Mathematical modeling of nanofiltration: the latest trends and developmental perpectives

Sherhii Huliienko, Svitlana Muzyka

Department of Machines and Apparatus of Chemical and Oil Refinery Productions, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", UKRAINE, Kyiv, Prosp. Peremohy, 37, 03056,
E-mail: sergii.guliienko@gmail.com

Abstract. The results of the analysis of the publications about mathematical modeling of the nanofiltration process are represented. The temdensy of the increasing of the punlications number is pointed out. It was defined, that the most perspective direction of the nanofiltration simulation include the expended Nernst-Plank equation and the molecular dymanics.

Keywords: nanofiltration, reverse osmosis, pressure-driven processes, mathematical modeling.

Introduction

The pressure-driven membrane processes are widely used in chemical industry, as well as in many other industries. The mathematical modeling of processes is an important area of research, which allows to increase the efficiency of design and operation of baromembrane equipment. In the XXI century, due to the development of computer technologies and specialized software, the efficiency of mathematical modeling methods increased. As a result, the number of such studies and publications dedicated to it is increasing. New approaches also arise and develop. Therefore, it would be expedient to systematize and summarize such investigations. In the work [1], such a generalization was made for the period from 2000 to 2010. Since in the coming decade, that is, from 2010 to 2020, the number of publications has increased significantly, it is advisable to make reviews of publications on mathematical modeling for individual processes. In particular, in the work [2], a review of works on modeling reverse osmosis for the period from 2010 to 2020 was made. The purpose of this work is to analyze the main directions of mathematical modeling of the nanofiltration process, which as reverse osmosis has a large number of practical applications.

Materials and methods

This paper considered theoretical studies of the nanofiltration process, which were published in leading thematic journals. First of all, the researcges publicated in *Journal of Membrane Science, Desalination, Mebranes, Separation and Purification Technology* were considered. Materials from other journals by *Elsevir* and *Springer* publishers, as well as publications available in the DOAJ database, are also considered in detail. The classification of mathematical models was carried out according to the principle used in the work [1].

Results and discussion

Among the materials published during the period under consideration, dedicated to the mathematical modeling of pressure-driven menbrane processes, more than 200 articles were found, where the nanofiltration process was considered. The distribution of publications by year is shown in Fig. 1. A slight decrease in the number of publications can be seen in 2017, but in general there is a clear tendency to increase the number of studies under consideration. In Fig. 2, shows the distribution of publications by model classes.

The information shown in Fig. 1 demostrate that, as in the previous period, the greatest number of theoretical investigations was carried out using the expanded Nernst-Planck equation and Donnan equilibrium. However, there has also been an increase in the number of studies using computational fluid dynamics (CFD) and molecular dynamics methods. As in 2000-2010, artificial neural networks for modeling nanofiltration were used very rarely.

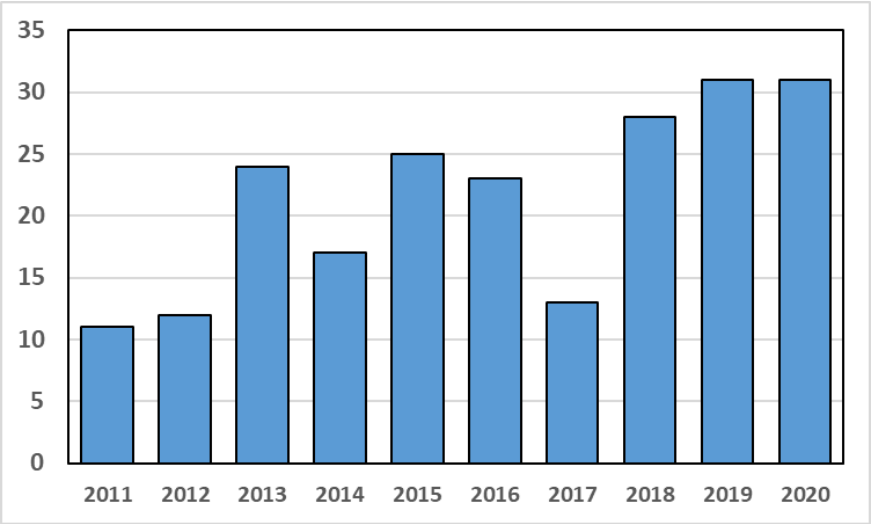

Fig.1. The distribution of publications dedicated to the simulation of nanofiltration by the years.

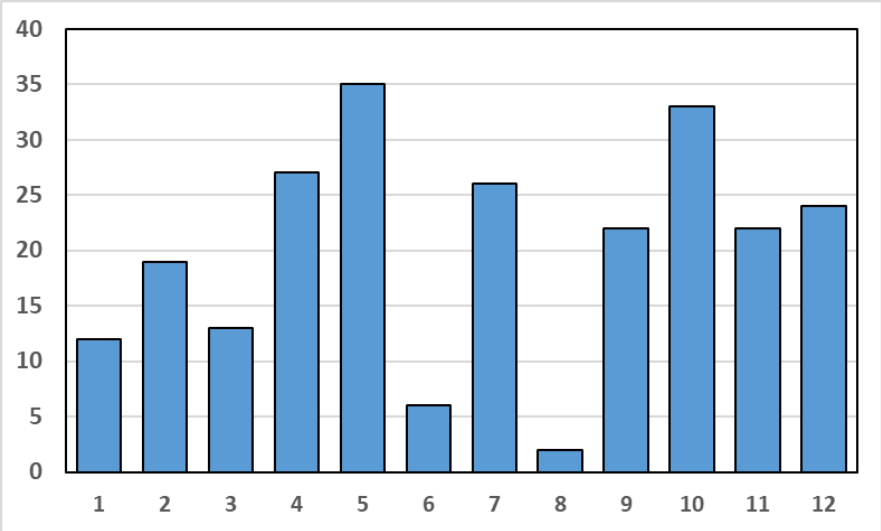

Fig.2. The number of NF models in the chosen articles by classes: 1 – irreversible thermodynamics models; 2 – diffusionbased models, 3 – pore models; 4 – Donnan equilibrium models; 5 – extended Nernst-Plank equations based models; 6 – Maxwell-Stephan equations based models; 7 – CFD models; 8 – ANN models; 9 – molecular dynamics; 10 –optimization; 11 – energy and economic analysis; 12 – other models.

Conclusion

The analysis of the distribution of publications on simulation the nanofiltration process shows that interest in this area is growing, and the most promising medods remain models based on the extended Nernst-Planck equation and molecular dynamics.

References

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