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Predictive membrane transport models for Organic Solvent Nanofiltration: How complex do we need to be?

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ABSTRACT

From feasibility tests at laboratory scale to large industrial scale processes, modelling can be applied to Organic Solvent Nanofiltration (OSN) for two purposes: (i) parameter estimation, when experimental data for standard solute + solvent systems are available, and it is desired to estimate relevant parameters for as yet uncharacterised systems, and (ii) prediction, when the model parameters for the solvent–solute are available, and modelling can be applied to describe the performance of a different solute + solvent system or operations at a different process scale. Both estimation and prediction require the choice of a transport model, to carry out regression and simulation, respectively. This paper reports a systematic comparison of a range of different transport models (irreversible thermodynamics, solution–diffusion, pore-flow and transient transport models, such as the solution–diffusion with imperfections model) using selected experimental data for various solutes and solvents through polymeric OSN membranes with different physico-chemical properties. Commercial integrally skinned asymmetric polyimide (PI, glassy) and thin film composite silicone-coated PI (rubbery) membranes from Evonik® MET were systematically tested in this study, with styrene oligomers and Safranin-O dye in different organic solvents under uniform operating conditions (temperature, pressure, cross-flow velocity and solute concentration). In addition, experimental data from the literature were taken for non-commercial thin film composite silicone-coated PI, glassy poly[1-(trimethylsilyl)-1-propyne] (PTMSP) and poly[4methyl2pentyne] (PMP) membranes, to include a broad spectrum of positive and negative rejection values. The different transport models were used to perform regression of experimental data and prediction at different pressure values, based on the regressed model parameters. The models were then compared in terms of regression performance and experimental/numerical effort required to use them for parameter estimation. Negative rejection data was used to further discriminate among the models. Solution–diffusion-based models gave a better description of permeation through flexible-chain glassy membranes than pore-flow models. On the other hand, pore-flow-based models gave a better description of permeation through glassy PTMSP and PMP membranes. For integrally skinned asymmetric PI membranes, the prediction of a concentration process using the best performing regression models (i.e. the Maxwell–Stefan and the classical solution–diffusion model) was also performed. Interestingly, no significant difference was observed between the two models for both a membrane with complete solute rejection (Duramem® 200) and a membrane with partial solute rejection (Duramem® 500). Process modelling by accounting for a classical solution–diffusion-type transport mechanism is therefore sufficient to obtain a reliable transport description for this membrane family.

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1. Introduction

Since the beginning of membrane development, a substantial amount of research has focused on the description of the transport mechanism through membranes, for the purpose of process understanding and development. The development of membrane processes usually involves several stages, starting from feasibility tests at laboratory scale, passing through pilot plant tests and finishing with large industrial scale processes [1]. As illustrated in Fig. 1, three levels can be distinguished within the general process modelling framework: (i) transport through the membrane, (ii) fluid dynamics and mass transfer in membrane modules, and (iii) design at the process scale.

Across the different scales, modelling can be applied for two purposes: *parameter estimation* and *prediction*, as shown in Fig. 2.

At the membrane scale, *parameter estimation* is performed when experimental data for standard solute + solvent systems are available (Y* in Fig. 2(a) for standard solute A and solvent B), and it is desired to estimate relevant parameters for as yet

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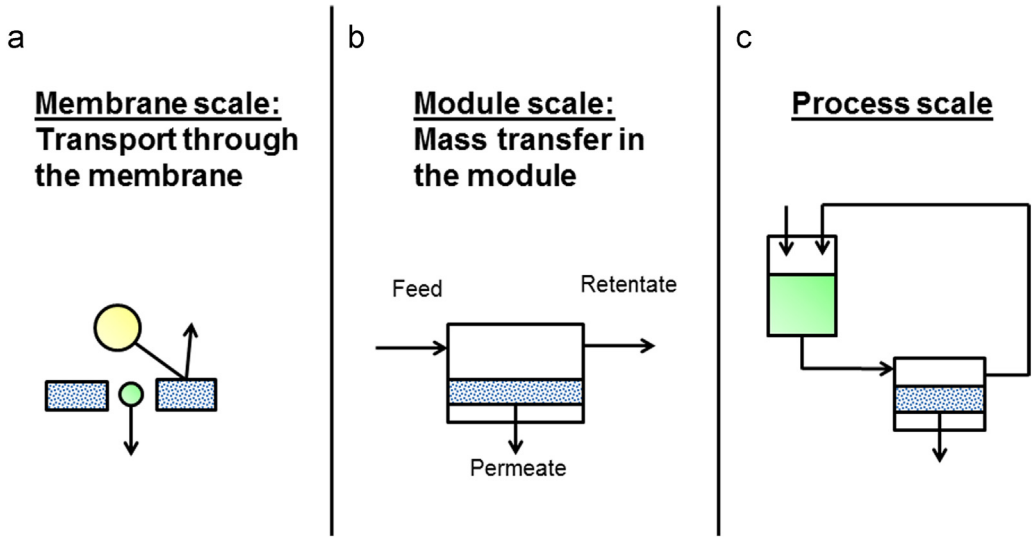

Fig. 1. Modelling levels for the development of a membrane process: (a) membrane scale; (b) module scale; (c) process scale. (Adapted from Peshev and Livingston [1]).

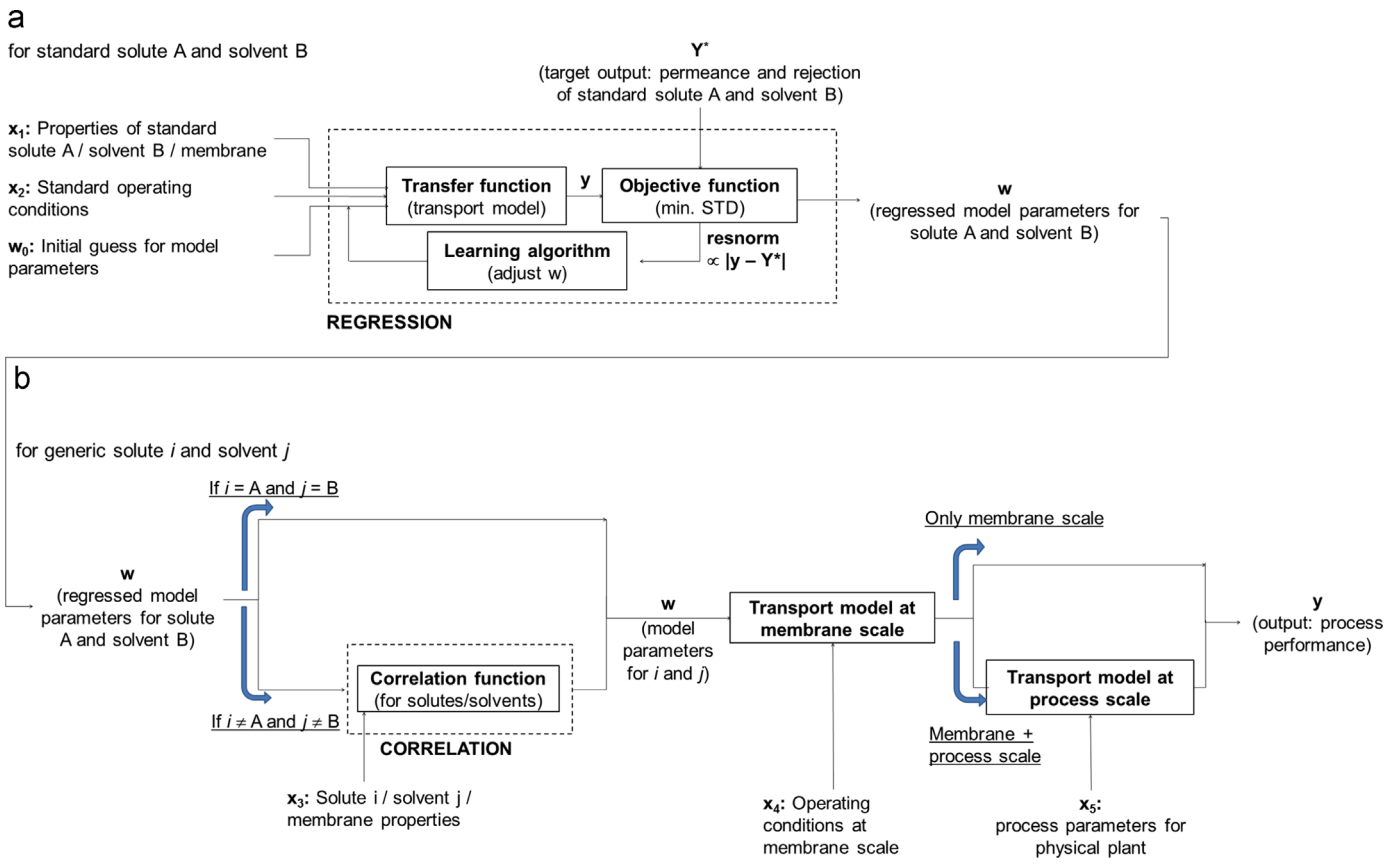

Fig. 2. Schematic representation of the modelling process: (a) parameter estimation; (b) prediction.

uncharacterised systems (w). Here, the unknown parameters, characteristic of the model (solute, solvent, membrane or interaction parameters) are obtained by linear or non-linear regression of the experimental data. The learning algorithm is designed so as to minimise an error measure between the model output (y) and the corresponding desired, or target, output (Y*), to find an optimal parameter vector (w) that provides the "best" approximation of $y(x)$ for a given transfer function (i.e. transport model). Once the model parameters for the solvent–solute system are available, modelling can be applied to perform *prediction* (cf. Fig. 2(b)):

- for the same solute + solvent system (i.e. when the generic solute i + solvent j mixture corresponds to the mixture of solute A and solvent B used to perform the parameter regression) at different operating conditions (pressure, temperature, cross-flow velocity, concentration, etc.);
- for the transport performance of a different solute + solvent system: in this case, fundamental or empirical correlations between model parameters and solute/solvent properties will be used to estimate the model parameters (w) for the new system i + j;

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