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Cell-element simulations to optimize the performance of osmotic processes in porous membranes

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ABSTRACT

We present a new module of the software tool PoreChem for 3D simulations of osmotic processes at the cell-element scale. We consider the most general fully coupled model (see e.g., Sagiv and Semiat (2011)) in 3D to evaluate the impact on the membrane performance of both internal and external concentration polarization, which occurs in a cell-element for different operational conditions. The model consists of the Navier–Stokes–Brinkman system to describe the free fluid flow and the flow within the membrane with selective and support layers, a convection–diffusion equation to describe the solute transport, and nonlinear interface conditions to fully couple these equations. First, we briefly describe the mathematical model and discuss the discretization of the continuous model, the iterative solution, and the software implementation. Then, we present the analytical and numerical validation of the simulation tool. Next, we perform and discuss numerical simulations for a case study. The case study concerns the design of a cell element for the forward osmosis experiments. Using the developed software tool we qualitatively and quantitatively investigate the performance of a cell element that we designed for laboratory experiments of forward osmosis, and discuss the differences between the numerical solutions obtained with the full 3D and reduced 2D models. Finally, we demonstrate how the software enables investigating membrane heterogeneities.

1. Introduction

Forward osmosis (FO) and pressure retarded osmosis (PRO) are industrial processes that rely on the osmotic pressure difference across a semi-permeable membrane [1]. The osmotic pressure difference drives both processes, but unlike in FO, PRO occurs in the presence of a non-negligible hydraulic pressure. FO is used in, for example, hybrid systems for waste water, in agriculture, in food processes [2–4], while PRO is used in, e.g., the technology for renewable power generation [5,6].

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Concentration polarization significantly affects the efficiency of both processes. Concentration polarization is a concentration gradient which occurs next to the surface of the membrane or inside the support layer. The main driving force in FO and PRO is the osmotic pressure which directly depends on the concentration difference across the separating membrane interface, the polarization phenomenon has a significant impact on the performance of these osmotic processes. There are two types of concentration polarization, internal (ICP), when the concentration gradient is found inside the support layer, and external (ECP), when the concentration gradient is found next to the membrane surface [2,7].

The membrane performance is usually evaluated using a cross-flow cell element, which is a lab-scale filtration unit designed to measure an accurate performance while using a minimal membrane area. Laboratory experiments for osmotic processes provide measurements only at the output of a cell element, while the details of the processes within the cell element are usually not accessible. In particular, concentration polarization cannot be easily measured because it occurs within the cell element, thus, it is usually evaluated indirectly. Mathematical modeling followed by computer simulations is a popular approach in the membrane community, which assists in the design and interpretation of the laboratory experiments and also helps to better understand the osmotic processes. A mathematical model which is correctly formulated and accurately applied provides a detailed 3D picture of the processes, leading to their adequate characterization.

Several factors control the concentration polarization, namely the shape of a cell element in the laboratory or a membrane module in industrial applications, the flow control parameters, and membrane characteristics [8]. These factors can be accounted explicitly or implicitly while studying concentration polarization. Below we review the models introduced in the literature, and comment on their advantages and limitations.

Modeling assumptions

To numerically represent concentration polarization, most of the studies (see for example [2,7,9–13]) use directly or modify the ICP model initially proposed for PRO phenomena by Lee et al. [14] and then extended for FO by Loeb et al. in [15]. The model describes the transport through the membrane taking into account ICP and membrane orientation. The model analytically solves the governing equations within the membrane while assuming that the osmotic pressure depends linearly on the concentration, that is, it assumes as ideal solution. The linearity assumption, however, can be applied only in limited number of cases, since several studies showed that the osmotic pressure–concentration relation is approximately linear only for low concentration solutions. For high concentration solutions, which are most relevant for FO and PRO processes, a more complex approximation is needed [2,16,17].

The limitations of the linearity assumptions inspired extensions of this simple model. Tang et al. [18] proposed an iterative model to account for the internal concentration polarization in forward osmosis that circumvents the linearity assumption between the osmotic pressure and the concentration. This method uses an analytical solution of the governing equations for the flow and the transport inside the membrane coupled with a nonlinear osmotic pressure–concentration relation. Since the governing equations are stated and solved only for the membrane, the proposed approach accounts only for internal effects of the concentration, but not for external ones. Nevertheless, the external concentration polarization has a significant impact on performance (see e.g., [2]). Later, this analytical model was incorporated into an FO model for the whole cross-flow setup that accounts for fluid dynamics and solute transport [16]. The latter approach accounts for the ECP influence, but has two limitations that cannot be overcome. First, the analytical solution in the membrane assumes that the hydraulic pressure is negligible, and therefore only the solute transport is accounted for in the support layer, while fluid flow effects are explicitly neglected from the model. Hence, the model cannot be directly applied to PRO processes. Second, all parameters of the support layer are averaged over its thickness, therefore, complex heterogeneities cannot be included.

To simulate forward osmosis processes Sagiv et al. [19,20] used a general model that does not rely on the linearity assumption and considers a resolved support layer of the membrane. This model generalizes the previously discussed approaches as it accounts for arbitrary osmotic pressure–concentration relations and has the potential to be further extended to model pressure retarded osmosis processes or to investigate membrane heterogeneities. Keeping in mind these advantages, we choose this mathematical model as a base model for our study.

Dimensionality of simulations

Another aspect which deserves discussion in connection with existing numerical simulations of FO and PRO processes is their dimensionality. The interpretation and design of experimental and of some numerical studies concerned with FO and PRO processes usually assume that the geometry of the cell elements produces a homogeneous tangential flow. Based on this presumption, the cell element geometry is assumed not to affect the membrane performance, i.e., any 3D effects are ignored. Under this homogeneity assumption, experimental studies rarely present or discuss the geometry of the cell elements that were used in the experiments (a notable exception is the experimental work [21]). Thus, it is difficult to evaluate the reliability of the parameters extracted from these experiments. While this presumption may be is valid in many cases, accepting it as always valid is dangerous.

A part of this paper describes our efforts to design a cell element for which the homogeneity assumption is not severely violated. But some cell elements might introduce a significant error if their 3D shape is neglected. Sagiv et al. [22] analyzed effects of the different factors on water permeation of the forward osmosis, and in particular, they found that improving the cell element design is beneficial for the forward osmosis performance for the parameters and regimes they investigated. We

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