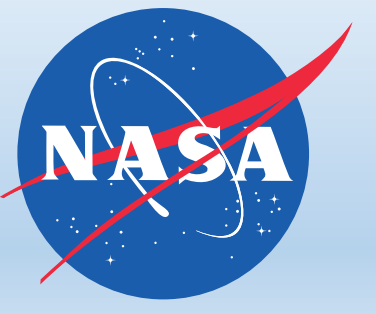


# Exploring Li-air batteries for high specific energy and high power applications: A simulation study

M. Mehta (mrmehta@nasa.gov)\*, J. Haskins\*, and J. W. Lawson§

\*AMA, Inc.; §Thermal Protection Materials Branch, NASA Ames Research Center, Moffett Field, California



## Introduction

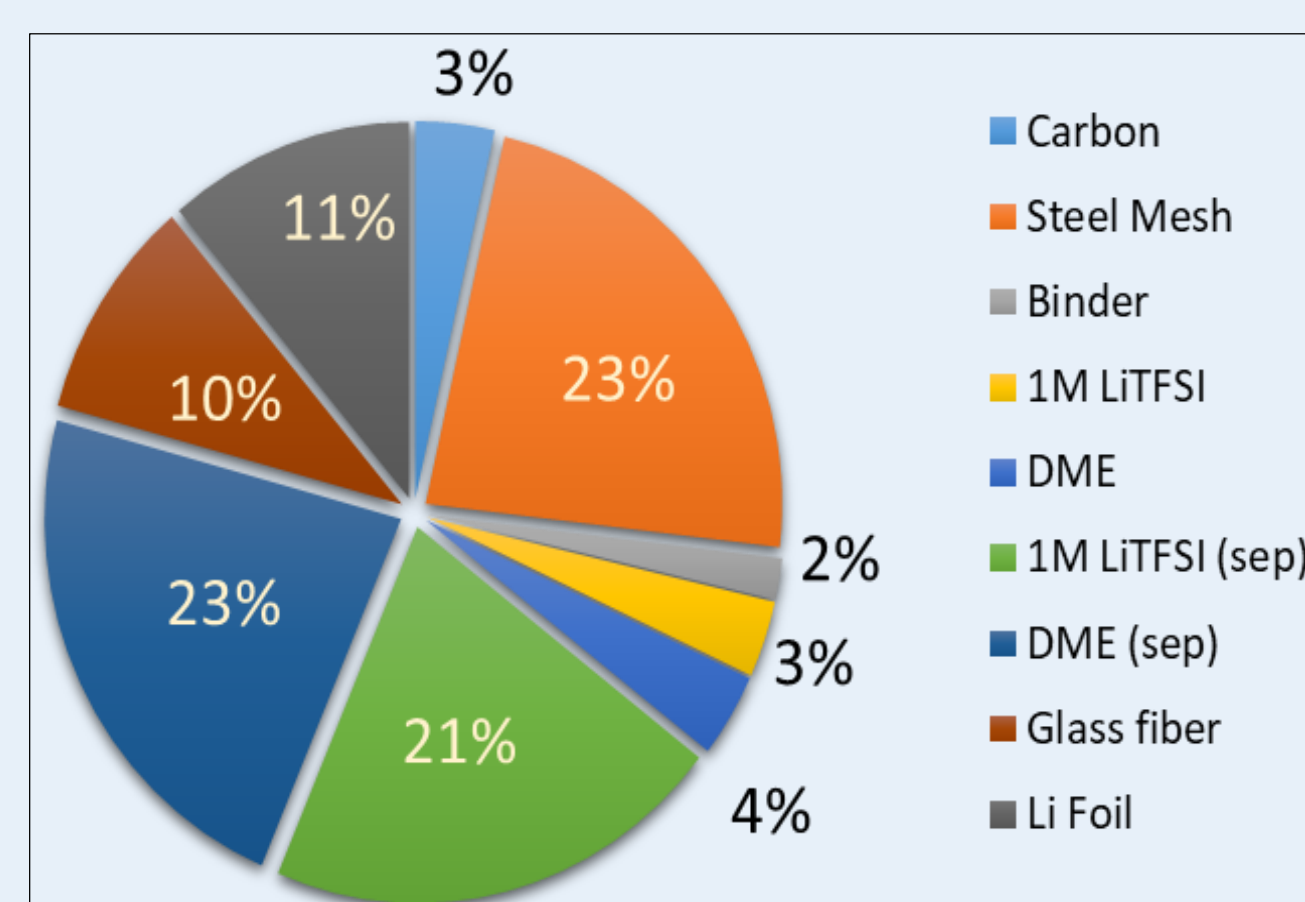
Commercialization of Li-air batteries for mass sensitive applications is more challenging due to additional constraints on battery mass in addition to order issues such as safety, electrolyte evaporation, high specific energy, and long discharge times. Here, we present our finite element simulation results comparing energy density, specific power, and discharge times for Li-air battery with some optimal designs. We use a finite element model and a discharge product model developed in [1], the electrolyte properties such as ion conductivity and ion diffusion were obtained from Molecular Dynamics (MD) simulations [3], and the other parameters for the finite element model were calibrated to match experiments at high discharge current densities ( $>1.5 \text{ mA/cm}^2$ ).

## Background

The finite element model adapted from refs. [1, 2, 4, 5] and it used:

1. Concentrated electrolyte theory for ion transport and electrolyte potential
2. Fickian diffusion for oxygen transport
3. Quantum tunneling for electron transport in  $\text{Li}_2\text{O}_2$
4. Ohm's equation for electron conduction in the cathode
5. Electron transport in the Butler-Volmer kinetics
6. Faraday's mass transfer relation for change in surface area

The mass distribution is taken from refs. [6] and [7]



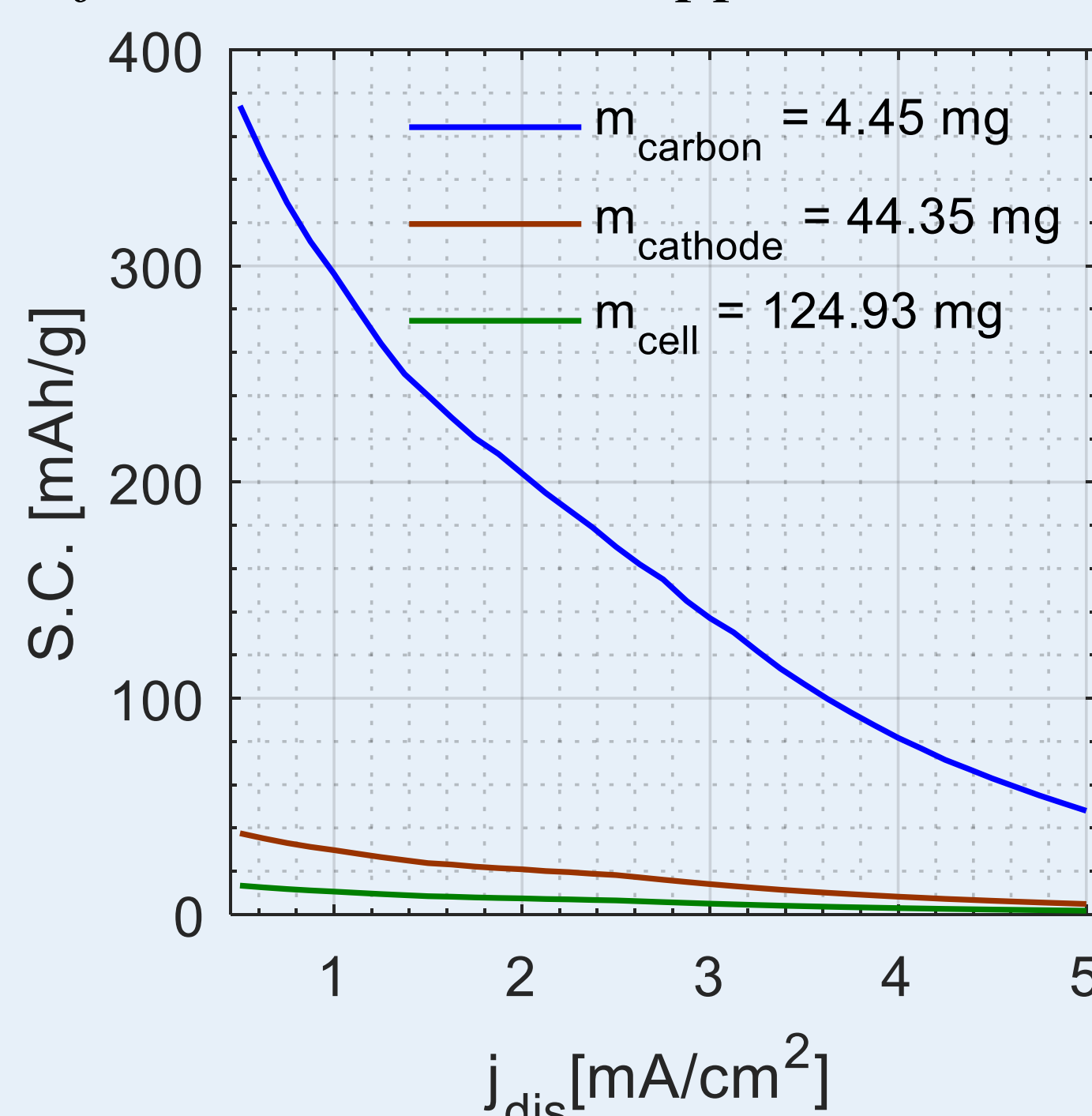
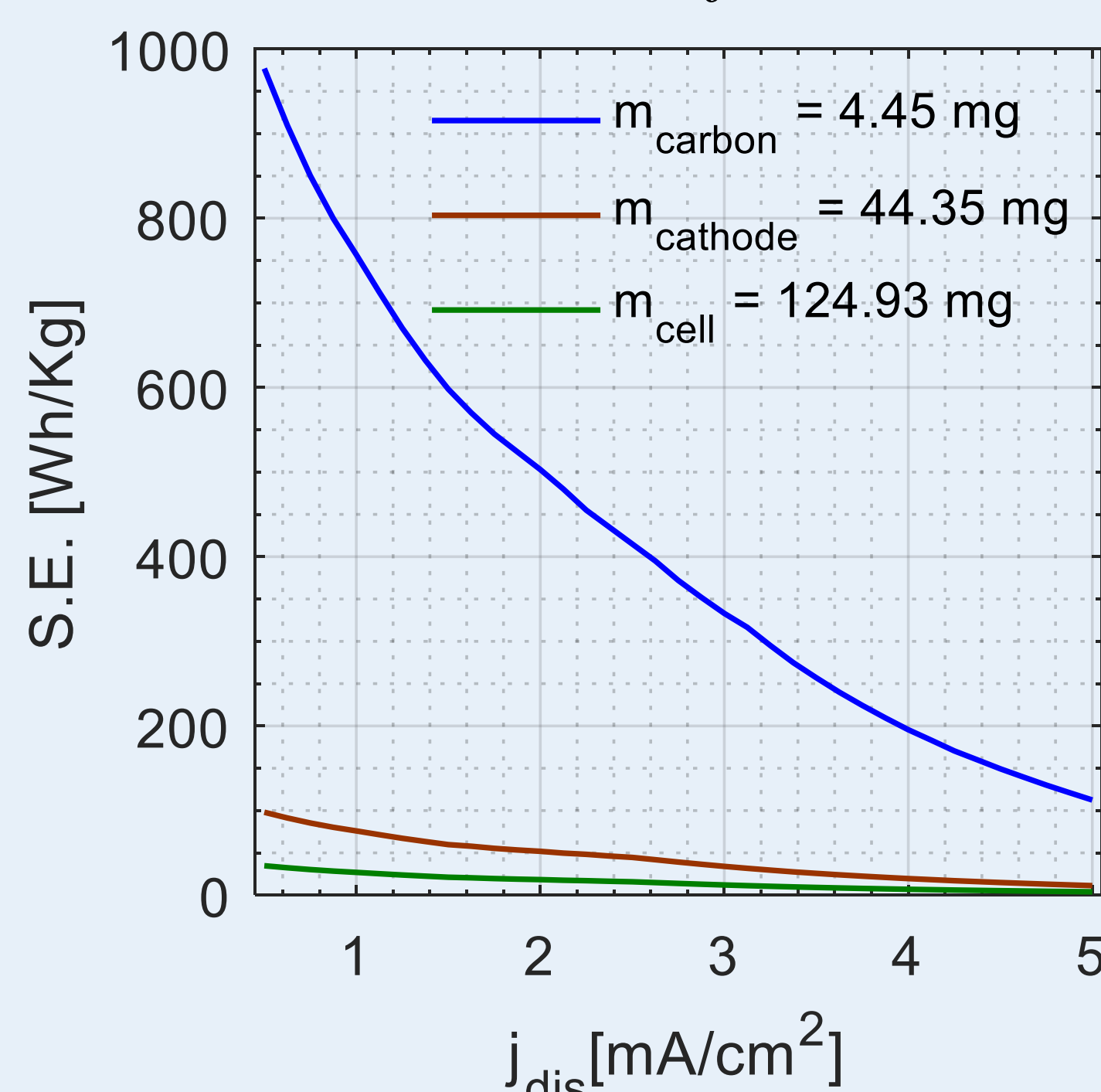
Thickness:

- Cathode:  $131 \mu\text{m}$
- Separator:  $450 \mu\text{m}$
- Anode:  $280 \mu\text{m}$

Diameter:

- Cathode:  $12 \text{ mm}$
- Separator:  $12.7 \text{ mm}$
- Anode:  $11 \text{ mm}$

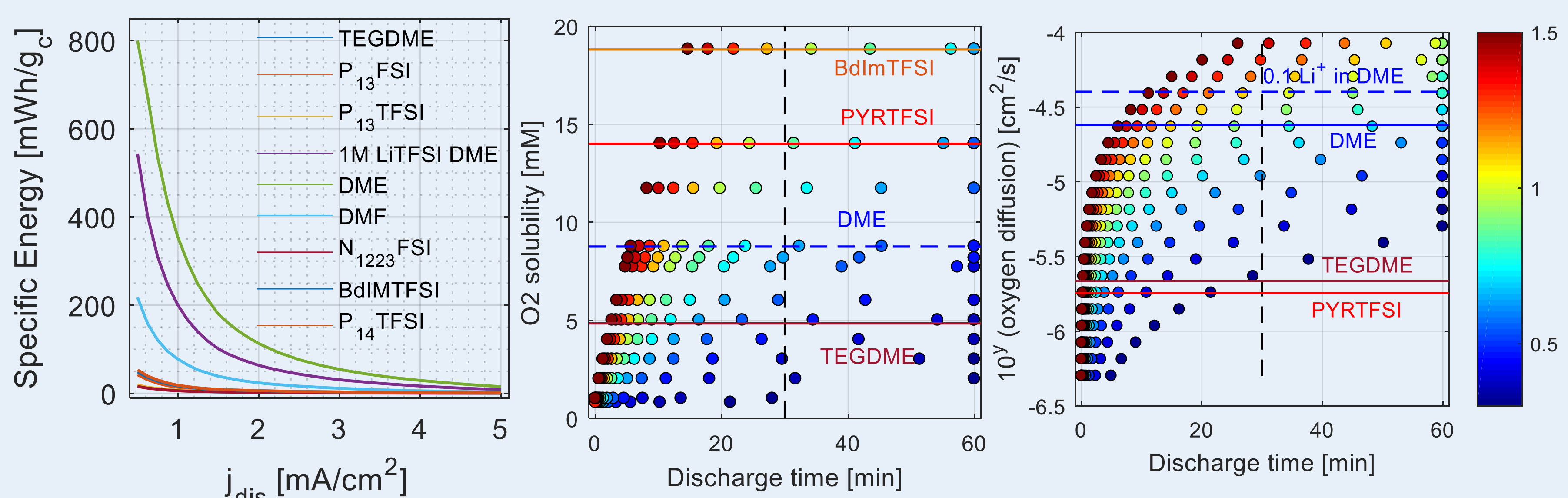
Reporting cell mass and normalizing performance with cell mass provide realistic estimation of Li-air batteries for mass sensitive applications.



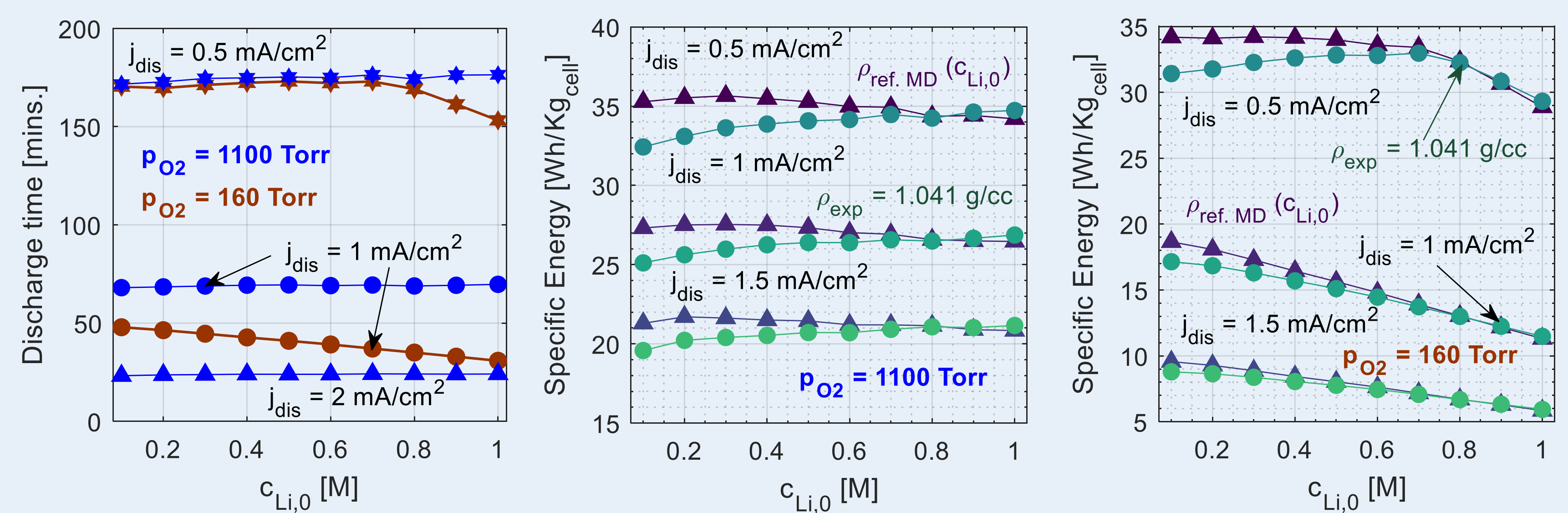
Large difference in performance parameters based on normalization mass.

## Results

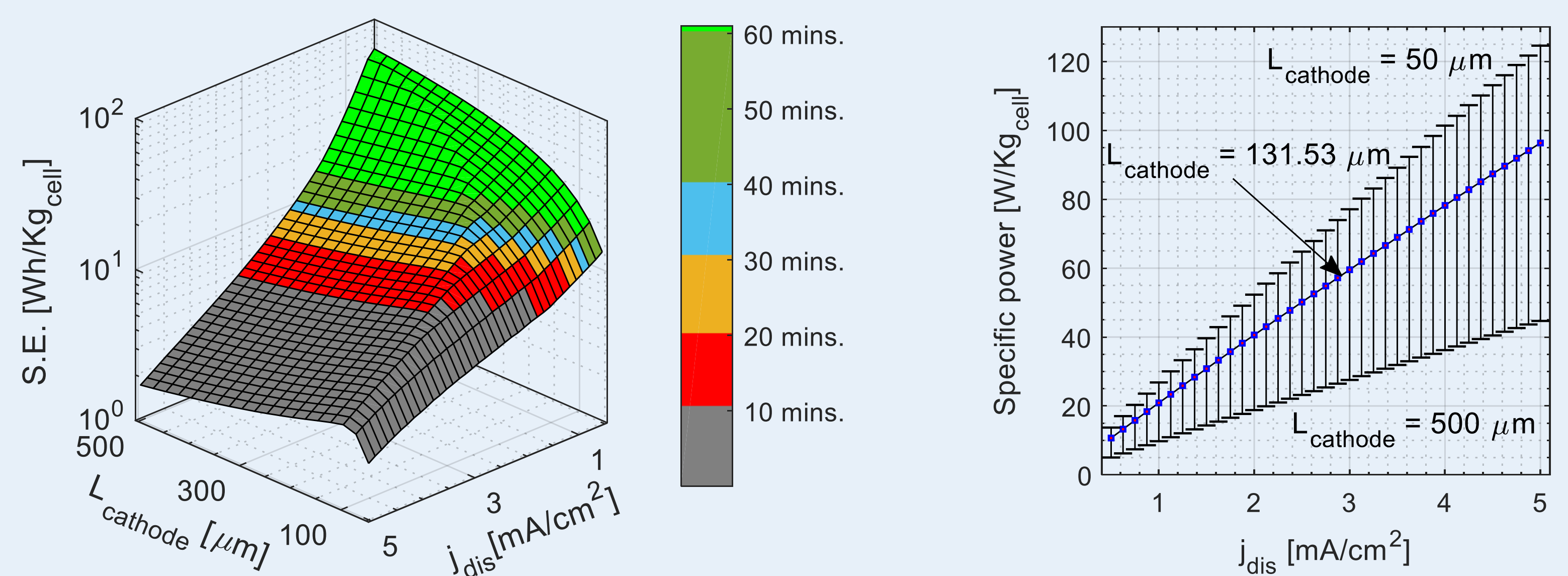
Effect of electrolyte on specific energy and the sensitivity of discharge time and maximum discharge current density to oxygen diffusion and solubility [9] in the electrolyte



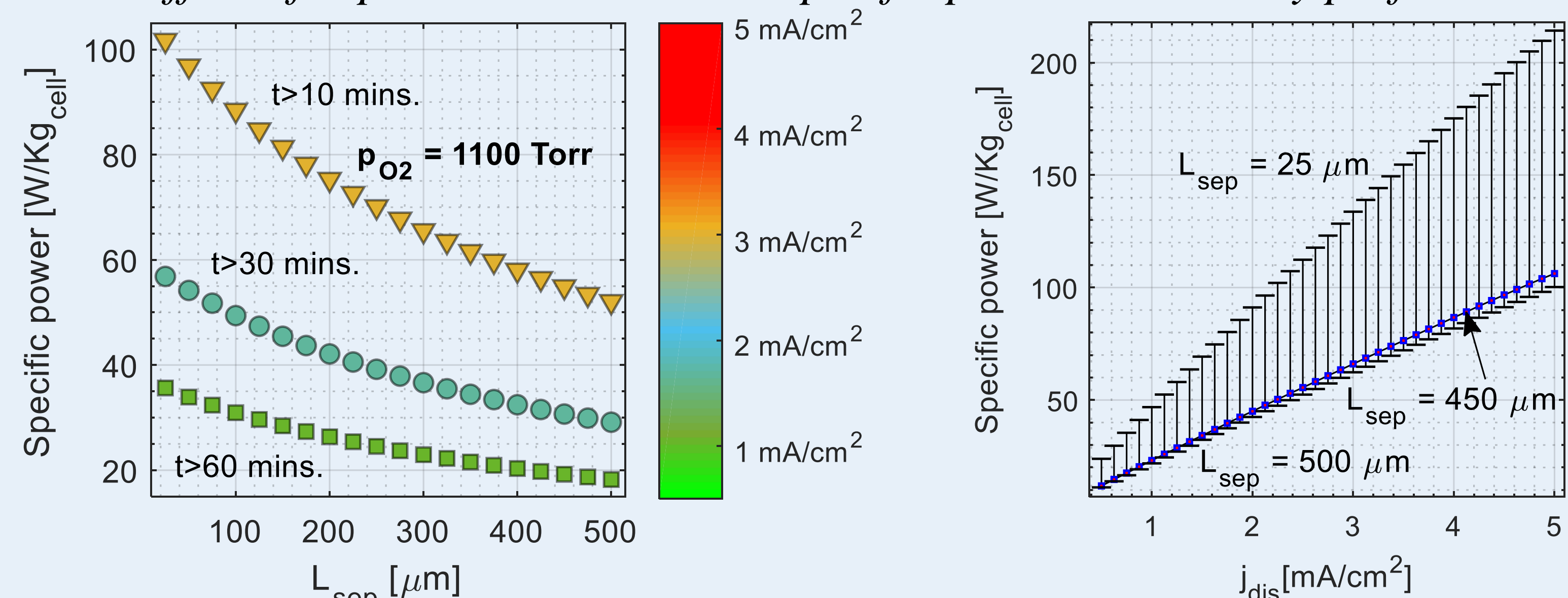
Effect of Li-ion concentration on discharge time and on specific energy for different current densities and different partial pressures.



Effect of cathode thickness on discharge time and max. current density

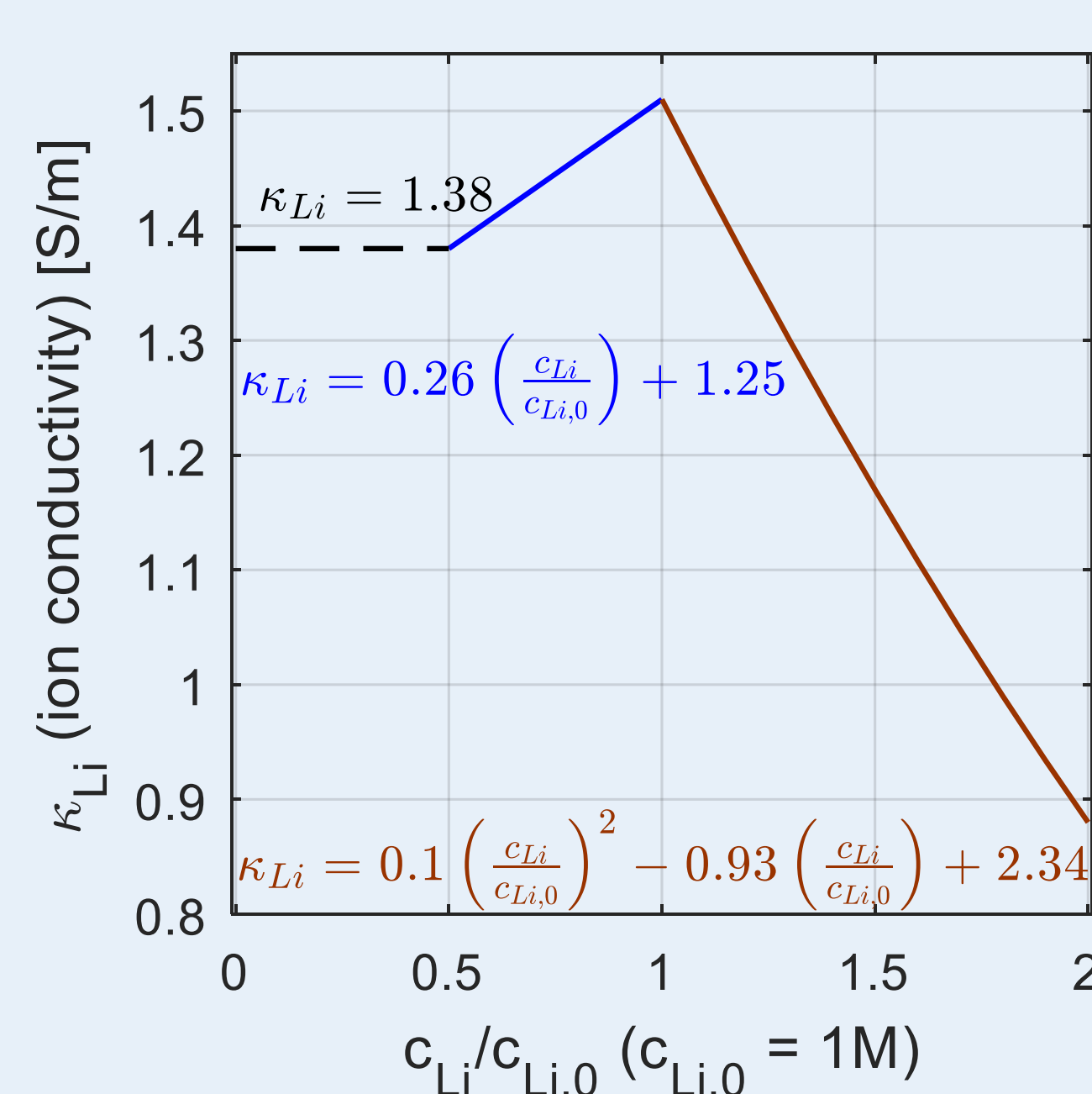
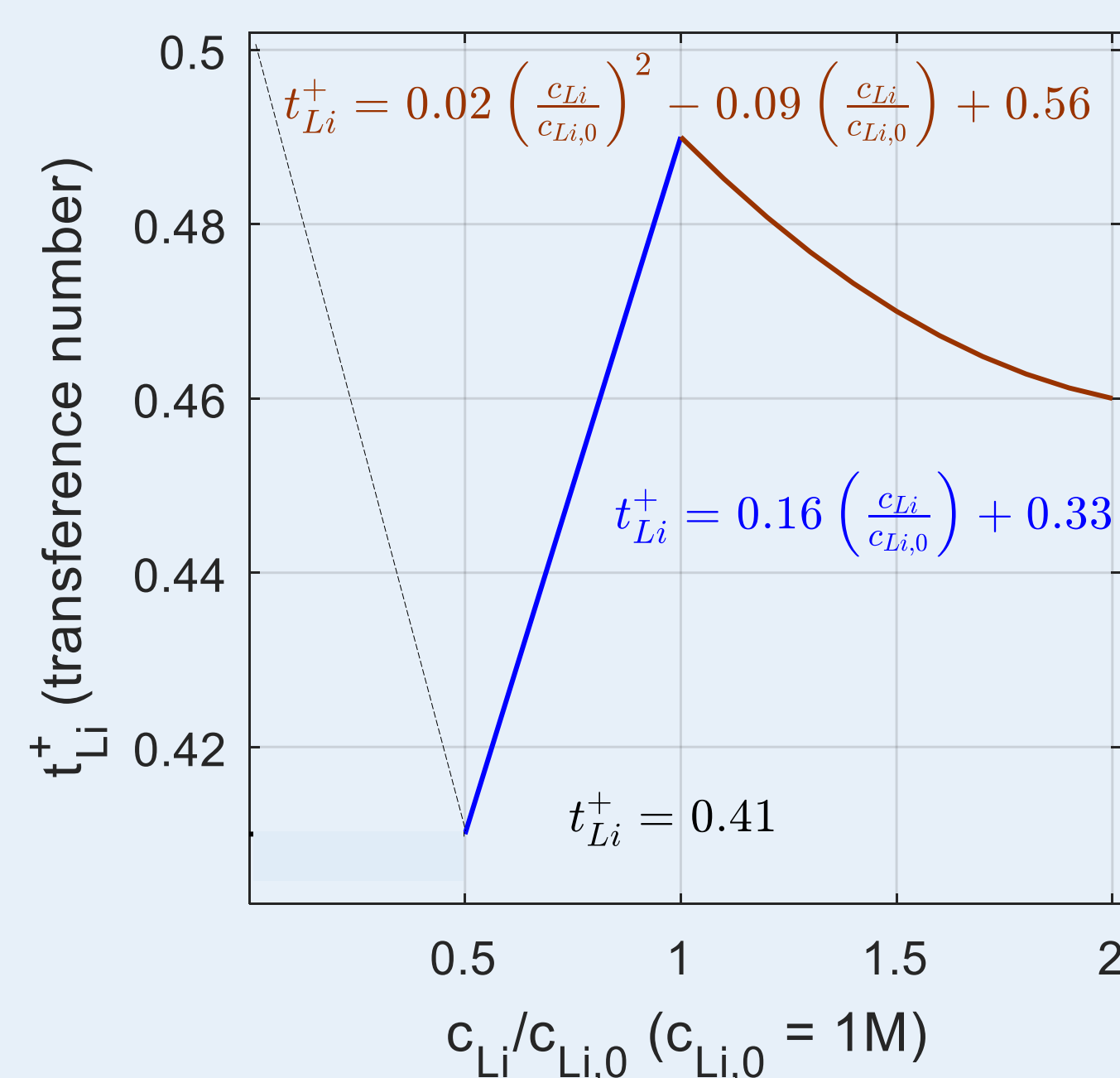


Effect of separator thickness on specific power and battery performance

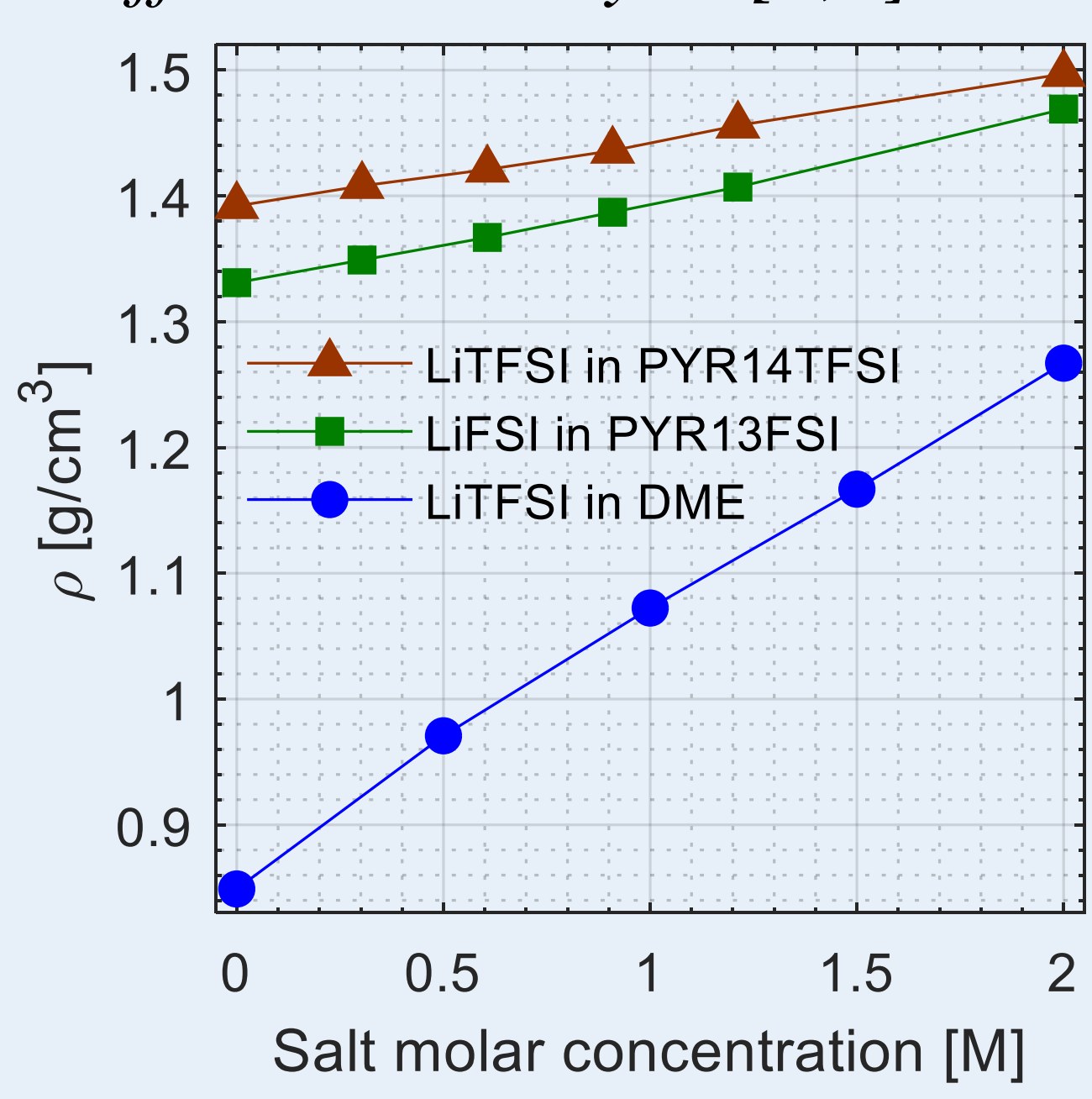
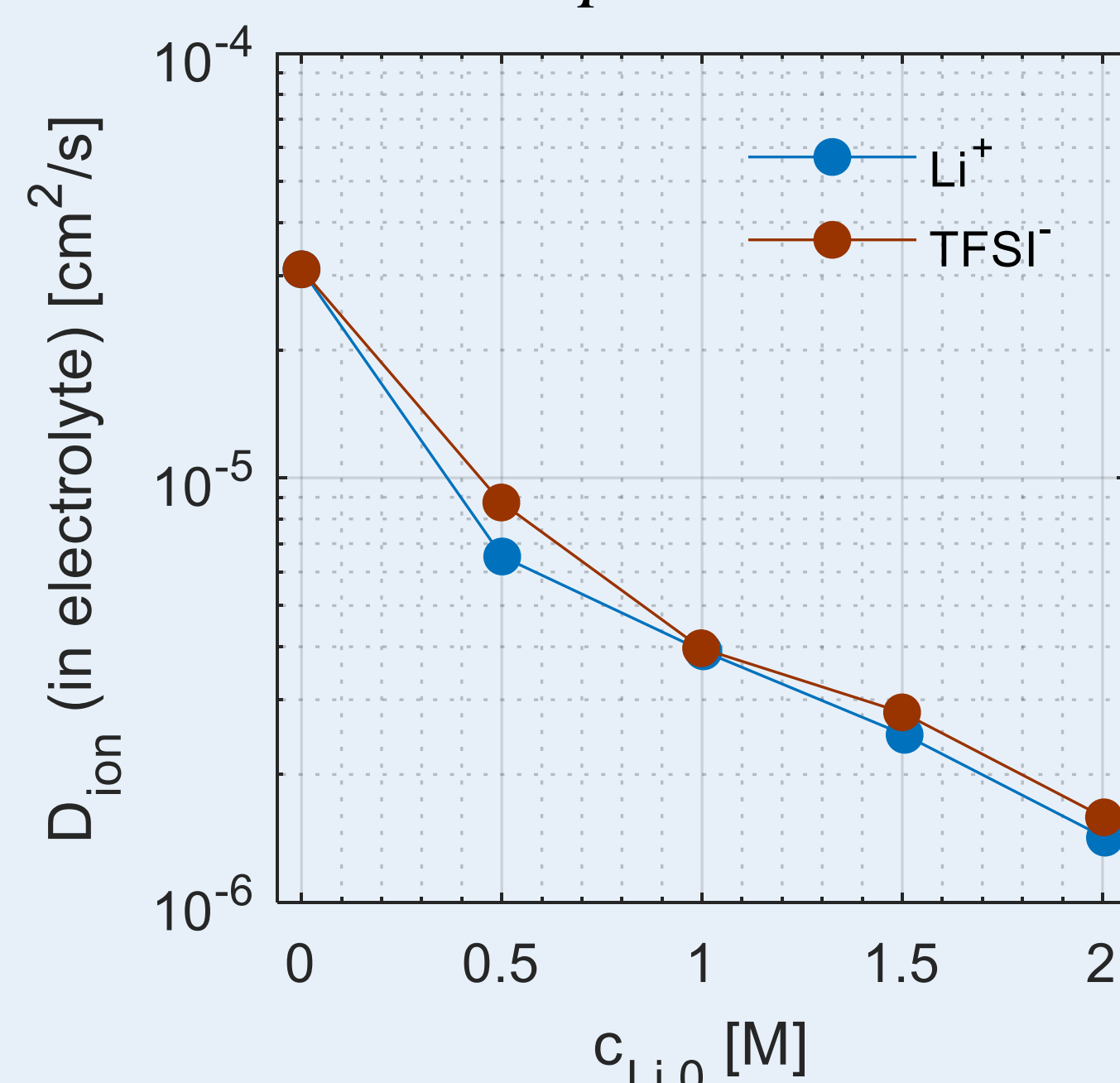


## Electrolyte parameterization from MD simulations

MD simulations [3] provided electrolyte properties for the Newman model



MD simulations provided mass densities for different electrolytes [3,8]



## Conclusions

- Reporting cell mass is important for real performance of these batteries
- Reducing cell mass increases specific energy by an order of two without performance compromise
- Choosing an optimal electrolyte with low mass and high oxygen diffusion and solubility can improve discharge times and discharge current density performance

## Future work

- Extend the current analysis to other electrolytes such as amides and nitrates
- Perform detailed power analysis on different commercial cathode and custom cathode structures to understand optimal cathodes architectures for power sensitive applications
- Study the effect of redox mediators on specific energy and discharge current densities

## References

1. Bevara, V. & Andrei, P. (2014), J. Electrochem. Soc. 161(14), A2068-A2079.
2. Mehta, M. & Andrei, P. (2015), J. Power Sources. 286, 299-308.
3. Liyana-Arachchi, TP, Haskins, J. et.al. (2018), J. Phys. Chem. C, Under Review.
4. Andrei, P. et. al. (2010), J. Electrochem. Soc. 157(12), A1287-A1295.
5. Sahapatombut, U., Cheng, H., & Scott K. (2013), J. Power Sources. 243, 409-418.
6. Knudsen, K. et.al. (2016), J. Electrochem. Soc. 163(9), A2065-A2071.
7. Mehta, M. et. al. (2018), In Preparation.
8. Haskins, J.; et. al. (2014), J. Phys. Chem. B. 118(38), 11295-11309.
9. Das, S. et. al. (2015), J. Phys. Chem. C 119, 18084-18090.

## Acknowledgements

Funding acknowledgement: NASA Aeronautics Research Mission Directorate (ARMD) Convergent Aeronautics Solutions (CAS) Project, LiON sub-project.