Multi-Scale Modeling of Electrochemical Separation: From Material Modeling to Process Optimization

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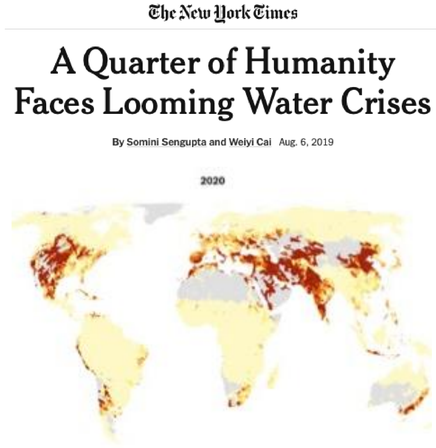
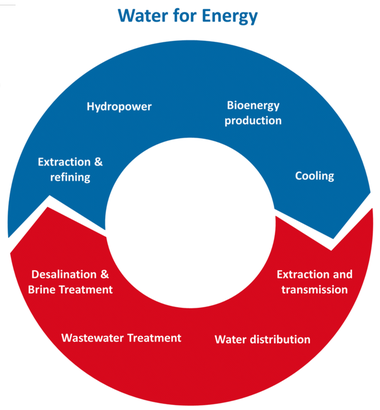
Internships

Water scarcity in 21st century



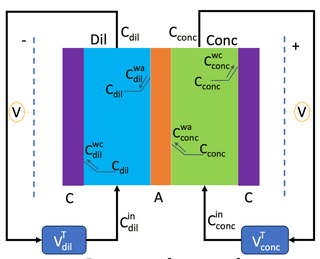


- Thermoelectric power plants use ~42% total freshwater in USA.
- ~12.6% of total energy consumption for water related purposes.
- Actively seeking simple electrified separation units (e.g. Electrodialysis, ED; Electrodeionization, EDI; Capacitive Deionization, CDI) with low pressure & energy requirement.

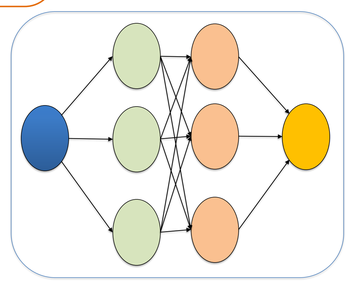
Computational Frameworks

Continuum model

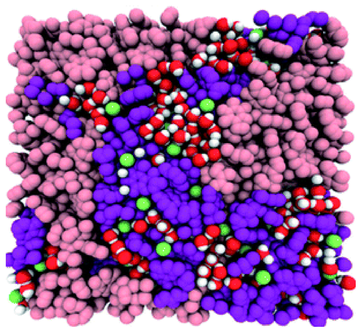
$$\frac{dC_i}{dt} = \frac{A}{V_k}\sum J_i \qquad V = \sum E_i$$



Separation unit

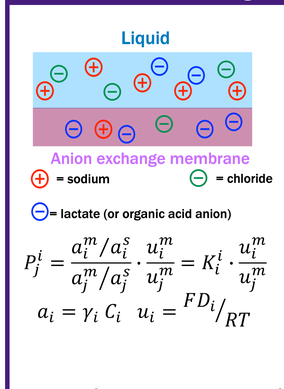


Data-driven modeling



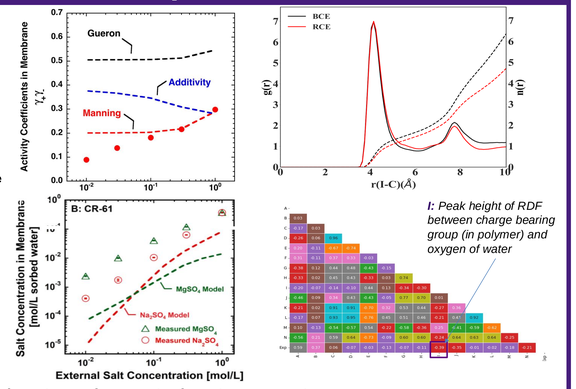
Molecular Dynamics (MD)

Modeling of ion transport in membranes

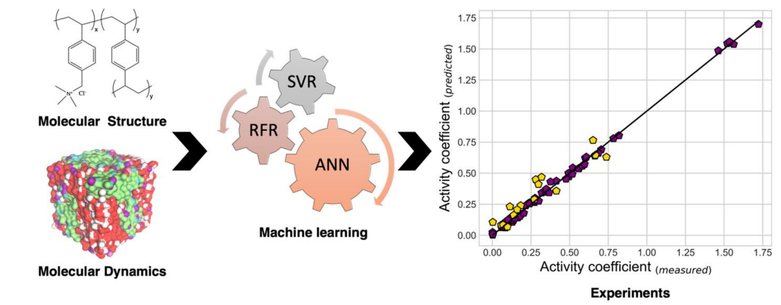


$$P_j^i = \frac{a_i^m/a_i^s}{a_j^m/a_j^s}\cdot\frac{u_i^m}{u_j^m} = K_i^i\cdot\frac{u_i^m}{u_j^m}$$

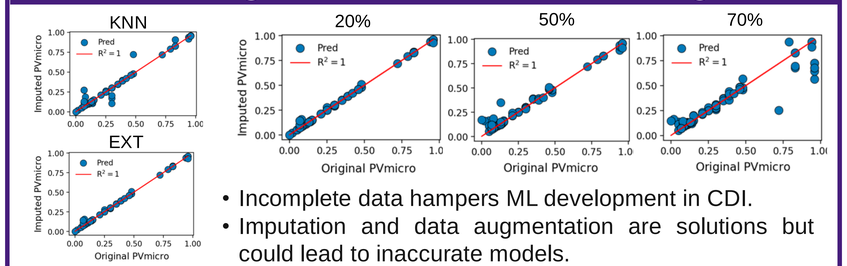
$$a_i = \gamma_i C_i \quad u_i = {FD_i}/{RT}$$



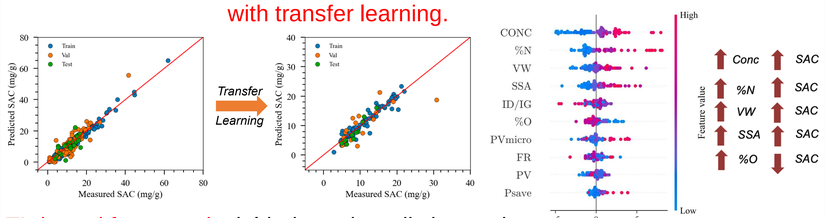
- Membrane structure & ion type impacts ion transport.
- Interest in ionic transport models applicable across different ionic systems.
- MD showed most counterions in (block or random) are inside the first solvation shell.
- Herein, combining MD and experiment can improve ion transport modeling.



Missing data in Data-driven modeling



- Incomplete data hampers ML development in CDI.
- Imputation and data augmentation are solutions but could lead to inaccurate models.
- Proposed 'ImputeNet' to resolve inaccuracy in model with transfer learning.

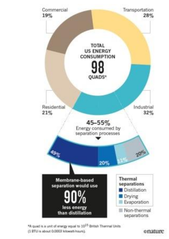


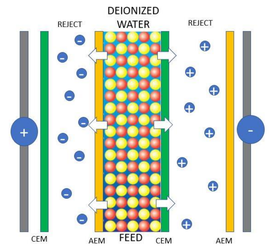
TL-based framework yielded good prediction and discovered new adsorption capacity with >200 mg/g.

Ongoing Works

- Physics-Informed Machine Learning for Electrochemical Separation.
- Investigating real-time control of electrochemical separation with reinforcement learning.

Discovering Energy Efficient Separation

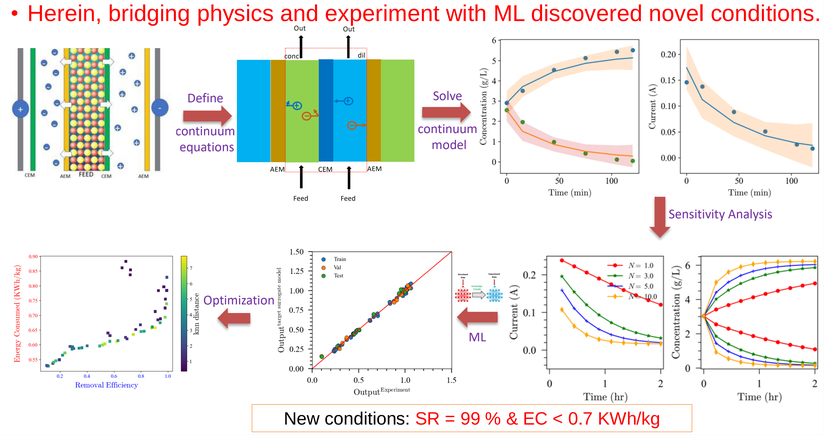




Operational:
Voltage, flowrate, stacks, spacer length.

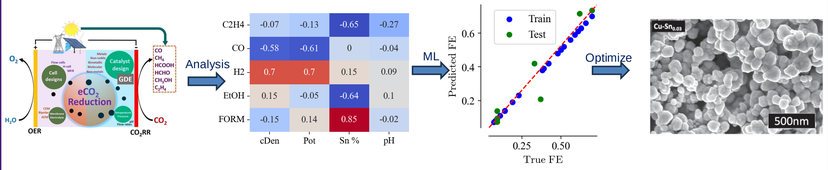
membrane/resin :
Packing density
Ion exchange capacity
Porosity

- Searching for best condition is expensive.
- Limited dataset & no data-driven optimization strategy.
- Herein, bridging physics and experiment with ML discovered novel conditions.



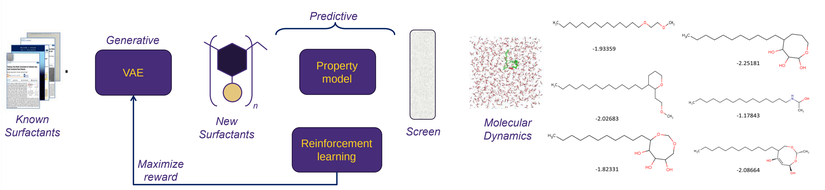
New conditions: SR = 99 % & EC < 0.7 KWh/kg

Electrochemical CO_2 conversion



Novel framework yielded experimentally verifiable optimized conditions with 55% C_2H_5OH FE, which surpasses experimental approach (~48%).

Tailored Molecular Design



Novel stable molecules verified with MD simulation were discovered.

Skillsets

Programming

python MATLAB git

- Numerical modeling
- Data analysis & visualization
- High performance computing

Machine Learning

PyTorch mlflow learn aws docker

Chem Eng & Chemistry

GROMACS FAST. FLEXIBLE. FREE. LAMMPS RDKit

- Process simulation
- Structure property modeling
- Polymer/surfactant simulations

Experiment: Catalyst synthesis & testing; CO Spectroscopy