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Input for process simulator

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Colophon

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Input for process simulator

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Contents

1 Indroduction

Scientists and engineers both need models for their work. However they have different ideas about models and use them for different purposes. While scientists use them for analysis, i.e. for a better understanding of a physical phenomenon, engineers are interested in their application for different purposes. Models enable him to calculate and design plants and to optimise their operation and design.

Their are three principle types of models (see figure 1):

- Empirical or "Black Box" models, which mathematically describe experimental results without considering the real phenomena taking place in the system, e.g. by regression analysis.

- Semi-empirical models, which are based on scientific laws. Since the phenomena taking place in a real system are usually quite complex and it is almost impossible to describe them exactly, the semi-empirical models use simplified forms of scientific laws. In order to have a good fit with experimental data, parameters are introduced into the scientific laws which are determined by comparison with experimental data. An example for a semi-empirical model is Fick´s first law which contains the diffusion coefficient as parameter.

- Physical models, which describe the phenomena accurately without need for experimental results, e.g. by solving the Navier-Stokes-equations.

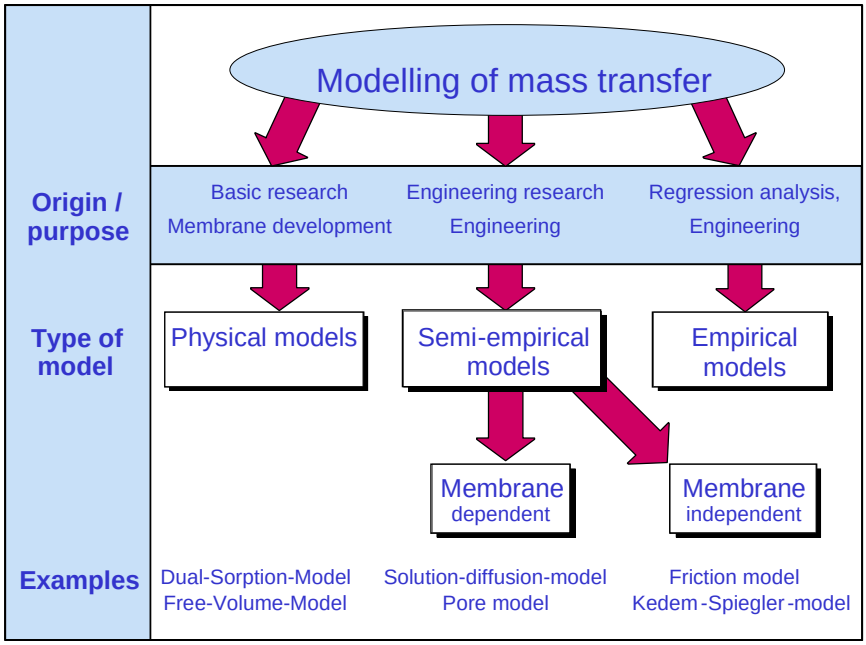

Figure 1: Survey of possible types of models for mass transfer[1]

While purely empirical models have the disadvantage of permitting no extrapolation into regions where no experiments have been performed, the main disadvantage of physical models is the extremely large effort which is required for more complicated systems. Examples for this would be the description of a column of bubbles by the Navier-Stokes equations or of a water droplet by the Schrödinger-equation for its molecules.

Semi-empirical models are neither a perfect solution. Often it is difficult to find a model which is accurate enough and does have a sufficiently small number of parameters, i.e. requires only a few experiments to determine the parameters. However, engineers usually choose semi-empirical models. The most important step in creating a semi-empirical model is to determine the degree to which reality is transferred to the model. Reality is always almost infinitely complicated and simplifications are inevitable. The difficulty is to find those physical dependencies which can be neglected without causing significant deviation and those which contribute the most to the behaviour of a system [1].

2 Modelling by using pore model

A semi-empirical model for the description of the mass transfer in pore membranes (ultrafilration and microfiltration membranes) is the pore model. The pore model assumes the membrane to be a system of pipes in a material which itself is impermeable for the permeating substances. The transported substances flow through the pipes (figure 2).

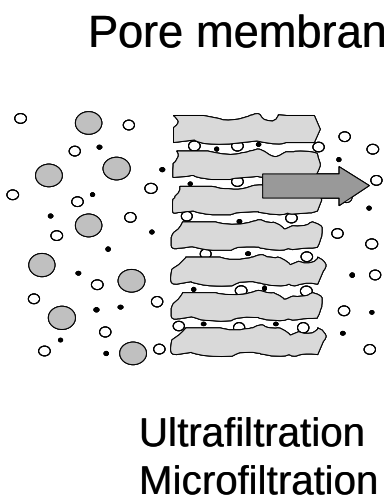

Figure 2: Pore membrane

The pore model consists of two parts. A first part deals with the flow of the considered liquid through the membrane while a second part deals with the rejection coefficient for the macromolecules which are dissolved in the liquid. In order to model the flux in pore membranes (see figure 3) the membrane is considered as a system of parallel capillaries with all the capillaries having the same diameter. Three parameters are introduced to characterise the membrane: the porosity ε, the surface area per unit volume $S_{(V)}$ and the ´detour´ factor τ.

$$\varepsilon = \frac{V_{Por}}{V_{tot}}, \tag{1}$$

$$S_{(V)} = \frac{A_{Por}}{V_{tot}}, \tag{2}$$

$$\tau = L / H \text{ ,} \tag{3}$$

where V_{por} and A_{por} are the volume and the surface of the pores in the considered membrane volume V_{tot} and L is the actual length of the capillaries and H the height of the membrane.

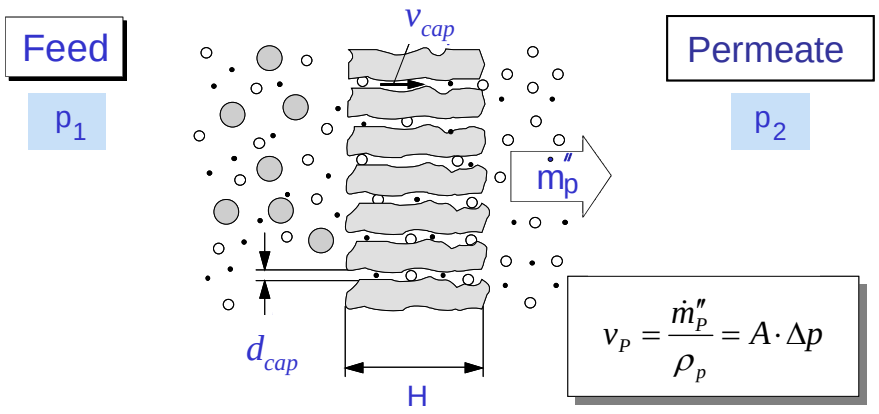

Figure 3: Model of a pore membrane

The model is based on the Hagen-Poiseuille law:

$$v_{cap} = \frac{d_h^2}{32\,\eta} \cdot \frac{\Delta\, p}{L}\,. \tag{4}$$

If the calculation is done for the whole surface of the membrane it reads:

$$v_p = \frac{\dot{m}''_p}{\rho_p} = A\,\Delta\, p\,, \tag{5}$$

where A is a membrane parameter characterising the membrane:

$$A = \frac{\varepsilon^3}{\eta \cdot (1-\varepsilon)^2\, S_{(V)}^2\; 2\,\tau\, H} \qquad \text{(Carman-Kozeny).} \tag{6}$$

Equation 6 is known as the Carman-Kozeny equation. The linear dependence of mass flow on the pressure difference over the membrane is confirmed by experiments. Since the porosity, the surface area per unit volume and the detour factor of a membrane are difficult to determine, the membrane parameter A is also determined by experiments [1].

The level of the pressure difference (TMP: Transmembrane pressure) depends of the used membrane system. While submerged systems (e.g. ZENON) usually with lower TMP are operated, the crossflow and dead-end systems are

operated with higher pressures [2]. Within WA 5 of the TECHNEAU project a survey on operational strategies of UF in the field of drinking water production has been conducted. The results are published in D. 5.3.5a and D.5.3.6.a. The results show that the TMP for submerged systems usually lies between 0.13 - 0.4 bar and for the other membrane systems between 0.13 - 2.0 bar [3, 4].

However, in practice the ultrafiltration is usually surface layer-controlled. In operation rejected compounds can lead to a fouling of the membrane. This fouling can affect the flux and retention behaviour much more than the membrane.

Few autors have been reported that beside of semi-empirical models also empiric models can be used for the modelling of micro- and ultrafiltration processes [5, 6, 7, 8]. An important group of these modelling tools are artificial neural networks (ANNs) [5]. ANNs are adaptive systems that changes their structure based on external or internal information that flows through the network during a learning phase. Theodosiu et al. 2000 show that the water flux in ultrafiltration membranes can be good described by using ANNs. Based on experimental data, in this study the artificial neural networks were trained to describe flux during ultrafiltration on hollow fibre membranes [7]. In another study Maelzer et al. (2006) show that the transmembrane pressure (TMP) in coagulation/microfiltration processes can be predicted by using ANNs. As input data for the artifical neutal network they have used water quality parameters such as temperature or turbidity as well as process parameters such as flocculation pH or backwashing conditions [8].

3 References

[1] Melin, T., Rautenbach. R.. et al., *Membranverfahren – Grundlagen der Modul- und Anlagenauslegung.* ISBN 3-540-00071-2. 2., vollständig bearbeitete und wesentlich erweiterte Auflage (2003).

[2] Lipp, P., Bestandsaufnahme zum Betrieb von MF/UF-Anlagen in der öffentlichen Wasserversorgung in Deutschland, Technolgiezentrum Wasser Karlsruhe (TZW), ISBN 1434-5765 (2007).

[3] Salehi, F., Wintgens, T., Melin, T., Ultrafiltration with pre-coagulation in drinking water production - Survey on operational strategies, Deliverable number 5.3.5a, Technology Enabled Universal Access to Safe Water (TECHNEAU), Integrated Project Funded by the European Commission under Sustainable Development, Global Change and Ecosystems Theamtic Priority Area, Contract Number: 018320, (2007).

[4] Salehi, F., Wintgens, T., Melin, T., Operational recommendations for pre-coagulation with ultrafiltration, Intermediate report Deliverable number 5.3.6a, Technology Enabled Universal Access to Safe Water (TECHNEAU), Integrated Project Funded by the European Commission under Sustainable Development, Global Change and Ecosystems Theamtic Priority Area, Contract Number: 018320, (2008).

[5] Geißler, S., *Modelle zur Beschreibung der Leistungsentwicklung von getauchten Membranen*, Dissertation, RWTH Aachen University (2008).

[6] Delgrange-Vincent, N., Cabassud, C., Cabassud, M., Durand-Bourlier, L., Laine, J. M., *Neural networks for long term prediction of fouling and backwash in ultrafiltration for drinking water production*, Desalination 131, 353-362 (2000).

[7] Teodosiu, C., Patravanu, O., Macoveanu, M., Neural network models for ultrafiltration and backwashing, Water Research Vol 34, No. 18, 4371 - 4380 (2000).

[8] Maelzer, H. J., Strugholtz, S., Ding, W., Recent Activities in Mechanistic, CFD and Neuronal Network Modelling at the IWW, Workshop on Developments in Drinking Water Treatment Modelling, 22-23 June 2006, TU Delft (2006).