# **465f Correcting the under-Prediction of Flux in Steady-State Ultrafiltration** *S.S. Vasan, S.R. Smith, R.W. Field, and Z.F. Cui*

#### Background and identification of the problem

Cross-flow ultrafiltration and microfiltration are used widely in the process industry (e.g. water production, wastewater treatment, food and pharmaceutical industries). The design of industrial filtration processes (especially that of new processes) relies heavily on pilot plant data which is expensive to generate due to the substantial costs involved (materials, research, engineering, labour and operating costs). Reliable process design models offer a solution to this problem by examining the feasibility of the process prior to the pilot stage, and thus giving a strong indication as to whether or not the investment of resources in pilot tests is warranted. Such predictive modes could also reduce the amount of pilot testing required, thus saving process design costs and reducing the time-to-delivery<sup>1</sup>. The most commonly employed predictive models for membrane processes involve the estimation of a convective mass transfer coefficient from the first principles, and combining this with a filtration model for flux prediction. Attempts to model membrane processes (such as ultrafiltration) using the classical non-porous flat-plate boundary layer approach has always led to an under-prediction of the permeate flux. While many researchers have attempted to solve this well-known problem since the 1970's (including the luminary T.K. Sherwood<sup>2</sup>), a simple non-empirical correction mechanism with broad applicability has so far remained elusive.

### The performed work

Recent theoretical developments<sup>3,4</sup> have identified three major effects that cause the under-prediction of flux in a steady-state system, and have individually corrected for these effects using simple non-empirical correction factors. This paper combines the correction mechanisms for all three effects into a flux prediction model (Figure 1).

INPUT Native membrane permeability System geometry (membrane length and diameter) Operating conditions (trans-membrane pressure, liquid velocity, temperature) Physical property relationships (with solute concentration)
MODEL COMPONENTS Driving force-resistance model for filtration mass transfer Film theory model for filtration mass transfer Boundary layer model for convective-diffusive mass transfer Such on correction if using non-porous transport equations Correction for edge effects (geometry) if using flat plate boundary layer model Accounting for the variation of fluid properties
OUTPUT Membrane flux estimate at stipulated input conditions

Figure 1: Flux prediction model flow chart

This model has been successfully validated in this work against benchmark experimental data from the cross-flow ultrafiltration of dextran (using commercial tubular and hollow-fibre membranes). The benchmark data spans Re  $\sim$  225 to 7950, thus demonstrating the broad flow-regime applicability of the proposed integrated flux correction mechanism for a steady-state pipe-flow membrane process.

#### Results and discussion

The three major effects that cause the under-prediction of flux in a steady-state system are: (i) wall suction, (ii) the concentration-dependence of physical properties, and (iii) edge effects. By combining the correction mechanisms for these effects and applying them to the benchmark data (from tubular and hollow-fibre ultrafiltration experiments), this paper is able to quantify the error accrued by neglecting these effects in a steady-state system (Figure 2). A brief description of each effect and its significance is given below<sup>5</sup>:

# (i) Wall suction

The most important effect is wall suction. The mass transfer coefficient obtained from non-porous hydrodynamics can be corrected for a given value of permeation (or wall suction) using a simple correction factor derived recently, on the basis of film theory<sup>3</sup>. This non-empirical suction correction factor improves (increases) the predictions substantially (Figure 2).

## (ii) Concentration dependence of physical properties

The second factor arises from neglecting the concentration-dependence of physical properties such as diffusivity, viscosity and density. For instance, the errors frequently encountered in membrane science literature are: (a) using the bulk values for these properties (illustrated in Figure 2), and (b) estimating these physical properties by assuming an arbitrary concentration profile, most often a linear profile (not illustrated). It has been shown<sup>3</sup> that a reliable method to correct the physical properties for the concentration effect is to use the concentration dependence determined using the boundary layer Peclet number. This approach is based on film theory, and as such, maintains consistency throughout the flux prediction model. It also has broad applicability in that the average concentration-dependence is considered for diffusivity only (as viscosity and density effects are not important for the benchmark data used). This results in an enhancement of the predictions if bulk properties were assumed originally (illustrated in Figure 2), or a decrease in the predictions if a linear concentration profile was assumed originally (not illustrated).

# (iii) Edge effects

The third factor (edge effects) is relevant to systems with internal, circular-conduit flows (such as tubular or hollow-fibre systems). Modelling such systems using flat plate boundary layer equations results in an under-prediction of the flux. This issue has been recently resolved<sup>4</sup> by imposing a simple geometric correction factor upon all flat plate boundary layer equations such that the constant width of the flat plate boundary layer is corrected for the axially changing widths of the developing pipe boundary layer. The fully developed pipe boundary layer mass transfer coefficient under-predicts by a fixed value of ~12% when compared to the flat plate analysis. Therefore, the permeate flux is also under-predicted by ~12% if the edge effects are neglected (Figure 2).



*Figure 2: Waterfall chart showing how the under-prediction of flux can be successfully corrected by considering the three effects described in the text* 

(Benchmark data spanning  $Re \sim 225-7950$ , normalised to 100% of experimental flux)

#### Closing remarks

This paper successfully achieves its objective of developing an integrated flux correction mechanism, which is simple, non-empirical and easy to integrate into calculations involving the gamut of membrane processes. Furthermore, the improved flux prediction model has broad applicability in terms of Reynolds number, and is not affected by the charge on the filtered solute. Unsteady state filtration effects, such as fouling and feed channel plugging are not considered in this work, as general models cannot be developed easily for these phenomena. However, experimentally derived fouling or channel plugging rates could be incorporated into the filtration model component of this work. This work has many practical applications in the membrane industry and could, for example, be employed for parametric studies to reduce the time and costs associated with conducting pilot trial runs.

<sup>1</sup> Pilot data will always serve to determine long-term fouling and other long-term flux decline effects because the general a priori models do not exist for these system-specific and fluid-specific phenomena.

<sup>2</sup> T.K. Sherwood, R.L. Pigford and C.R. Wilke, Mass transfer, McGraw-Hill, 1975.

<sup>3</sup> S.S. Vasan, D.Phil Thesis, Trinity College, Oxford, 2005.

<sup>&</sup>lt;sup>4</sup> S.R. Smith, D.Phil Thesis, Keble College, Oxford, 2003.

<sup>&</sup>lt;sup>5</sup> Detailed derivations can be found in Vasan (2005), Smith (2003), and related journal articles.