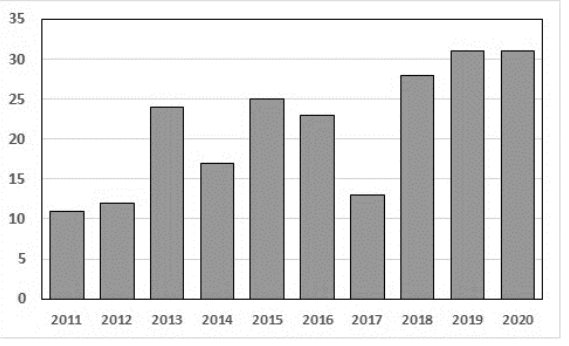

Fig. 1. The distribution of publications dedicated to the simulation of nanofiltration by years

The aims of this paper include: (i) the review and systematization of the theoretical investigation of the nanofiltration process based on mathematical simulation published from 2011 to 2020; (ii) the determination of the areas of effective applications of different approaches to the simulation of nanofiltration; (iii) the comparison of the development trends in mathematical simulation with those

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fulfilled in the previous period and with trends regarding other pressure-driven membrane processes, primarily reverse osmosis.

Like the previous publications[6,7], this review does not claim to be exhaustive but it has the same advantages, namely, it allows us to sufficiently assess the current state and prospects for development. It should be noted that all equations were written in the same form as in the original papers, so a description of symbols and dimensions is given below each equation.

2. Research Methodology

During carrying out the review, the published researches were grouped by the type of applied approach (taking into account that in one work more than one approach can be used). In this case, the choice of classification of the mathematical models of the NF process becomes an important issue. In paper[6], the classification of models was chosen based on the conventional classification of models, which was described in the earlier review works and was extended with accounting for the novel approaches, which were reported in research articles. In the work[7], the classification of the reverse osmosis models was also extended accounting for the works published in the considered period. Since in the period from 2011 to 2020 several review works, in which the issue of simulation of the NF process was considered, were published, it is reasonable to consider data from these articles during choosing the classification of the approaches to the simulation.

The most complete consideration of the issue of the NF simulation was done by Yaroshchuk *et al.*[8], Agboola *et al.*[9], Marchetti and Livingston[10], Schmidt and Lutze[11], and to some extent by Zhang *et al.*[12]. Also, the question of simulation was considered in general in some other reviews[5,13,14]. Moreover, nanofiltration was mentioned in the reviews dedicated to the simulation of the desalination processes[15,16], transport through the composite[17] and osmotic[18] membranes, computational fluid[19] and molecular[20–21] dynamics. Also, the publication[22] should be mentioned, in which the software applied for the simulation of NF was reviewed.

Despite the quite wide representation of the simulation of the NF issue in review works during 2011–2020, none of them gives the complete picture of this question, therefore the current review is reasonable.

In work[6], the classification of mathematical models of the NF process was proposed, which includes the irreversible thermodynamics-based models, the diffusion-based models, the pore flow-based models, the Donnan equilibrium-based models, the extended Nernst–Planck equation-based models, the Maxwell–Stepan equation-based models, the computational fluid dynamics (CFD)-based models, the artificial neuron networks (ANN)-based models, the optimization and economic analysis-based models, as well as other models which cannot be attributed to the previous classes. In work[7], it was pointed out, that molecular dynamics methods began to be intensively applied in the simulation of the reverse osmosis process. In the simulation of the nanofiltration process, such a method, is also, being actively implemented, as shown in works[20–21]. It also should be noticed that in work[6], it was pointed out that artificial neuron networks are rarely used for the simulation of the NF process, they will not be considered here as other rarely used approaches. Since the issues of optimization and economics have no principal differences with the reverse osmosis case, they will not be considered in the current work. Therefore, the classification shown in Fig. 2 was accepted.

Within each class of models, a review of relevant works was carried out, and the advantages, range of applications, and further perspectives of each approach were defined. Furthermore, the full generalization about the range of applications of the mathematical simulation of NF process simulation and perspective of development was made.

3. Results and Discussion

3.1. Irreversible Thermodynamics-Based Models

In this case, the transport of material through the membrane is assumed to be an irreversible process, during which the free energy continuously dissipates and entropy increases. The models of this class describe the NF process by the phenomenological equations and the membrane itself is considered as a “black box”. Therefore, these models are not applicable to the characterization of the structure and electrical properties of membranes[10].

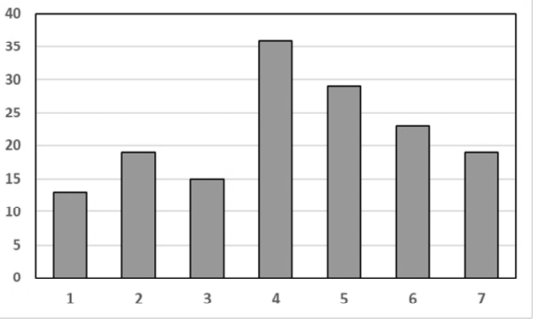

Fig. 2. The distribution of the NF process models by classes: 1 – irreversible thermodynamics-based models; 2 – diffusion based-models; 3 – pore flow-based models; 4 – extended Nernst – Planck equation-based models; 5 – Donnan equilibrium-based models; 6 – CFD; 7 – molecular dynamics

According to Marchetti and Livingston[10], the main models include the Kedem–Katchalsky model and the Spiegler–Kedem model. In the articles published during the period from 2011 to 2020, both models were mentioned; moreover, in some works, they were examined simultaneously.

The Kedem–Katchalsky model is the earliest and the simplest model. The solvent J_w and solute J_s fluxes are described according to the following equations ($m^3/(m^2 \cdot s)$)[10]:

$$J_w = L_p \left(\Delta p - \sigma \cdot \Delta \pi \right), \quad (1)$$

$$J_s = L_s \Delta c_i + \left(1 - \sigma\right) J_w \overline{c}_i, \quad (2)$$

where L_p is the local permeation coefficient ($m^3/(m^2 \cdot s \cdot Pa)$); L_s is the solute permeation coefficient ($m^3/(m^2 \cdot s)$); σ is the reflexion coefficient; Δp is the applied pressure (Pa); Δc_i is the concentration (molar fraction) difference between feed and permeate; $\overline{c}_i$ is the average solute concentration (molar fraction) in the membrane; $\Delta\pi$ is the osmotic pressure difference (Pa).

For the evaluation of selectivity, the value of the rejection coefficient (R) is applied. Abejon *et al.*[23] proposed the following equation for its calculation:

$$R = 1 - \frac{c_p}{c_f} = \sigma \frac{J_w}{J_w + \omega}, \quad (3)$$

where c_p is the solute concentration in permeate (mol/m^3); c_f is the solute concentration in feed solution (mol/m^3); ω is the solute permeability coefficient ($m^3/(m^2 \cdot s)$).

It should be noticed that in most works where the Kedem–Katchalsky model was mentioned, the issue of selectivity is covered quite briefly. The same goes for the issue of osmotic pressure.

In the considered period, the Kedem–Katchalsky model was mainly applied for the description of the NF of organic components[10,12,23,24], including the recovery of organic solvents in the pharmaceutical industry[23], the separation of glucose amines and the removal of organic dyes[24]. Moreover, this model was also applied for the analysis of the process of the recirculation of water with high salinity[25]. It also should be noted, that in considered works, only ASPEN[23] was mentioned among the special software.

The Spiegler–Kedem model was used in a wider range of applications. According to Shahmansouri and Bellona[26], this model was derived by the integration of the differential forms of the irreversible thermodynamics equations by the membrane thickness. The solvent flux is described by the following equation ($m^3/(m^2 \cdot s)$)[27]:

$$J_w = -P_w \cdot \left(\frac{dp}{dz} - \sigma \frac{d\pi}{dz} \right), \quad (4)$$

where P_w is the solvent permeability ($m^3/(m^2 \cdot s \cdot Pa)$); dp/dz is the pressure gradient (Pa); $d\pi/dz$ is the osmotic pressure gradient (Pa); σ is the reflexion coefficient.

The solute flux, correspondingly, may be described as ($m^3/(m^2 \cdot s)$)[27]:

$$J_s = -P_s \frac{dc_s}{dz} + \left(1 - \sigma\right) \cdot c_s \cdot J_w, \quad (5)$$

where P_s is the solute permeability ($m^3/(m^2 \cdot s)$); dc_s/dz is the concentration (molar fraction) gradient through the membrane; c_s is the solute concentration (molar fraction).

For the description of the process selectivity, the following equation was applied[27]:

$$R = 1 - \frac{1 - \sigma}{1 - \sigma \cdot \exp\left(\frac{\left(\sigma - 1\right) \cdot J_w}{P_s / z} \right)}, \quad (6)$$

where z is the membrane thickness, m. Other symbols are described above.

The Spiegler–Kedem model also had a wider range of practical applications in comparison with the previous model. During 2011–2020, it was used for the description of the process of ammonium lactate removal[28], smart water production[29], the removal of succinic acid from sodium hydroxide solution[27], and the organic solvent nanofiltration[26,30]. Among the software in considered articles, only MATLAB was mentioned in the work[26].

It also should be noted that the united Spiegler-Kedem–Katchalsky was proposed by Hidalgo *et al.*[24].

The thermodynamics methods were also applied in other approaches. ten Kate *et al.*[31] analyzed the negative effects during NF of concentrated NaCl solution based on the concept of chemical potential. The methods of classical thermodynamics were also used by Minelli and Sarti[32].

3.2. Diffusion-Based Models

It was pointed out in paper[7], that during 2011–2020 the models of this class were widely applied for the analysis of the reverse osmosis process, moreover, to a significantly greater extent in comparison with the previous decade. However, from Fig. 2 it is seen that in the case of NF, this approach was applied to a lesser extent. Also, it should be noticed, that during the analysis of the NF process, the application of the diffusion-based models was somewhat more diverse in comparison with reverse osmosis. Although the solution-diffusion model is still the most widely used, the solution-diffusion-imperfection model was applied more frequently. Also, some specific models were proposed.

In the conventional solution-diffusion model, it is assumed that the solute and the solvent are sorbed and diffuse through the non-porous active layer, and one of the basic assumptions of this model is that the reflection coefficient (Eq. (1)) for all solutes is equal to one[33].

According to this model, the solvent (water) flux through the membrane can be expressed in the following form ($m^3/(m^2 \cdot s)$)[33]:

$$J_w = C_f \cdot L_p \cdot (\Delta p - \Delta\pi), \quad (7)$$

where C_f is the feed concentration (molar fraction); L_p is the permeation constant ($m^3/(m^2 \cdot s \cdot Pa)$); Δp is the applied pressure (Pa); $\Delta\pi$ is the osmotic pressure difference (Pa).

As in the case of reverse osmosis[7], the Van't Hoff equation is widely used for the evaluation of the osmotic pressure value[33].

The solute flux is described by Eq. (8) ($m^3/(m^2 \cdot s)$)[34]:

$$J_s = \frac{DK}{\delta}(C_m - C_p), \quad (8)$$

where D is the diffusion coefficient (m^2/s); K is the partition coefficient; δ is the membrane thickness (m); C_m is the solute molar fraction in membrane; C_p is the solute molar fraction in the permeate.

For the evaluation of the rejection coefficient value, the following equation was proposed[33]:

$$R = \frac{J_w - \Delta p \cdot L_p}{J_w - R_G \cdot T \cdot C_f \cdot L_p \cdot \exp(J_w / k)}, \quad (9)$$

where k is the mass transfer coefficient (m/s); R_G is the gas constant (J/(mol·K)); T is the temperature (K); C_f is the feed concentration (molar fraction).

Li *et al.*[34] used the alternative form of the equation for calculating the rejection coefficient value.

In paper[7], a significant number of relationships for the determination or correction of permeation constant values, however, in the publication dedicated to the NF, such data are represented to a much lesser extent. For example, Abels *et al.*[35] represented the equation for the permeation constant in the following form:

$$L_p = \frac{DvK}{R_G T \delta}, \quad (10)$$

where v is the molar volume (m^3/mol); other symbols are the same as in Eq. (8) and Eq. (9).

Furthermore, Shi *et al.*[36] listed correlation relationships for physical properties.

The practical application of the solution diffusion model was concerned mainly with the organic solvent NF, and is shown in several works[10,22,36–39]. Also, this model was used for the analysis of the NF process performance in the water treatment systems[40–42]. The other applications include the separation of ionic solutions[33,35], the concentration of grape juice[34], and the performance of the ceramic membrane[43]. As in the case of reverse osmosis, this model was applied for the analysis of hybrid systems[37,41].

For carrying out the calculation according to this model, software such as ASPEN[22,36,37], MATLAB[22,36], OSN Designer[22], and CAPE OPEN[22] was applied. It should be noticed, that above-mentioned review and comparison of the software made by Peshev and Livingston[22] considered exactly the solution-diffusion model.

The solution-diffusion-imperfection model for the case of NF was applied in the wider range compared to reverse osmosis. This model was an early modification of the solution-diffusion model, according to which the transport mechanism can be described by the combination of diffusion through the dense active layer and transport in pores due to the small imperfections or defects in the active layer of the membrane[44].

In this model, the second term, which takes into account the viscous transport, is added. The equation for the description of the flux of the substance (J_i) through the membrane, in this case, may be written in the following form (mol/(m^2·s))[45]:

$$J_i = \frac{D_i K_i C_{tot}}{l}\left(x_{i.F} - x_{i.P}\exp\left(-\frac{v_i \Delta p}{R_G T}\right)\right) + \frac{B_0 C_{tot}}{l}\frac{x_{i,F}}{\eta_F}\Delta p \quad (11)$$

where K_i is the sorption coefficient; D_i is the diffusivity (m^2/s); C_{tot} is the feed concentration (mol/m^3); l is the membrane thickness (m); $x_{i,F}$ is the feed molar fraction; $x_{i,P}$ is the permeate molar fraction; B_0 is the specific permeability (mol/m^2); η_F is the feed viscosity (Pa·s).

At the same time, in the publication dedicated to the application of this model, the topic of the determination of selectivity is not described in detail.

During the considered period, this model was applied for the cases of the organic solvent NF[11,44] and the treatment of fat and oil industry effluents[39,45]. The application of the ASPEN for the work with this model[11] should be highlighted.

Also, the other modifications of the solution-diffusion model were applied. They include the solution-diffusion-film model[46], the homogenous solution-diffusion model[47], and the solution-diffusion-electromigration model[48]. However, these approaches were single.

It should be also noticed that Werth *et al.*[39] compared the accuracy of several models, and defined that among the models of the current class, the solution-diffusion-imperfection model appeared to be the most accurate.

3.3. Pore Models

Despite the membranes for NF are classified as porous[5], as can be seen from Fig. 2, such models are applied not often during the considered period. Moreover, its number is even less than the number of the diffusion-based models. It also should be noticed that, unlike the case of reverse osmosis, where several models were used[6,7], such diversity was not observed for NF.

In some works, such models were simply called the pore flow models[22,39,44,49] or the steric exclusion models[12,29,50,51]. Herewith, the solvent flux through the pores can be described by Eq. (12) (mol/(m^2·s))[39]:

$$J_w = P_i \frac{\Delta p}{\mu}, \quad (12)$$

where P_i is the permeability (mol/(m^2·s)); μ is the dynamic viscosity coefficient (Pa·s); Δp is the applied pressure (Pa).

The osmotic pressure also can be taken into account. In this case, Eq. (12) takes the form (m^3/(m^2·s))[52]:

$$J_w = A(\Delta p - \Delta\pi), \quad (13)$$

where A is the permeability coefficient (m/(s·bar)). Δp and $\Delta\pi$ are described above.

In some works, the concretization about the type of the main equation is presented. In particular, it was pointed out in works[10,53] that the flux through the pores is described by the Darci law, which can be represented in a form of Eq. (14) (m^3/(m^2·s))[53]:

$$J_w = \frac{\Delta p - \Delta\pi}{\mu_p R_m} \quad (14)$$

where R_m is the membrane resistance (m^{-1}); μ_p is the permeate dynamic viscosity coefficient (Pa·s).

In a slightly larger number of works, the Hagen–Poiseuille equation was mentioned[10,11,29,43,52,54]. According to Kong *et al.*[52], this equation can be written in the form (m^3/(m^2·s)):

$$J_w = \frac{r_p^2 (\Delta p - \Delta\pi)}{8\mu\delta} \quad (15)$$

where r_p is the average pore radius (m); δ is the effective membrane thickness (m). Other symbols are described previously.

It should be noted, that Eq. (15) was also applied by Labban *et al.*[55], however, in this case, its name was not mentioned.

For the prediction of selectivity, Xu *et al.*[51] applied the following equation:

$$R = 1 - \frac{K_{i,c}\Phi}{1 - \exp(-\mathrm{Pe})\left[1 - K_{i,c}\Phi\right]}, \quad (16)$$

where $K_{i,c}$ is the convective hindrance factor; Pe is the Peclet number; Φ is the steric partition factor. The relationships for the determination of $K_{i,c}$ and Φ are represented by Liu *et al.*[50] and Xu *et al.*[51].

As in the case of diffusion-based models, the pore flow models are mostly used for the analysis of organic solvent NF[10,11,22,39,44], the organic compounds removal[52], the purification of polysaccharides[50,53], the water softening[55], the ethylene glycol removal[50], the wastewater treatment (the pesticides removal)[49], the purification of the pharmaceutical and personal care products[51] and the purification of N-acetyl glucosamine[12].

It can be seen, that among applications of these models, the traditional nanofiltration applications such as water treatment are represented in a small number. Probably, this is due to the fact, that for the analysis of such a process, the extended Nernst–Planck equation-based equation is often used, which also considers the NF membranes as porous ones.

3.4. Extended Nernst−Planck Equation

During 2011–2020 years the majority of researches dedicated to the NS process simulation considered this approach. In the previous decade, also the biggest number of theoretical studies of NF process were carried out with using of the extended Nernst–Planck as it was shown in work[6].

This approach is based on the concept of the ions transport, which combines their transport into the membrane pores and the equilibrium distribution in pores at the input and output[56]. In this case, the transport of each ion i with charge z_i is described by an equation, which takes into account the diffusion under the influence of the concentration gradient, its electrical migration due to spontaneous formation of the electrical field, and its convection by the flow inside the membrane pores. Taking into account the hindrance factors to diffusion and convection, the extended Nernst–Planck equation can be adopted for the specific case of nanofiltration membranes[57]. The explanation of the pore model with the use of this equation is based on several assumptions[9], namely: (i) the solution is assumed to be ideal, this allows to neglect the conjugation effects among the solution components; (ii) all ions present in membranes can be transported; (iii) the charge capacity is uniform at any point in the separational zone of the membrane; (iv) the Donnan equilibrium occurs on the membrane-solution interface.

If it is possible to assume that the activity of the solution is constant, the extended Nernst-Planck equation can be written in the following form (mol/(m^2·s))[58]:

$$J_s = K_C c_s v - K_d D \frac{dc_s}{dx} - \frac{c_s K_d D}{RT} \bar{V}_s \frac{dp}{dx}, \quad (17)$$

where K_c is the hindrance factor for convection; c_s is the solute concentration (mol/m^3); v is the solvent velocity; K_d is the hindrance factor for diffusion; D is the diffusivity coefficient (m^2/s); x is the axial coordinate in pore (m); R is the universal gas constant (8.314 J/(mol·K)); T is the absolute temperature (K); $\bar{V}_s$ is the molar volume of solute (m^3/mol).

More generally this equation can be written as follows[9]:

$$J_s = -D_i \frac{dc_i}{dx} - \frac{z_i c_i D_i}{RT} F \frac{d\psi}{dx} + K_{ic} c_i J_v, \quad (18)$$

where F is the Faraday constant (C/mol); ψ is the electrical potential into the membrane (V), z_i is the ion valence; K_i is the partitioning coefficient. Other symbols are described above.

Fadaei *et al.*[59] show the relationships for the determination of the main parameters in the extended Nernst-Planck equation. The relationships between the factors and the auxiliary variables are also represented in some other works[60–64].

Eqs. (17) and (18) describe the solute flux. The Hagen–Poiseuille equation (Eq. 15) can be applied to describe the solvent flux[58].

For the evaluation of selectivity, the following equation was proposed by Blumenschein *et al.*[58]

$$R = 1 - \frac{(K_c - Y)\phi}{1 - [0 - (K_c - Y)\phi]\exp(-\mathrm{Pe}')}, \quad (19)$$

where

$$Y = \frac{K_d D}{RT} \bar{V}_s \frac{8\mu}{r_p^2}. \quad (20)$$

In Eq. (19) φ is the partition coefficient; μ is the solvent dynamic viscosity (Pa·s); K_d, K_c are the hindrance factors; $\bar{V}_s$ is the solute molar volume (m^3/mol) Pe' is the modified Peclet number.

The relationships for the determination of the rejection coefficient are represented by several authors[60,65,66]. However, for this purpose, most often the Donnan equilibrium-based approach was used, which will be considered in the next section.

During the review of the above approaches to simulate the NF process, it was noted that they are most common in the case of organic solvents and/or dissolved substances. The extended Nernst–Planck equation also can be used for such purposes, as it was done in works[52,58,67]. However, in general, it has a wider area of application. In particular, the considered model was used for describing the water treatment processes[9,55,68–73]. On the other hand, the problem of treatment of hazardous effluent was also considered[62,65,66,74,75]. In several works, the authors restricted the theoretical investigation of the ions transport through the membrane[60,76] or the removal of salts[56,57,61,64,68,69,77–80]. The other applications include the separation of monosaccharides[81,82], the removal of lactic acid from the fermentation broth[60], and removal of antibiotics[83].

The extended Nernst–Planck equation-based models were also applied in combination with other theoretical concepts such as the Poisson equation[84], the concentration polarization models[59], the method of economic analysis[62] and optimization[80], as well as the computational fluid dynamics[19,59,84]. However, the combination of the extended Nernst–Planck with the Donnan equilibrium in one investigation was the most common practice[9,56,57,59–61,64,65,69–71,75–77,81–82,85–87]. This approach will be discussed in detail below.

Among the software, that was used in publications considered in this section, the application of COMSOL Multiphysics[59,84], MATLAB[76,82], and also the programming languages Visual Basic[68,75] and Python[72] should be noticed.

In a significant number of works the processes were analyzed in plate and frame modules[60,71,78,79] and/or the lab cells[67,70,79,86], whereas the widely used spiral wound modules were considered quite rarely, for example in work[71], as well as tube modules[56,77] and ceramic membranes[58,86].

3.5. Donnan Equilibrium

During the consideration of the extended Nernst-Planck equation, it was pointed out that the Donnan equilibrium-based method was often applied in combination with that approach. By the conjunction of this method, important models were developed, namely the Donnan Steric Pore Model (DSPM) and the Donnan Steric Pore Model with dielectric exclusion (DSPM-DE). These models were quite widely used during the considered period. Moreover, the number of applications of DSPM was approximately equal to the use of DSPM-DE. In particular, the DSPM was applied in works[59,60,63,78,82,88–90], and the DSPM-DE was used in works[9,65,71,76,81,85,91–92]. Furthermore, in some works both models were mentioned, for example in works[64,87,93]. Also, in some theoretical investigations of the NF process, the Donnan equilibrium was applied without references to the abovementioned models, in particular in works[56,61,68–70,77,94–97].

Since the DSPM and DSPM-DE approaches have a significant practical value, they should be considered in more detail.

The Donnan Steric Pore Model (DSPM) was first used for the description of the ion particles transport through the NF membranes. This model is based on the extended Nernst–Planck equation and includes diffusion, convection, the mechanism based on the electric potentials, and ionic distribution between solute and membrane surface, which is described by the Donnan equilibrium and steric effects. This is one of the most effective approaches for the cases of non-charged solutes and monovalent electrolytes[65].

According to Ortiz-Albo *et al.*[89], the DSPM includes a set of equations that involve the mass balance, the equilibrium distribution of the components, the equation for the description of the concentration polarization phenomena, the solute transport through the membrane, and the electroneutrality conditions. With the exception of the full set of equations for the DPSM, the paper[89] describes the physical content of all the variables considered and the limits of the calculation formulas. Therefore, they will not be presented here.

In the considered period, this model was successfully used for the description of the separation of electrolytes[63], in particular the removal of the sulfate-ions[78],

nitrates and heavy metals[88], the desalination processes[89], the separation of monosaccharides[82] and lactic acid[60], and the purification of succinic acid[90].

Despite its advantages, DPMS is not as accurate in the case of dissolving mixtures of electrolytes or multivalent ions. Therefore, dielectric exclusion is involved in the separation mechanism[89].

The approach developed in this way was called the Donnan Steric Pore Model with dielectric exclusion (DSPM-DE). Despite its complexity, the thoroughness of this model determined its wide application for the simulation of the NF process, it was successfully used, and it has a good agreement with experimental results[76].

The distribution among ions on the solution-membrane interface depends on the ionic size (steric distribution), the ionic and membrane charge (Donnan distribution), and the dielectric constant insight the pores, which determine the solvation energy (dielectric distribution). This mechanism of exclusion is widely used for the simulation of NF and many investigations were carried out to define the influence of the membrane parameters (pore radius, membrane thickness, dielectric constant of pore, and charge density) on the NF performance[91].

The equilibrium distribution on the solution membrane interface can be described for the feed and permeate sides by the corresponding equations in the following forms[91]:

$$\frac{\gamma_{i,1}^{m} C_{i,1}^{m}}{\gamma_{i}^{bm} C_{i}^{bm}} = \varphi_i \varphi_{B_i} \exp\left(-\frac{z_i F}{RT} \Delta\psi_{D,feed} \right), \quad (21)$$

$$\frac{\gamma_{i,N}^{m} C_{i,N}^{m}}{\gamma_{i}^{p} C_{i}^{p}} = \varphi_i \varphi_{B_i} \exp\left(-\frac{z_i F}{RT} \Delta\psi_{D,perm} \right), \quad (22)$$

where φ_i is the steric coefficient; φ_{Bi} is the Born coefficient of solvation; C is the concentration (mol/m^3); γ is the activity coefficient; z_i is the ion valence; F is the Faradey constant (C/mol); R is the universal gas constant J/(mol·K); T is the absolute temperature (K); $\Delta\psi$ is the Donnan potential (V). Superscripts *m*, *bm*, and *p* denote the membrane, bulk-membrane interface, and permeate correspondingly.

The Donnan potential can be calculated according to the following equation (*V*)[65]:

$$\Delta\psi_d = -\frac{RT}{F}\left\{ \ln\left(\frac{c_{p,m}}{\varphi_p C_{p.B}} \right) \right\} = \frac{RT}{F}\left\{ \ln\left(\frac{c_{n,m}}{\varphi_n C_{n,B}} \right) \right\}, \quad (23)$$

where $c_{p,m}$ is the concentration of the positive ions in membrane (mol/m^3); $C_{p,B}$ is the concentration of the positive ions in solution (mol/m^3); $c_{n,m}$ is the concentration of the negative ions in membrane (mol/m^3); $C_{n,B}$ is the concentration of the negative ions in solution (mol/m^3); φ_p, φ_n are steric partition coefficients. The symbols *R*, *T*, and *F* have the same meaning as in Eq. (22).

In the considered period, the DSPM-DE was applied for the description of the processes of the tannery effluent purification[65], the water treatment[9], the separation of mono- and disaccharides[81], the wastewater treatment[91], the seawater desalination[71], and the organic solvents removal[92].

The Donnan equilibrium was also mentioned in works dedicated to the removal of salts[61,79], in particular from multicomponent solutions[56,95–97], the removal of arsenic[68] and fluoride[69], the water treatment[87], and the wastewater desalination[70]. The paper[94] devoted to the study of electric effect on the membrane should also be pointed out.

Among the software, applied for the calculations according to the models of this class, the following products should be pointed out: Visual Basic[68], Comsol[59], MATLAB[82] and gPROMS[88].

3.6. Computational Fluid Dynamics-Based Models

The significant influence of the hydrodynamic conditions on the course of the mass transfer processes, including the case of pressure-driven membrane processes was noted in papers[6,7]. Nanofiltration is not an exception, however, it was mentioned in paper[6] that during 2000–2010, the computational fluid dynamics method was applied in a relatively low number of publications. This fact was explained by the high efficiency of describing this process using the extended Nernst–Planck equation, which was discussed above. Nevertheless, during 2011–2020 the number of investigations in this direction considerably increased, as shown in Fig. 2.

The CFD method is based on the mass conversion, the Navier–Stocks equations, and the continuity equation[98]. These equations are often written in the operator form[99]:

$$\rho(\vec{u}\cdot\nabla)\vec{u} + \nabla P - \mu\nabla^2\vec{u} = 0, \quad (24)$$

$$\nabla\cdot\vec{u} = 0, \quad (25)$$

$$D\nabla^2 C = \vec{u}\cdot\nabla C. \quad (26)$$

In these equations $\vec{u}$ is the velocity vector (m/s); *P* is the pressure vector (Pa); *C* is the concentration vector (mol/m^3); ρ is the density (kg/m^3); *D* is the diffusivity (m^2/s); μ is the dynamic viscosity (Pa·s).

Also, in works[100–102] the two-dimensional equations were used, and in work[19] the cylindrical coordinates were considered. The unsteady state conditions were taken into account in works[102,103].

In work[7], some turbulence models were discussed in detail, which were represented in the set of publication dedicated to the reverse osmosis simulation by the CFD methods. However, in the case of NF the detailed description of the turbulence models was not found. Only pa-

pers[104,105] mentioned the application of the *k*-ε turbulence model but without a detailed explanation. Therefore, in the current paper, the descriptions of these models are not represented.

For defining an unambiguous solution, it is necessary to formulate the initial and boundary conditions, which are described in most of the considered in the current section works. In particular, the detailed descriptions are represented in papers[98,103].

Taking into account the complexity of the solution of equations that are used in the CFD method, the special software is particularly important for the application of this approach, as it was shown in the previous reviews[6,7]. In the chosen for this review papres the most widely used software includes the ANSYS Fluent package[98,101,104-113] and COMSOL Multiphysics[59,99,114-117]. Also, in some works, the open software OpenFOAM[102] and the programing language Visual Basic[118] were applied.

Since the geometrical shape has significant importance during the analysis using the CFD methods[6,7], considerable attention is paid to the module design. It should be noticed that in the case of nanofiltration, in the substantial number of publications, the laboratory cells of different constructions[99–101,105, 106,112,114,115] and the rotating modules[104] were considered. Among the conventional modules, the most attention is paid to the spiral wound modules[98,100,107,108,111,117,118]. To a lesser extent, the plate and frame[103,110] and hollow fiber[109] modules were considered. Also, the performance of the multichannel inorganic membranes[113] and patterned membranes[116].

3.7. Molecular Dynamics-Based Models

As in the case of reverse osmosis, among the relatively new simulation methods, the molecular dynamics (MD) methods showed considerable development for the simulation of NF. The most comprehensive concept of this approach is described by Ebro *et al.*[20], who considered in general the membrane methods of water treatment. According to these authors, the concept of molecular dynamics is based on Newtonian mechanics. Following the second Newton's law the force applied to particle *i* is equal to the product of mass of this particle times its acceleration. Also, the force can be represented in the form of a potential energy gradient (N):

$$F_i = m_i a = m_i \frac{d^2 r_i}{dt^2} = -\nabla_i U\left(r_i\right) = -\frac{\partial U\left(r^N\right)}{\partial r_i}, \qquad (27)$$

where m_i is the particle mass (kg); a_i is the particle acceleration (m/s^2); r is the distance between particles (m); U is the potential energy (J); t is time (s).

By using Eq. (27), it is possible to obtain the trajectories of all atoms, which are described by their consistent coordinates, velocities, and momentuma. These trajectories are used as feed data for forecasting the conditions of the whole system with the following association with physical phenomena[20].

An example of the determination of the system's general energy is represented by Yao *et al.*[119].The energy of molecules interaction was determined as the difference between the system's general energy and the net energy of the membrane and solute component (monosaccharides).

Suk[120] calculated the non-bounded interactions between the water molecules and membrane using the Lennard–Jones interaction (J/mol):

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad (28)$$

where ε is the depth of the potential well (J/mol); σ is the distance between atoms at which the potential is equal to zero (Å); r is the distance between two atoms (Å).

As in the case of CFD, the molecular dynamics methods require a significant number of calculations, therefore, for its effective application, it is reasonable to use special software. In the considered period, the most applied program products include GROMACS[94,120–124], NAMD[125,126], and Materials Studio[119,127]. Also, for the force field analysis, such software as OPLS[121,124], CHARMM[126], and COMPASS[119] was used.

The MD methods were supplemented by the application of the Maxwell–Stephan equation[32,119], the Donnan equilibrium[94], the Hagen–Poiseuille equation[128], the relationships for the electric fields[129], and the Navier–Stocks equation[128,130]. In addition to the above-mentioned study[120], the potential of Lennard–Jones was considered by Sofos *et al.*[131]

It has been noted by the authors previously[7] that CBM methods are often used to account for the influence of membrane materials. In the considered period during the NF process simulation, in some works, several materials were investigated, including cellulose derivatives[122], polybenzimidazole[124], and novel materials such as graphene[120,125], liquid crystals[126], and the membranes from nanotubes[127].

The MD methods were the most often applied for the analysis of the organic solvents NF[32,121,123,132], the removal of salts[9,4] heavy metals[131], magnetic particles[126], monosaccharides[119], and also for water treatment and desalination[125].

4. Conclusions

The great practical importance of the nanofiltration process and the advantages of theoretical research methods have led to a large number of publications on the mathematical modeling of this process. In this study, we reviewed the papers on the mathematical modeling of the NF process published during 2011–2020.

It has been determined that the most commonly used approaches for this purpose are those based on the extended Nernst–Planck equation and Donnan equilibrium, as well as methods of computational fluid dynamics and molecular dynamics. These methods are likely to remain the most common due to their efficiency. At the same time, approaches based on irreversible thermodynamics, diffusion, and pore flow have been used to a much lesser extent.

The software used to solve the mathematical models was analyzed.

The presented results can be useful for choosing the mathematical modeling strategy of systems that include nanofiltration units.

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МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ПРОЦЕСУ НАНОФІЛЬТРАЦІЇ: АНАЛІТИЧНИЙ ОГЛЯД

Анотація. *Проведено огляд публікацій, присвячених математичному моделюванню процесу нанофільтрації, встановлено переваги, обмеження та сфери застосування різних підходів до моделювання. Виявлено, що найефективніші підходи ґрунтуються на розширеному рівняння Нернста-Планка, рівновазі Доннана, а також методах обчислювальної гідродинаміки та молекулярної динаміки. Розглянуто використання програмного забезпечення для вирішення завдань моделювання нанофільтрації.*

Ключові слова: *мембрана, нанофільтрація, математична модель, оптимізація, програмне забезпечення.*