

# Effect Of Intercalation Diffusivity When Simulating Mixed Electrode Materials In Li-Ion Batteries

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# Outline

- **Background**
- **Physics based modeling**
- **Mixed electrode material**
- **Results**
- **Conclusions**



Photo: Volvo

# Background



**Volvo Cars Corporation  
Battery Systems**

Theresa Granérus  
Henrik Markusson



UPPSALA  
UNIVERSITET

**Uppsala University  
Ångström Advanced Battery Center**

Prof. Kristina Edstöm  
Prof. Daniel Brandell  
Erik Björklund



**ABB AB  
Corporate Research**

Tomas Tengnér  
Antonis Marinopoulos



CHALMERS

**Chalmers University of Technology  
Electric Power Engineering**

Prof. Torbjörn Thiringer  
Evelina Wikner

# PhD project

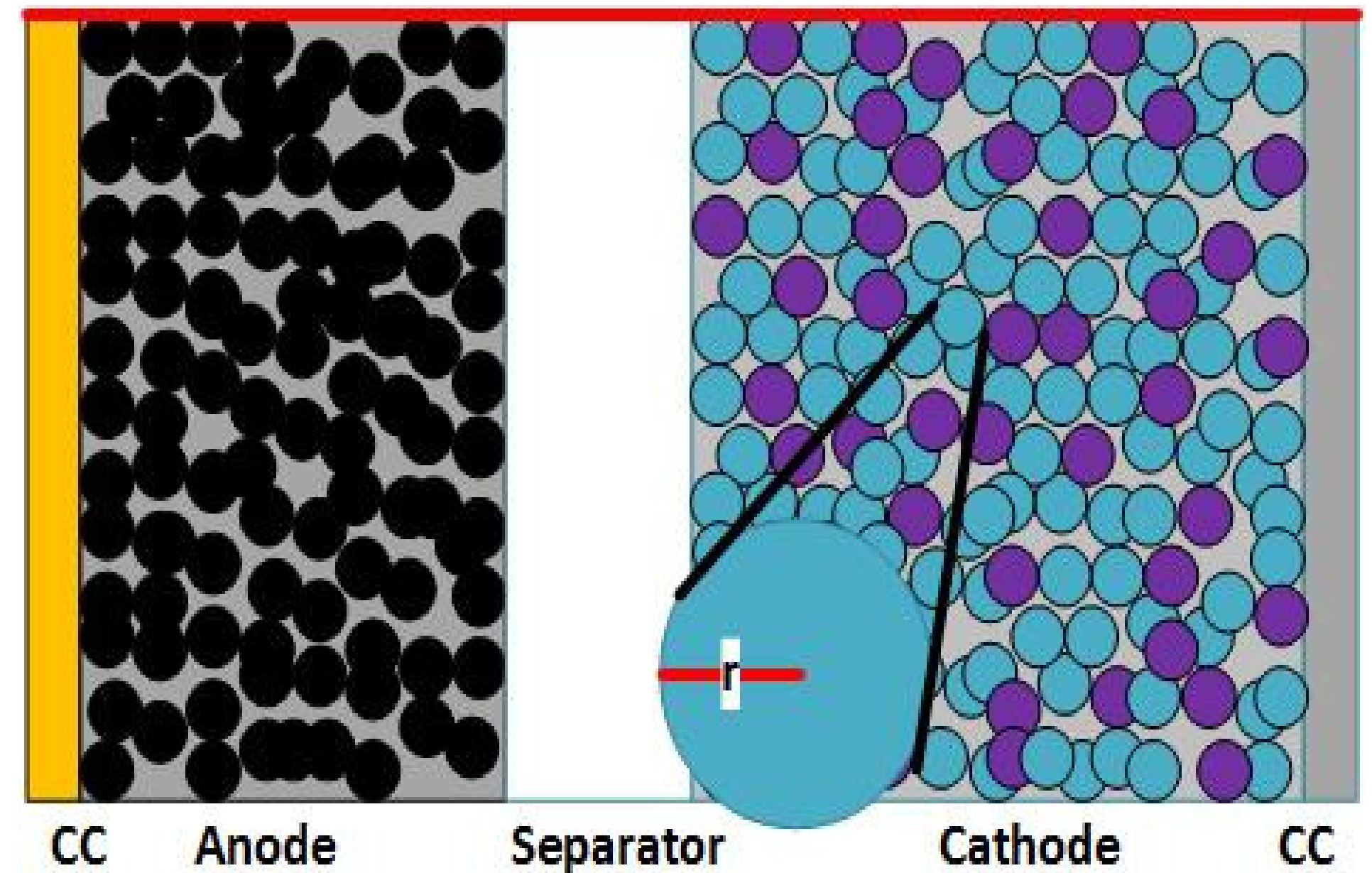
- **Aging mechanisms**
- **Simulation of chosen mechanisms**
- **Predict aging**
- **Improve battery utilization**

**Funded by:**



# Physics based battery model

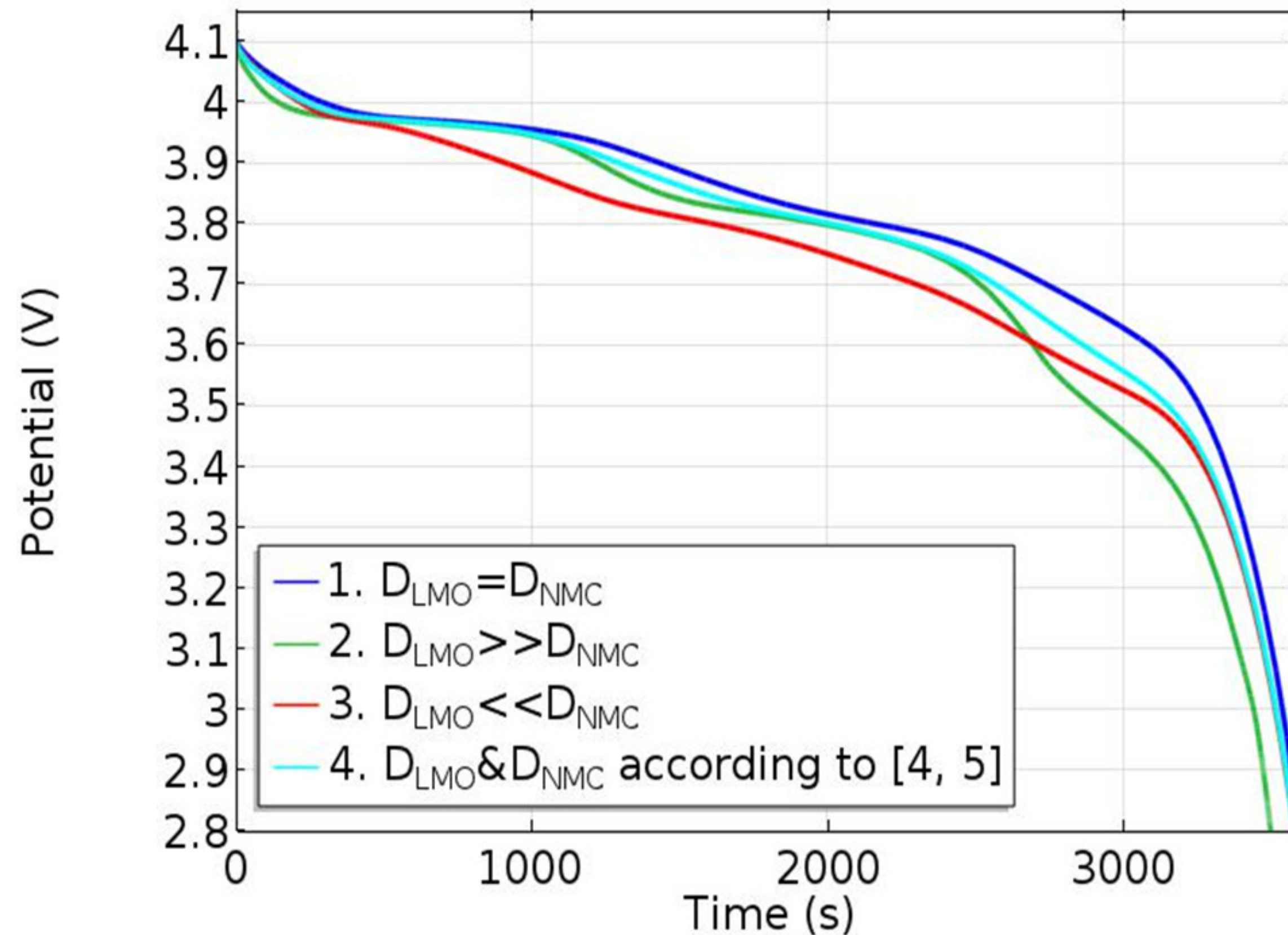
- More than 80 parameters!
- Difficult to measure several of the parameters
- Concentration and temperature dependence



# Mixed electrode materials

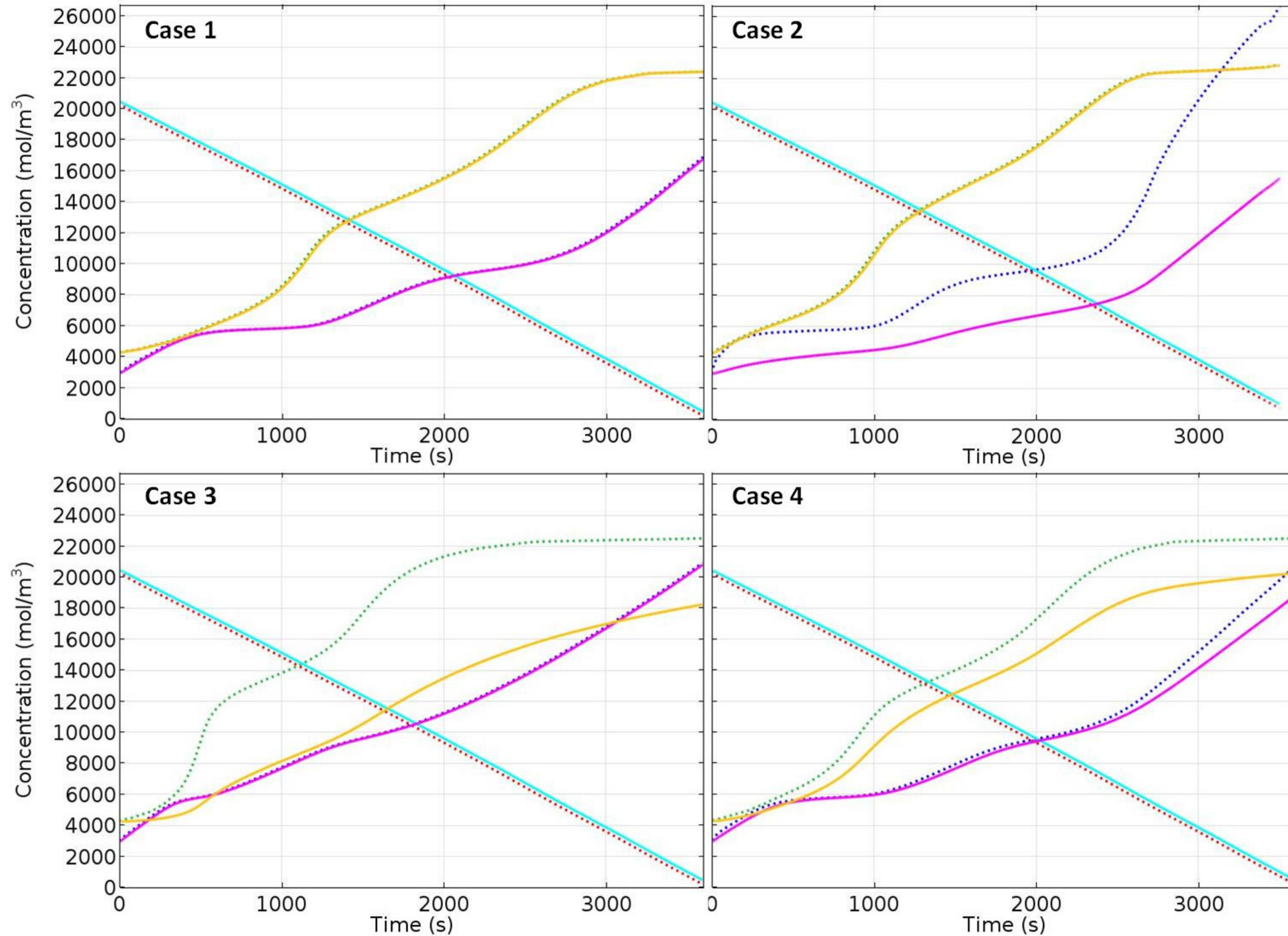
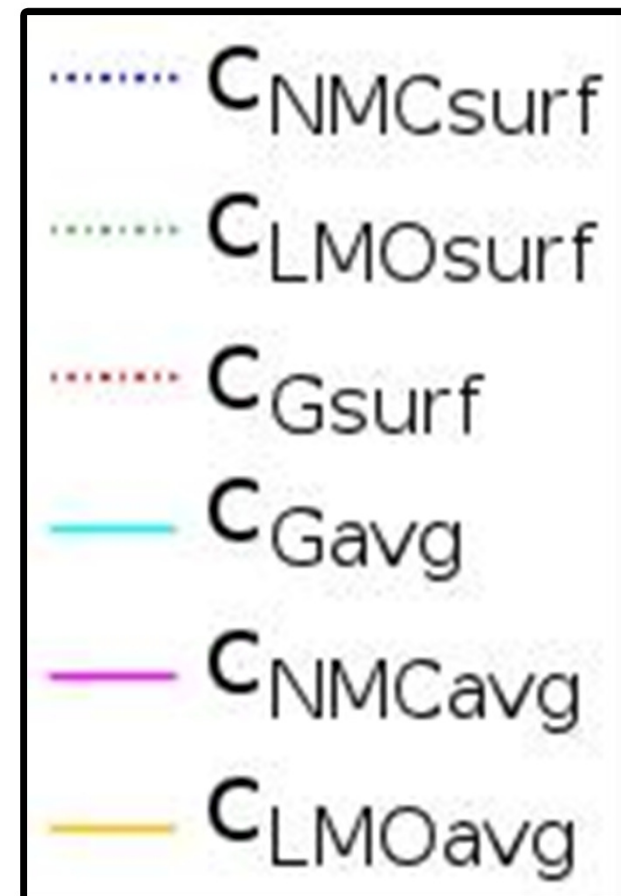
- **Higher complexity**
- **More parameters**
- **Higher impact of diffusion coefficient**

# Results



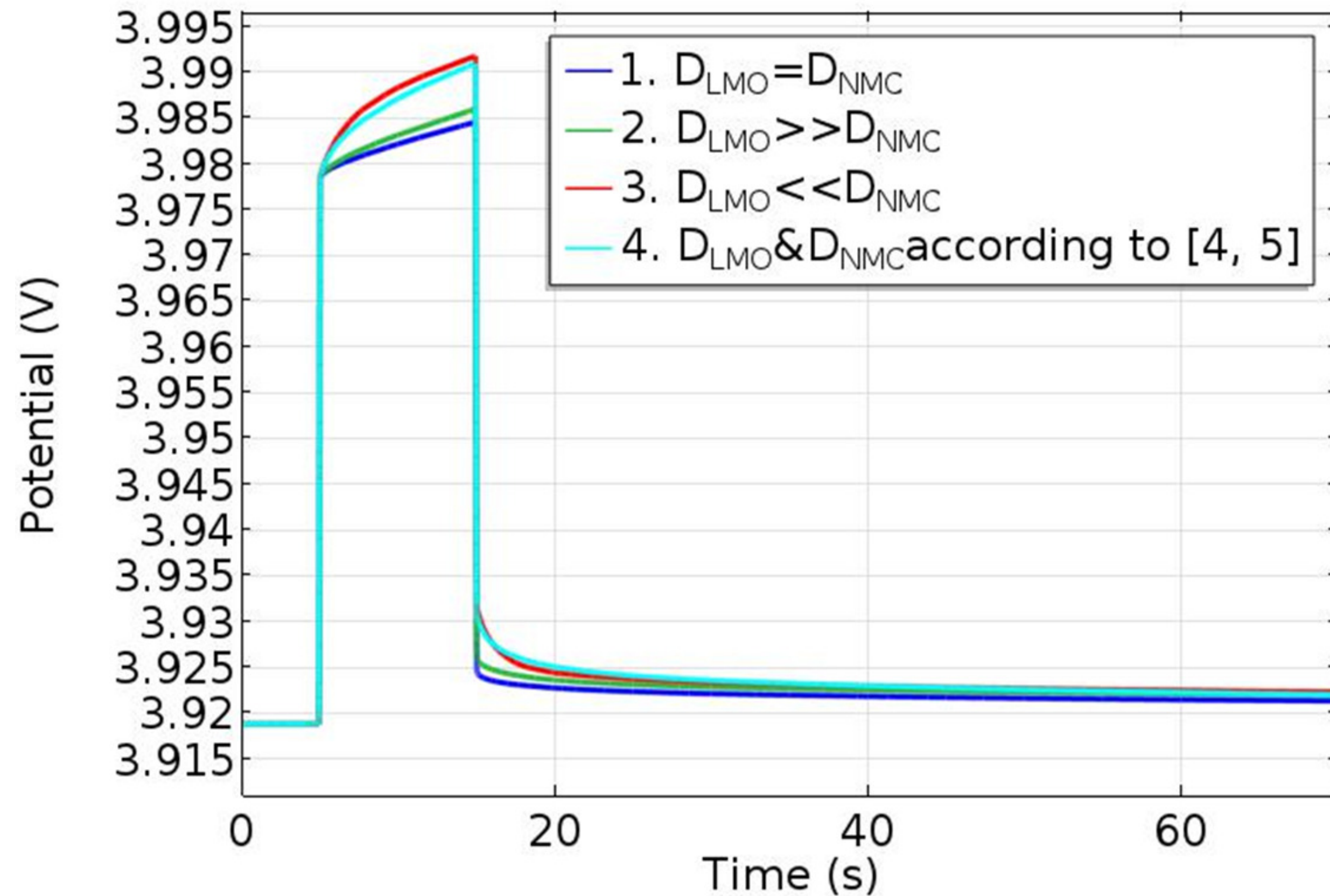
4. P. C. Goonetilleke, J. P. Zheng and D. Roy, "Effects of Surface-Film Formation on the Electrochemical Characteristics of  $\text{LiMn}_2\text{O}_4$  Cathodes of Lithium Ion Batteries", *Journal of the Electrochemical Society*, **vol. 156**, pp. A709-A719 (2009)
5. Wu, Shao-Ling, Wei Zhang, Xiangyun Song, Alpesh K. Shukla, Gao Liu, Vincent S. Battaglia, and Venkat Srinivasan, High Rate Capability of  $\text{Li}(\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3})\text{O}_2$  Electrode for Li-Ion Batteries, *Journal of the Electrochemical Society*, **vol. 159**, pp. A438-A444 (2012)

# Results



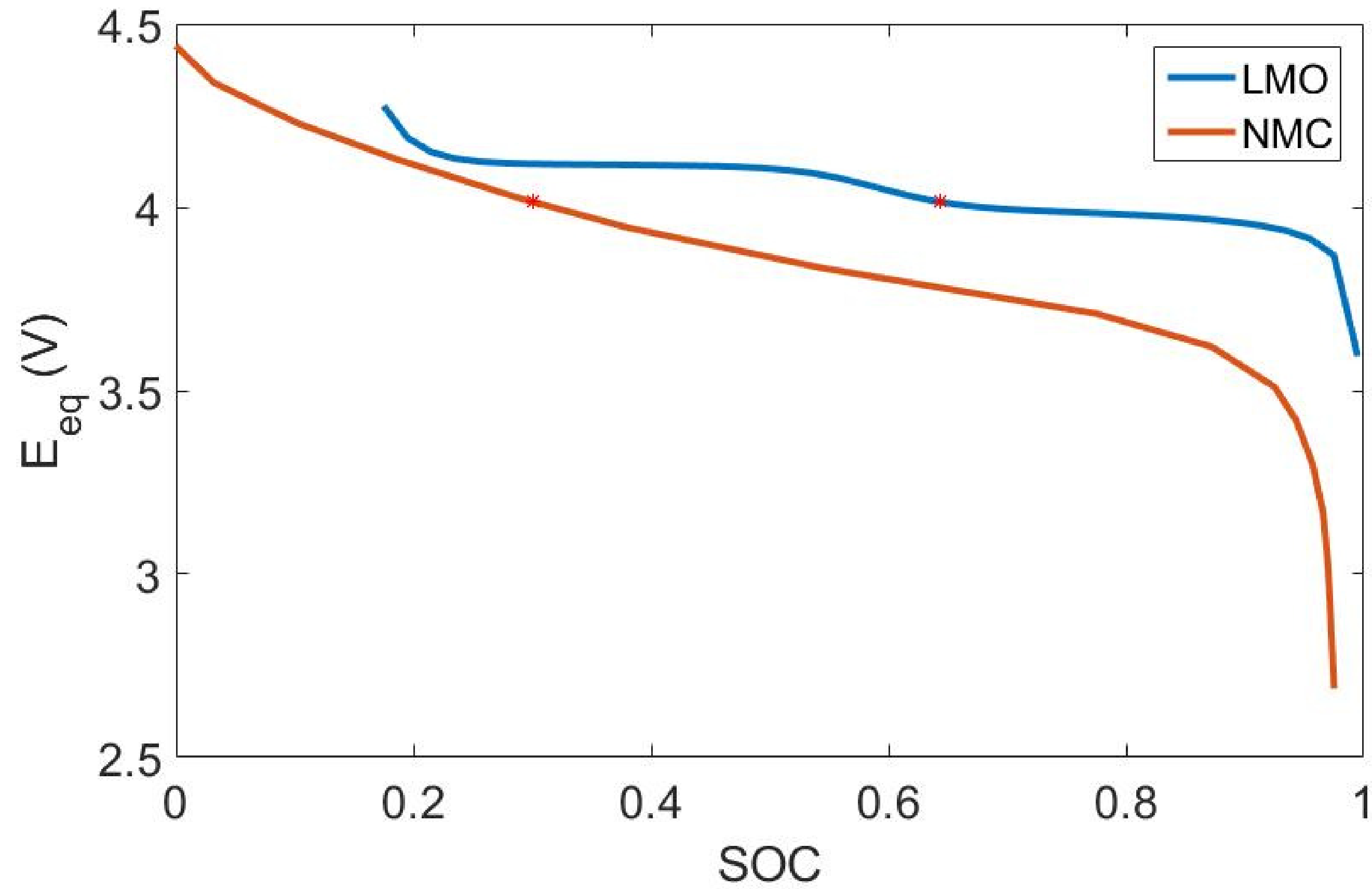


# Results



4. P. C. Goonetilleke, J. P. Zheng and D. Roy, "Effects of Surface-Film Formation on the Electrochemical Characteristics of  $\text{LiMn}_2\text{O}_4$  Cathodes of Lithium Ion Batteries", *Journal of the Electrochemical Society*, **vol. 156**, pp. A709-A719 (2009)
5. Wu, Shao-Ling, Wei Zhang, Xiangyun Song, Alpesh K. Shukla, Gao Liu, Vincent S. Battaglia, and Venkat Srinivasan, High Rate Capability of  $\text{Li}(\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3})\text{O}_2$  Electrode for Li-Ion Batteries, *Journal of the Electrochemical Society*, **vol. 159**, pp. A438-A444 (2012)

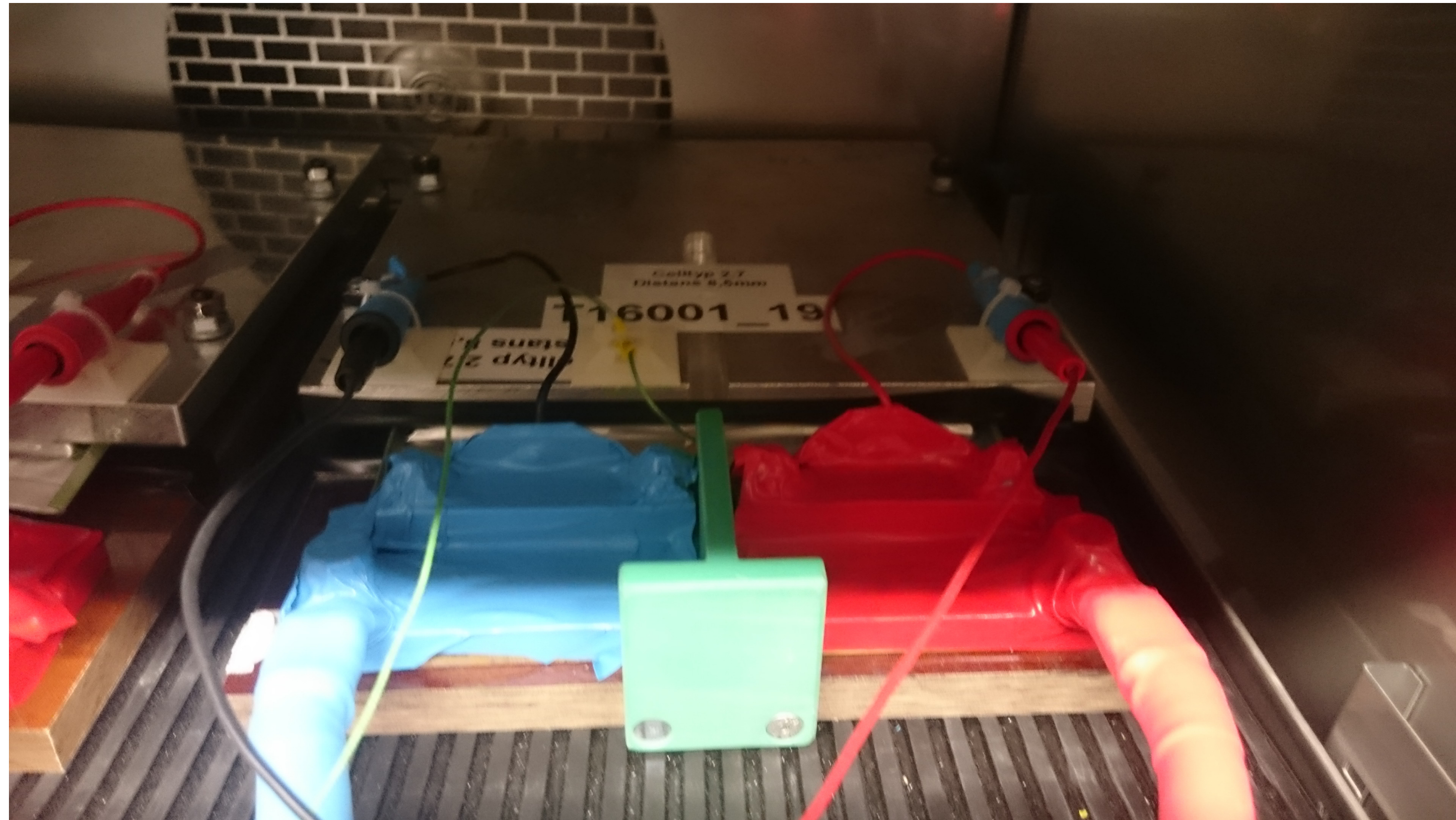
# Results



# Conclusions

- **Special care needs to be taken when simulating mixed electrode materials.**
- **The diffusion coefficient's concentration dependence should not be neglected.**
- **The model can be used to find optimal mix of two electrode materials.**

# Thank you for your attention!





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