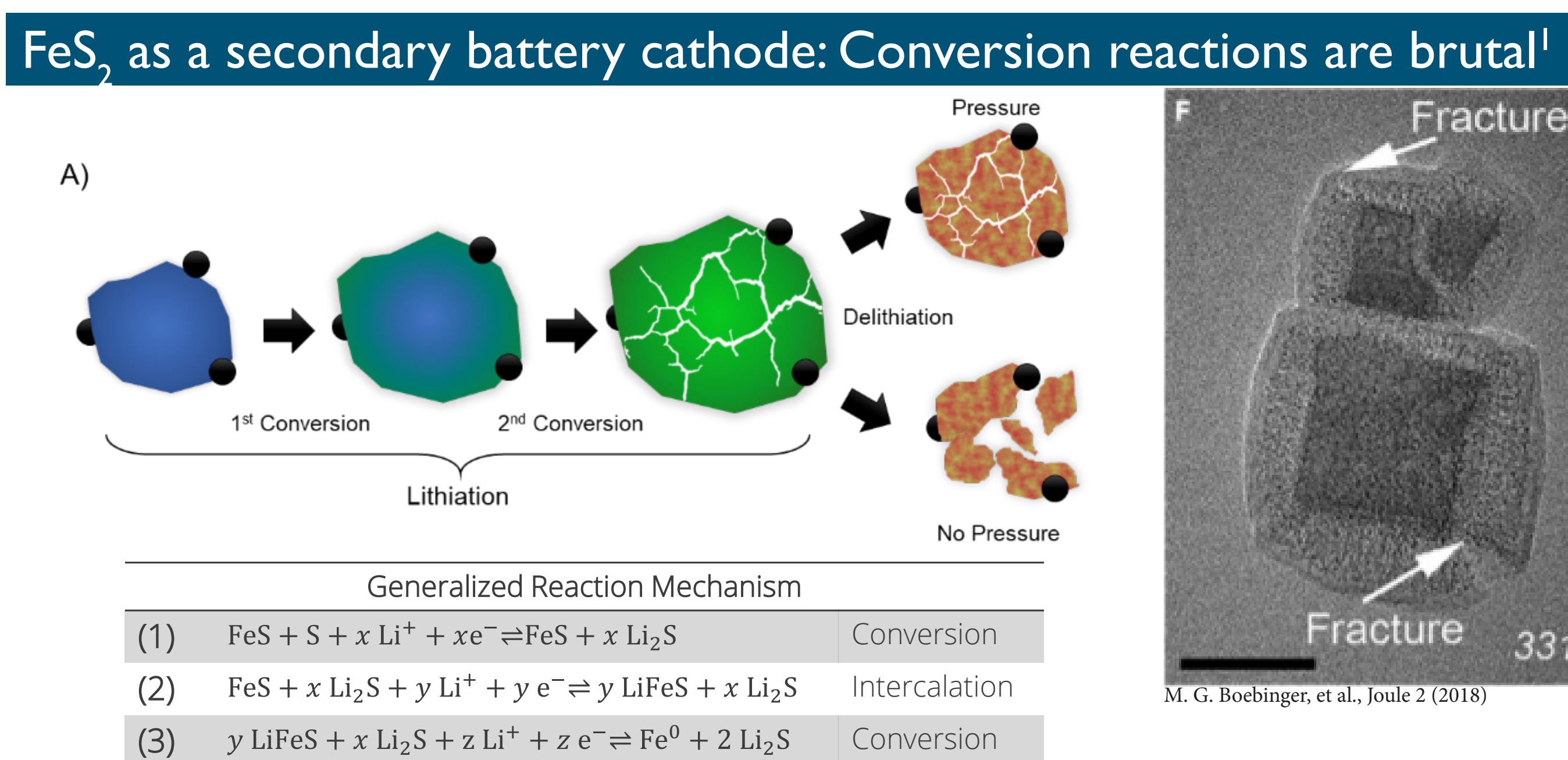
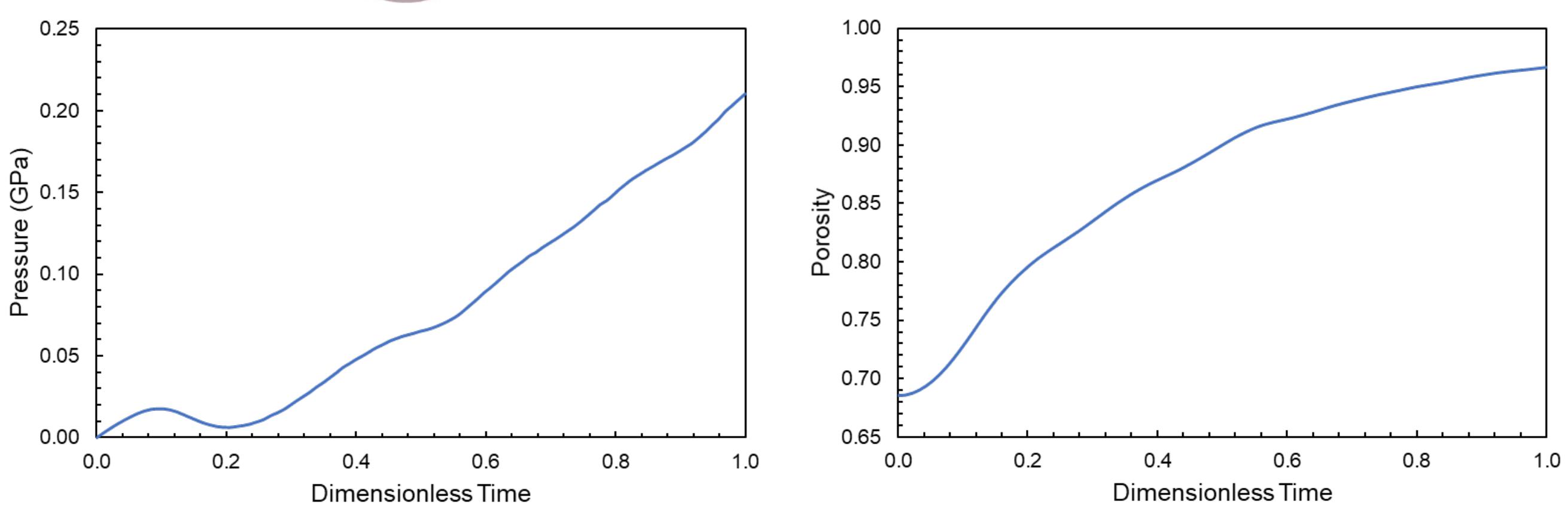
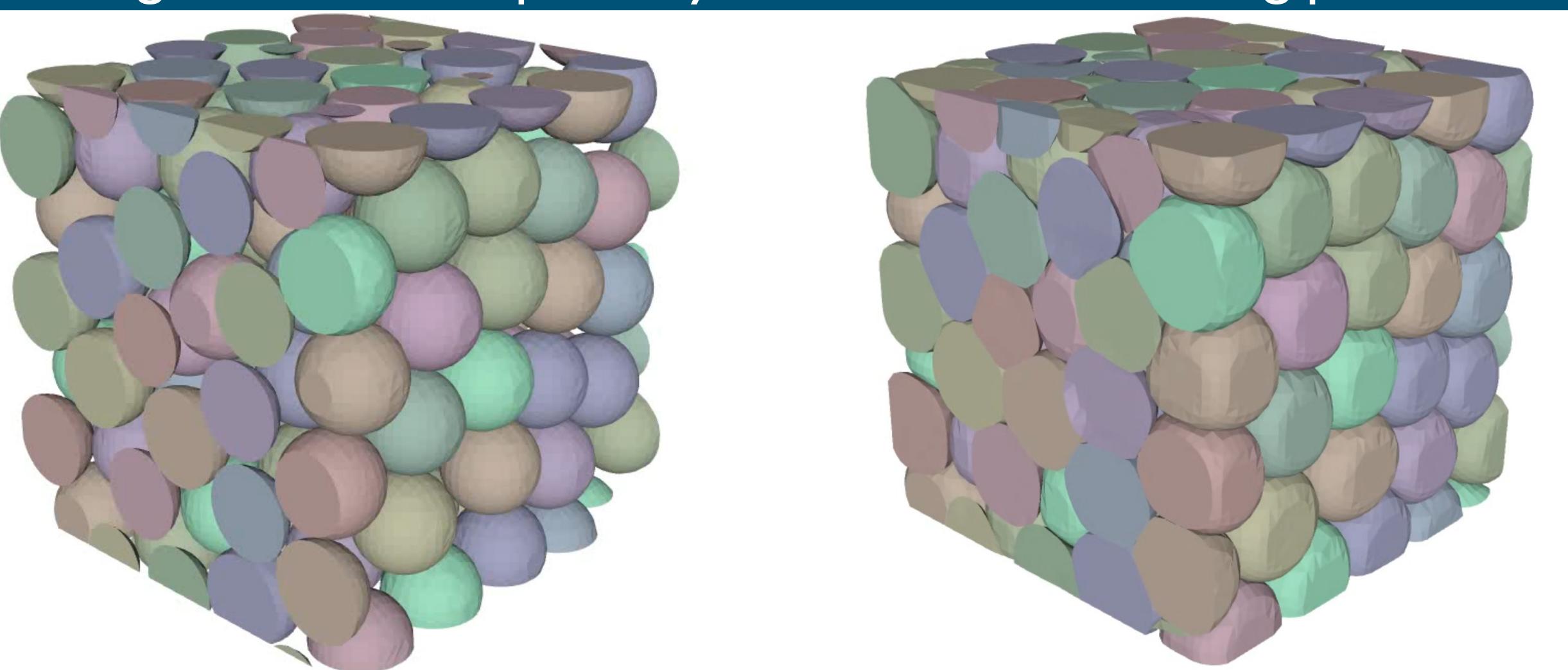


Modeling Coupled Electrochemistry and Mechanics for Conversion Cathodes

Scott A. Roberts (srober@sandia.gov) and Jeffrey S. Horner

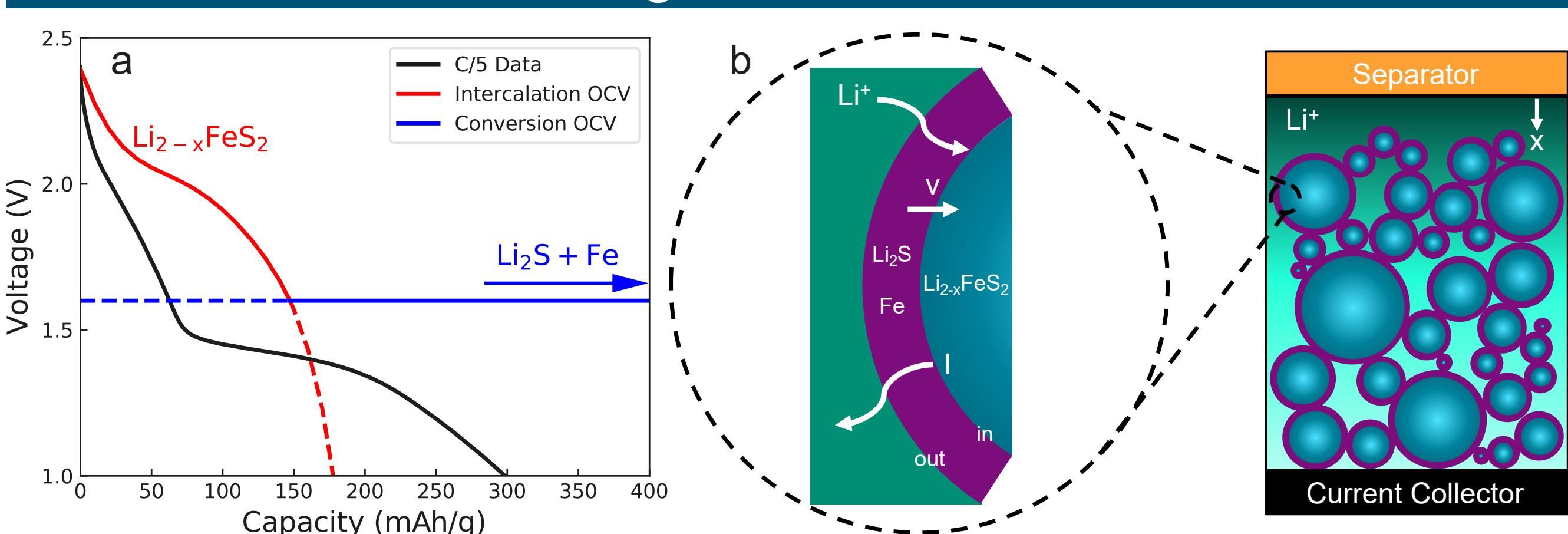


Stress generation and porosity evolution in converting particles^{1,4}



Pressure and porosity evolution during conversion highly nonlinear, requiring contact mechanics model

P2D modeling for conversion cathodes²



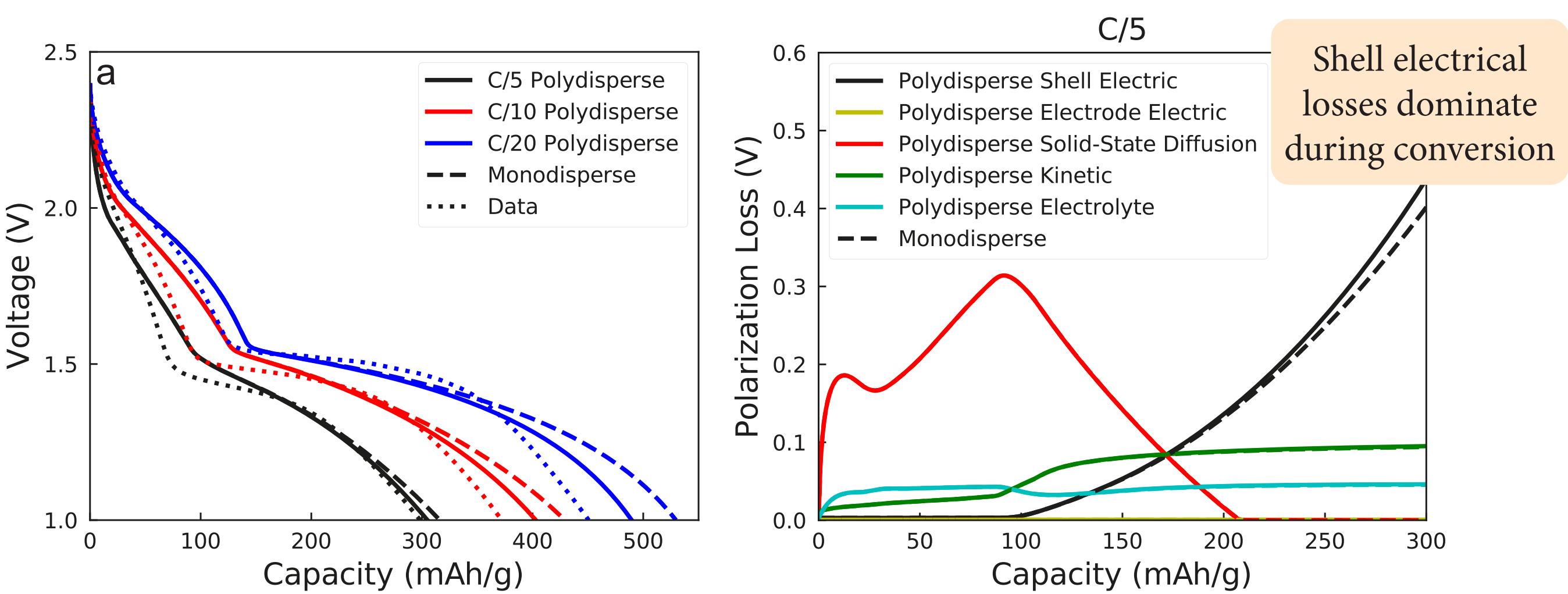
Additional equations specified for the converted particle shell region (purple Li₂S in above image)

$$\frac{\partial \delta}{\partial t} = -\frac{j_{\text{conv}} M_{\text{FeS}_2}}{\rho \left(4 - 2 \frac{C_{\text{Li}}}{C_{\text{max}}} \right)}$$

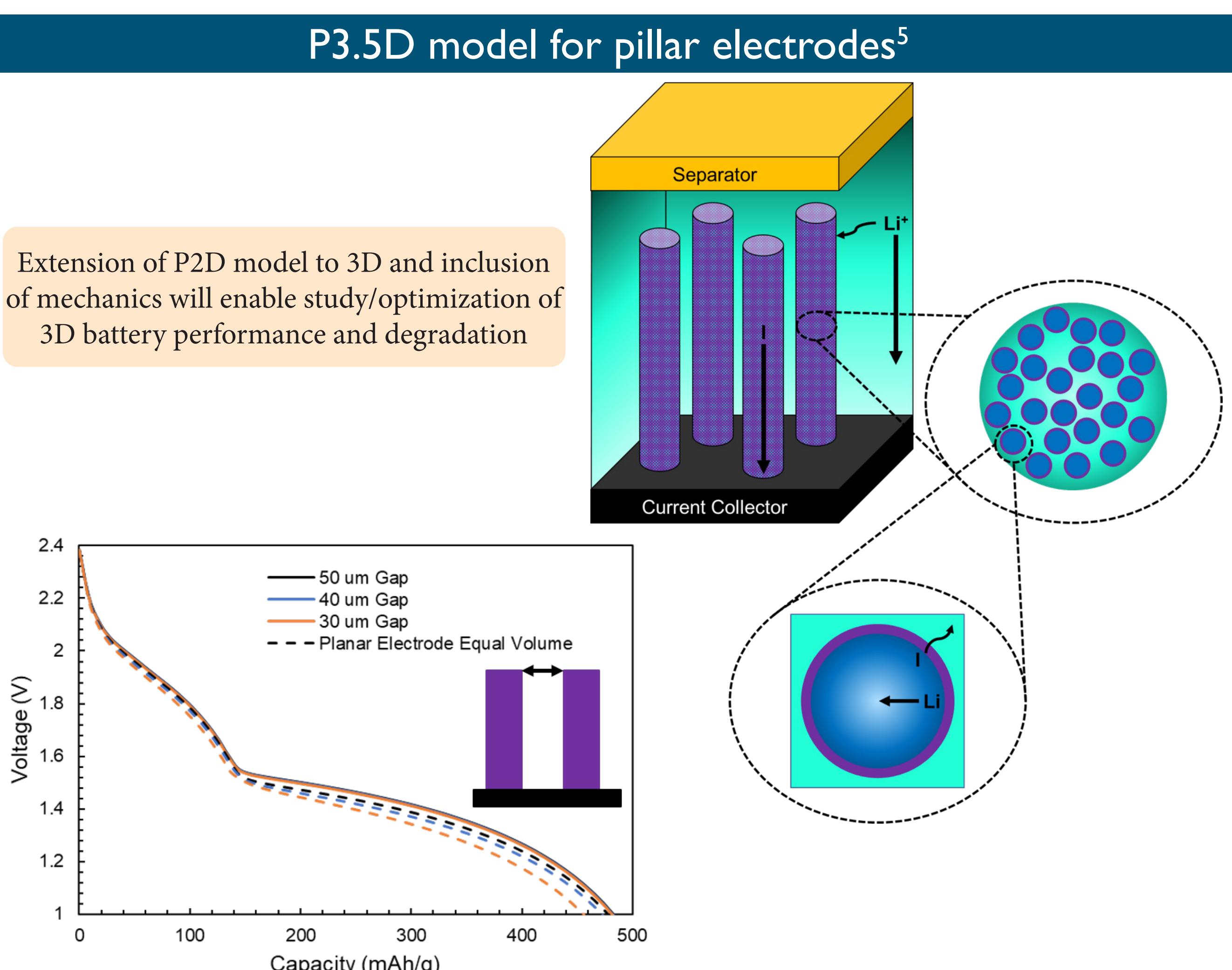
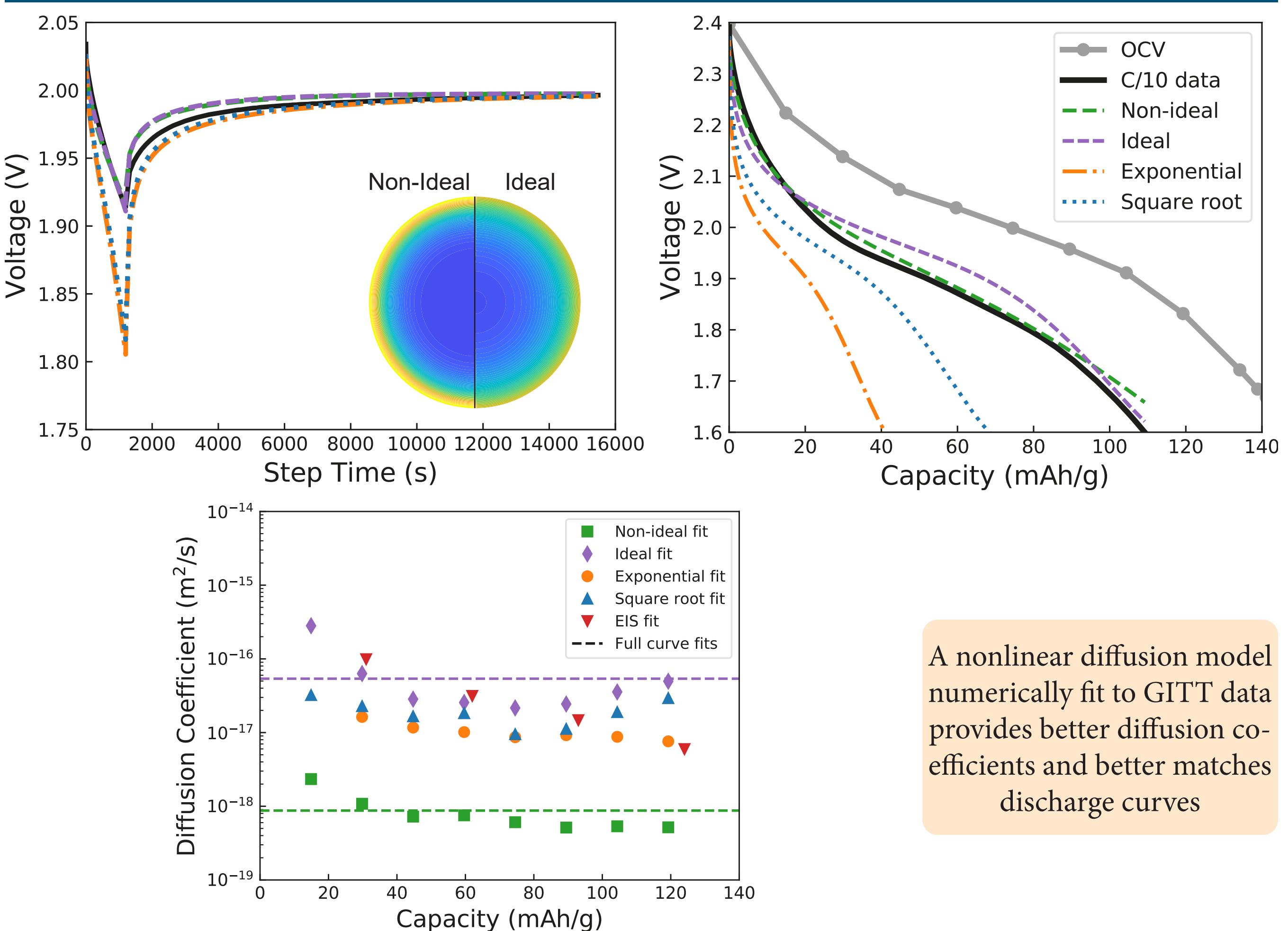
$$V_{s,\text{in}} = V_{s,\text{out}} - \frac{jFR_c^2}{\kappa_{\text{shell}}} \left(\frac{1}{R_c} - \frac{1}{R_p} \right)$$

$$V_{l,\text{in}} = V_{l,\text{out}} + \ln \left(\frac{C_{\text{Li}^+,\text{in}}}{C_{\text{Li}^+,\text{out}}} \right) \frac{RT}{F}$$

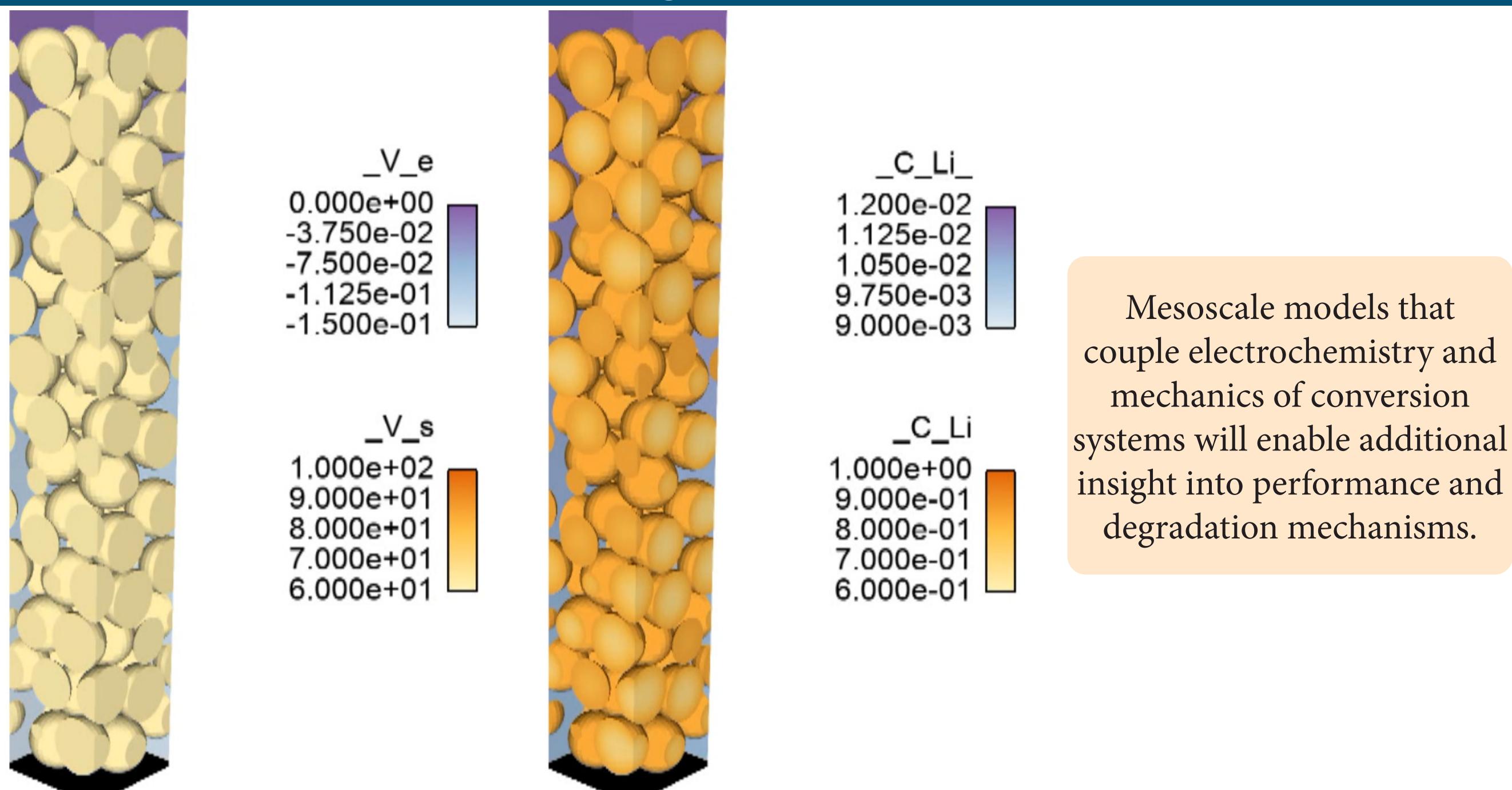
$$C_{\text{Li}^+,\text{in}} = C_{\text{Li}^+,\text{out}} + \frac{jR_c^2}{2D_{\text{shell}}} \left(\frac{1}{R_c} - \frac{1}{R_p} \right)$$



Improved extraction of diffusion coefficients from GITT³



Mesoscale modeling of conversion electrodes⁴



References

1. D. S. Ashby, et al., "Understanding the Electrochemical Performance of FeS₂ Conversion Cathodes," in press at ACS Applied Materials & Interfaces
2. J. S. Horner, et al., "A Pseudo-Two-Dimensional (P2D) Model for FeS₂ Conversion Cathode Batteries," under review
3. J. S. Horner, et al., "Electrochemical Modeling of GITT Measurements for Improved Solid-State Diffusion Coefficient Evaluation," ACS Applied Energy Materials (2021), doi: 10.1021/acsami.1c02218
4. J. S. Horner, et al., To be a FeS₂ mesoscale modeling paper submitted this year
5. J. S. Horner, et al., To be a P3.5D FeS₂ modeling paper submitted this year