A Multi-Physics Study on High-Specific Power Li-O_2 Batteries for Electric Aircraft

Mohit Mehta, Kristian Knudsen, Brian McCloskey, John Lawson

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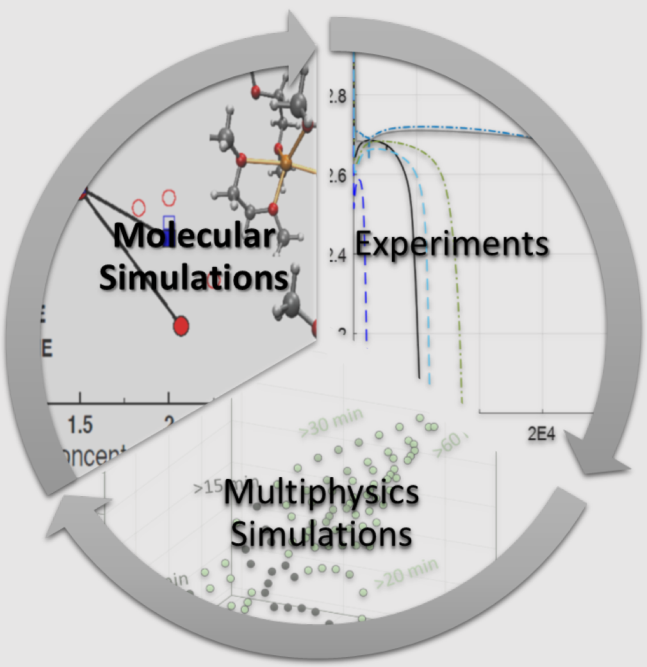


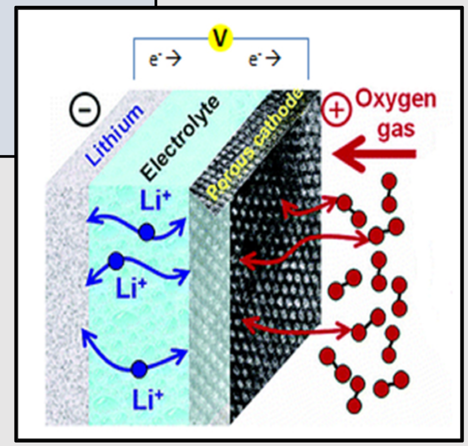
1. Introduction
2. Model calibration
3. Parametric Study
4. Simulation Based Optimization

NASA Strategic Plan for Green Aviation

Strategic Thrust 4: Transition to Low Carbon Propulsion

Alternate Propulsion Demonstrators

Li-Air Battery



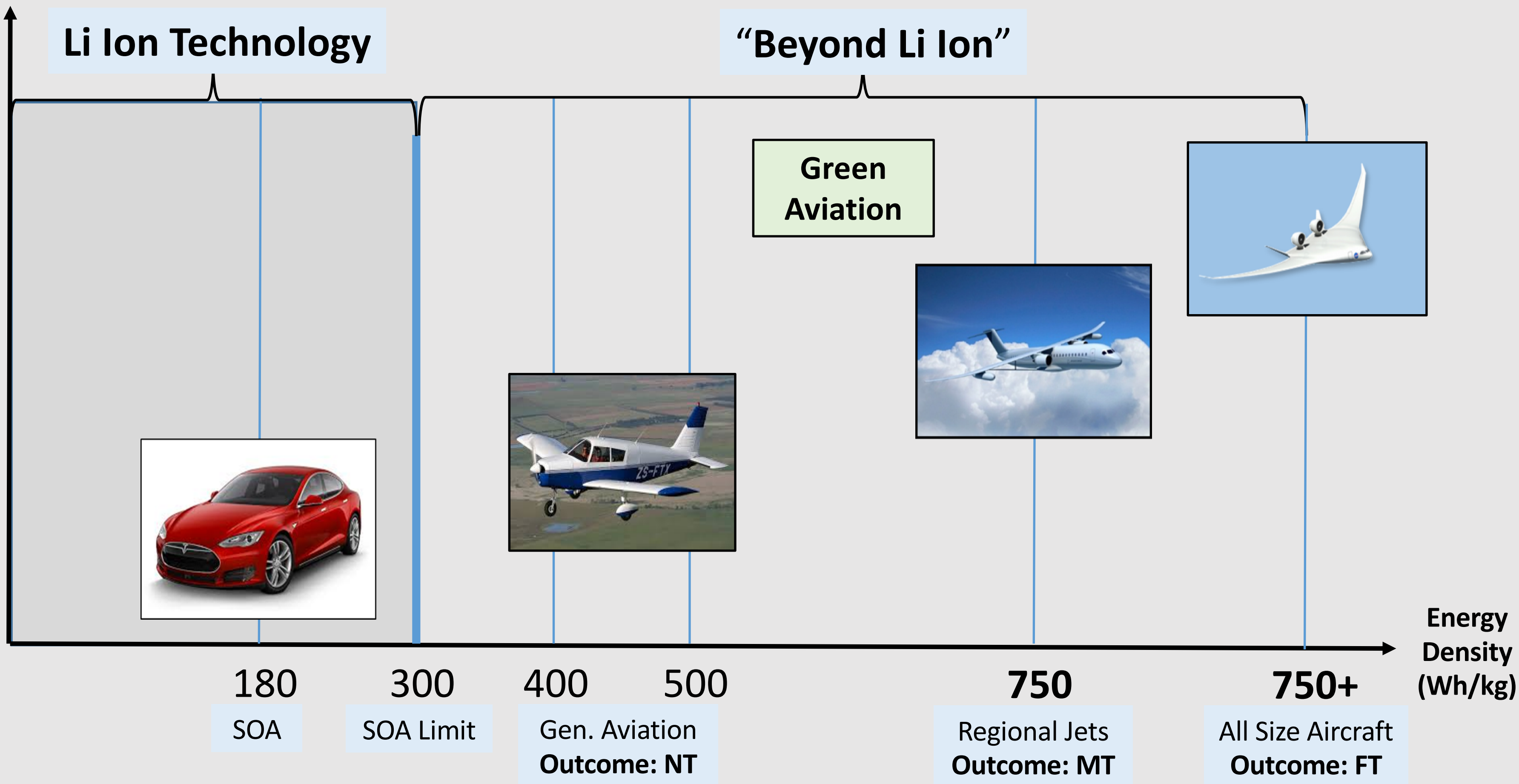
- Zero emissions
- Low noise
- Energy efficient

Batteries are a critical enabler for electric aircraft

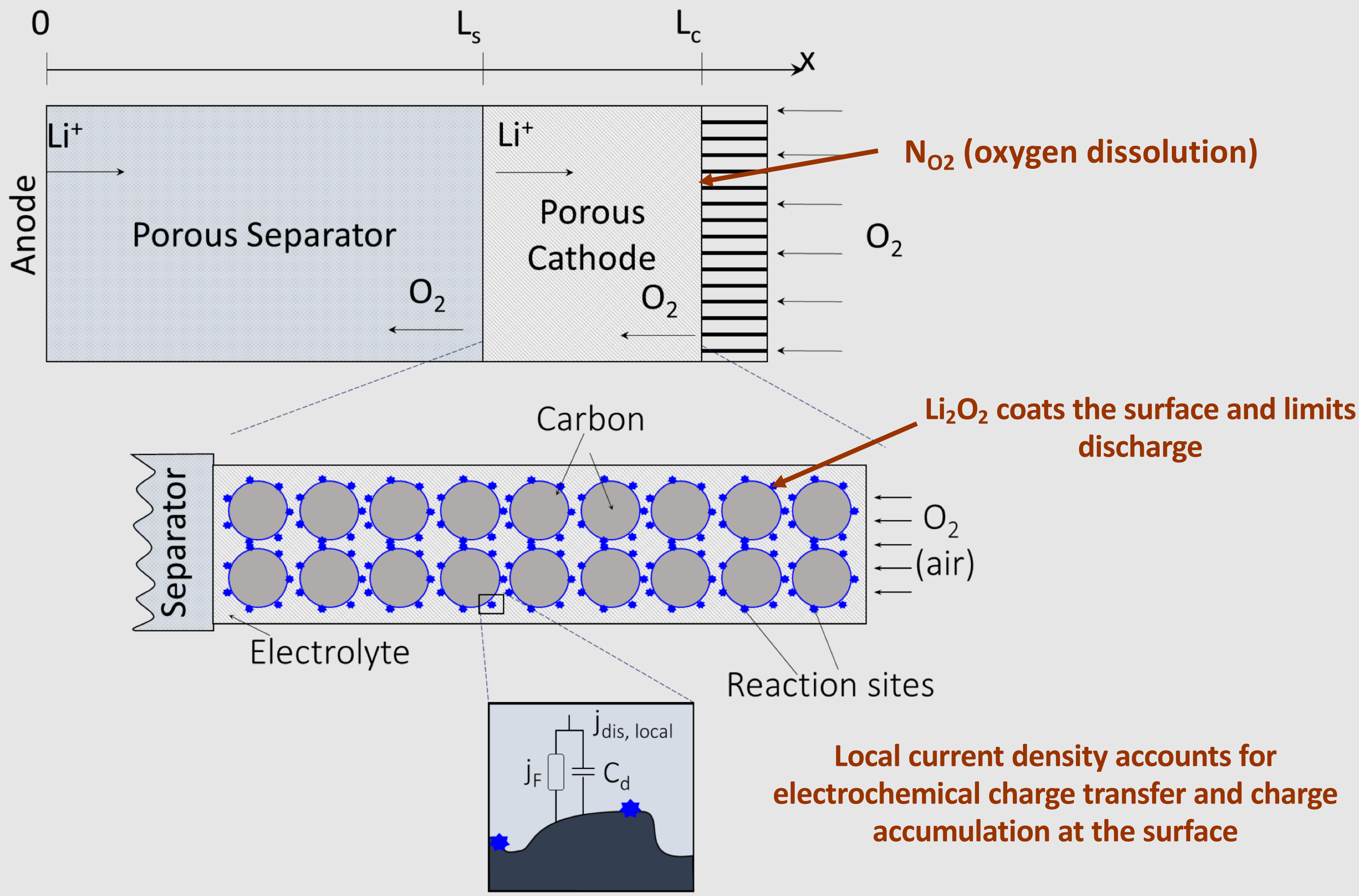
Green Aviation Battery Requirements

Major requirement is: High Energy Density

Other requirements are **rechargeable**, **safety**, power, recharge time, cost, etc.

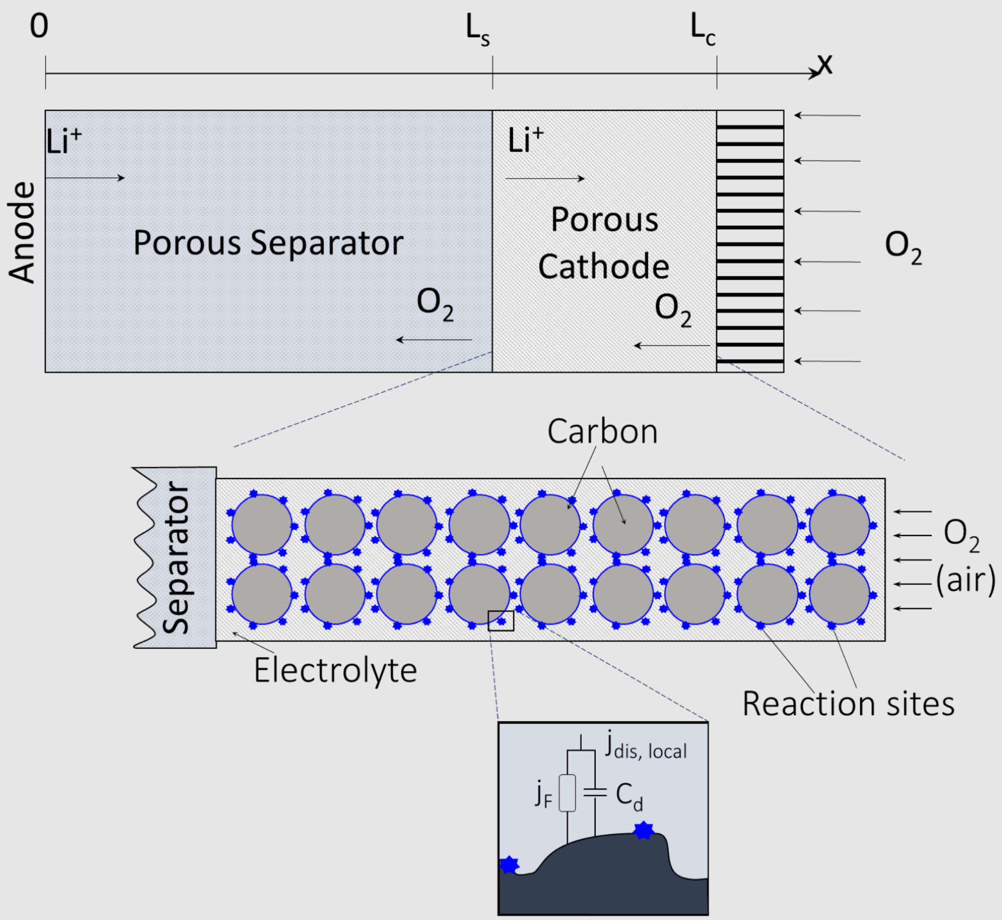


Working of a lithium-oxygen battery



Local current density accounts for electrochemical charge transfer and charge accumulation at the surface

Modeling a lithium-oxygen battery



Over-voltage, thermodynamic

$$\eta = \phi_{\mathrm{Li}} - \phi - E^0 - V_{\mathrm{discharge}}$$

electrolyte, electrode, Li_2O_2

$-I$ (electron current)

$$\nabla \cdot \left(\sigma_{\mathrm{eff}} \nabla \phi\right) + R_C = aC_d \frac{\partial\left(\phi - \phi_{\mathrm{Li}}\right)}{\partial t}$$

$-I_{\mathrm{Li}}$ (electrolyte current)

$$\nabla \cdot \left(\kappa_{\mathrm{eff}} \nabla \phi_{\mathrm{Li}} + \kappa_D \nabla \ln c_{\mathrm{Li}}\right) - R_C = aC_d \frac{\partial\left(\phi - \phi_{\mathrm{Li}}\right)}{\partial t}$$

$-I_{\mathrm{Li}}$ (electrolyte diffusion flux)

$$\frac{\partial\left(\epsilon c_{\mathrm{Li}}\right)}{\partial t} = \nabla \cdot \left(D_{\mathrm{Li,eff}} \nabla c_{\mathrm{Li}}\right) - \frac{1 - t^+}{F} R_C - \frac{I_{\mathrm{Li}} \cdot \nabla t^+}{F}$$

$-I_{O2}$ (O_2 diffusion flux)

$$\frac{\partial\left(\epsilon c_{O_2}\right)}{\partial t} = \nabla \cdot \left(D_{O_2,\mathrm{eff}} \nabla c_{O_2}\right) - \frac{R_C}{nF}$$

ϵ (porosity change -from Li_2O_2 deposition)

$$\frac{\partial \epsilon}{\partial t} = -R_C \frac{M_{\mathrm{discharge}}}{nF\rho_{\mathrm{m,discharge}}}$$

$$V_{\mathrm{discharge}} = j_{\mathrm{dis}} \delta_{Li_2O_2} \rho_{\mathrm{Li_2O_2}} \exp\left(\alpha_{j_{dis}} \frac{-\delta_{Li_2O_2}}{10\mathrm{nm}}\right)$$

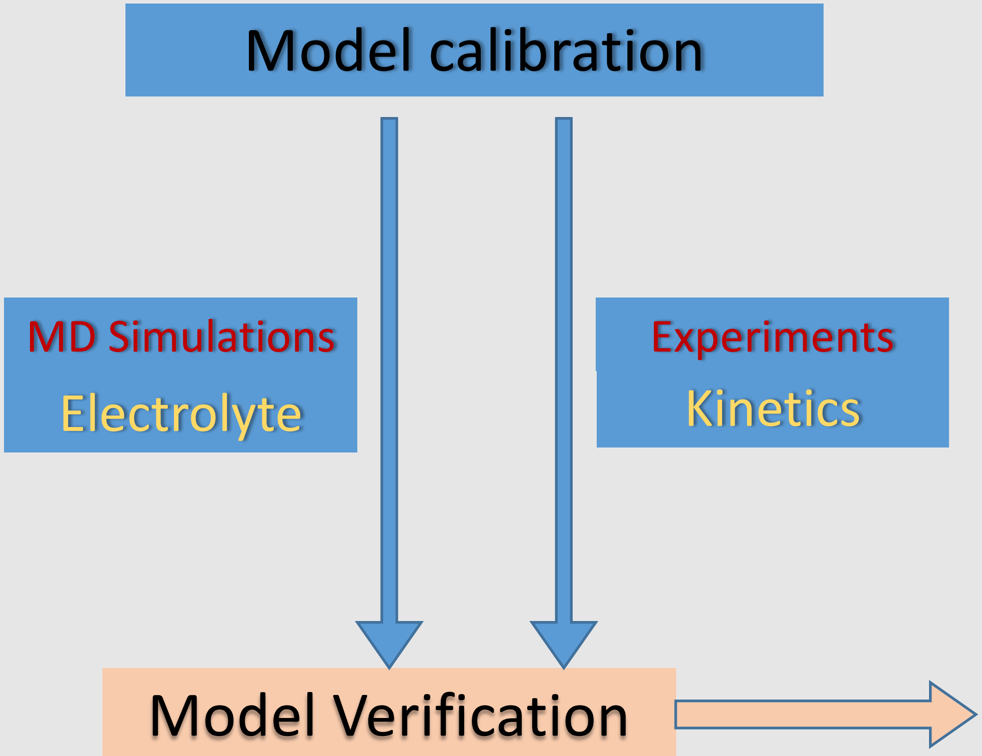
Reaction rate

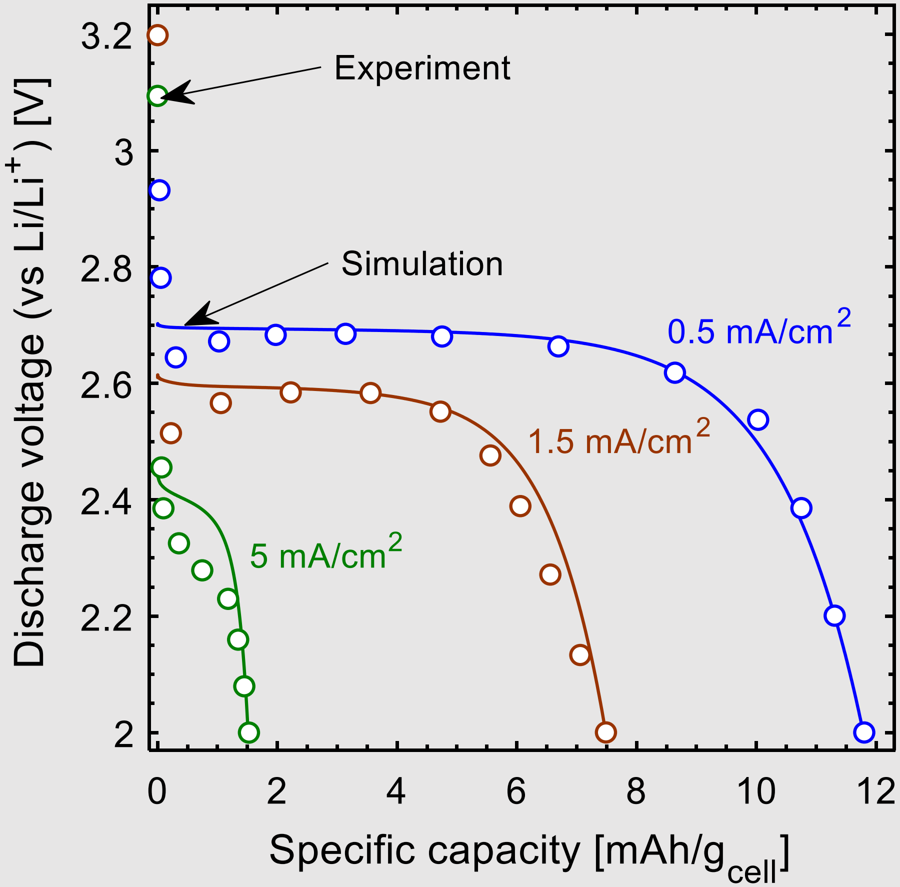
$$R_C = nFc_{O_2} k_0 a \left(e^{\frac{(1-\beta)n}{V_T}\eta} - e^{\frac{-n\beta}{V_T}\eta}\right)$$

Oxygen dissolvation

$$c_{O_2}(L_c) = N_{O2} = k_f\left[p_{O2} - k_H c_{O2}(0)\right]$$

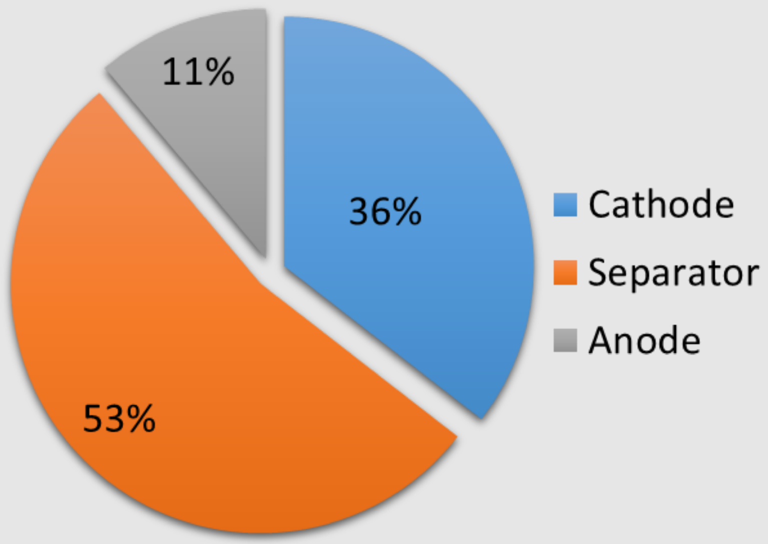
Model calibration for simulating high current



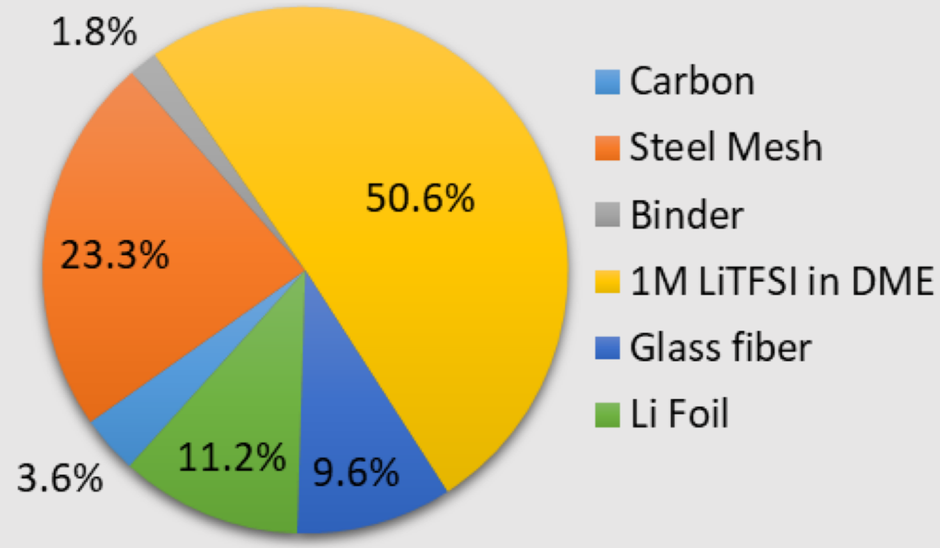


Simulating cells for high power cell needs accurate electrolyte properties and current dependent kinetics

Electrochemical mass distribution



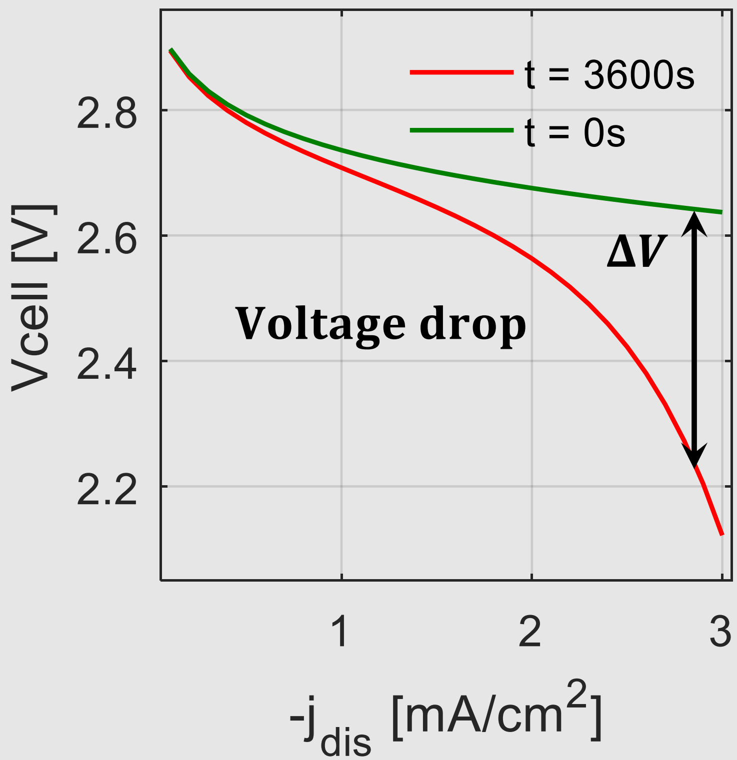
Cell mass distribution

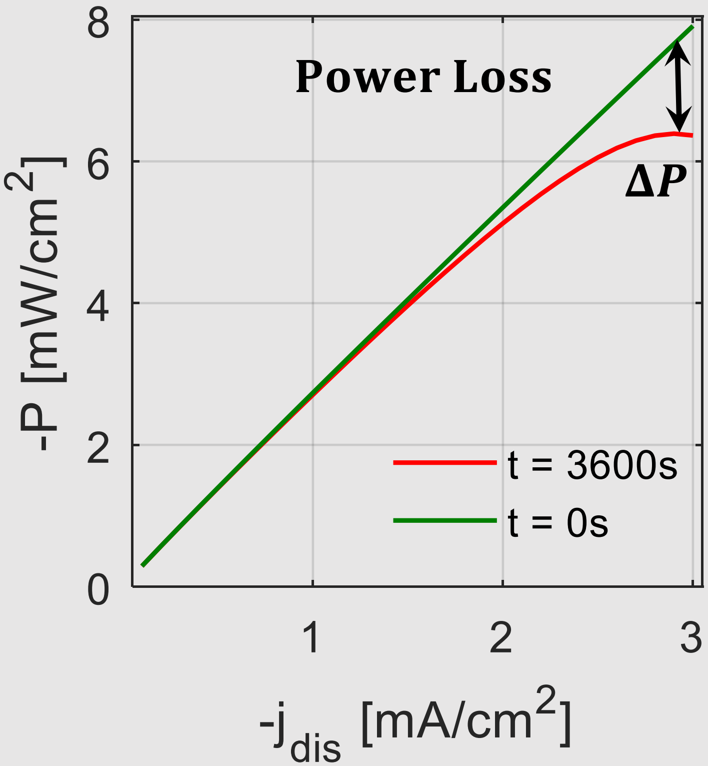


Mass distribution separated into solid and liquid phases

All three components of Li-O_2 cell can be optimized to achieve high specific power

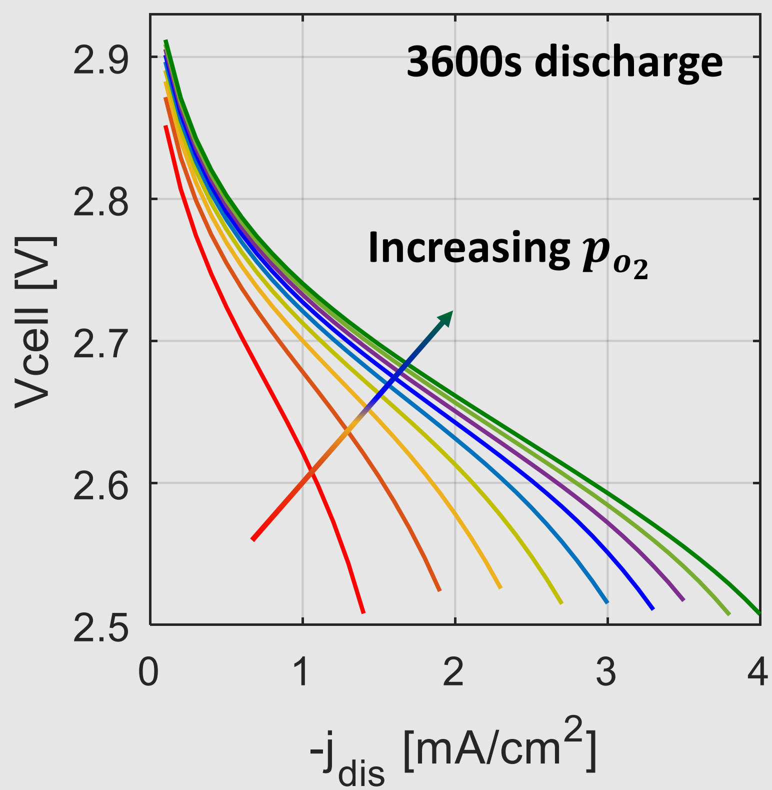
Polarization test: The effect on power

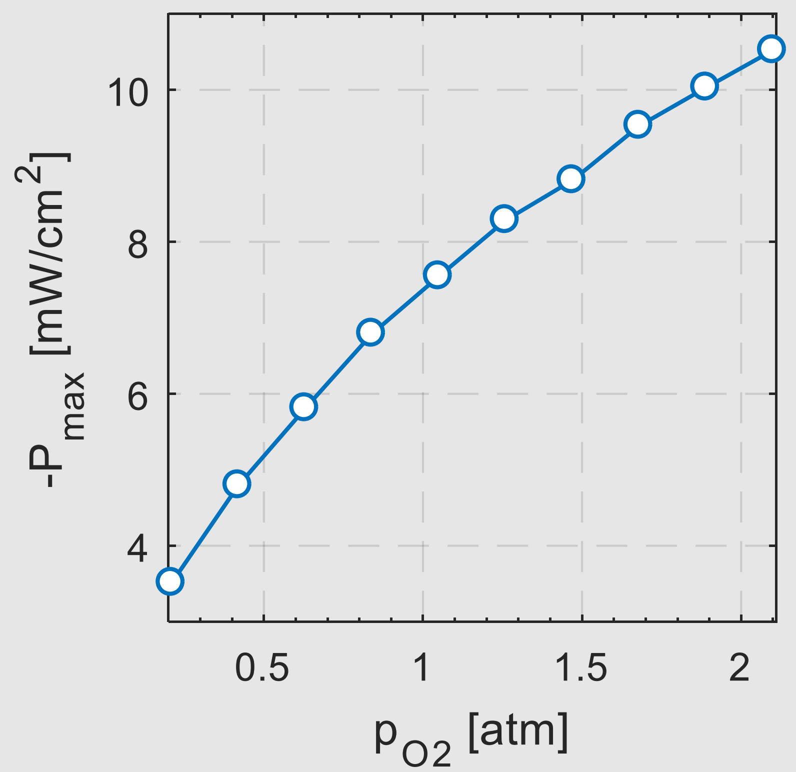




Operating at "high" current densities can lead to 25% power loss during 1hr discharge

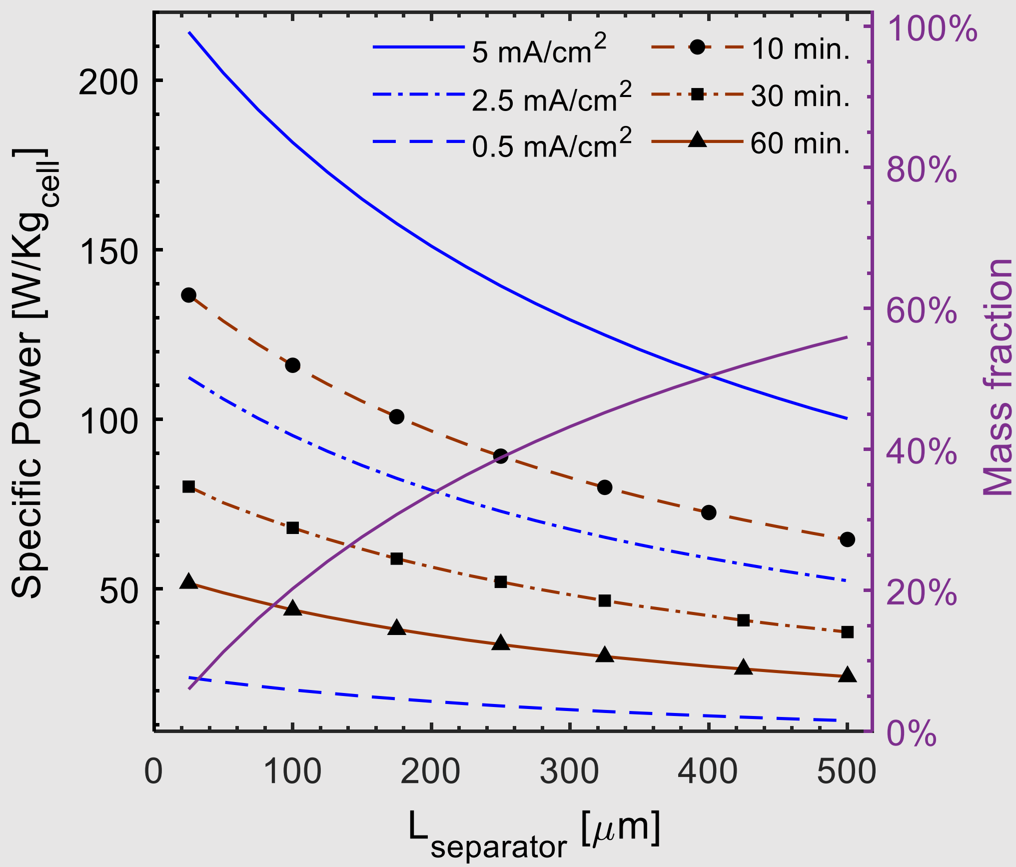
Polarization test: Oxygen Partial Pressure





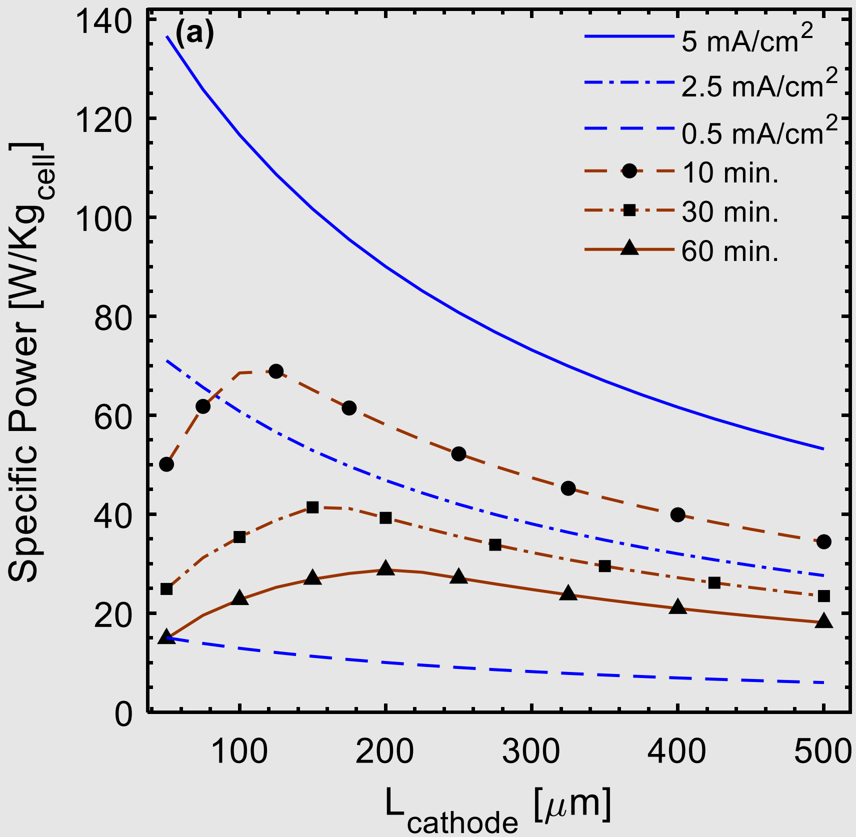
Increasing oxygen partial pressure improves power as well as non-electrochemical mass

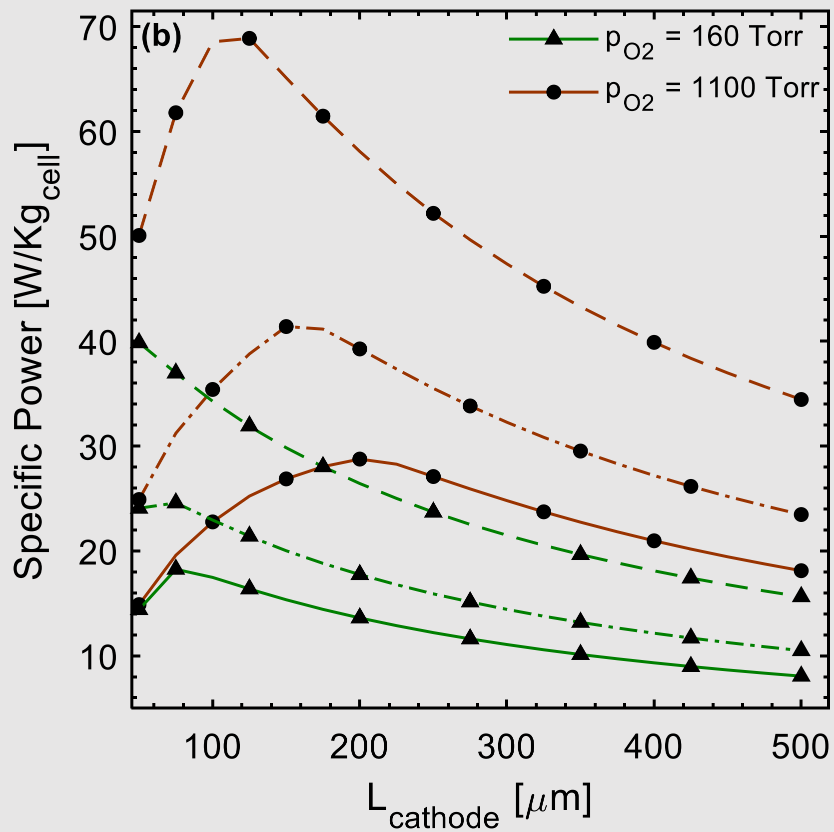
Influence of separator on performance



Separator does not contribute to battery performance at high current densities

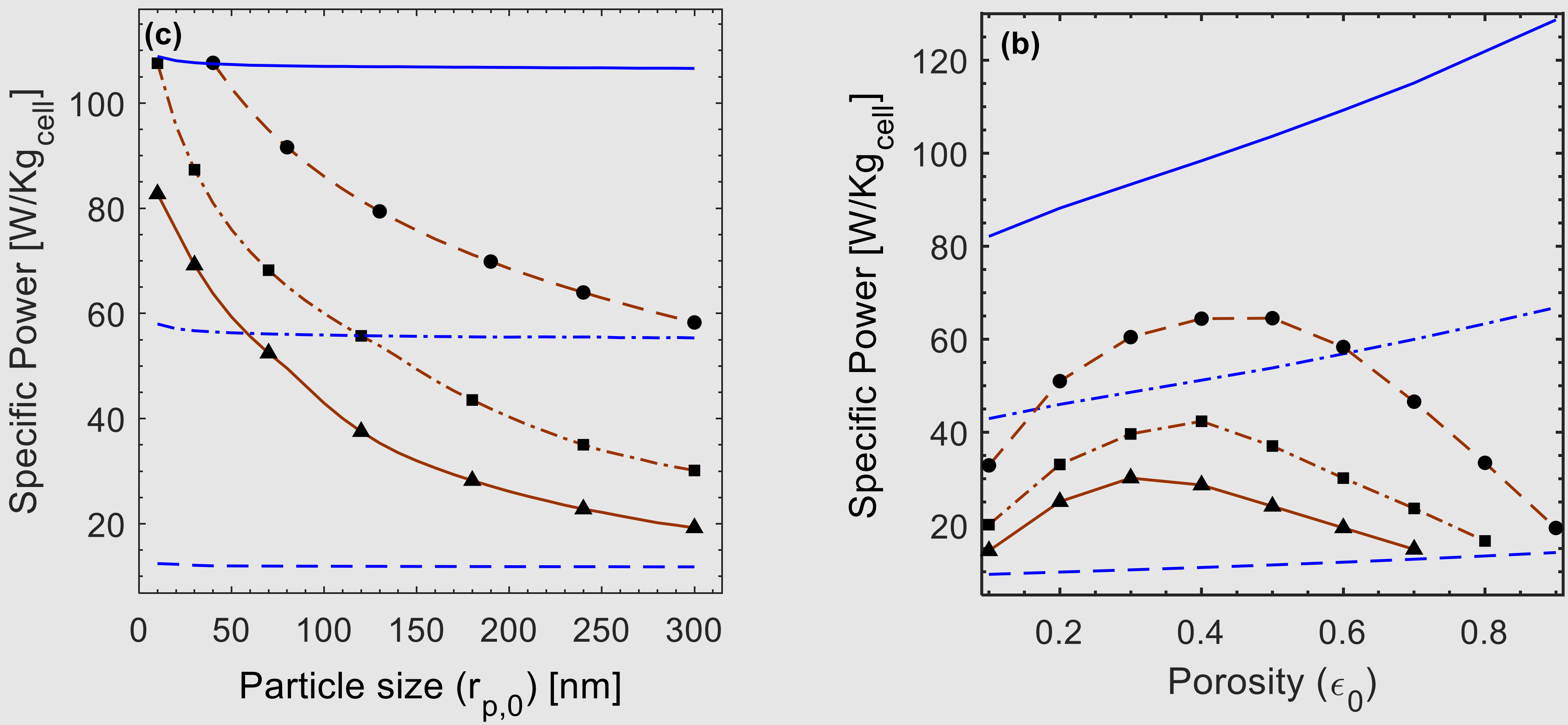
Effect of cathode thickness on performance





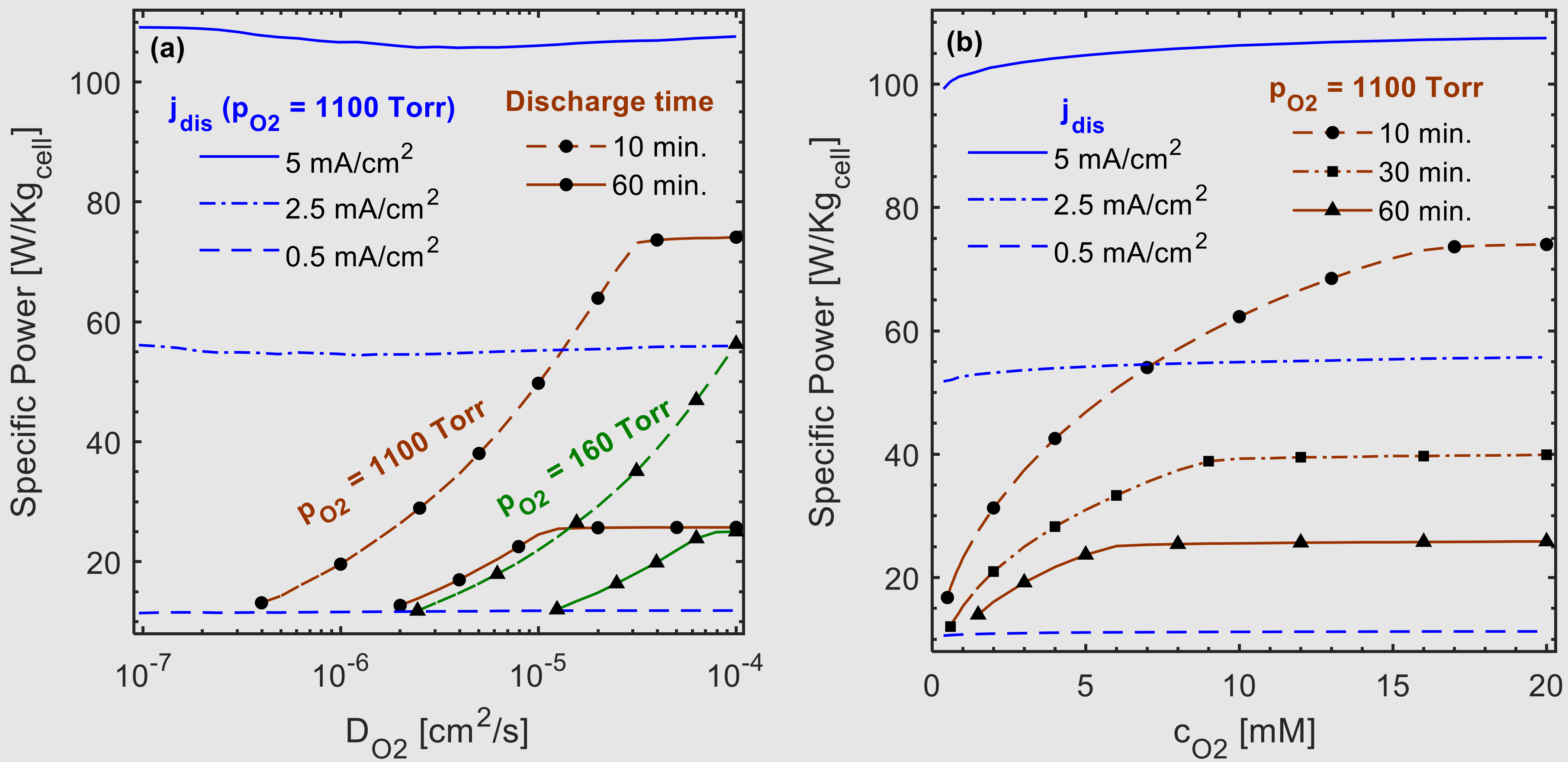
Oxygen diffusion length determines the optimal cathode thickness

Influence of microstructure on performance



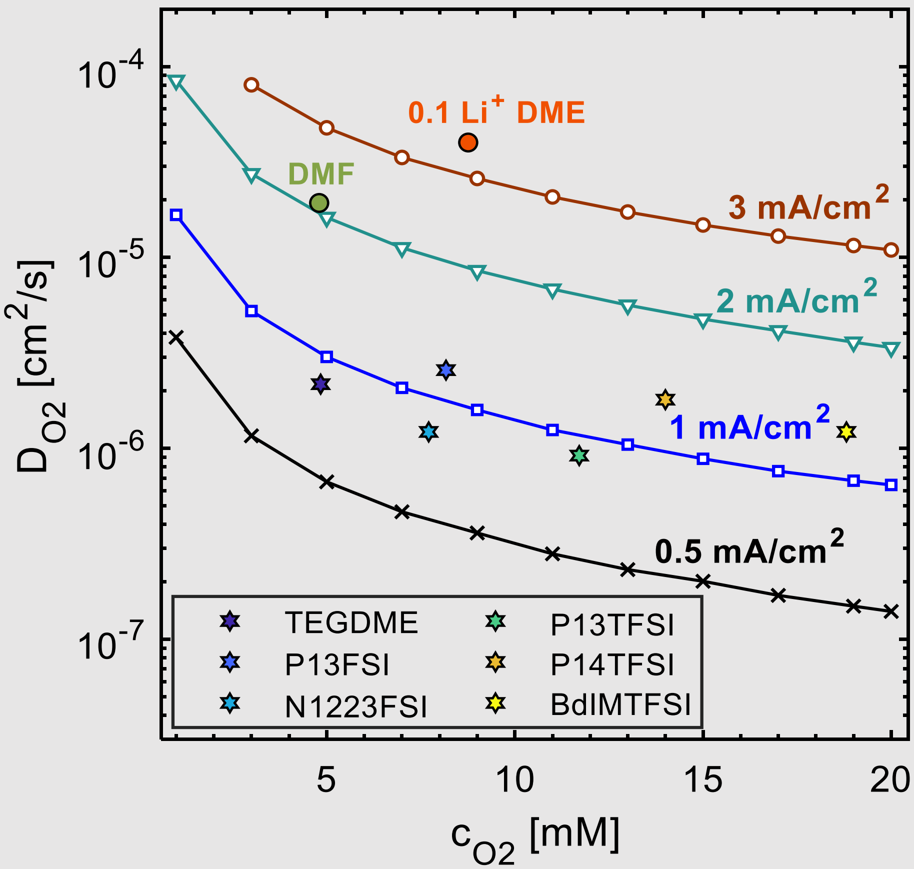
Optimal values for porosity, particle size, and tortuosity depend on discharge current density and discharge time

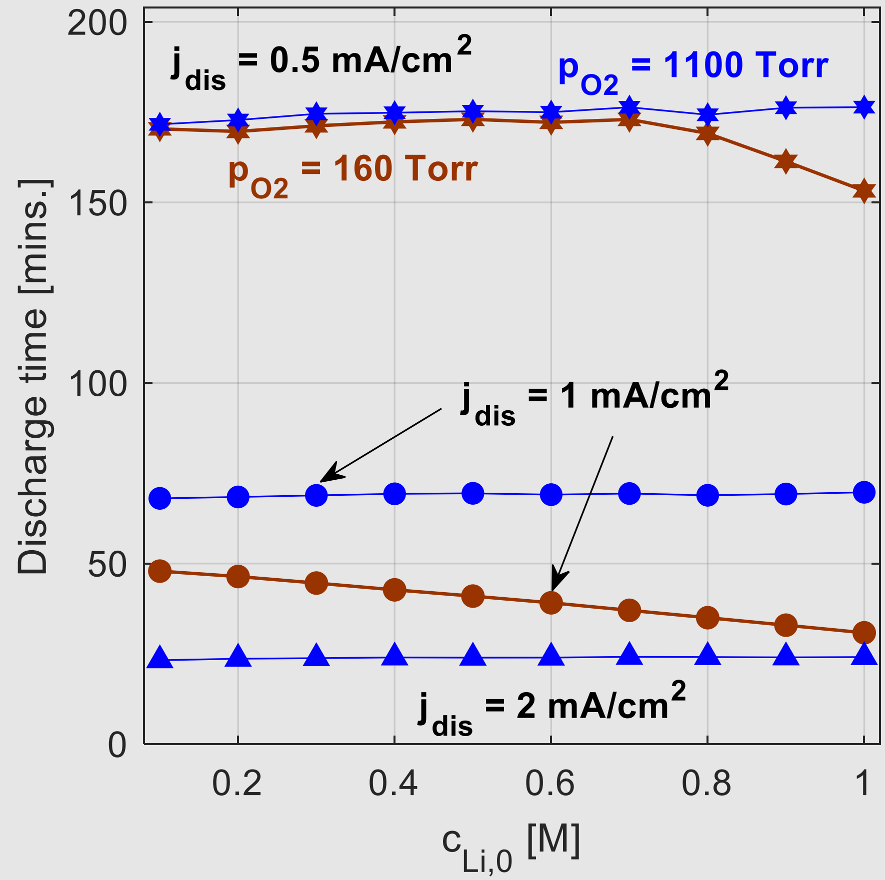
Influence of electrolyte properties



Requirement for electrolyte properties changes with application needs

Influence of electrolyte properties –cont.



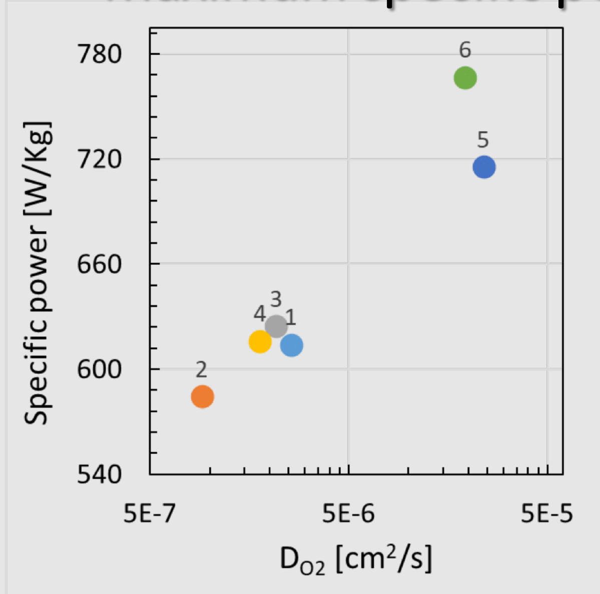


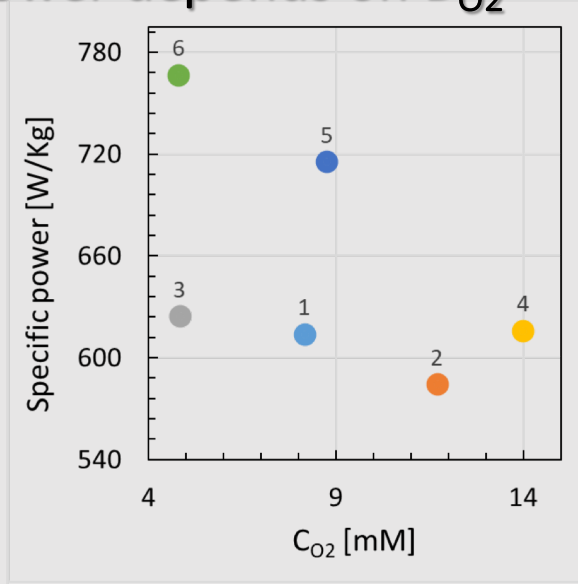
Diffusion requirements can be relaxed based by changing operating partial pressure and choosing lower salt concentration

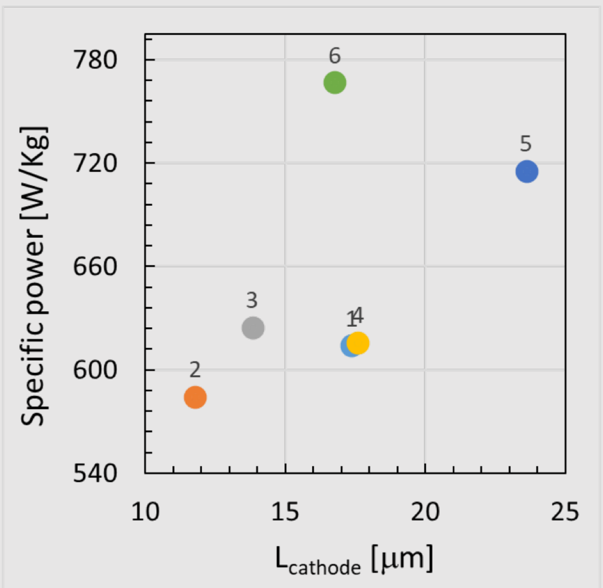
Simulation-based optimization

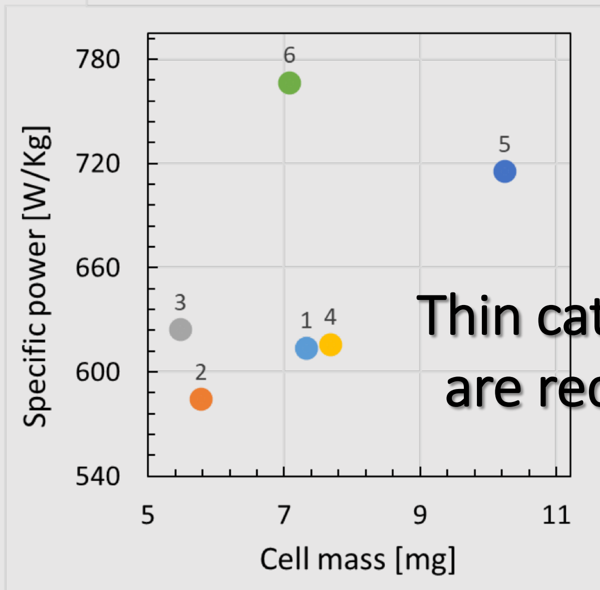
1 • 0.3M LiTFSI P_{13}FSI
2 • 0.3M LiTFSI P_{13}TFSI
3 • 0.1M LiTFSI TEGDME
4 • 0.3M LiTFSI P_{14}TFSI
5 • 1M LiTFSI DME
6 • 0.1 TEAP DMF

Maximum specific power depends on D_{O2}





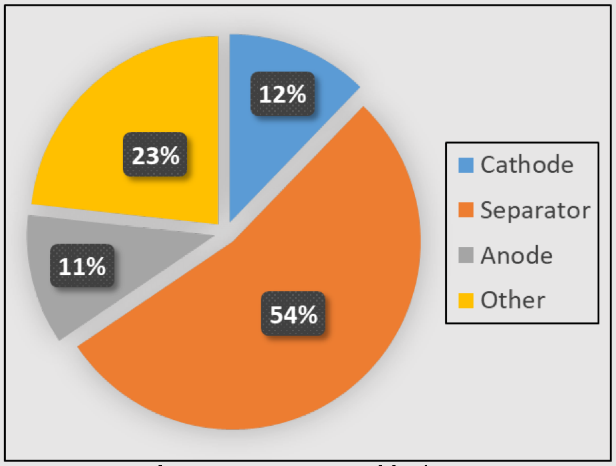




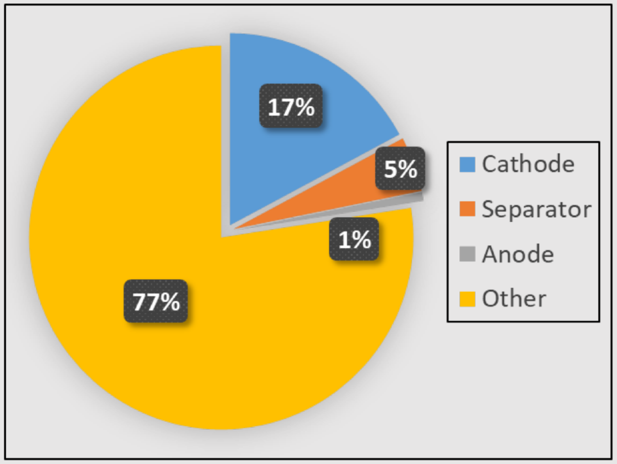
Thin cathodes and very low mass cells are required for high specific power

Summary

- To achieve high specific power, both, current density and cell mass needs to be optimized
- Reducing mass of the separator improves specific power without decreasing the power performance
- Optimal cell design changes based on discharge time, discharge current density, and operating conditions
- Electrolytes with high oxygen diffusivity results in cell with high specific power (promoting better oxygen distribution can mitigate this requirement)



Laboratory cell (not optimized)



Cell optimized for low electrochemical mass

Acknowledgements

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