# Master's Thesis Engineering Technology

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# *Model-based optimization of electrodes for lithium-ion batteries*


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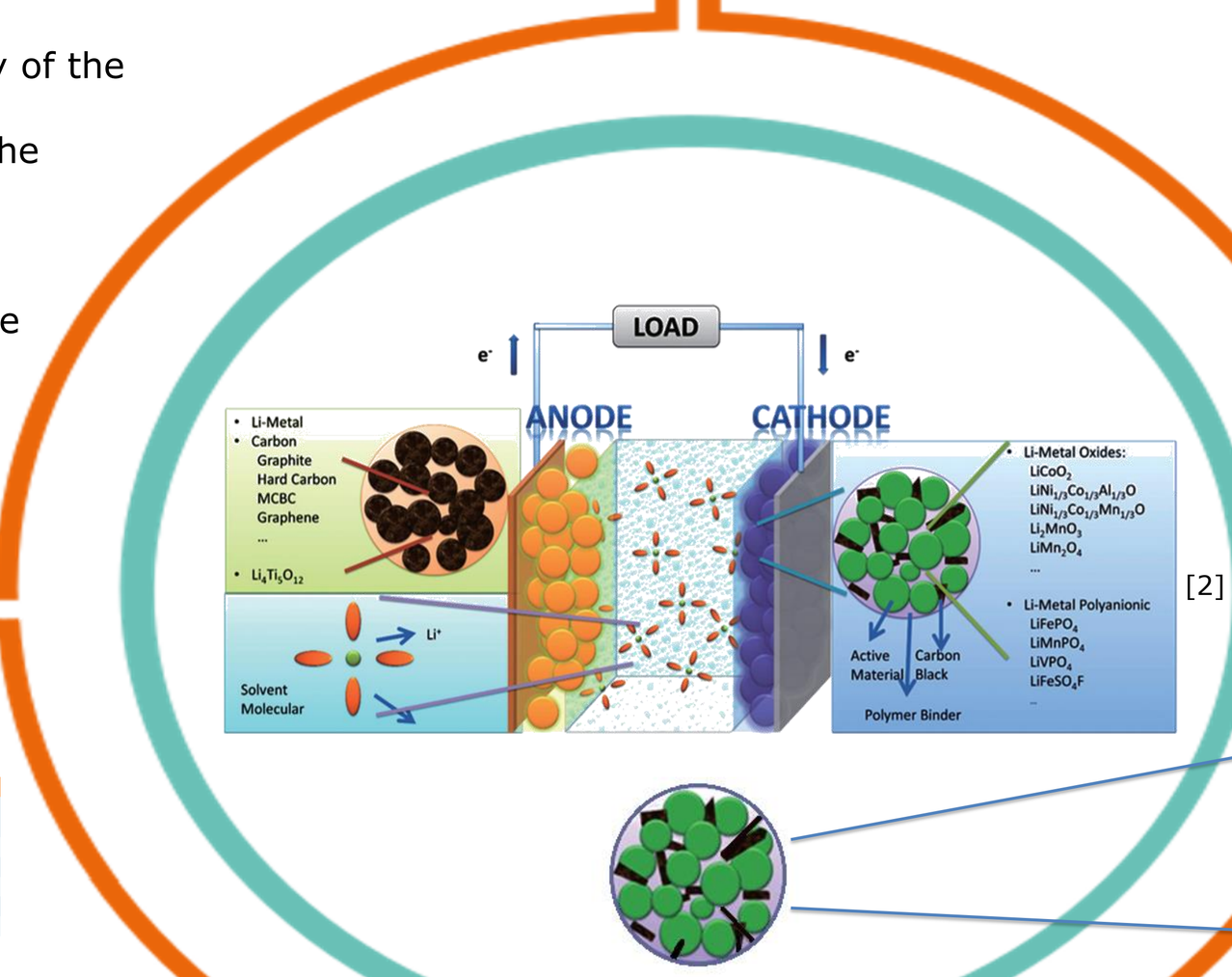
## Objective

The objective is to perform a systematic investigation of the influence of the main adjustable design parameters on the performance of a LIB. LMO, NMC, LCO, and LFP are the cathode materials considered in this study and the following design parameters are studied in the sensitivity analyses:

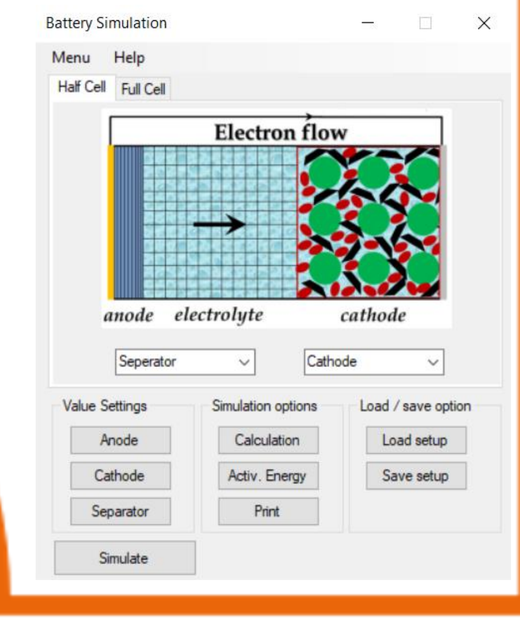
- Solid-state Li diffusion coefficient in cathode material
- Electronic conductivity of the cathode
- Ionic conductivity of the electrolyte
- Cathode thickness
- Cathode composition
- Porosity of the cathode

## Approach and methods

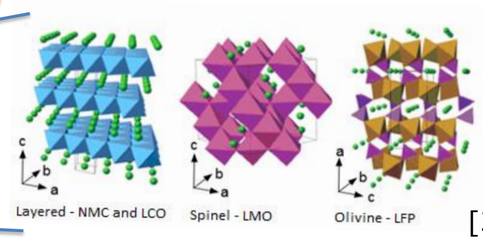
Sensitivity analyses are done with the aid of Physics-based modeling and simulation. To simplify the analyses, a half-cell setup is used where a lithium foil is used as the anode electrode. Here, Doyle's Dualfoil program [1] is used as the source code and further elaborated to create a user-friendly program for fast and efficient simulation of lithium-ion batteries.




[2]



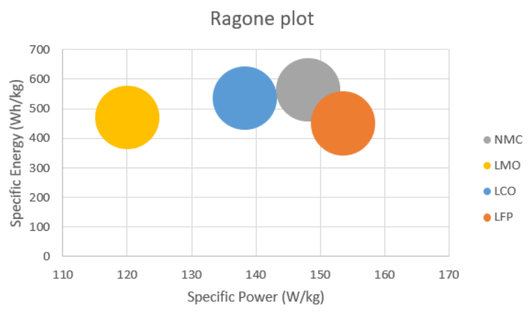

## Structures



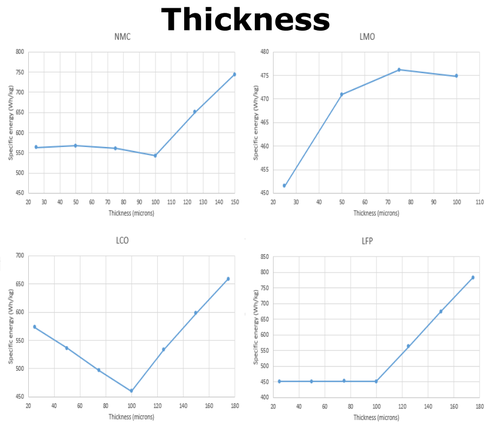

[3]

## Results

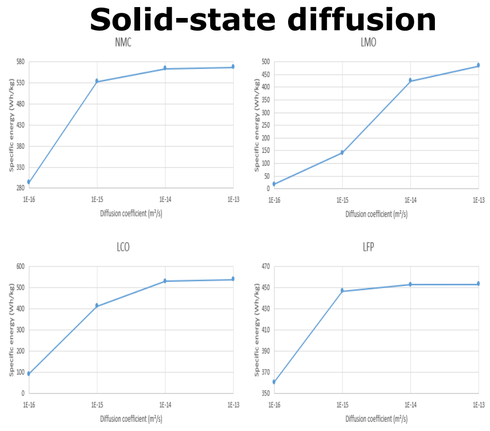
| Parameters | Values range |
|---|---|
| **Cathode thickness** | 25 – 50 – 75 – 100 – 125 – 150 – 175 ($\mu$m) |
| **Active material wt%** | 80 – 85 – 90 – 95 (%) |
| **Diffusion coefficient** | e-13 – e-14 – e-15 – e-16 ($m^2/s$) |
| **Electronic conductivity** | 0.1 – 1 – 10 – 100 (S/m) |
| **Ionic conductivity** | 0.1 – 1 – 10 – 100 (S/m) |
| **Porosity** | 0.3 – 0.4 – 0.5 – 0.6 |



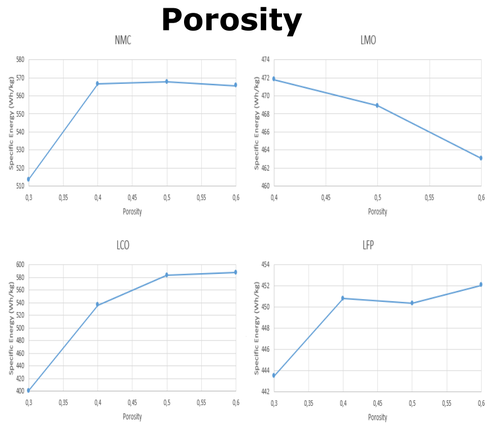

### Thickness




### Solid-state diffusion




### Porosity




## Conclusion

The performance of a battery is sensitive to many parameters. Here, modeling and simulation proves to be a powerful tool to reduce the complexity and save time in finding the optimum set of parameters to reach the specific needs of the user.

## References


[1] J. Newman, "cchem.berkeley.edu," 1998. [Online]. Available: http://www.cchem.berkeley.edu/jsngrp/dualfoil5.2.f. [Accessed 1 05 2018].

[2] J. Gao, S.-Q. Shi en H. Li, „Brief overview of electrochemical potential in lithium ion batteries," Chinese Physical society and IOP Publishing Ltd., vol. 25, nr. 1, pp. 018210-2 , 2015.

[3] C. M. Julien, A. Mauger, K. Zaghib and H. Groult, "Comparative Issues of Cathode Materials for Li-Ion Batteries," inorganicas, no. 2, pp. 132-1254, 2014.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