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Predictive pressure drop models for membrane channels with non-woven and woven spacers

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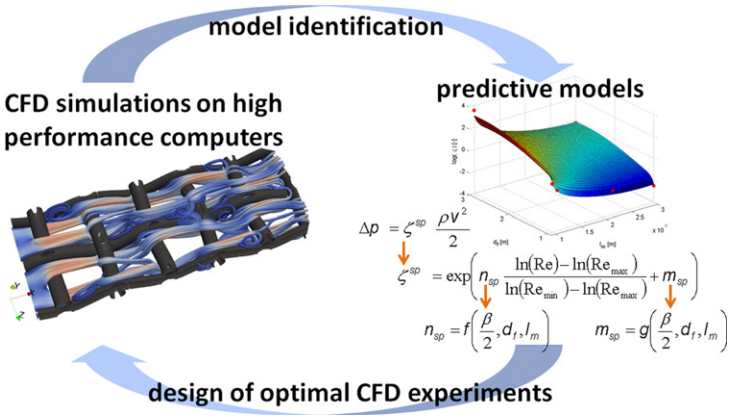
HIGHLIGHTS

- Predictive pressure drop models have been identified for woven and nonwoven spacers.
- Quantitative description of the pressure drop for a wide range of design parameters
- Work flow is presented for the identification of models with a minimal effort.
- A new Lattice–Boltzmann-based tool is used for CFD simulations on HPC clusters.

GRAPHICAL ABSTRACT



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ABSTRACT

Predictive pressure drop models have been identified for membrane channels with both woven and non-woven spacers as found in plate and frame or spiral wound membrane modules. The models allow for the first time the thorough quantitative description of the pressure drop for a wide range of design parameters specifying the thickness and orientation of the spacer filaments. A systematic work flow has been developed efficiently integrating detailed computational fluid dynamics (CFD) simulations on high-performance computing (HPC) systems with established optimization-based model identification methods. The work-flow efficiently handles the complexity arising from the large number of design parameters and allows for the model identification with minimal number of CFD simulations. The resulting models facilitate for the first time a thorough sensitivity analysis of the pressure drop with respect to all important design parameters elucidating strongly nonlinear patterns in the sensitivities. This indicates that the generalization of trends from a small number of CFD simulations, frequently used in previous work to simplify the spacer design problem, can yield inaccurate results.

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Greek symbols

α	flow attack angle [°]
β	angle between filaments [°]
$\Delta\theta_k$	confidence intervals [–]
ρ	density $[\frac{kg}{m^3}]$
σ	standard deviation of measurements [–]
ζ^{MUSUBI}	friction factor predicted by MUSUBI [–]
ζ^{sp}	friction factor of the spacer [–]

Roman symbols

ϕ	least squares objective [–]
AIC_i	Akaike criterion [–]
$\Delta AIC_{i,c}$	relative Akaike criterion w.r.t. model c [–]
c_f	correction factor [–]
d_f	filament diameter [m]
d_g	characteristic diameter [m]
F	Fischer information matrix [–]
H	Hessian matrix [–]
h_{ch}	channel heights [m]
J	Jacobian matrix [–]
l_{ch}	channel length [m]
l_m	orthogonal distance of filaments [m]
n^{sp}, m^{sp}	empirical model parameters [–]
Δp	pressure drop [Pa]
p	total pressure [Pa]
$\hat{p}^k$	empirical model parameters [–]
$p_{tp,i}$	averaged total pressure at tracking plane i [Pa]
Re	Reynolds number [–]
RSS	residual sum of squares [–]
$RSSCV$	averaged root mean square error [–]
u^k	geometric design parameters [–]
$\check{u}_k$	scaled model inputs
v	velocity vector $[\frac{m}{s}]$
v_{ch}	mean velocity $[\frac{m}{s}]$
w_{ch}	channel widths [m]
$w_{i,c}$	Akaike weights w.r.t. model c [–]

1. Introduction

Modules used for membrane processes, such as reverse osmosis, nanofiltration or electrodialysis, are typically realized in spiral wound or plate and frame configuration. A common characteristic of both configurations is the use of structural components called spacers [1]. The main functionality of the spacers is the separation of adjacent membranes. A second functionality of the spacer is to influence the hydrodynamics in the flow channels in a favorable manner.

The local hydrodynamic conditions in the spacer-filled channels determine important design objectives governing the performance of a membrane process: (i) the pressure drop over the membrane module, (ii) the wall shear-stress rate at the membrane surface and (iii) lateral mixing resulting from the formation of steady or turbulent vortices. A high pressure drop results in a loss of driving force in nanofiltration or reverse osmosis [2]. In electrodialysis the pressure drop is directly proportional to the energy demand of the pumps [1]. Zones characterized by a low wall shear-stress rate are likely to act as initiation points for the formation of fouling films [3]. Lateral mixing increases the local mass transfer intensity by reducing concentration polarization effects [4,5]. Zamani et al. [6] emphasize the increasing importance of these design objectives concomitant with the advances in the development of a new generation of ultra-permeable membranes for reversed osmosis processes.

The hydrodynamics in spacer-filled membrane channels have been investigated in numerous studies using either experimental (e.g.,[7–9]) or computational fluid dynamics (CFD) techniques (e.g.,[10–16,3]). An excellent review is provided in [3]. The focus of the majority of CFD studies [4,5,14,17,16] has been directed to a qualitative description of the flow fields arising in different Reynolds regimes.

In more detailed studies, the simulation of the hydrodynamics in the channel is extended to include additional physical phenomena. The simulation of simultaneous diffusive and convective mass transport in the channel, for example is included in a few simulation studies reported in [18,4,3]. Similarly, Picioreanu et al. [19] and Radu et al. [20] employ coupled simulations of hydrodynamics and biofilm growth in the channel to study the formation of fouling. Simulations of coupled phenomena require a significantly increased computational effort and thus limit the number of simulations in a model-based analysis.

Improved insight into the transport mechanisms have led to the development of numerous innovative spacer structures (e.g.,[3,21, 14,22]). Some of these innovative spacer structures have shown an improved performance with respect to different design objectives in model-based and experimental studies. However, despite this improvement, commercially available spacer structures are still based on the established non-woven or woven spacer geometries. One reason for the apparently difficult translation of innovative structures into industrial processes relates to the higher effort in the spacer manufacturing.

The quantitative effect of important design parameters on the design objectives, i.e., pressure drop, shear-stress pattern and mass-transport efficiency, has been investigated in [23,11,15,24]. All studies emphasize the strong sensitivity of the design objectives with respect to the design parameters. Most of them vary one parameter and fix all the others to nominal values to analyze the dependency of design objectives on design parameters. However, the extrapolation of the identified trends beyond the nominal values gives only adequate results, if the variation in the sensitivities is small.

The evaluation of experimentally measured or simulated pressure drop and mass-transfer rates is commonly assisted by simple algebraic models [25,4,18]. These models correspond to power laws relating well-known dimensionless quantities such as friction factors, Reynolds, Sherwood and Schmidt numbers by empirical parameters. The comparison of the empirical parameters in these power laws for different spacer geometries allows for a reasonable evaluation of the geometries in the entire range of Reynolds or Schmidt numbers. However, these models are restricted to a fixed spacer geometry. A general model for the prediction of the pressure drop or mass-transfer rate for a wide range of design parameters is still missing [3].

This contribution addresses this gap and aims at the identification of predictive models for the design objectives in the entire space spanned by the design parameters. To handle the complexity arising from this multi-dimensional design space, a work-flow is proposed guiding the execution of specific CFD simulations by means of optimization-based model identification techniques. With this, the approach yields predictive models by a minimal number of CFD simulations. In a first step, we restrict our consideration to the pressure drop constituting one central objective for the spacer design. As the primary result, the contribution presents a generalization of the established pressure drop models by accounting for varying design parameters. For the first time, this allows a thorough quantitative description of the pressure drop in the entire design space.

The remainder of this publication is organized as follows: Section 2 introduces a systematic work flow and the model-based and experimental methods employed. In Section 3 CFD simulation results are discussed and compared to experimental data. Section 4 presents the results of the identification of the generalized pressure drop models.