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Extending potential flow modelling of flat-sheet geometries as applied in membrane-based systems

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ABSTRACT

The efficiency of chemical reactors can be analysed using the residence time distribution. This research focusses on flat-sheet geometries applied in membrane-based systems. The residence time distribution depends mainly on the 2D velocity field, parallel to the membrane. The velocity average over the transversal direction is calculated using potential flow theory. A combination of real and virtual sources and sinks are used to model the internal inlets and outlets. Furthermore, a novel method is presented to calculate the residence time distribution. By ignoring diffusion and dispersion, every streamline is modelled to have a fixed residence time, which can be calculated with a simple quadrature based on a coordinate transformation. The model predicts the impact of the two-dimensional geometry on the residence time distribution, but it is demonstrated that large zones of nearly stagnant flow have only a limited impact on the residence time distribution. The new model can predict the travelling time from the inlet to each interior location, providing a better tool to analyse spatially distributed chemical reactions. The models agreed highly with pressure measurements (R^2 = 0.94–0.98) and they agreed well with tracer experiments for the residence time (R^2 = 0.73–0.99).

1. Introduction

The efficiency of many chemical and biological plants is determined by the residence time distribution, see, e.g. one of the standard textbooks [1]. The residence time distribution depends on the velocity field, which is determined by the system geometry [2]. Therefore, a careful design of the system geometry can improve the system efficiency [3,4]. This article focusses on membrane technology systems that have a flat-sheet geometry. The efficiency of membrane-based systems, which can be analysed based on the residence time distribution, is influenced by velocity gradients transversal to the membranes [4–6], but velocity gradients in the two spatial directions parallel to the membranes may also be relevant [7]. These effects can be modelled based on local mass, momentum and energy balances, expressed in partial differential equations with three space dimensions [7]. Computational fluid dynamical (CFD) modelling [8] is a numerical method to solve these local balances. However, the problem is that three-dimensional CFD models generally require long calculation times. Furthermore, CFD modelling requires expert knowledge, because the geometry has to be meshed and the mesh quality determines the solution accuracy.

In order to develop a relatively simple tool, the three-dimensional problem may be reduced to two dimensions by averaging the three-dimensional local balances over the limited height [9,10]. This way, the two-dimensional superficial velocity vector remains to be modelled. The membranes are typically very close to each other (1 mm or less), causing the Reynolds number to be low. Therefore, the superficial velocity field may be modelled as a potential flow [7]. Potential flow theory calculates the pressure and the velocity field based on a conformal map [7,11], which maps the physical plane onto the infinite strip. However, membrane-based systems often are not single-connected, because the inlet and the outlet of a cell (area between membranes) are not located on the boundary. The research questions are: (a) can potential flow theory be applied to bounded geometries with internal inlets and outlets as in flat-sheet geometries; (b) can potential flow theory be extended to model the residence time distribution?

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2. Theory

2.1. Modelling the velocity field

The example that motivates this research is reverse electrodialysis [12–14], an experimental method for electricity generation. The hydrodynamic design requirements of a reverse electrodialysis stack differs from that of a conventional electrodialysis stack. The design of a conventional electrodialysis stack intended for turbulent flow conditions in order to obtain a reasonable limiting current. These turbulent conditions are obtained with relatively big distances between the membranes of 1 mm or more, relatively high-cross-flow velocities in the range of 20–40 cm s^{-1}, and the use of screen spacers for turbulence promotion. For reverse electrodialysis, however, it is not likely and, in fact, not preferred to operate the system with high-Reynolds numbers. It is not likely, given that the distance between the membranes should be decreased to less than 1 mm in order to cut down the internal ohmic resistance and the cross-flow velocities should be lower to keep the parasitic energy losses for pumping to a reasonable level. It is not preferred, given that the diffusion layers do play a minor role in reverse electrodialysis [15] as there exists no limiting current. The spacers in a reverse electrodialysis are, therefore, not applied for turbulence promotion but only to keep distance between the adjacent membranes. Although these differences are recognized, the current design of a reverse electrodialysis is still based on the common stack design of electrodialysis. However, the stack design would be reconsidered when the technology comes beyond its experimental phase. This research on the applicability of the potential flow, would provide a relatively simple tool for this redesign process.

The goal of reverse electrodialysis is to generate energy. Therefore internal losses should be minimized. These losses are both electrical and mechanical, due to the electrical resistance perpendicular to the cells and the fluid resistance in the lateral direction through the water compartments, respectively. The electrical and mechanical requirements are counteracting. The optimum thickness of the compartments is below 1 mm. Fluid dynamics in this thin layer is very important. However, to study these flow direct measurements of fluid velocities and pressures in real reverse electrodialysis cells are needed, which is difficult in practice. More details on the experimental setup can be found in Section 3.

The distance between the membranes is typically 1 mm or less, which is small compared to the membrane area. Therefore, the flow can be considered to be two-dimensional, and the small membrane distance causes the Reynolds number to be small. Low-Reynolds number two-dimensional flows can be modelled using potential flow theory [7,16]. The friction force is determined by the velocity being 0 on the membrane surfaces (no-slip condition), introducing transversal velocity gradients. The impact of these gradients can be modelled based on the theory of parallel flow between flat plates, which states that [17]

$$\frac{\mathrm{d}p}{\mathrm{d}s} = -\frac{12\eta}{\delta^2}u \tag{1}$$

with $\mathrm{d}p/\mathrm{d}s$ the pressure drop in the streamwise direction (N m^{-3}) (averaged over the transversal direction), η the viscosity (Pa s), δ the distance between the plates (m), and u is the average velocity (m s^{-1}). Eq. (1) models one dimension parallel to the membranes (the s-direction), and the second parallel dimension is added by replacing the scalar velocity u with the two-dimensional average velocity vector $\vec{u}$, and by replacing $\mathrm{d}p/\mathrm{d}s$ with grad p.

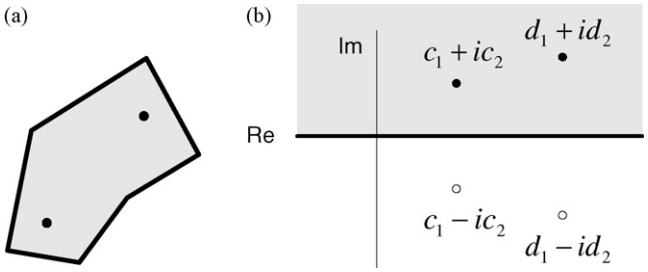

Fig. 1. Transformation of a low-Reynolds number (creeping) flow inside the gasket (left) to its conformal map (right).

The average velocity $\vec{u}$ can be modelled by defining a potential function ϕ (m^2 s^{-1}) as

$$\phi = -\frac{\delta^2}{12\eta}p \tag{2}$$

which transforms Eq. (1) to grad $\phi = \vec{u}$. According to the continuity equation [7], the potential function ϕ must satisfy Laplace's equation:

$$\text{div grad } \phi = 0 \tag{3}$$

The boundary condition for Eq. (3) comes from the requirement that there is no fluid flow through the boundary of the two-dimensional domain, which is expressed as the boundary condition that grad ϕ is parallel to the two-dimensional boundary.

Laplace's equation (Eq. (3)) can be solved using complex function theory. The two spatial coordinates x_1 and x_2 (m) are combined in a complex number $z = x_1 + ix_2$, with i the imaginary unit. Furthermore, a function ψ (the stream function, m^2 s^{-1}) is introduced that has its gradient perpendicular to grad ϕ. Using this notation, Laplace's equation (Eq. (3)) transforms to the requirement that the complex function $z \to \phi + i\psi$, is differentiable (satisfies the Cauchy–Riemann equations) [11]. The geometric meaning of the Cauchy–Riemann equations is that small area elements are not deformed, and hence differentiable complex functions are conformal maps. The boundary condition on grad ϕ transforms to the requirement that the stream function ψ is constant on the boundaries. When the volumetric flow rate is F_V (m^3 s^{-1}), the corresponding area flow rate must be $\psi_A = F_V/\delta$ (m^2 s^{-1}). Therefore, flows in single-connected channels are characterized by the boundary conditions $\psi = 0$ on one wall, and $\psi = \psi_A$ on the other wall, see Fig. 2.

However, reverse electrodialysis cells are characterized by multiply connected domains, because the inlet and the outlet are holes in the membranes. Extra boundary conditions are required for the boundaries of the holes. This problem can be solved by modelling

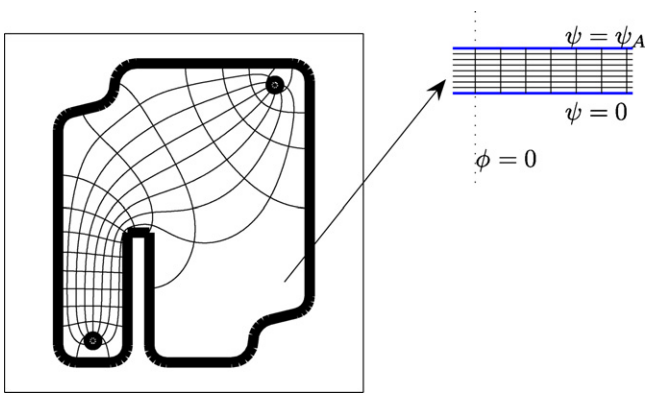

Fig. 2. Conformal map from physical domain (a) to the upper half-plane ζ (b).