Model identification of pressure drop in membrane channels with multilayer artificial neural networks

JIANGHANG GU*, School of Chemical Engineering and Technology, Sun Yat-sen University, China
JIU LUO*, School of Materials Science and Engineering, Sun Yat-sen University, China
MINGHENG LI, Department of Chemical and Materials Engineering, California State Polytechnic University, America
YI HENG†, School of Data and Computer Science, Guangdong Province Key Laboratory of Computational Science, National Supercomputing Center in Guangzhou (NSCC-GZ), Sun Yat-sen University, China

This paper presents the work of identifying a data-driven model of pressure drop in spacer-filled reverse osmosis membrane channels and conducting CFD simulations. The established model by applying multilayer artificial neural networks (ANN) method correlates the pressure drop with a wide range of design objectives, which enables a quantitative description of the geometric structures and operation conditions for improvement. A large number of CFD models with respect to different geometry parameters are efficiently calculated with high throughput calculation (HTC) strategy in this work. The optimal design of spacer geometry can then be transformed into solving a minimization problem of the obtained pressure drop model, which is easy to handle. In a word, that the proposed strategy coupling with multilayer ANN method and HTC strategy can be considered as a new optimization idea to solve the intricate optimal problems involving CFD simulations.

CCS Concepts: • Computing methodologies → Neural networks; Distributed algorithms; • Applied computing → Engineering.

Additional Key Words and Phrases: Reverse Osmosis, High-Throughput Calculations, Pressure-Drop Model, Multilayer Artificial Neural Networks

1 INTRODUCTION

Facing with the threat of usable fresh water shortage, the development of efficient desalination techniques [1, 2] is crucial. Reverse osmosis (RO), as one of the most widely applied technology to purify water in industry, has attracted more and more attention [3]. In recent years, the hydrodynamics in spacer-filled membrane channels of reverse osmosis desalination has been intensively studied [4–6]. For example, many research works on CFD modeling of spacer membrane channels have been focused on the optimization of spacer geometry and the fouling process so as to reduce flow resistance and boost mass transfer [6–10]. However, most of the efforts are limited to a single-factor analysis due to high computational cost to conduct CFD simulations [5–7]. Model-based design of membrane channels are performed and the pressure drop model is derived with a large number of design parameters by applying the optimization-based model identification methods in [11]. Different from these studies, this work aims at establishing an algebraic data-driven pressure-drop model for industrial brackish water RO (BWRO) with a wide range of design parameters and operation conditions through multilayer artificial neural networks (ANN) with high-throughput calculations. Besides, the more accurate CFD models for the commercial feed spacers are built in this work than those simplified model considered cylinders of equal diameter such as in [11]. To handle the intractable computational task in the identification procedure and CFD simulations, a high-performance computing (HPC) strategy is employed to obtain massive data for different design parameters. The identified model of $\Delta p/\Delta L$ by the ANN can then be used to design membranes and guide experiments.

2 PROBLEM FORMULATION AND CFD SIMULATIONS

For BWRO, the applied pressure is appreciably higher than the osmotically pressure that ignoring the effect of concentration polarization (CP) does not compromise modeling accuracy. Navier-Stokes equation (1) and continuity equation (2) are the governing equations considered in the computational domain. $\rho$, $\mu$ denote the density and viscosity of fluid, respectively. $\mathbf{u}=(u,v,w)$ represents the velocity vector along $x$, $y$ and $z$ coordinates.

$$\rho \left(\mathbf{u} \cdot \nabla\right) \mathbf{u} = \nabla \cdot \left[-P I + \mu \left(\nabla \mathbf{u} + \left(\nabla \mathbf{u}\right)^T\right)\right]$$

(1)

$$\rho \nabla \cdot \mathbf{u} = 0$$

(2)

For the CFD simulations and identification procedure, we adopt the geometric structure and operation parameters reported in [6, 10] (cf. Figure 1), which imitates the typical spacer structure available for commercial use.

3 HIGH-THROUGHPUT CALCULATIONS

The CFD simulations adopt a hybrid parallel strategy combining a high-throughput computing approach and a high-performance computing approach to obtain massive data. The used operating environment is TH-Starlight HPC system established by the National Supercomputing Center in Guangzhou. To maximize the utilization of computing resources, a series of scalability tests are conducted.

---

# Both authors contributed equally to this research.
* Corresponding Author: hengyi@mail.sysu.edu.cn.
to explore the potential capability of parallelizing the codes with respect to a single RO CFD model. In this work, 72 cores (3 nodes) are chosen for each RO CFD model including 10 parameters combinations, which intends to balance the computational efficiency and computational time. In total, the whole computation needs 3600 cores for 50 RO CFD models with 500 parameter groups that are generated by a uniform random function in the whole target parameter space. This leads to a total computational cost of about 10000 core hours.

4 A DATA-DRIVEN PRESSURE-DROP MODEL

In the mathematical theory of ANN, the universal approximation theorem states that a feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of \( \mathbb{R}^n \), under mild assumptions on the activation function [12, 13]. Therefore, the ANN can be considered as a favorable surrogate model to find the complex relationship between multi-dimensional design space \( X \) and \( \Delta p/\Delta L \). The detailed information about the structure and the formulation of the used multilayer ANN is shown in the poster. According to the sensitivity analysis of design parameters mentioned in Section 2, 7 design variables are ascertained as influential factors of attributive variable \( \Delta p/\Delta L \) for all 16 parameters. So here \( X \) is a \( 7 \times n \) matrix (\( n \) stands for sample size that is 473 in this work).

5 SIMULATION RESULTS

In this work, we generate a three layers feed-forward neural network, applying the hyperbolic tangent transfer function (tansig) in the hidden layers and the linear transfer function (purelin) in the output layer. The formula of \( \Delta p/\Delta L \) is shown below in equation (3).

\[
\Delta p/\Delta L = \text{purlin}(LW^{3,1} \times \text{tansig}(IW^{2,1} \times \text{tansig}(IW^{1,1} \times X + b^1) + b^2) + b^3)
\]

(3)

6 CONCLUSIONS AND FUTURE WORK

The decreasing of driving force caused by flow resistance dominates and the effect of CP phenomenon can be ignored in BWRO and the effect of CP phenomenon can be ignored in BWRO process due to the fact that its concentration is sufficiently low and thus the osmotic pressure is significantly lower than the applied pressure in industrial operation. Therefore, in this work we only consider the hydrodynamic effect and establish a pressure-drop model with a wide range of design parameters in the reverse osmosis of industrial brackish water by using the ANN. The simulation results show that the model can yield satisfactory results. In our future work, we will consider the following points:

1. A much larger scale problem will be conducted. The CFD models coupling the hydrodynamics and transport processes simultaneously are considered in the future when the CP phenomenon can’t be ignored for feedwater with higher concentration.

2. The obtained data-driven model of pressure drop in microscale can be further combined with a system-level model in macroscale to derive the pressure drop, water yield with different design parameters for the whole RO membrane systems.

3. Further optimization towards the optimal experiment design is expected. The optimal design of geometric structures and operational conditions can be obtained by applying the aforementioned predictive models for salt water of a specific concentration.

ACKNOWLEDGMENTS

The authors acknowledge support from the National Supercomputing Center in Guangzhou for providing the computing resources.
REFERENCES


