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

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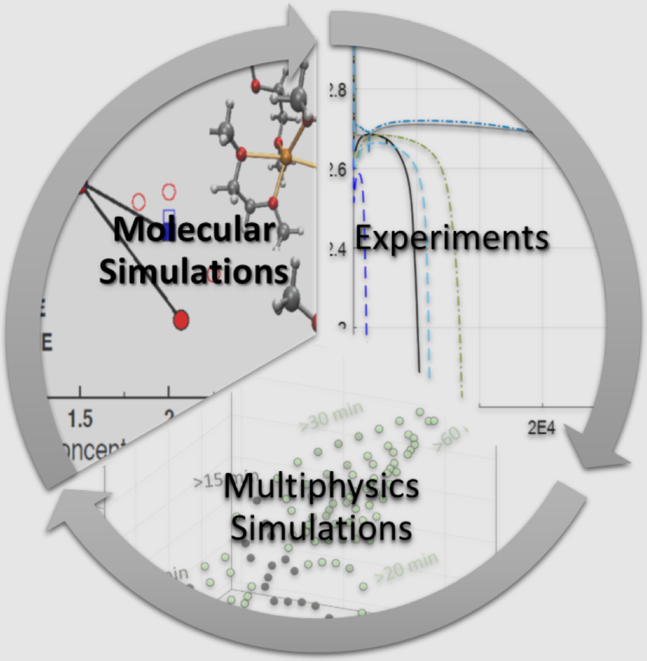

1. Introduction
2. Model calibration
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NASA Strategic Plan for Green Aviation

National Aeronautics and Space Administration

NASA AERONAUTICS

Strategic Implementation Plan

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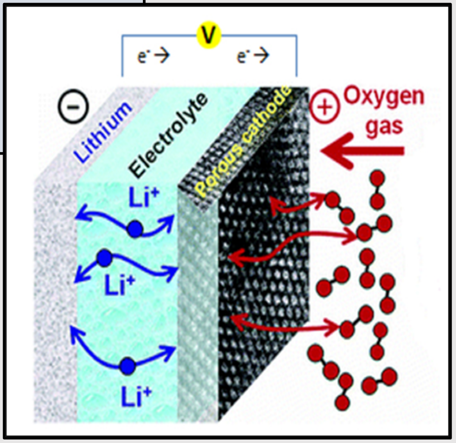
<u>Strategic Thrust 4</u>:
Transition to Low Carbon Propulsion

Alternate Propulsion Demonstrators

Li-Air Battery



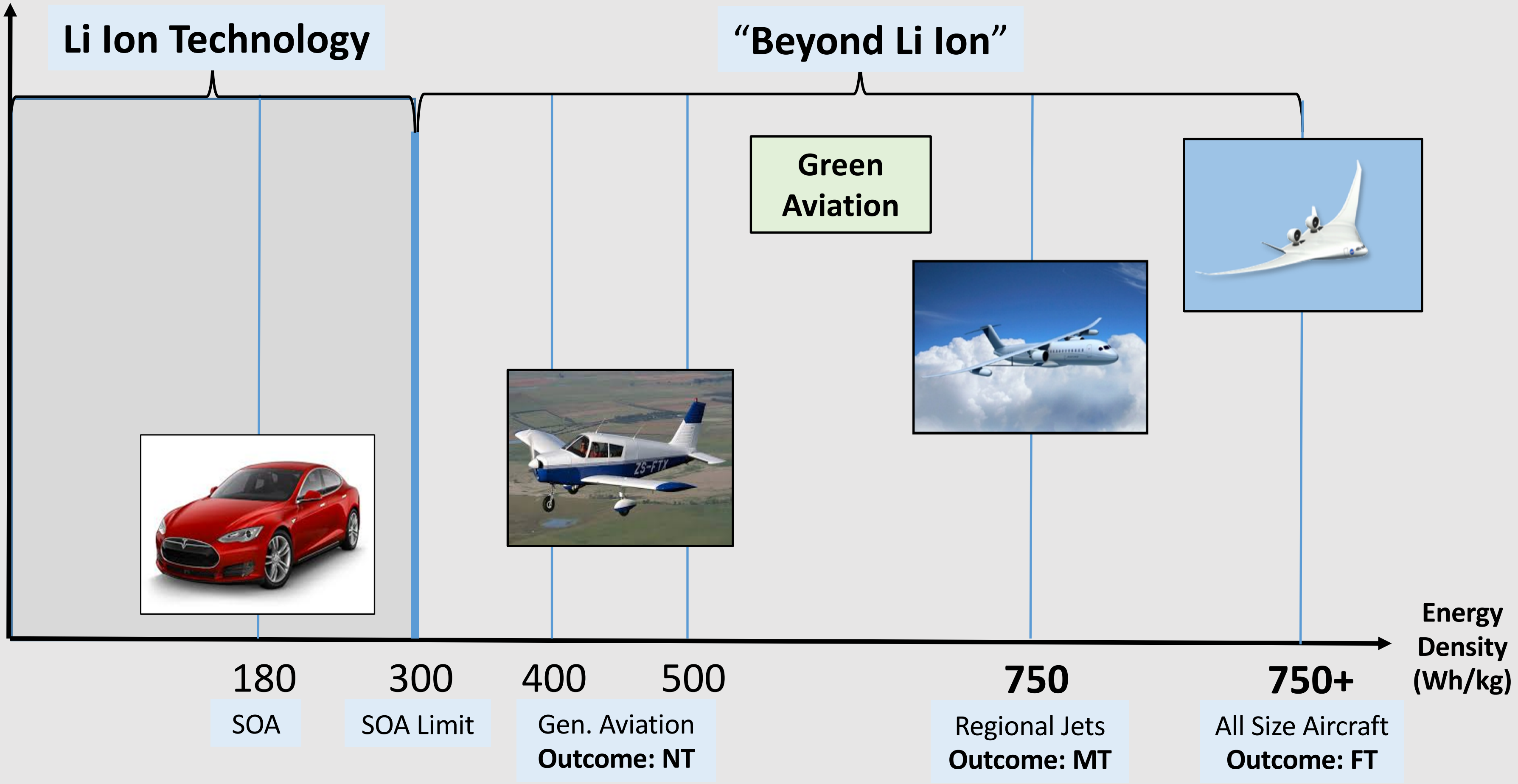
- **Zero emissions**
- **Low noise**
- **Energy efficient**

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.



Li Ion Technology

"Beyond Li Ion"

Green Aviation

180
SOA

300
SOA Limit

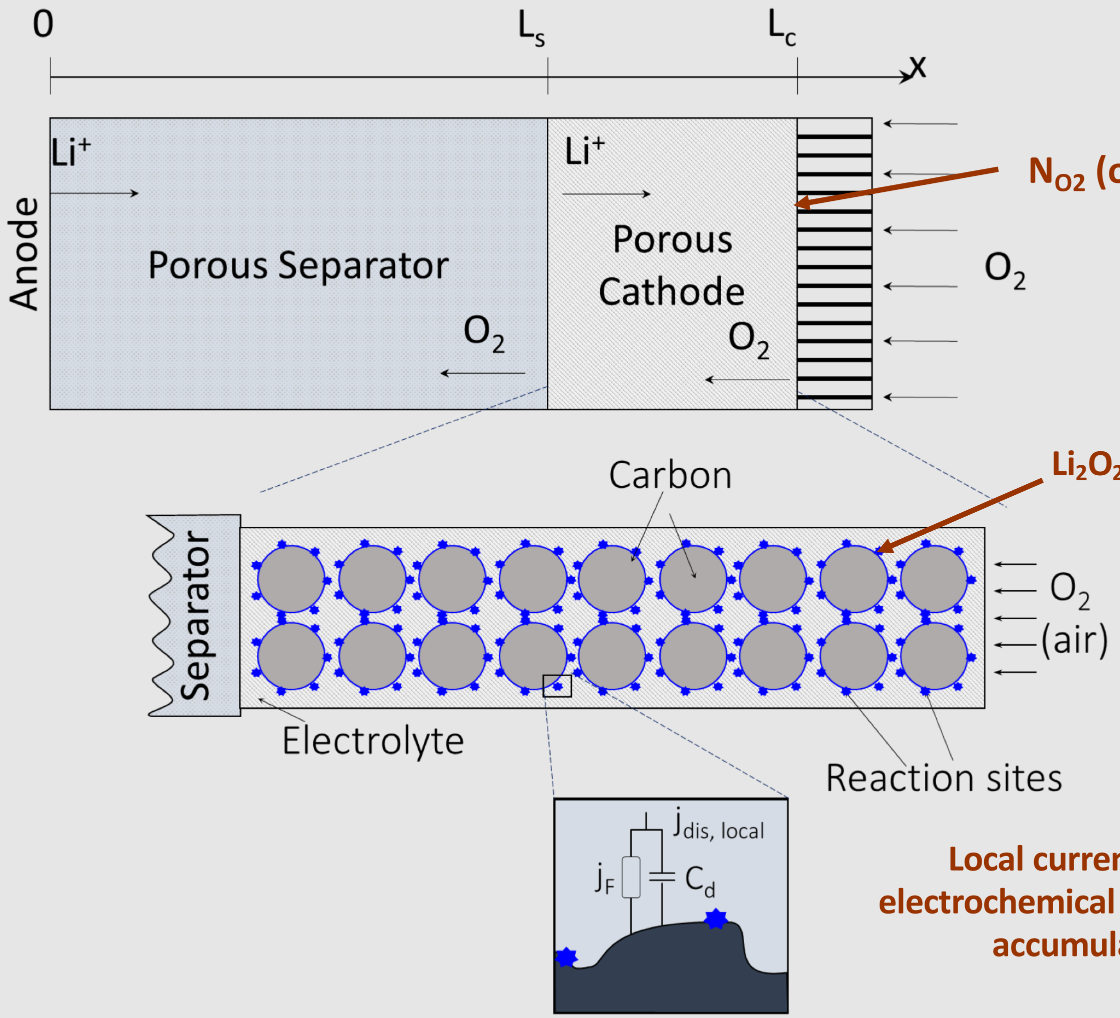
400 500
Gen. Aviation
Outcome: NT

750
Regional Jets
Outcome: MT

750+
All Size Aircraft
Outcome: FT

Energy Density (Wh/kg)

Working of a lithium-oxygen battery

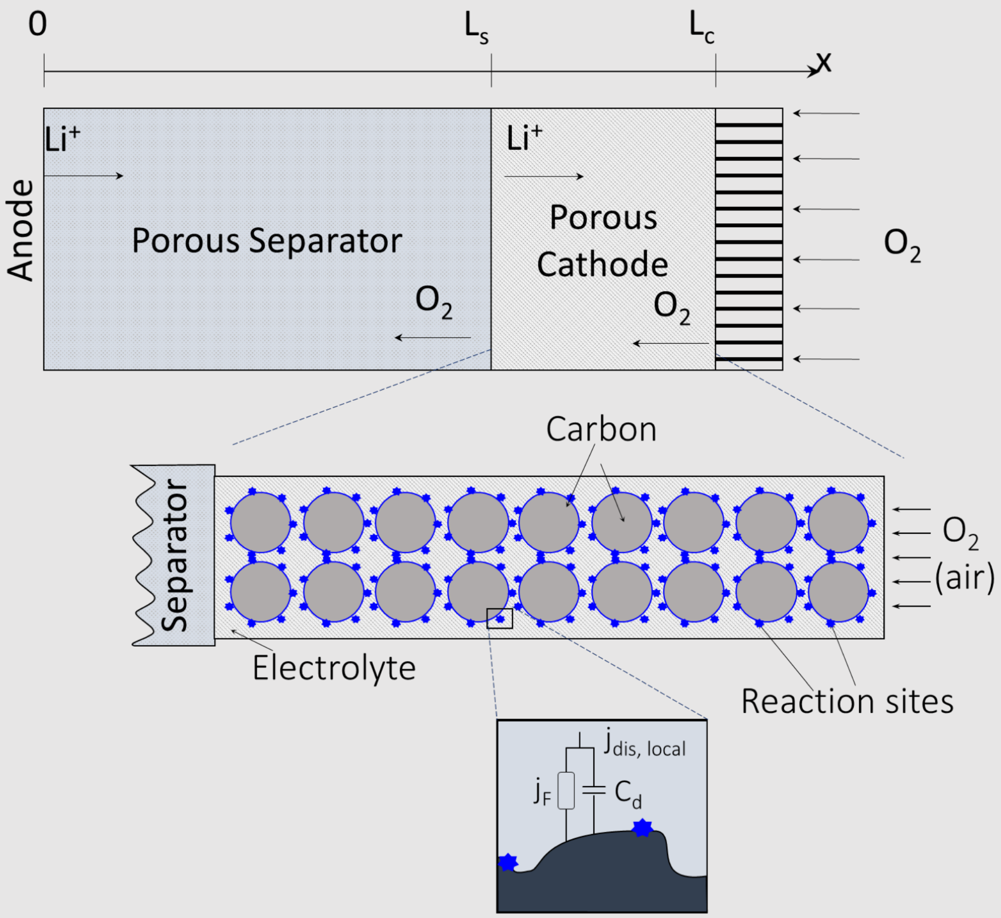


N_{O2} (oxygen dissolution)

Li_2O_2 coats the surface and limits discharge

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

Modeling a lithium-oxygen battery



$$\overbrace{\eta}^{\text{Over-voltage}} = \underbrace{\phi_{\mathrm{Li}}}_{\text{electrolyte}} - \underbrace{\phi}_{\text{electrode}} - \overbrace{E^0}^{\text{thermodynamic}} - \underbrace{V_{\mathrm{discharge}}}_{\mathrm{Li_2O_2}}$$

$$\nabla\cdot\Big(\overbrace{\sigma_{\mathrm{eff}}\nabla\phi}^{-\boldsymbol{I}\text{ (electron current)}}\Big) + R_C = aC_d\frac{\partial\left(\phi-\phi_{\mathrm{Li}}\right)}{\partial t}$$

$$\nabla\cdot\Big(\overbrace{\kappa_{\mathrm{eff}}\nabla\phi_{\mathrm{Li}} + \kappa_D\nabla\ln c_{\mathrm{Li}}}^{-\boldsymbol{I}_{\mathrm{Li}}\text{ (electrolyte current)}}\Big) - R_C = aC_d\frac{\partial\left(\phi-\phi_{\mathrm{Li}}\right)}{\partial t}$$

$$\frac{\partial\left(\epsilon c_{\mathrm{Li}}\right)}{\partial t} = \nabla\cdot\big(\overbrace{D_{\mathrm{Li,eff}}\nabla c_{\mathrm{Li}}}^{-\boldsymbol{I}_{\mathrm{Li}}\text{ (electrolyte diffusion flux)}}\big) - \frac{1-t^+}{F}R_C - \frac{\boldsymbol{I}_{\mathrm{Li}}\cdot\nabla t^+}{F}$$

$$\frac{\partial\left(\epsilon c_{\mathrm{O_2}}\right)}{\partial t} = \nabla\cdot\big(\overbrace{D_{\mathrm{O_2,eff}}\nabla c_{\mathrm{O_2}}}^{-\boldsymbol{I}_{\mathrm{O2}}\text{ (}\mathrm{O_2}\text{ diffusion flux)}}\big) - \frac{R_C}{nF}$$

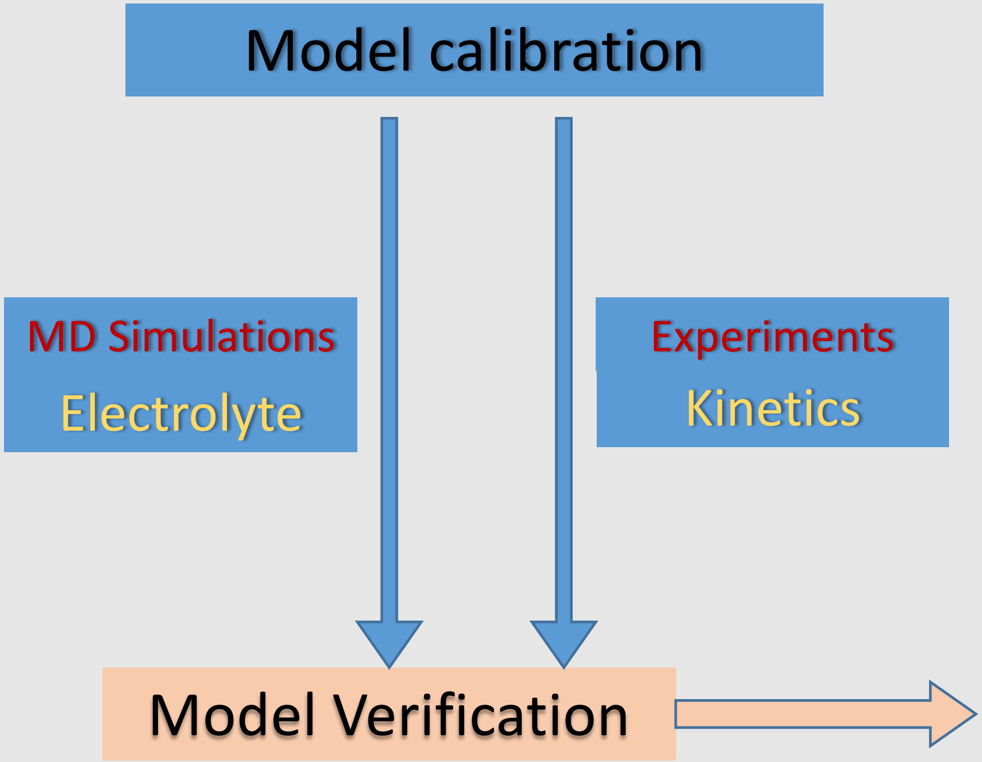
$$\overbrace{\frac{\partial\epsilon}{\partial t}}^{\epsilon\text{ (porosity change -from }\mathrm{Li_2O_2}\text{ deposition)}} = -R_C\frac{M_{\mathrm{discharge}}}{nF\rho_{\mathrm{m,discharge}}}$$

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

Reaction rate $R_C = nFc_{\mathrm{O_2}}k_0a\left(e^{\frac{(1-\beta)n}{V_T}\eta} - e^{\frac{-n\beta}{V_T}\eta}\right)$

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



Model calibration

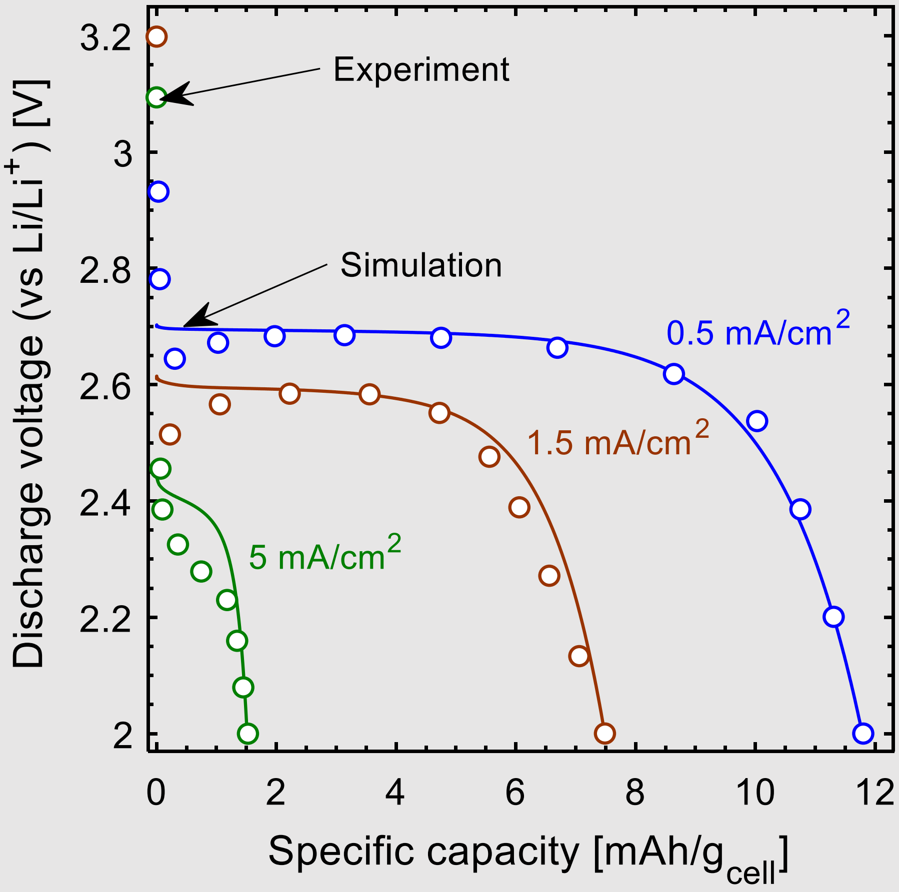
MD Simulations

Electrolyte

Experiments

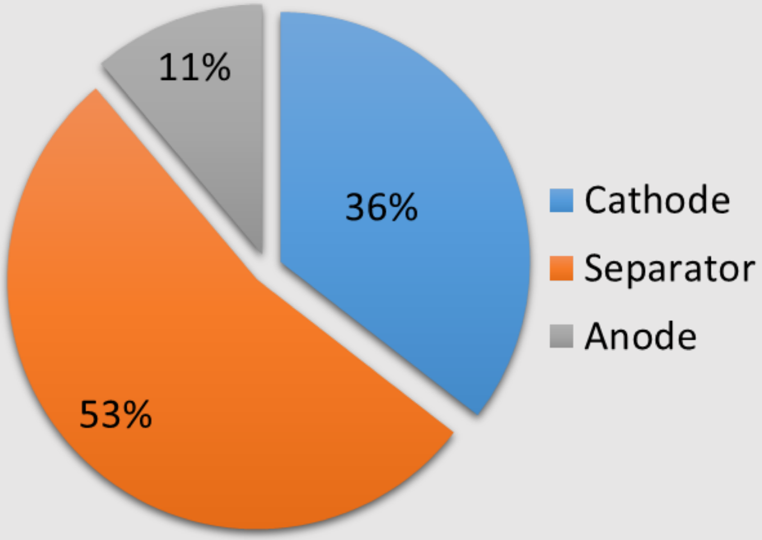
Kinetics

Model Verification

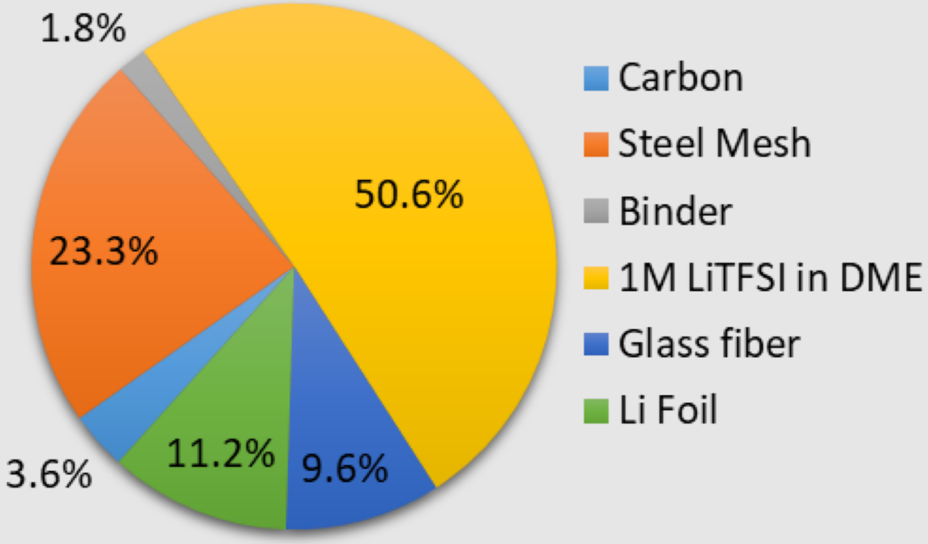


Simulating cells for high power cell needs accurate electrolyte properties and current dependent kinetics

Electrochemical mass distribution



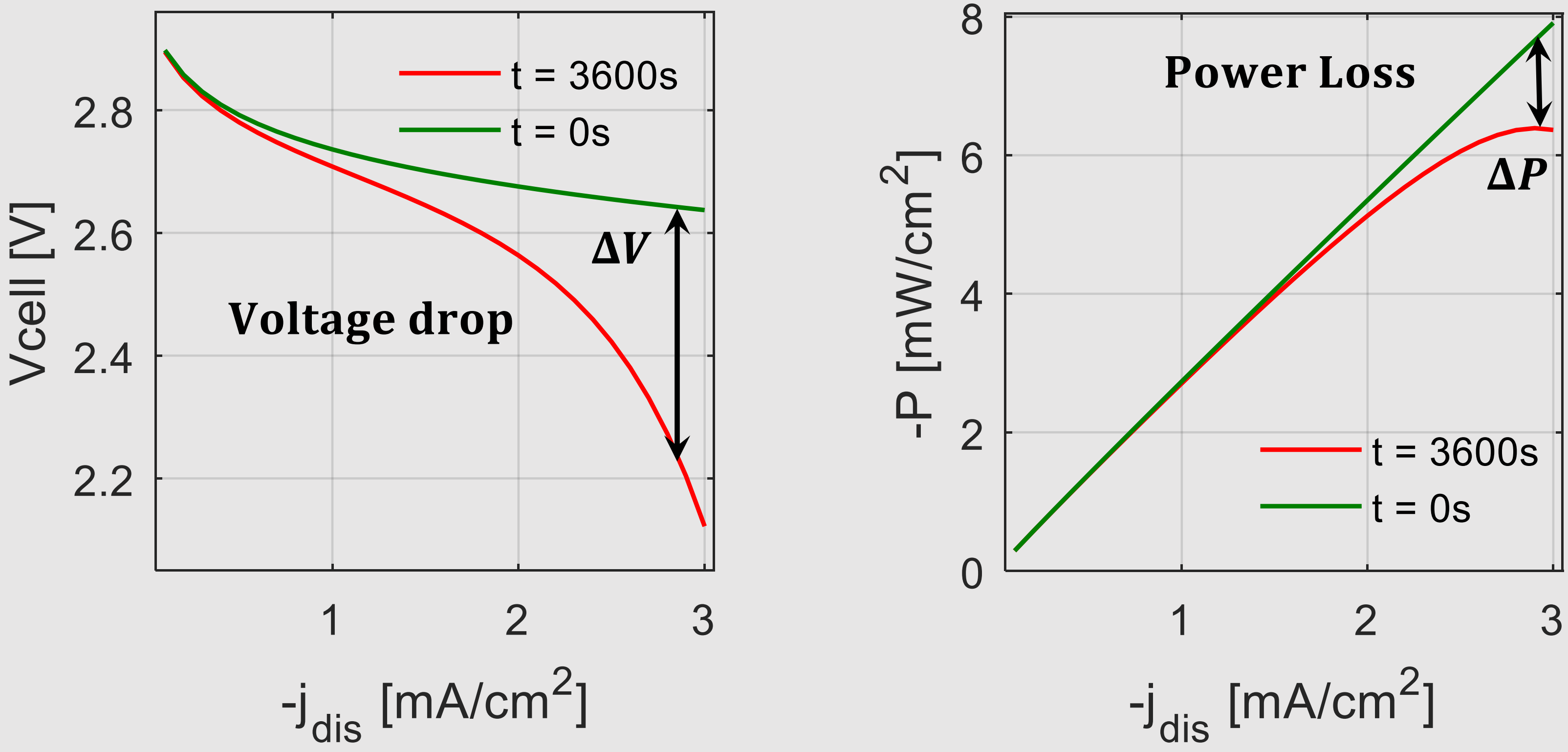
Cell mass distribution



Mass distribution separated into solid and liquid phases

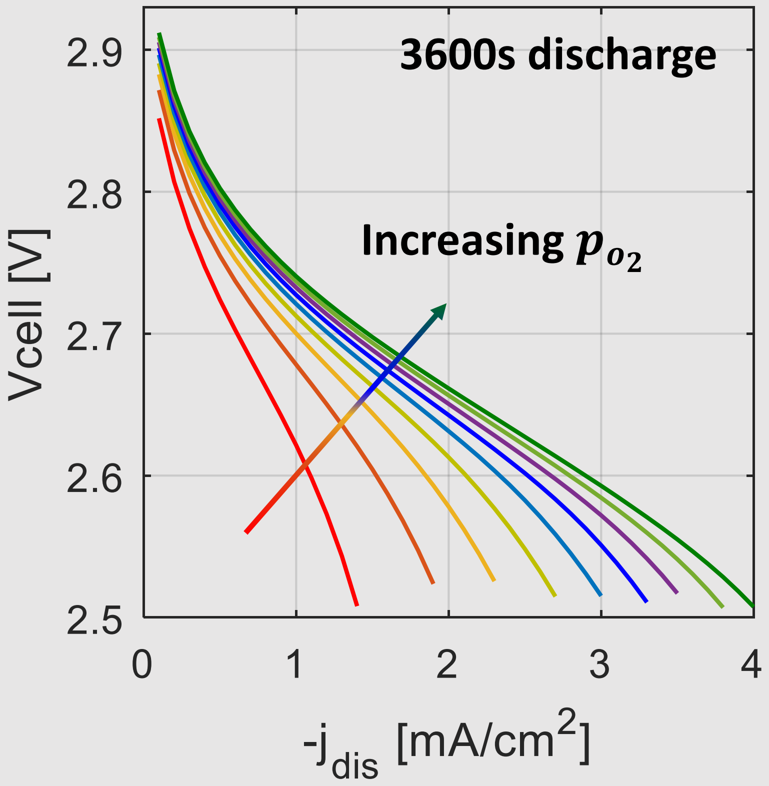
All three components of Li-O_2 cell can be optimized to achieve high specific power

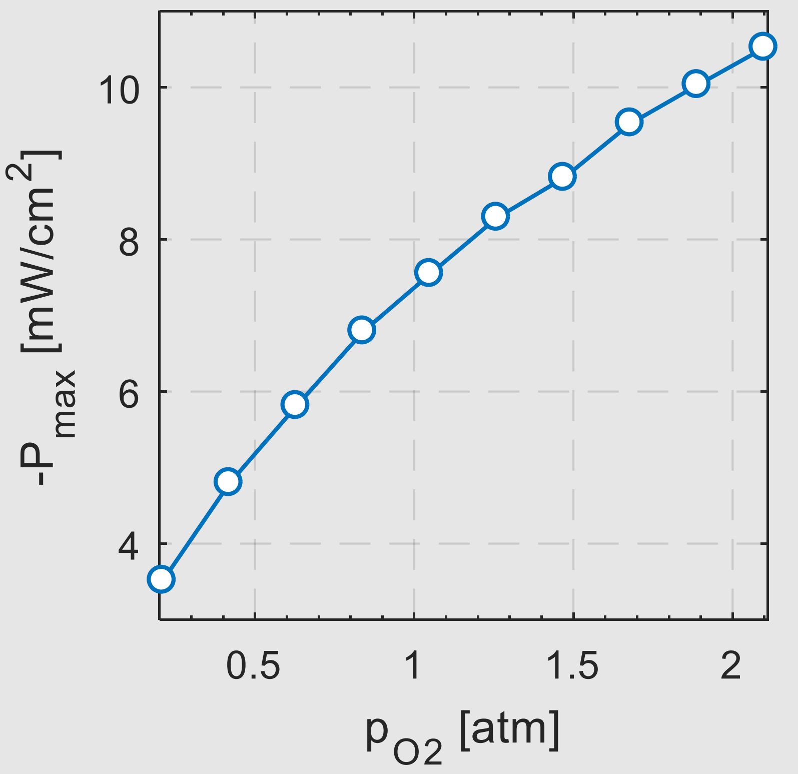
Polarization test: The effect on power



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

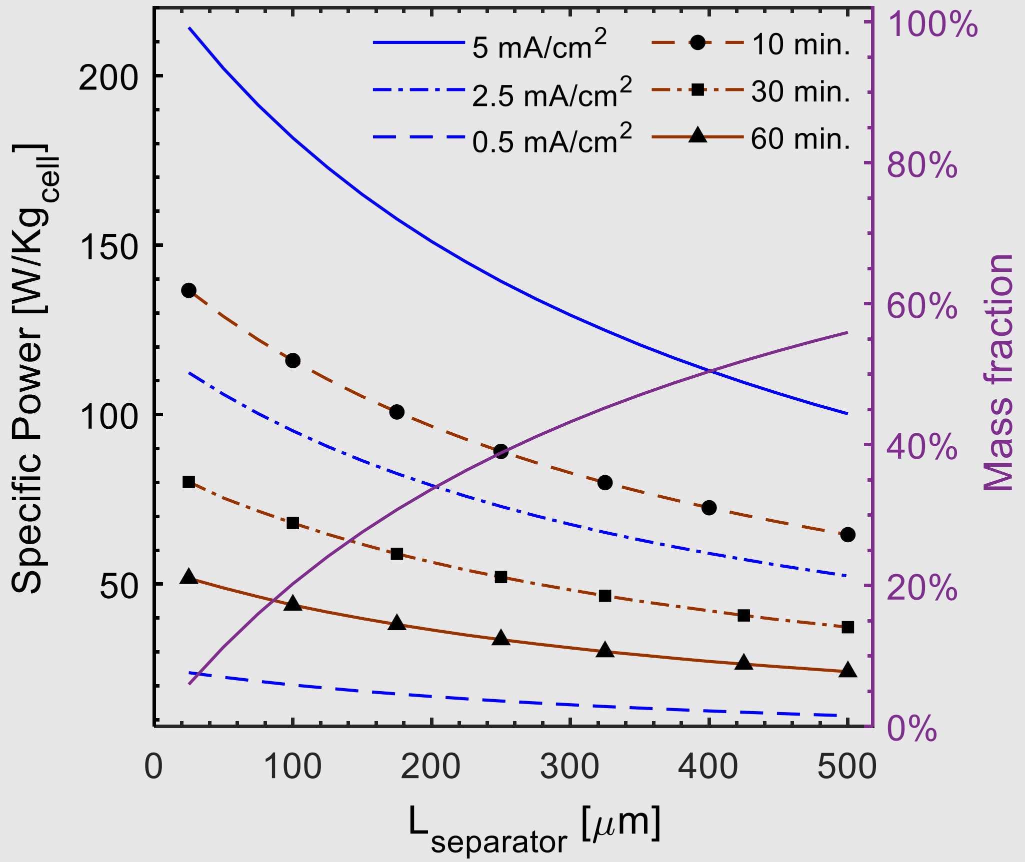
Polarization test: Oxygen Partial Pressure





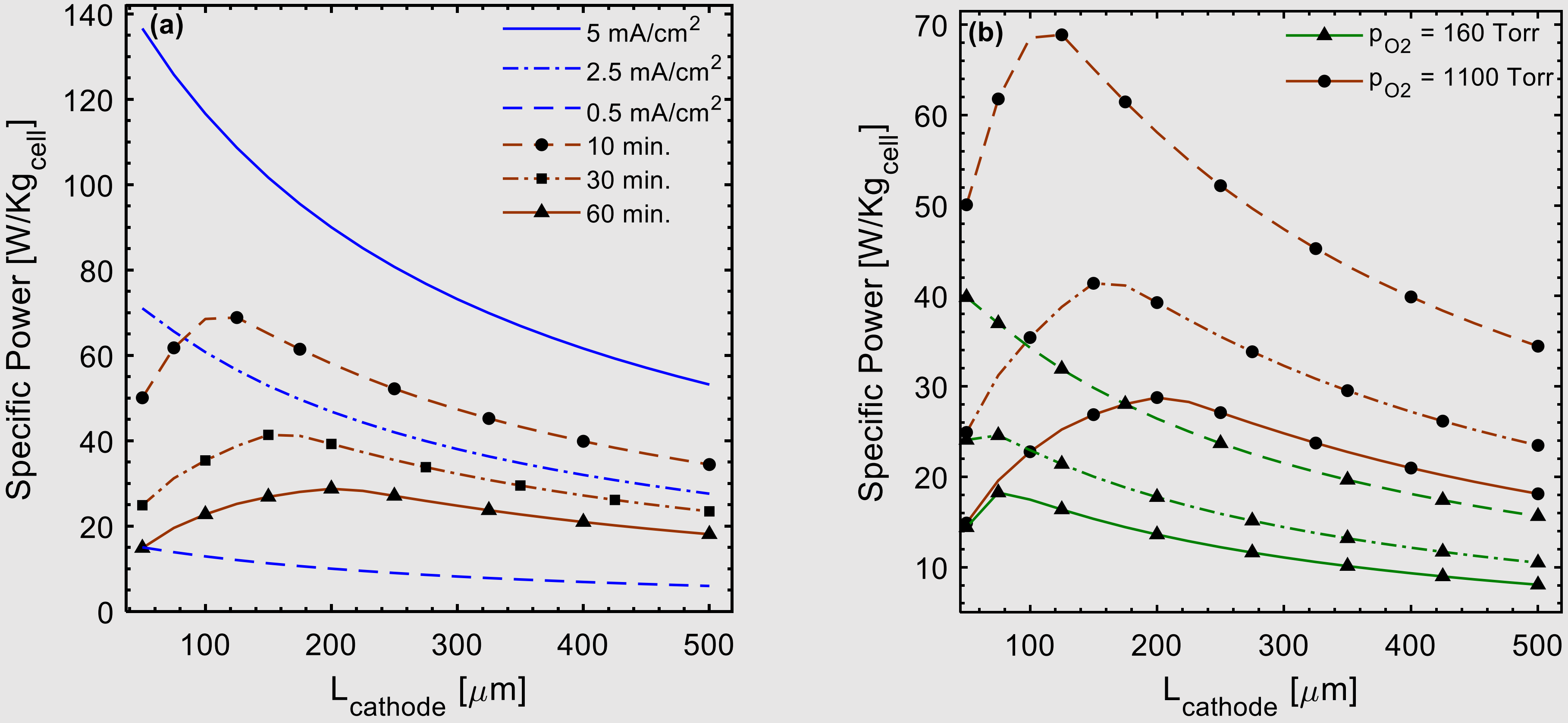
Increasing oxygen partial pressure improves power as well as non-electrochemical mass

Influence of separator on performance



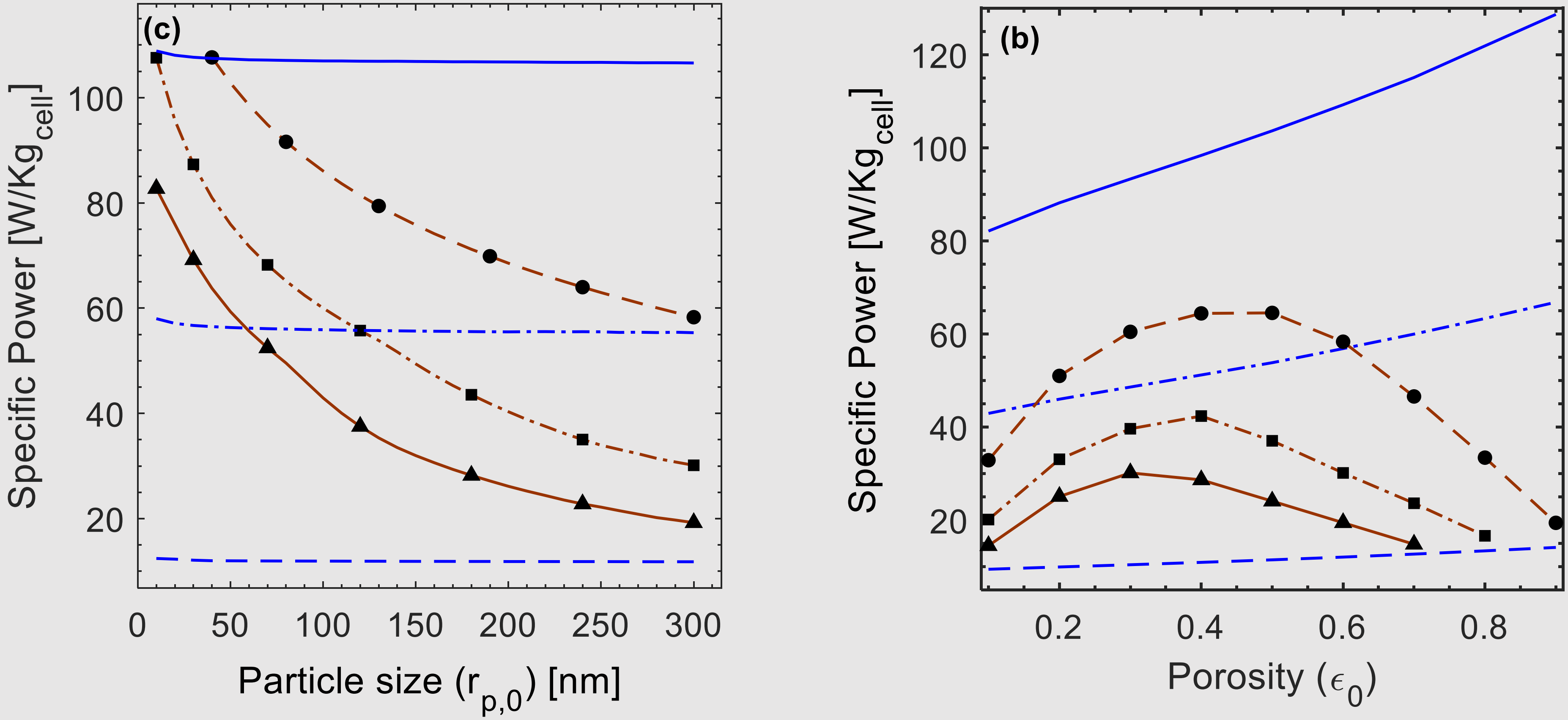
Separator does not contribute to battery performance at high current densities

Effect of cathode thickness on performance



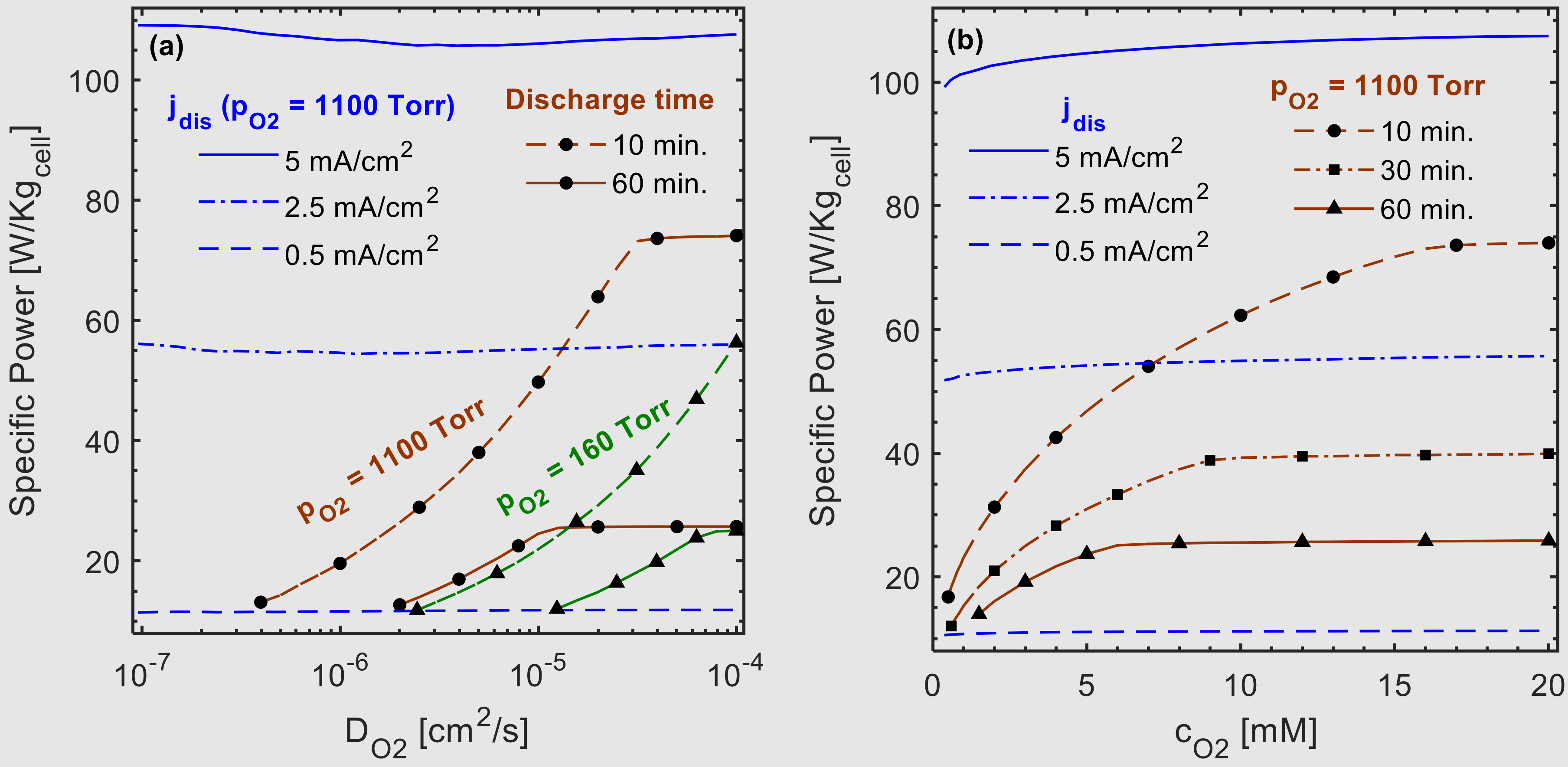
Oxygen diffusion length determines the optimal cathode thickness

Influence of microstructure on performance



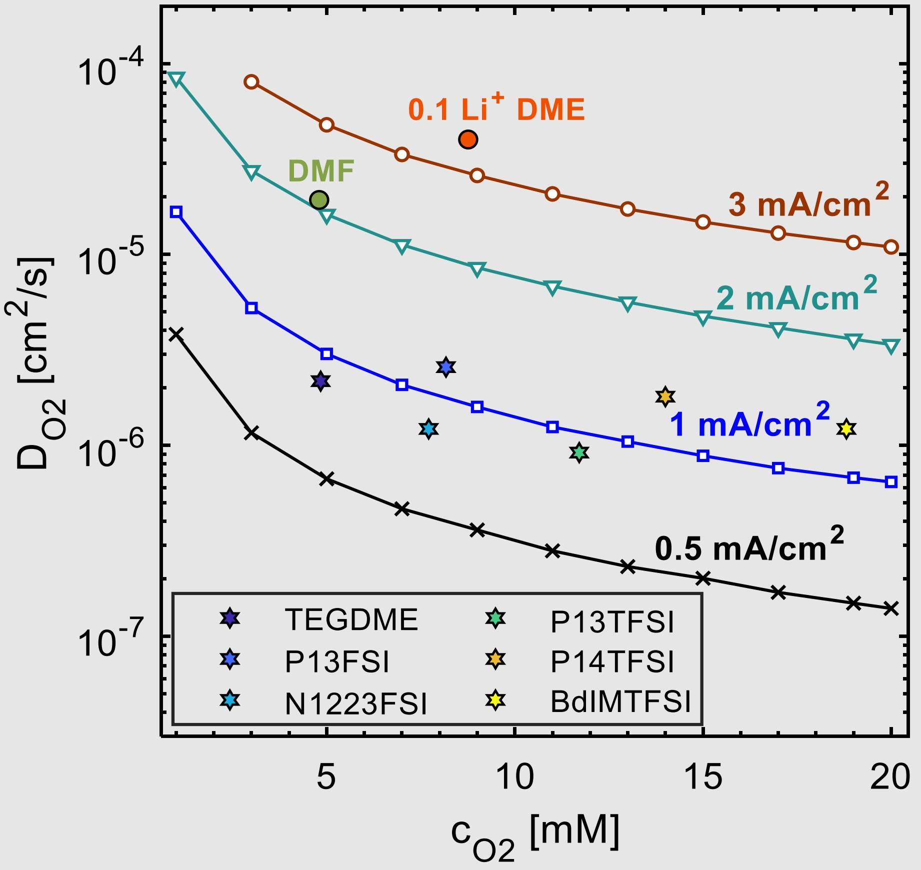
Optimal values for porosity, particle size, and tortuosity depend on discharge current density and discharge time

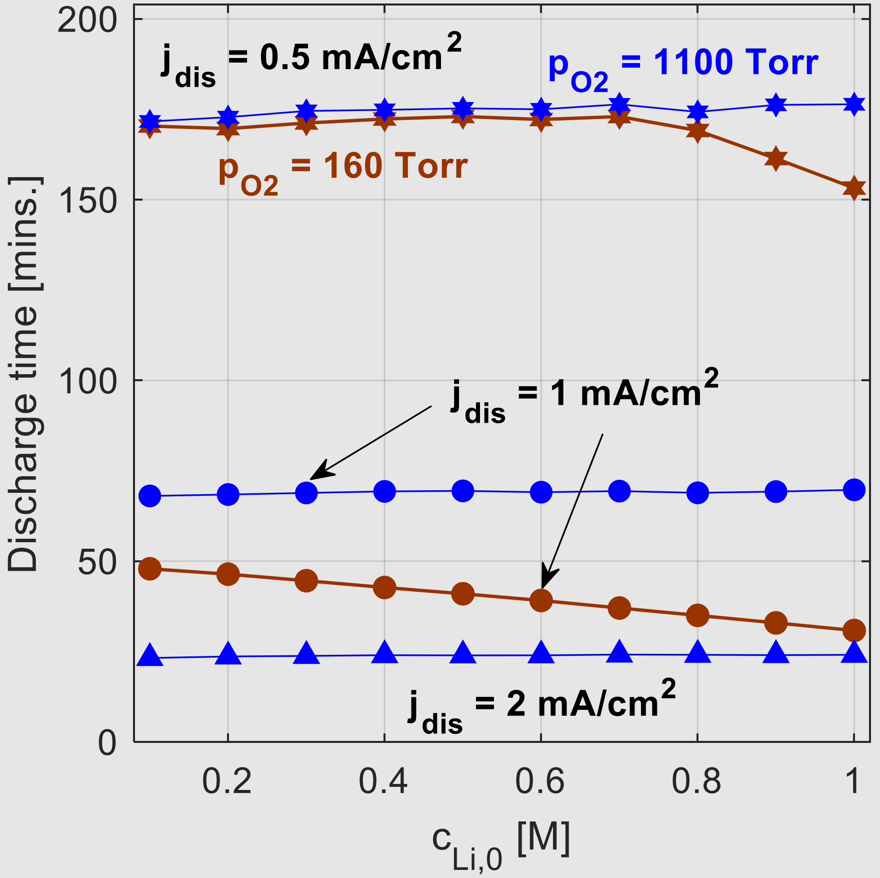
Influence of electrolyte properties



Requirement for electrolyte properties changes
with application needs

Influence of electrolyte properties –cont.



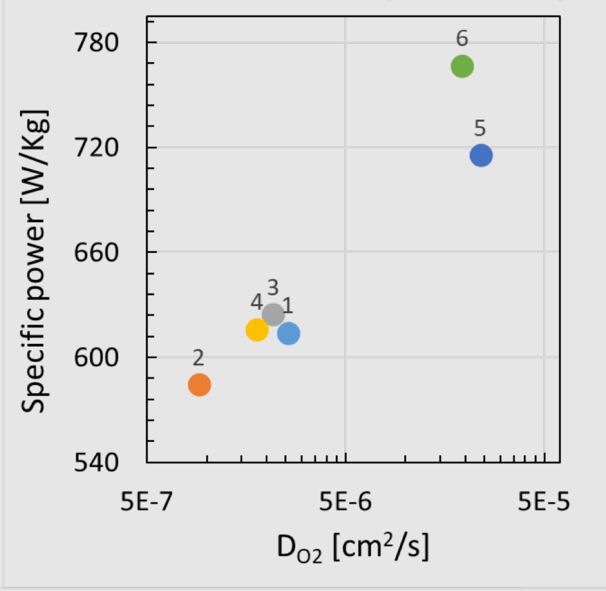


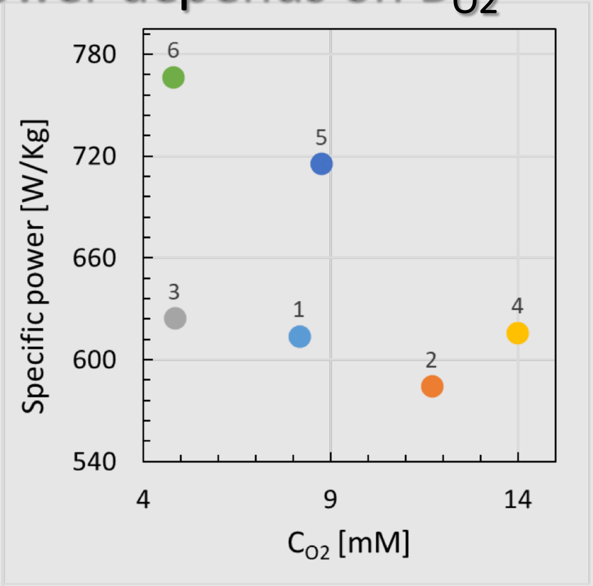
Diffusion requirements can be relaxed based by changing operating partial pressure and choosing lower salt concentration

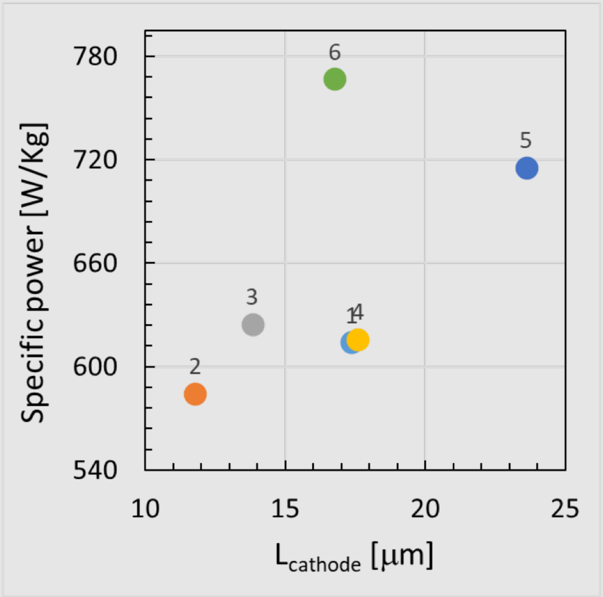
Simulation-based optimization

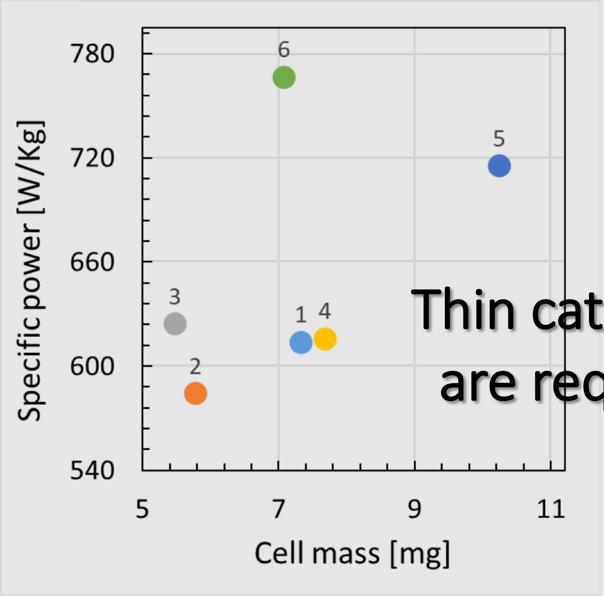
1 ● 0.3M LiTFSI P_{13}FSI
2 ● 0.3M LiTFSI P_{13}TFSI
3 ● 0.1M LiTFSI TEGDME
4 ● 0.3M LiTFSI P_{14}TFSI
5 ● 1M LiTFSI DME
6 ● 0.1 TEAP DMF

Maximum specific power depends on D_{O2}





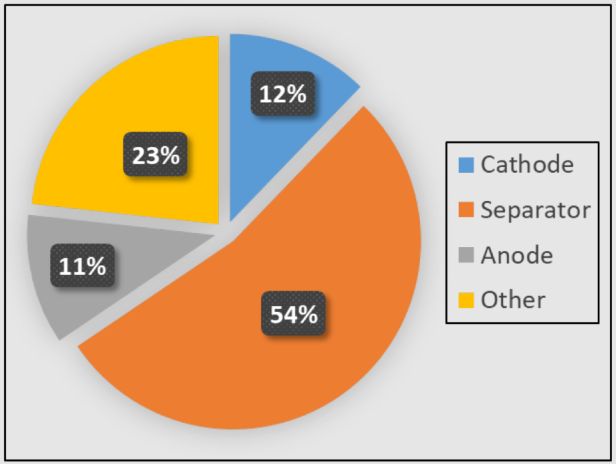




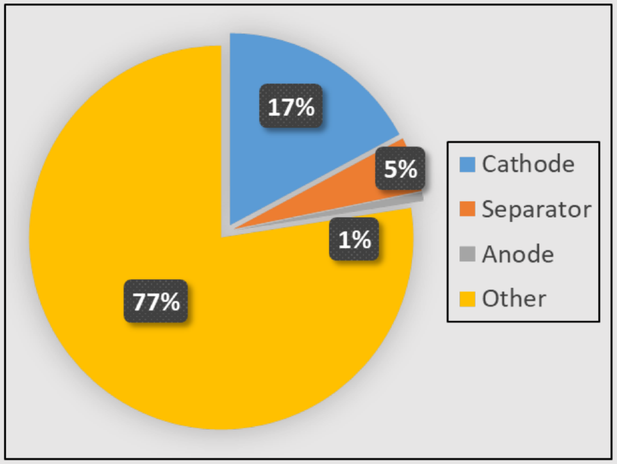
Thin cathodes and very low mass cells are required for high specific power

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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