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

Jianghang Gu[2#], Jiu Luo[3#], Mingheng Li[4], Yi Heng[1*]

1 School of Data and Computer Science, 2 School of Chemical Engineering and Technology, 3 School of Materials Science and Engineering, Sun Yat-sen University, China; 4 California State Polytechnic University, America.

* Corresponding Author: hengyi@mail.sysu.edu.cn (Yi Heng) # Authors contributed equally to this work

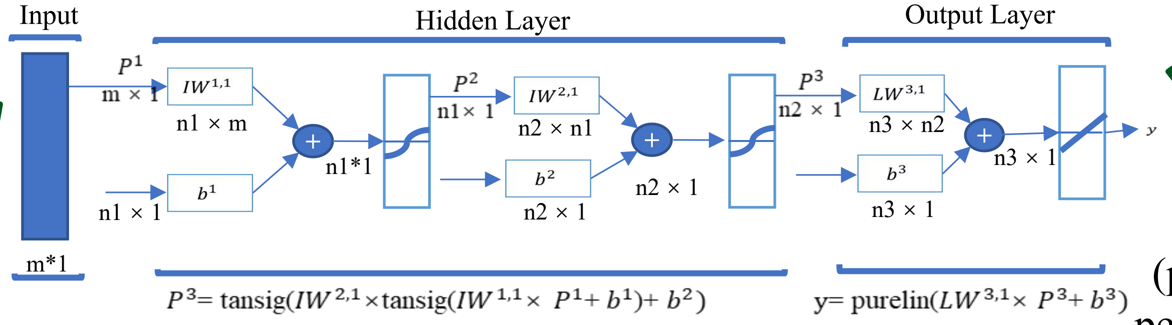
Motivation and introduction:

Reverse osmosis (RO) desalination process

- one of the most widely used technology to purify water;
- intensively influenced by geometric structures of spacers between membranes and operation conditions;
- most researches are limited to a single-factor analysis due to high computational cost of CFD simulations;
- development of a data-driven pressure drop with a wide range of design parameters and operation conditions by using multilayer artificial neural networks.

Work-flow:

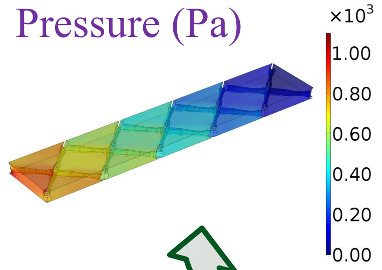
$\frac{\Delta p}{\Delta L}\Big|_{\mathbf{D},\alpha,u_0}$



Surrogate model (pressure drop per unit length)

CFD simulations

Pressure (Pa)



ANN method

- 70% of data for training;
- 15% of data for validation;
- 15% of data for test.

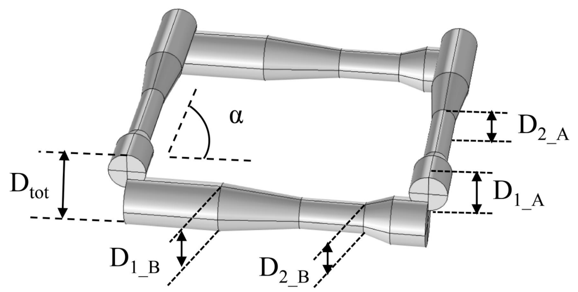
Design parameters ($\mathbf{D}$, α, u_0)

- About 500 groups.

$$\frac{\Delta p}{\Delta L} = f(\mathbf{D},\alpha,u_0)$$

Supercomputing, Tianhe-2

High performance computing



Optimal Experiment Design

Conclusions and future work:

A data-driven pressure-drop model

- is built by the ANN method based on CFD simulation data with high-performance computing (accounts for 3600 cores that result in about 10000 core hours);
- realizes a thorough quantitative description to geometric structure based on the real commercial spacer for RO processes;
- is applied to the optimal experiment design for RO process in the future work.

Problem formulation:

Momentum and continuity equations:

For Brackish Water RO (Incompressible fluid)

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-P\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] \quad \rho\nabla\cdot\mathbf{u} = \mathbf{0}$$

Inlet velocity $u_{in} = 1.5u_0\left[1-\left(\frac{2z}{H}\right)^2\right]$

Data driven pressure-drop model :

For two layers neural network :

(using the Neural Net Fitting App of MATLAB)

$$\frac{\Delta p}{\Delta L} = \text{purelin}(LW^{3,1}\times\text{tansig}(IW^{2,1}\times\text{tansig}(IW^{1,1}\times X + b^1) + b^2) + b^3)$$

HPC-based numerical simulation:

CFD parallel computing

CFD Parallel Computing

- Pre-processing
  - Flow field meshing
  - Domain decomposition
  - Boundary expansion
- Parallel algorithm
  - Process allocation
  - Parallel solution
  - Data exchange
- Post-processing
  - Flow fields' visualization
  - Hydrodynamic data's visualization

High-throughput computing

Uniform random generation by SPSS

Parameter groups (1-500)

Import

CFD Modeling by Comsol Multiphysics

1-10	11-20	......	471-500
Nodes 1-3	Nodes 4-6	......	Nodes 147-150

Results and discussion:

The accuracy and the generalization performance:

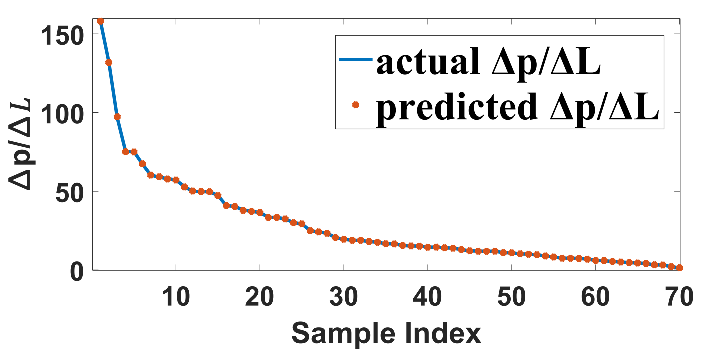


Figure 1. The actual $\frac{\Delta p}{\Delta L}$ and the predicted $\frac{\Delta p}{\Delta L}$

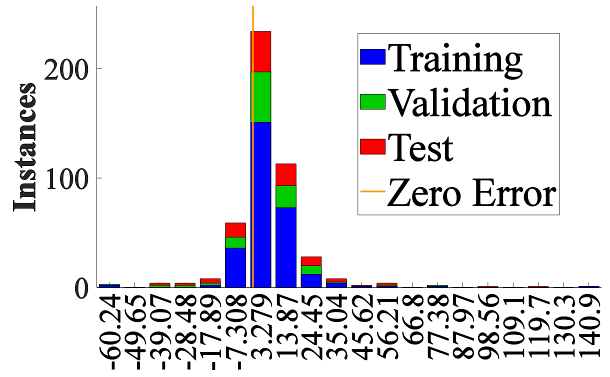


Figure 2. Error histogram with 20 Bins

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