NAWI National Alliance for Water Innovation

Evaluating the Design & Operation of an Electrodialysis Desalination System

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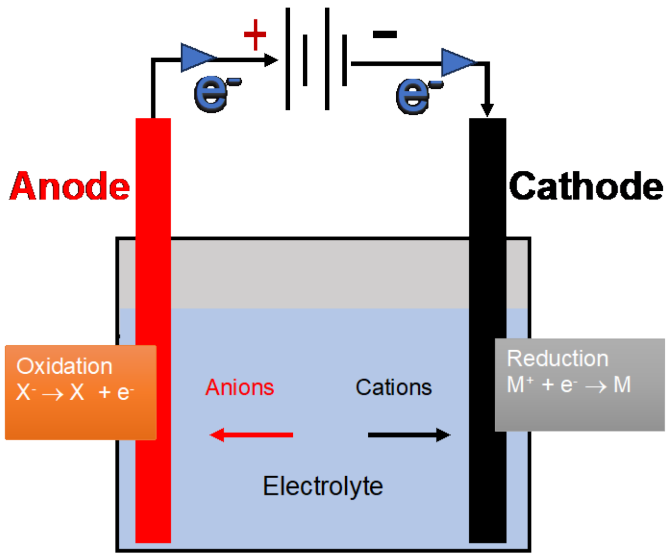
Context: electrochemical processes and WaterTAP



A generalized electrochemical cell.

- ❑ Driven by electricity.
- ❑ Electrode reactions for chemical processes.
- ❑ Electrical fluxes for physical processes.

Advantages

- Clean energy.
- Integrated physical and chemical processes.
- Competitive performance in certain cases.

Performance prediction

Technoeconomic assessment

Deepen insight into the system

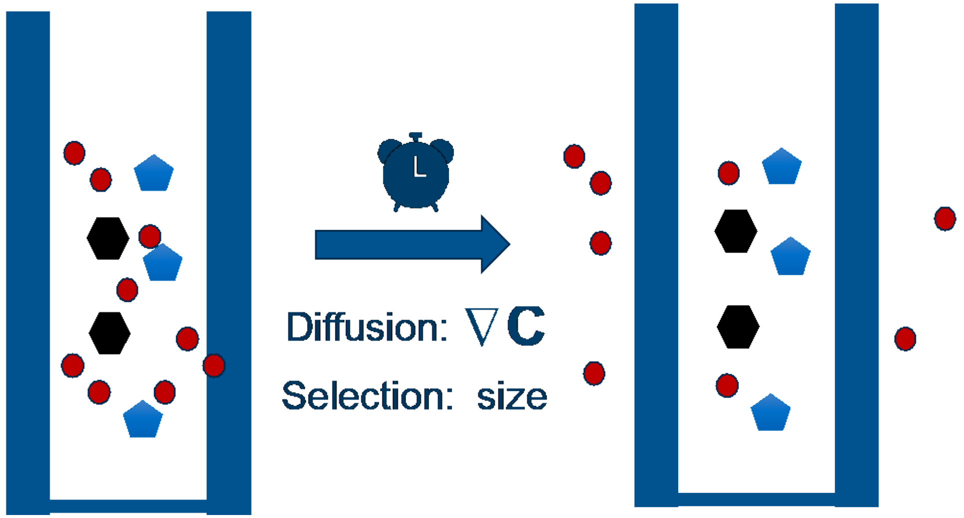
WaterTAP

Guide engineering design and operation

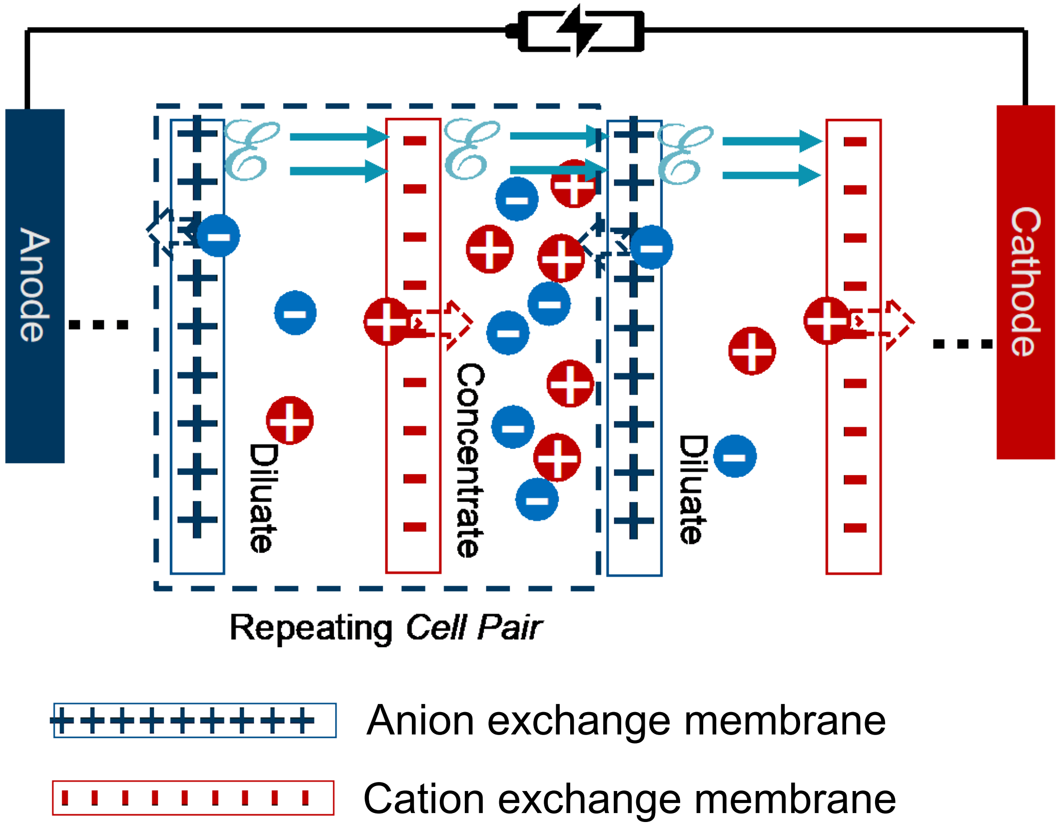
Guide research

What is electrodialysis (ED)?

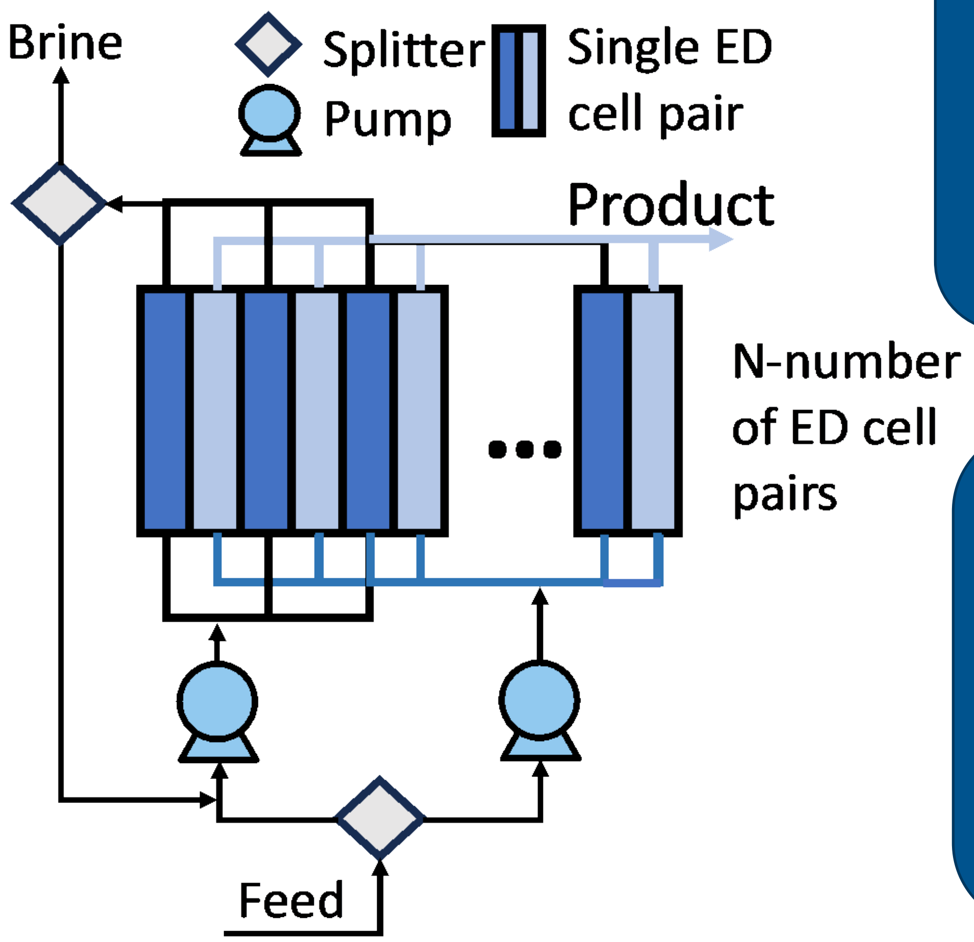
1 Dialysis



2 Electrodialysis stack



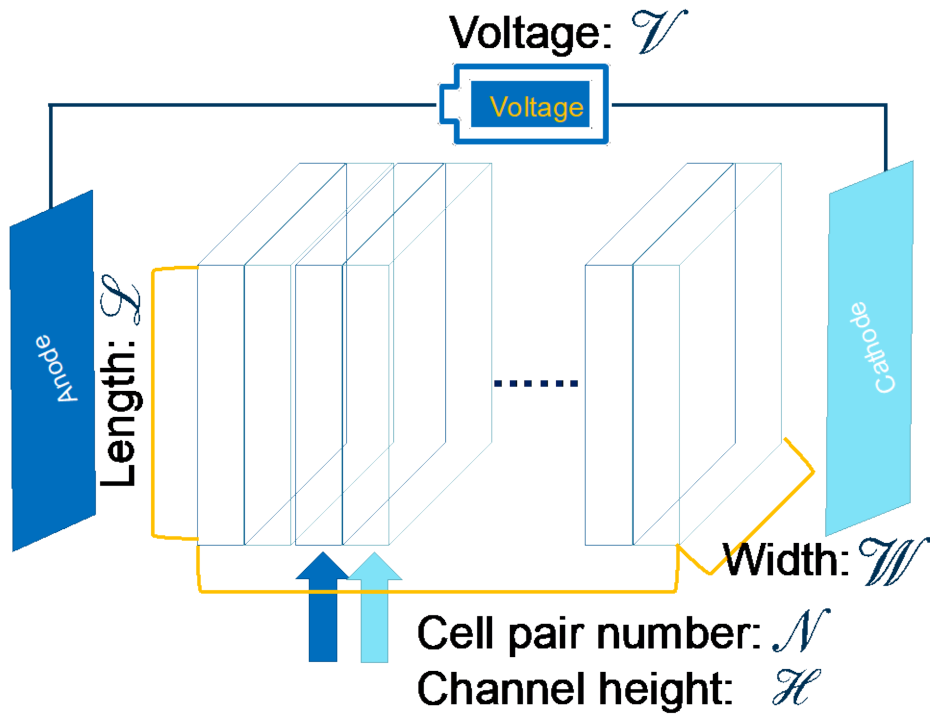
Goal: a cost-effective ED desalination system



A defined treatment task:
Feed salinity.
Water recovery.
Product salinity.

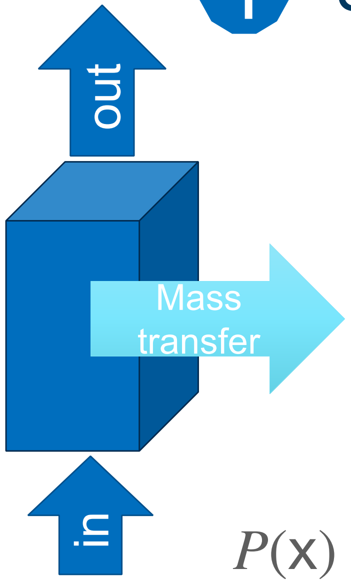
Objectives:
Configured system.
Cost estimation.
Performance satisfaction.
Minimized cost.

Key designing and operation parameters

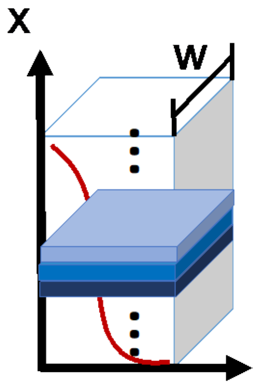


Approach: model construction

1 Unit model: all physical processes.



$P(x) = P$



Finite difference to solve 1-D ODE.

Mass transfer mechanisms

Ions	Electrical flux	Diffusion
water	Osmosis	Electro-osmosis

$$QC_i - QC_e + J_S A = 0$$

Other phenomena simulated

- Potential gradients in solution, diffusion layers, and membranes.
- Frictional pressure.

2 Costing model: capital investment and operation cost.

- Electricity
- Ion exchange membranes
- Electrodes
- Other stack materials
- Pumps
- Power supply device

$$\text{LCOW}\left([\$\ \text{m}^{-3}]\right) = \frac{\text{total annual cost}}{\text{annual product water volume}}$$

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Approach: Constrained Optimization

$$\min_{x \in \mathbb{R}^n} f(x)$$ → $$\min_{\mathbf{x}} \text{LCOW} = f(\mathbf{x}, \mathbf{P})$$

$$\text{subject to} \begin{cases} c_i(x) = 0, & i \in \mathcal{E}, \\ c_i(x) \geq 0, & i \in \mathcal{I}, \end{cases}$$ →

$$QC_i - QC_e + J_S A = 0$$

$$J_e = \left(\sum_{i^+} t_{i^+}^{cx} - \sum_{i^-} t_{i^-}^{cx}\right)(\xi i(z)/F)bdz$$

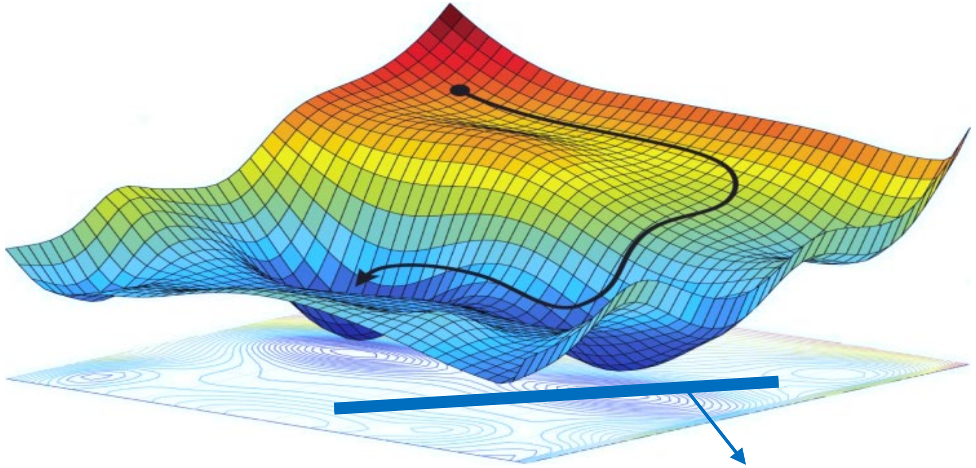
$$J_D = \sum_i [P_i(n_i^C(z) - n_i^D(z))](b/\delta^{cx})dz$$

...

All process and costing model equations except LCOW.

Proper *scaling* and *initialization*

Nonlinear Programming (NPL)
Interior-point filter line-search algorithm
IPOPT (Interior Point OPTmizer) solver



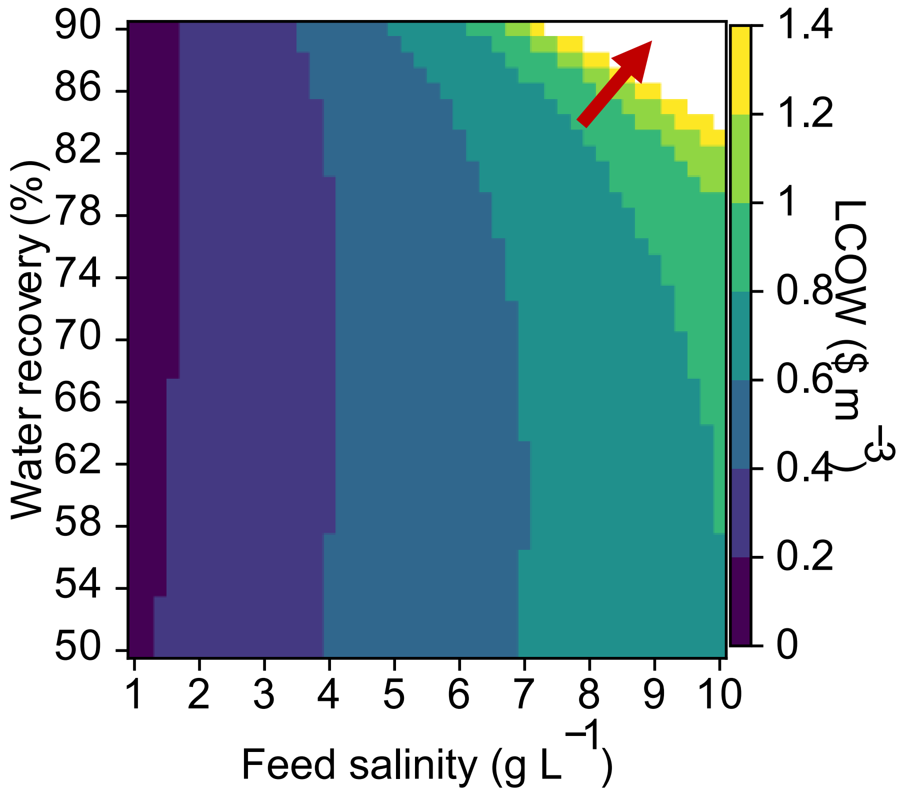
Outcomes: minimized cost for varying treatment load

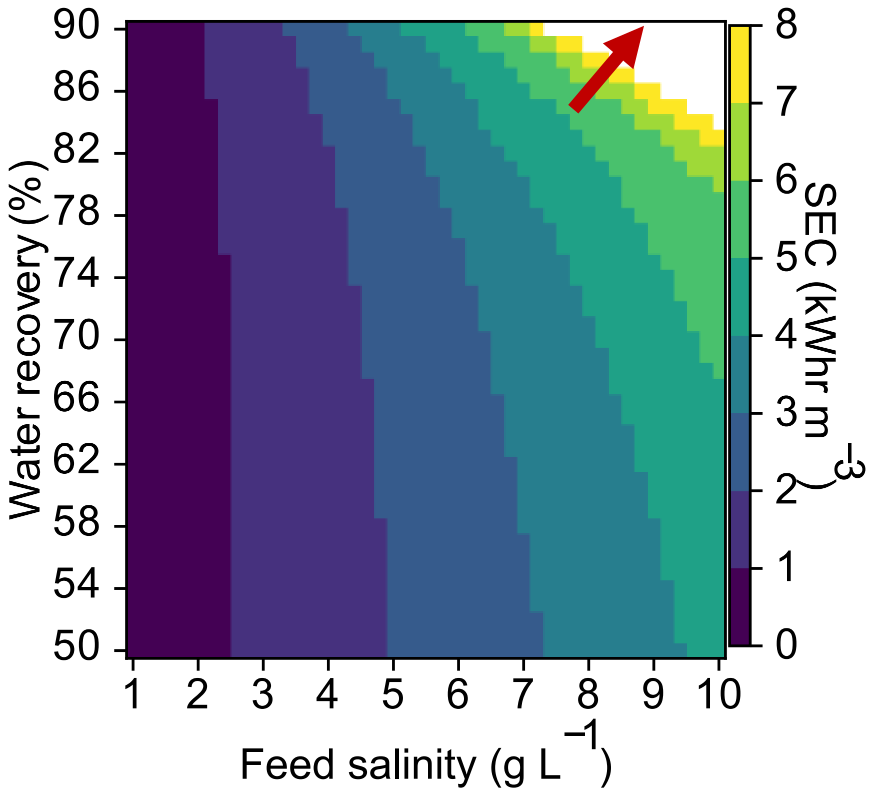
Treatment load

Feed Salinity (g L^{-1})	1-10
Product Salinity (g L^{-1})	0.5
Water Recovery	50% - 90%

Optimizer

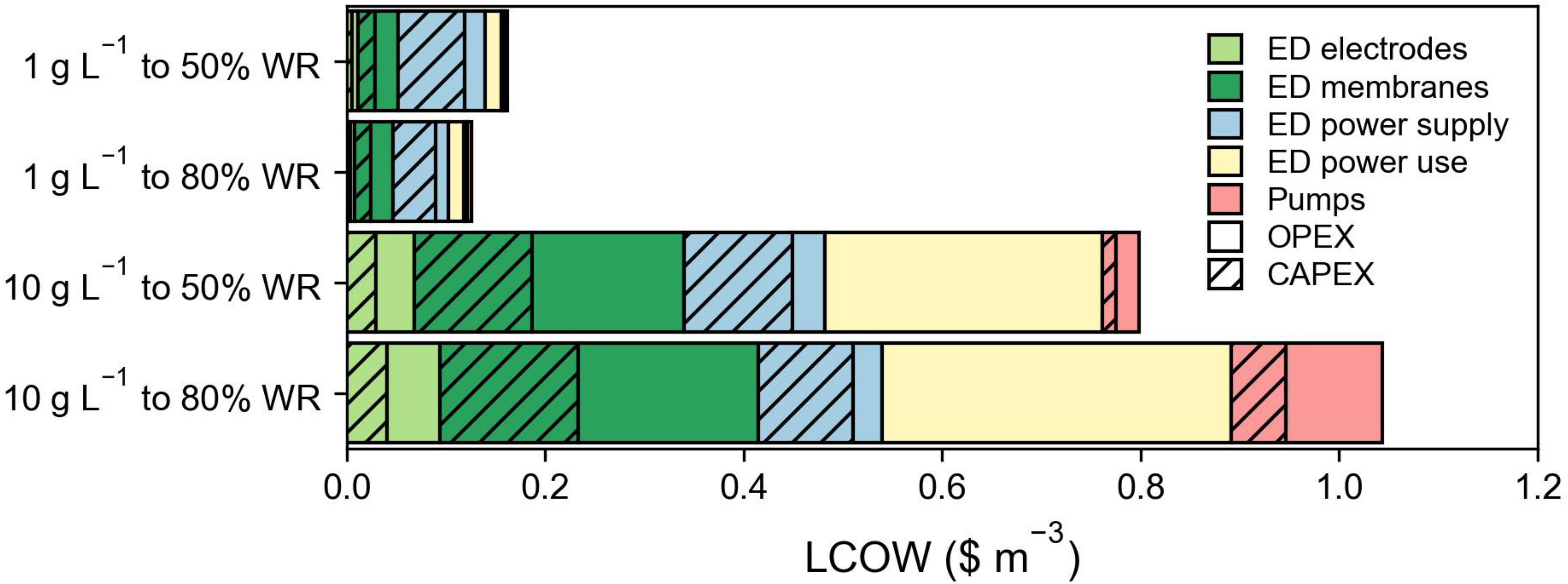
Var	Initial value	Bounds
Stack voltage (V)	10	0-3000
Cell pair number	100	10-10000
Cell length (m)	1.68	0.1-10





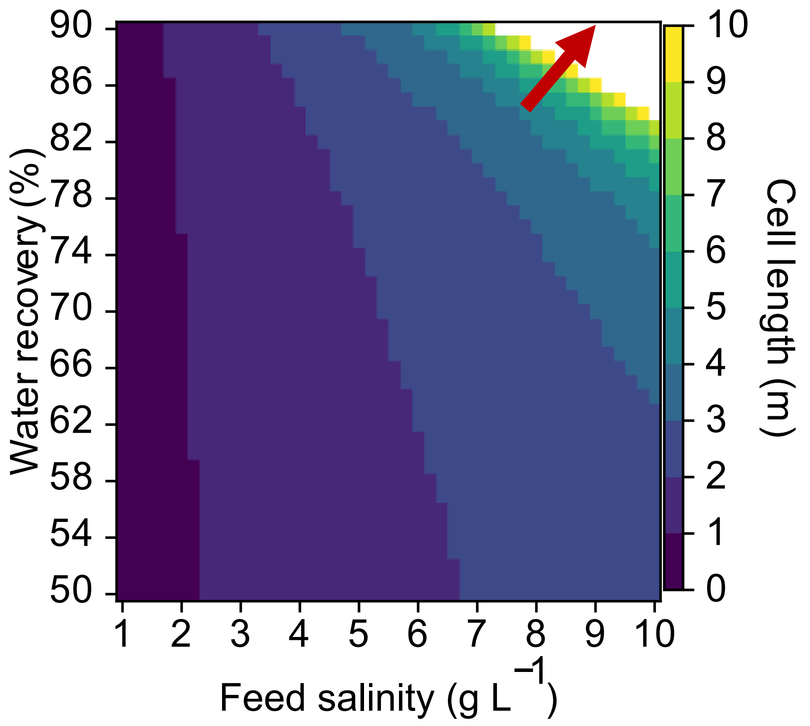
The contour line density suggests variation gradient.

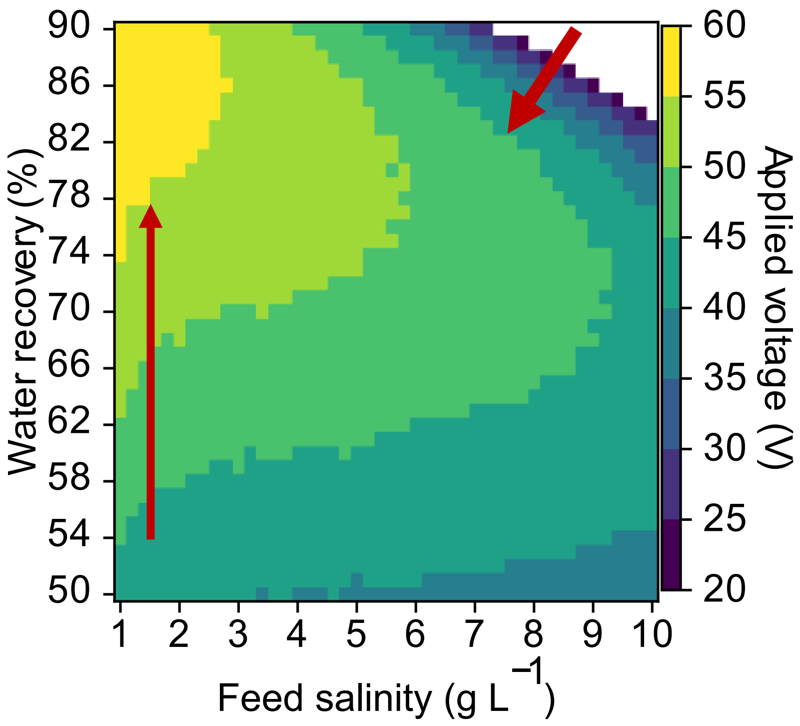
Outcomes: itemization of cost

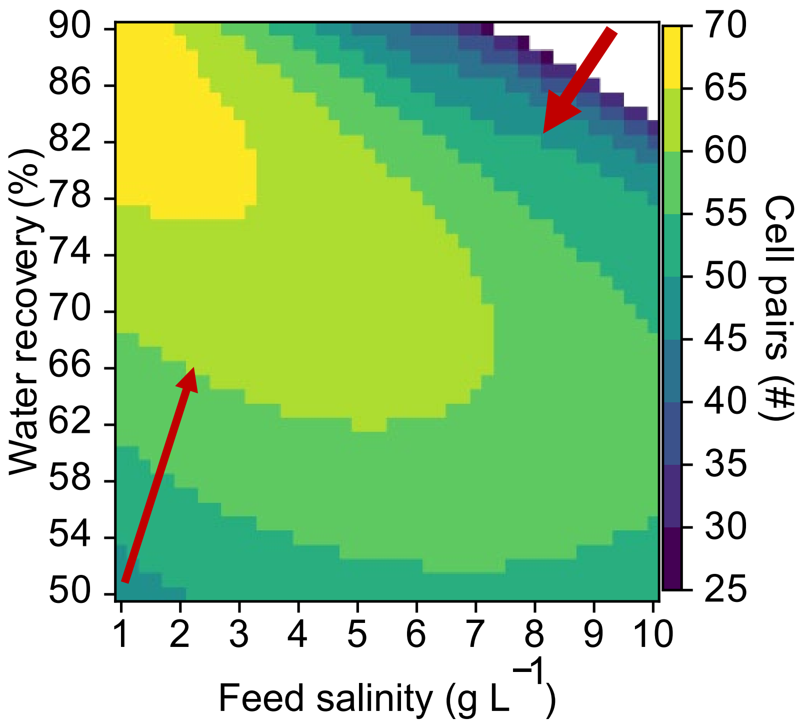


Low load	Material cost > power cost. Investment capital > operation cost.
High load	Power cost becomes competitively important. Operation cost becomes important.

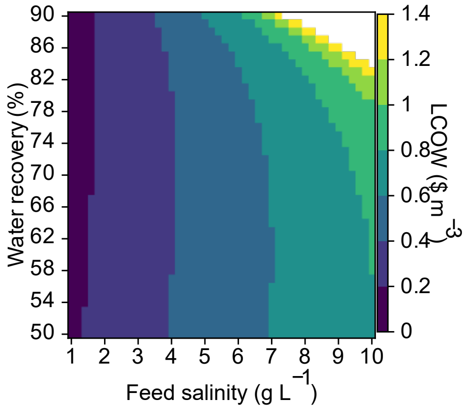
Outcomes: contours of optimizer variables







LCOW:



- Voltage (V) ~ cell pair number (N).
- Cell length (L) ~ LCOW.
- Increase V and N for low salinity's higher recovery.
- Increase L for high salinity and high recovery.
- Cell length appears to be the most important designing parameter.

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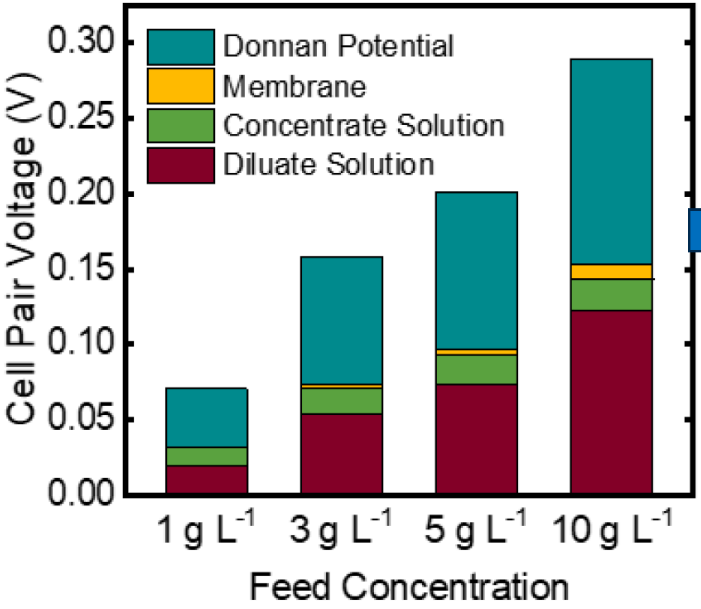
Outcomes: the importance of cell length vs. voltage

High voltage for high loads is a tempting intuition or "fact".



A fixed ED stack.

- "Increasing the extent of salt removal in ED inherently requires the application of larger voltage."

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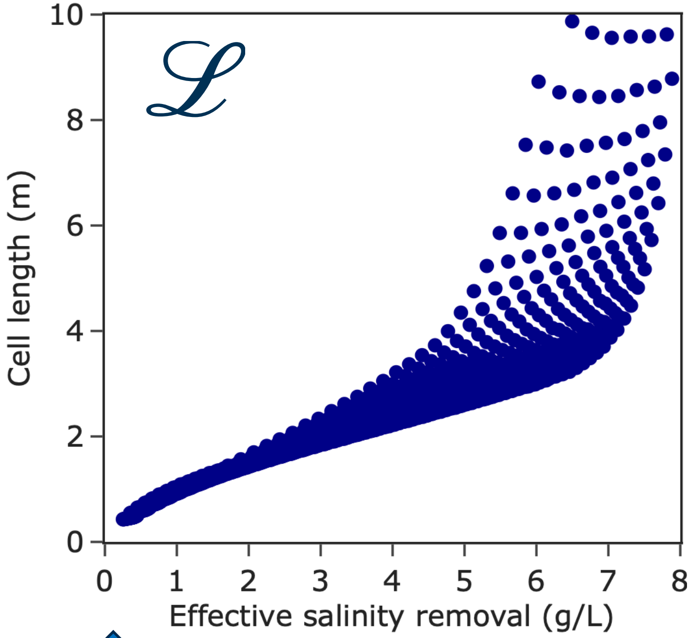
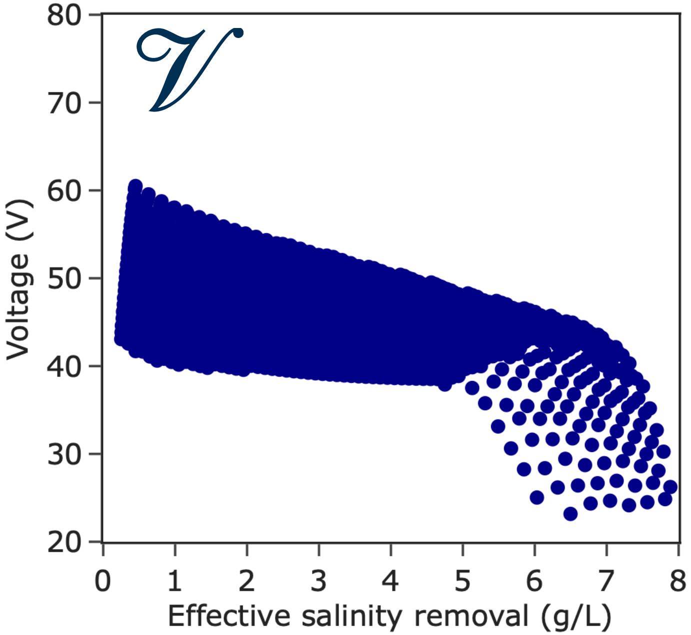
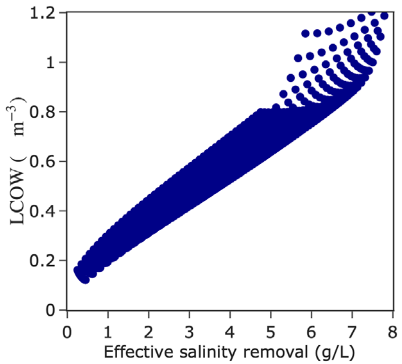
Cell length, rather than voltage, is the cost-effective solution.





Correlative trend.

LCOW:



- Multivariate optimization yields more accurate cost-effective design/operation.
- High loads should rely on more cell length.

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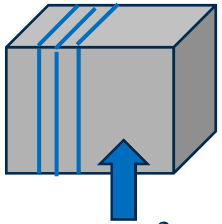
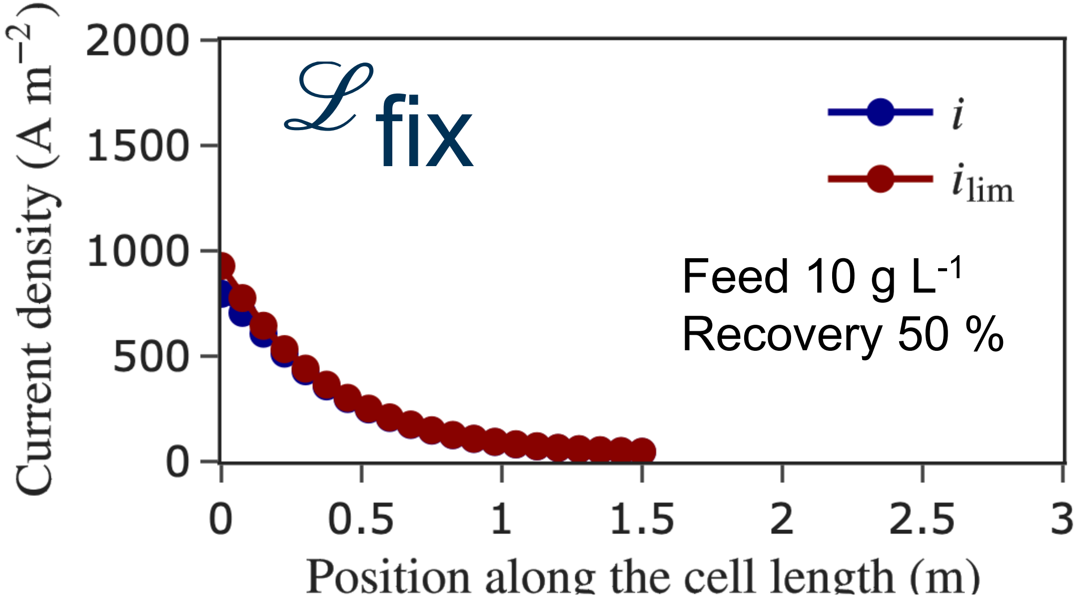
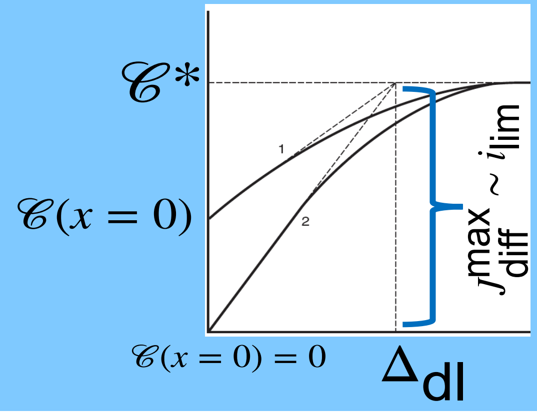
Why is length critical for a cost-effective design?

$\mathscr{L} = 1.50$ m
$\mathscr{N} = 150$
$\mathscr{V} = 123.46$ V
SEC = 4.91 kWh m^{-3}
LCOW = 1.00 \$ m^{-3}
$\Delta^{D}_{\text{dl, cem}} = 47\mu$m

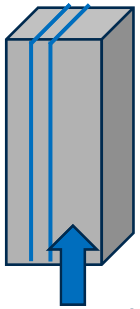


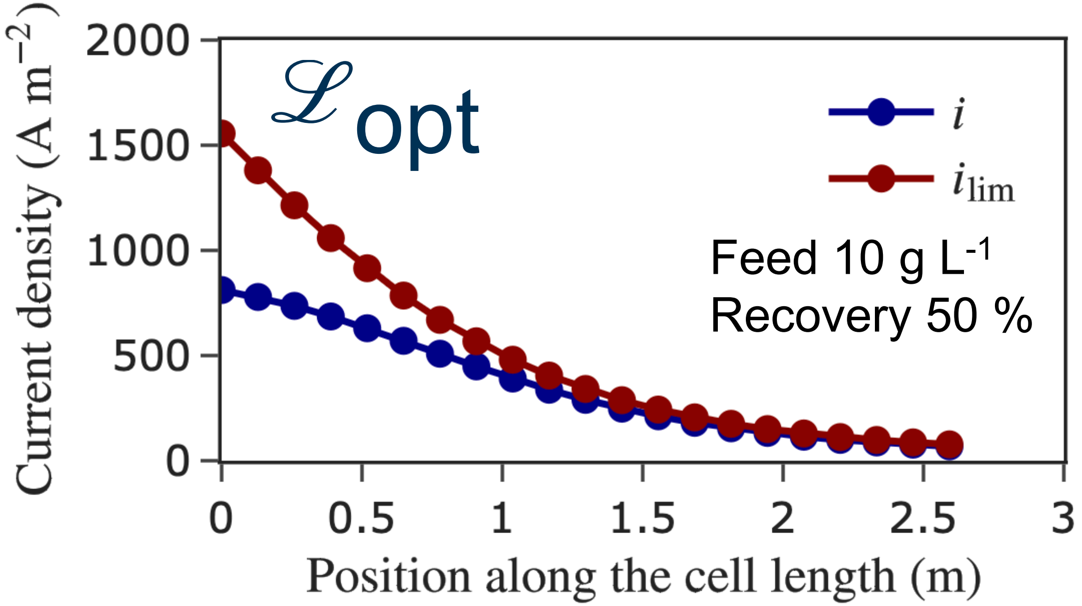


Limiting current density ~ largest near-surface diffusion



$\mathscr{L} = 2.59$ m
$\mathscr{N} = 53$
$\mathscr{V} = 38.51$ V
SEC = 4.26 kWh m^{-3}
LCOW = 0.80 \$ m^{-3}
$\Delta^{D}_{\text{dl, cem}} = 28\mu$m





- The optimized (longer) cell length operates more underneath the limiting current density, mitigating the limitation of diffusion.

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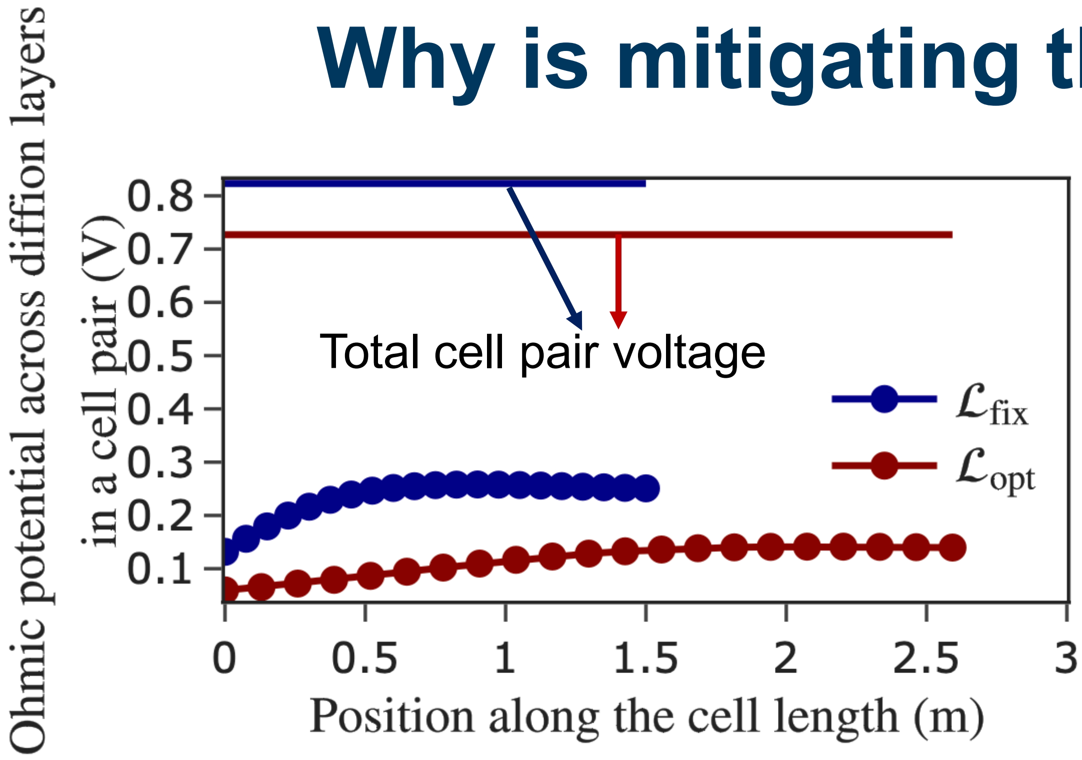
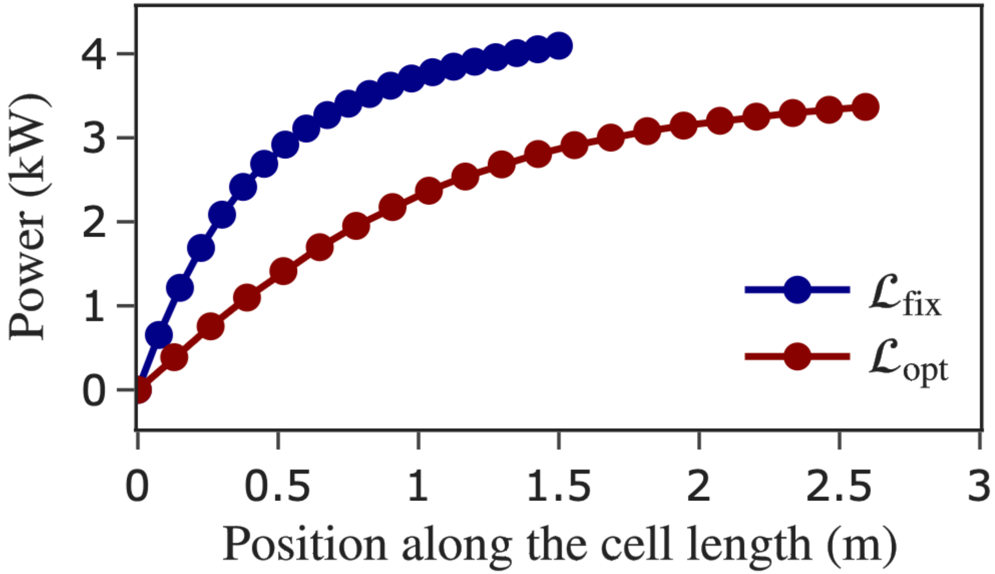
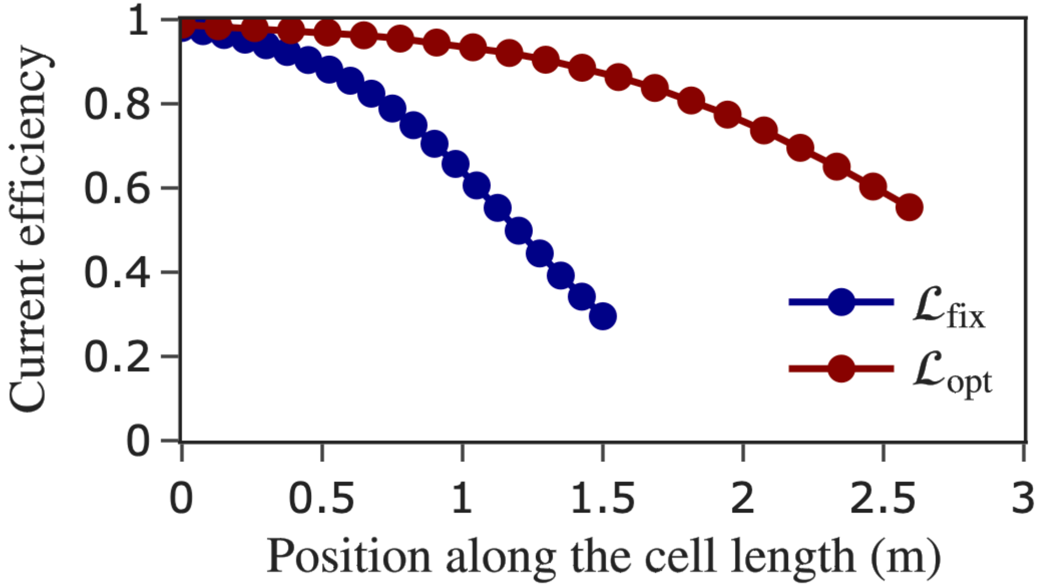
Why is mitigating the diffusion limitation better?





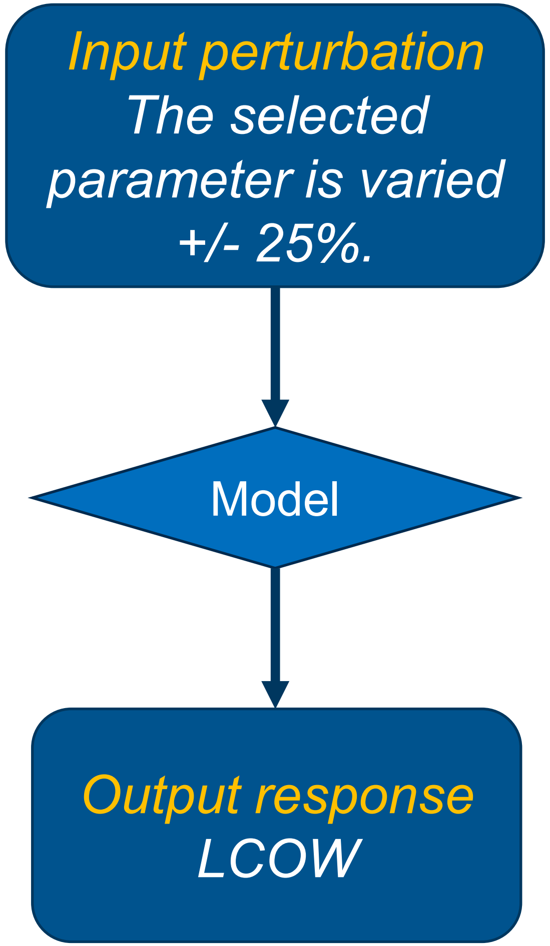


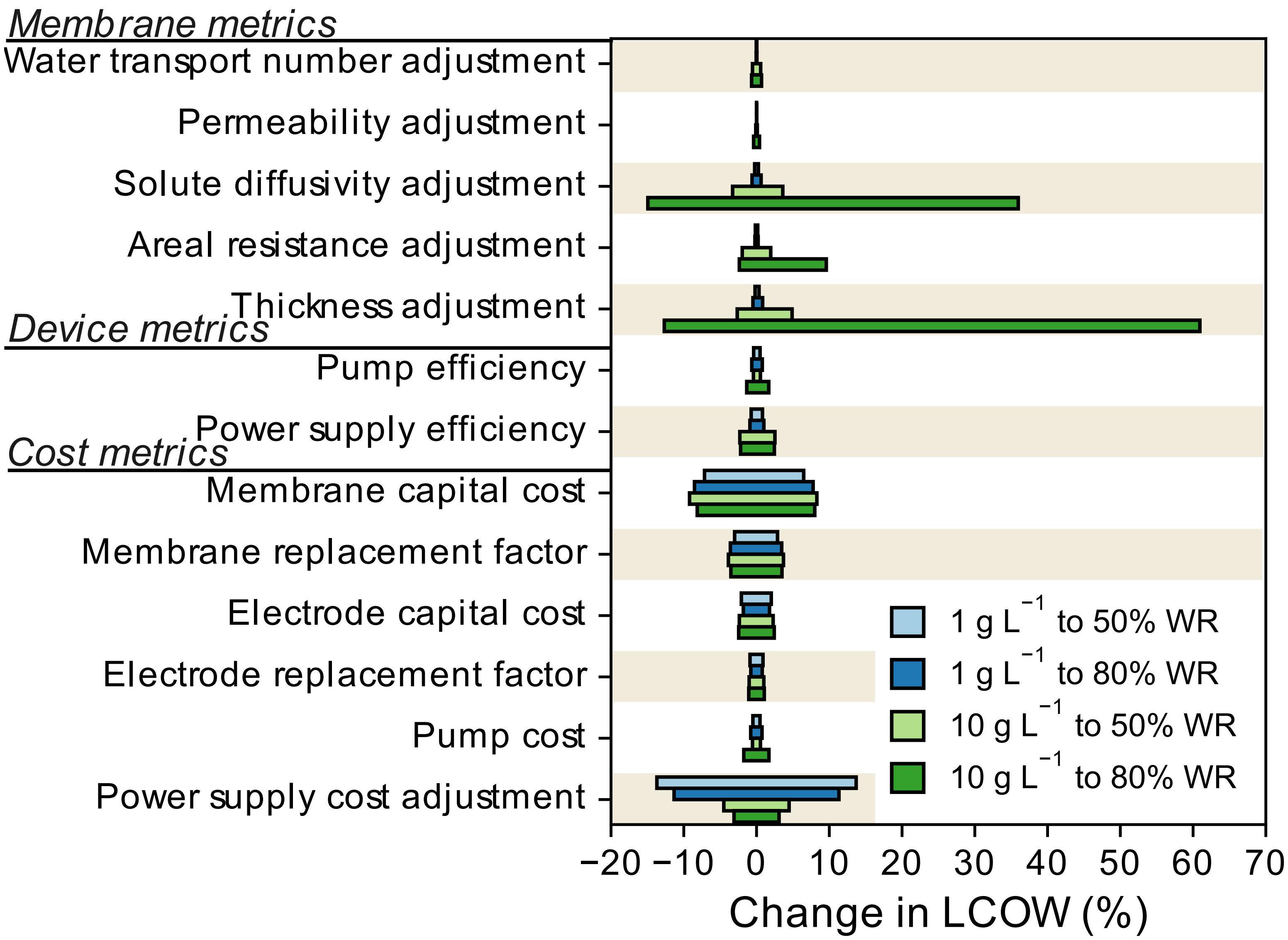
- Larger ohmic potential of DL suggests larger resistance.
- Current efficiency =

$$\frac{\text{Current used to drive ion fluxes}}{\text{Total current}}$$

- $P(x) = \int_0^x u(x) i(x) b \, \mathrm{d}x$

Outcomes: sensitivity of key params to optimized LCOW





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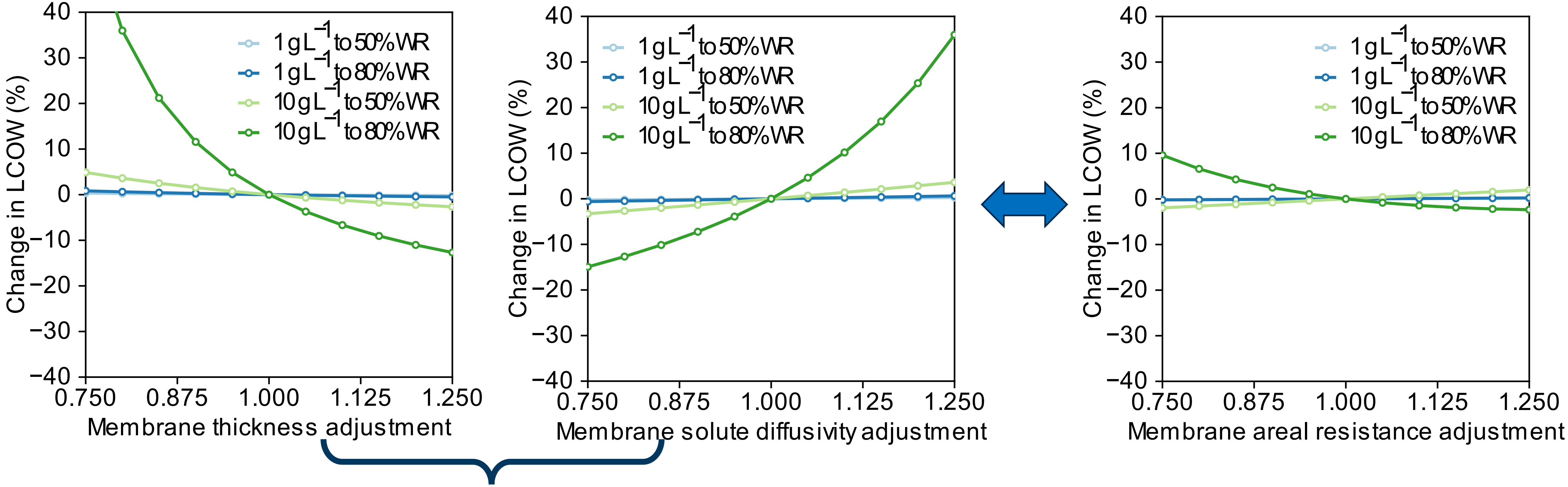
Outcomes: detailed sensitivity of LCOW's response to membrane properties



Guidance to membrane development:

- Consider the leverage between resistance and and diffusivity.
- Our sensitivity suggests diffusivity is more dominating for LCOW.

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Summary

Water TAP

Performance prediction

Technoeconomic assessment

Guide engineering design and operation

Deepen insight into the system

Guide research

ED

- Major mass transfer schemes simulated to predict performance.
- TEA in categories of power, materials and supplies and of capital and operational cost.
- Multivariate optimization by NPL to reveal more accurate cost-effective design.
- In-depth understanding of length’s importance and current use.
- Guided research in ion exchange membrane development.

Future work and acknowledgement

- Opportunities to support users in research and other communities.
  - Collaborating with experimental teams (NMSU) on ED pilot systems.
- Other ED functionalities
  - Selective desalination.
  - Bipolar membrane ED for chemical generation
  - Others as needed.

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  - Kejia Hu (LBNL)

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