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Optimization of porous reactors morphology based on pore network modeling and metaheuristic algorithms

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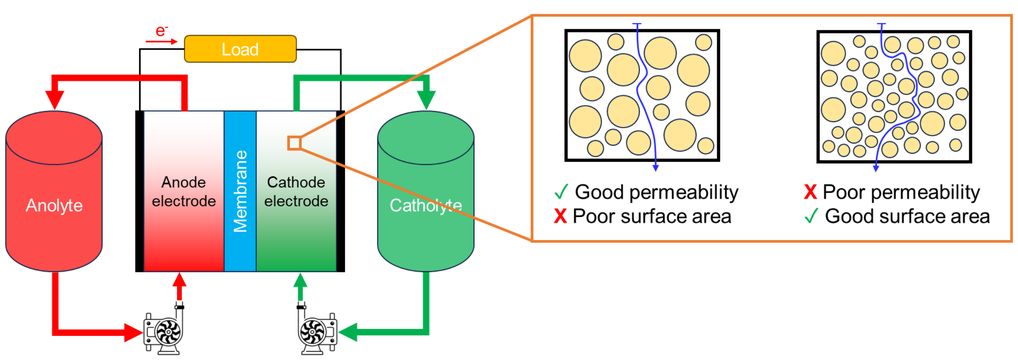
Introduction

➢ **What systems do we study?** Electrodes of electrochemical energy devices (e.g., secondary batteries)



➢ **What is an electrode?** A porous medium (e.g., carbon paper) where several physical phenomena are taking place and electricity is generated (or consumed)

➢ **What physical processes?** Electrochemical reaction and transport phenomena (fluid flow, mass transport, electric charge transport, heat transfer)

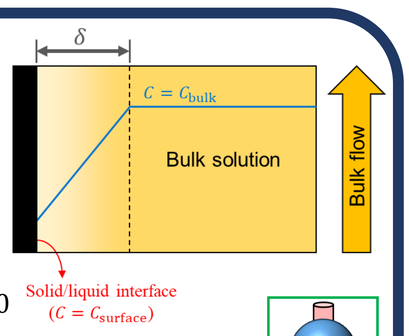
➢ **Challenge?** Low electrode performance

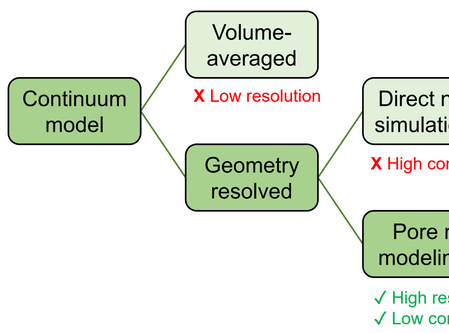
➢ **What is needed for better performance?** Balancing transport and rate phenomena through a better structural design

➢ **Research objective:** Finding an optimal structure with higher permeability and higher surface area

Methods

Modeling: A pore network model of an advection-diffusion-reaction system is developed to characterize the reactor performance.





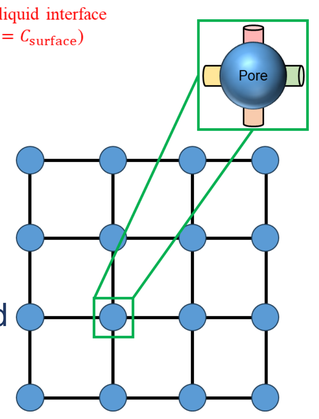
$$\nabla \cdot (\rho \boldsymbol{v}) = 0$$

$$-\boldsymbol{v} \cdot \nabla C_{\mathrm{bulk}} + D\nabla^2 C_{\mathrm{bulk}} - R = 0$$

$$R = k_{\mathrm{rxn}} A C_{\mathrm{surface}}$$

$$C_{\mathrm{surface}} = \frac{k_{\mathrm{mt}}}{k_{\mathrm{mt}} - k_{\mathrm{rxn}}} C_{\mathrm{bulk}}$$

$$Sh = a\, Re^{b} Sc^{c} \qquad k_{\mathrm{mt}} = Sh \times D/L$$



Mass balance (Stokes flow) and species conservation is solved around all pores:

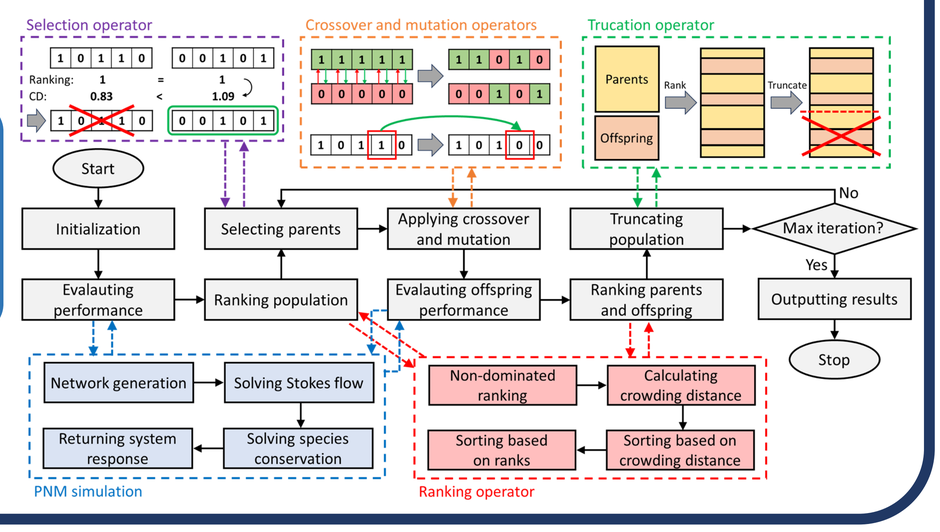
$$-\sum_{j=1}^{N_{\mathrm{neighbors}}} \rho u_{ij} S_{ij} = 0 \qquad -\sum_{j=1}^{N_{\mathrm{neighbors}}} m_{ij} S_{ij} = R_i = K_i A_i C_i$$

Optimization formulation:

$$\max_{V_g} F^1_{\mathrm{obj}} = \sum_{i=1}^{N_{\mathrm{pore}}} R_i$$

$$\min_{V_g} F^2_{\mathrm{obj}} = Q \times \Delta p$$

$$\text{s.t. } V_{g,j} \in \{0,1\} \text{ for } j = 1, 2, \ldots, n_g$$

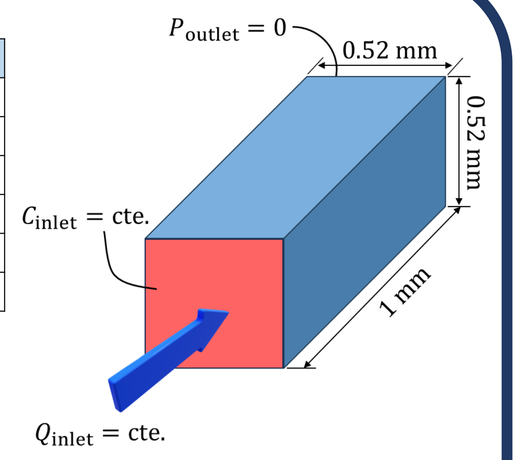


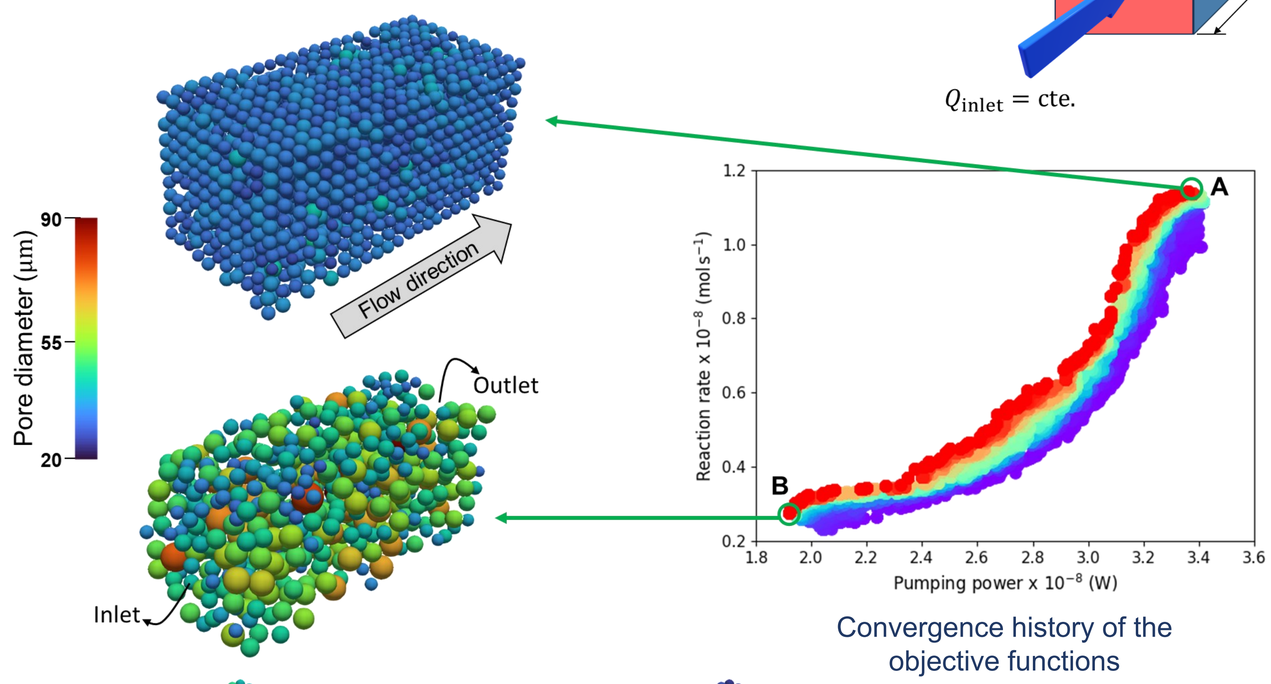
❖ Model details can be found in [1].

Results

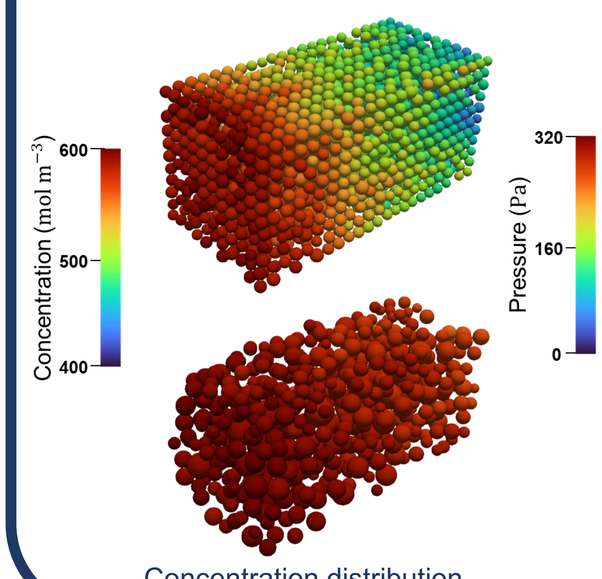
Optimization on a background grid with a shape of $25 \times 13 \times 13$ and pore spacing of $40\ \mu\mathrm{m}$ (NSGA-II algorithm for 1000 generations and 500 individuals):

Model parameter	Value
Density ($\mathrm{kg\ m^{-3}}$)	1350
Viscosity ($\mathrm{Pa\ s}$)	0.005
Diffusivity ($\mathrm{m^2 s^{-1}}$)	3.9×10^{-10}
Inlet flow rate ($\mathrm{m^3 s^{-1}}$)	10^{-10}
Inlet concentration ($\mathrm{mol\ m^{-3}}$)	600
Kinetics constant ($\mathrm{m\ s^{-1}}$)	1.72×10^{-4}

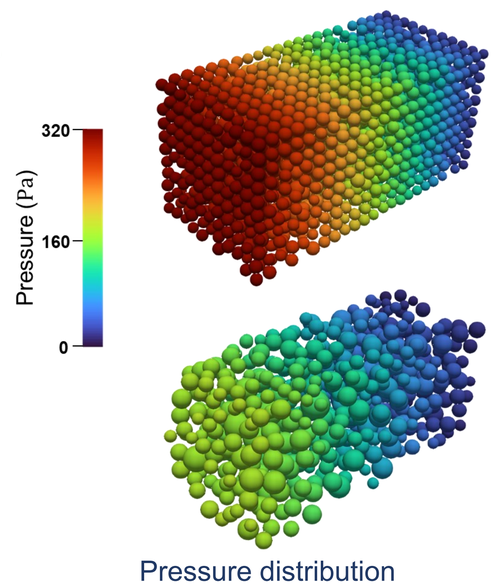




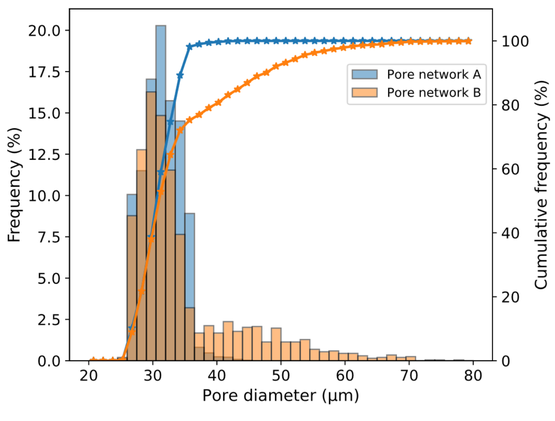
Convergence history of the objective functions



Concentration distribution



Pressure distribution



Pore size distribution (PSD)

Summary

- A pore network model of an advection-diffusion-reaction system was developed considering the effect of mass transfer at a local level.
- A general framework for optimizing pore network morphology has been proposed to make tailored microstructure at pore-level resolution.
- Thanks to the improved permeability and active surface area, the conversion (reaction) rate was increased while the pumping requirements (cost) was decreased.

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This work was supported by Grant-in-Aid for JSPS Fellows number **22KJ2198**, JSPS KAKENHI Grant number **21H04540**, JSPS Invitational Fellowship for Research in Japan number **L23534**, and Initiative on Recommendation Program for Young Researchers and Woman Researchers, Information Technology Center, The University of Tokyo.

References

[1] M. Alizadeh, et al., *Comput. Struct.*, **301**(2024): 107452.

[2] N. Misaghian, et al., *J. Electrochem. Soc.*, **170**(2023): 070520.

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