Inadequecy Representation in Models of Supercapacitor Batteries

Danial Faghihi

Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin

PECOS Inadequecy Meeting
Wednesday May 24, 2017

Outline

Outline

1. **Model Description**
2. Inadequecy Representation

Governing Equations

electrode

Current density following Ohm's law:

- Matrix phase : $\mathbf{i}_1 = -\sigma \nabla \phi_1$
- Solution phase: $\mathbf{i}_2 = -\kappa \nabla \phi_2$

ϕ_1, ϕ_2: potentials,
σ, κ: electronic/ionic conductivity.

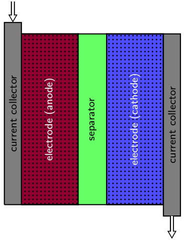
Conservation of charge:

$$-\nabla \cdot \mathbf{i}_1 = \nabla \cdot \mathbf{i}_2 = a i_n$$

a: interfacial area per unit volume
i_n: current transferred from the matrix to the electrolyte

$$i_n = \underbrace{C \frac{\partial}{\partial t} \eta}_{\text{double-layer}} + \underbrace{i_0 \left(\exp\left(\frac{\alpha_a F}{RT} \eta\right) - \exp\left(-\frac{\alpha_c F}{RT} \eta\right) \right)}_{\text{faradaic}}$$

overpotential: $\eta = \phi_1 - \phi_2$



collector

$$\mathbf{i}_1 = -\sigma \nabla \phi_1$$

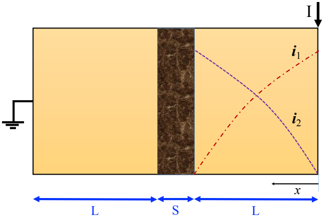
$$-\nabla \cdot \mathbf{i}_1 = 0$$

seperator

$$\mathbf{i}_2 = -\kappa \nabla \phi_2$$

$$-\nabla \cdot \mathbf{i}_2 = 0$$

High Fidelity Model



- $\eta(\xi, \tau)$ = overpotential in electrode
- $\gamma = \dfrac{\kappa}{\sigma}$: conductivity ratio
- ξ, τ : dimensionless distance/time
- $I(\tau)$: dimensionless current

Modeling Assumptions (Sins)

i. No Faradaic processes: current transferred from matrix to the solution phase goes towards only charging the double-layer at the electrode/electrolyte interface.

ii. ϕ_1 is uniformly distributed over the current collector domain (collector is sufficiently thin)

iii. There is no electron/ion fluxes cross the top and bottom boundaries

iv. The material properties are constant within each layer

High Fidelity (1D) model

$$\frac{\partial \eta}{\partial \tau} = \frac{\partial^2 \eta}{\partial \xi^2}$$

$$\begin{cases} \dfrac{\partial \eta}{\partial \xi}\Big|_{\xi=0} & = & -\dfrac{\gamma}{1+\gamma} I(\tau) \\ \dfrac{\partial \eta}{\partial \xi}\Big|_{\xi=1} & = & \dfrac{1}{1+\gamma} I(\tau) \\ \eta\Big|_{\tau=0} & = & \eta_0(\xi) \end{cases}$$

Low Fidelity Model

Modeling Assumptions (Sins)

i. Assuming a quadratically varying profile for overpotential inside the electrodes

$$\eta_{LF}(\xi,\tau) = a(\tau)\xi^2 + b(\tau)\xi + c(\tau)$$

where a, b, and c can be obtained from PDE+BCs of HF model.

Low Fidelity (0D) model

$$\eta_{LF}(\xi,\tau) = \frac{1}{2}I(\tau)\xi^2 - I(\tau)\frac{\gamma}{1+\gamma}\xi + \eta^{avg}(\tau) - \frac{I(\tau)}{6} + \frac{I(\tau)}{2}\frac{\gamma}{1+\gamma}$$

η^{avg} is the solution of following ODE given appropriate initial condition. Spatially averaging the governing equation over the entire domain length

$$\eta^{avg} = \int_0^1 \eta d\xi \qquad \Rightarrow \qquad \frac{\partial \eta^{avg}}{\partial \tau} = I(\tau)$$

QoI : cell voltage

Quantity of Interest

Potential drop across the system

$$\begin{aligned} V^{\text{cell}}(\tau) &= \phi^{L}_{\text{collector}} - \phi^{R}_{\text{collector}} \\ &= 2V_0 - 2V^{\text{elect.}} - V^{\text{sep.}} \end{aligned}$$

where

$$V^{\text{elect.}}(\tau) = \phi_1|_{\xi=0} - \phi_2|_{\xi=1} = \frac{1+2\gamma}{1+\gamma}\eta|_{\xi=1} - \frac{\gamma}{1+\gamma}\eta|_{\xi=0} - \frac{\gamma}{(1+\gamma)^2}I$$

and

$$V^{\text{sep.}}(\tau) = I\frac{L_s}{\kappa_s}$$

Outline

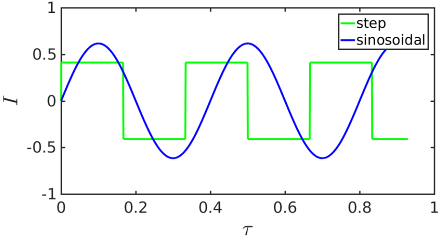
Inadequacy Representation

Objective:

Based on what we know about the models, develop a representation of inadequacy (*error in QoI*, ϵ) as a parametric model $\mathcal{P}(\boldsymbol{\theta})$ such that

$$V^{\text{cell}}_{\text{HF}} \equiv V^{\text{cell}}_{\text{LF}} + \mathcal{P}(\boldsymbol{\theta})$$

- Parameters of inadequacy model, $\boldsymbol{\theta}$, needs to be calibrated using the data furnished by HF model for simple scenarios, e.g.

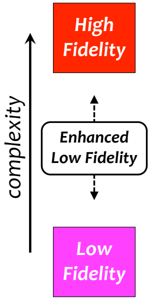


- $\mathcal{P}(\boldsymbol{\theta})$ enables predicting V^{cell} for more complex scenarios outside of the HF data domain along with the associated uncertainty.

Inadequacy Representation

Inadequacy model $\mathcal{P}(\boldsymbol{\theta})$ involves:

- *Deterministic counterpart:* Encapsulates our information about the models.
- *Stochastic counterpart:* Represents the remaining uncertainty due to lack of information about features of full HF system.



- The goal is to construct a class of enhanced low fidelity models (intermediate complexities) based on our knowledge about the system, thus,
  - Deterministic part of $\mathcal{P}(\boldsymbol{\theta})$: $V_{\text{ElF}}^{\text{cell}} - V_{\text{LF}}^{\text{cell}}$
  - Stochastic part of $\mathcal{P}(\boldsymbol{\theta})$: $V_{\text{HlF}}^{\text{cell}} - V_{\text{ELF}}^{\text{cell}}$
- The more complex ELF model:
  - more complex deterministic $\mathcal{P}$ i.e. more parameters
  - more HF data might be required to calibrate
  - less uncertainty in prediction.

Summary of Models and QoI

HF model

$$\frac{\partial \eta}{\partial \tau} = \frac{\partial^2 \eta}{\partial \xi^2}$$

$$\begin{cases} \frac{\partial \eta}{\partial \xi}|_{\xi=0} = & -\frac{\gamma I}{1+\gamma} \\ \frac{\partial \eta}{\partial \xi}|_{\xi=1} = & \frac{I}{1+\gamma} \\ \eta\big|_{\tau=0} = & \eta_0(\xi) \end{cases}$$

LF model

$$\eta = \frac{1}{2} I \xi^2 - \frac{I\gamma}{1+\gamma}\xi + \eta^{avg}(\tau) - \frac{I}{6} + \frac{I\gamma}{2(1+\gamma)}$$

QoI: $V_{\mathrm{LF}}(\tau) = \eta^{avg}(\tau) + C_{\mathrm{LF}} I(\tau)$ where

$$\frac{\partial \eta^{avg}}{\partial \tau} = I(\tau)$$

What do we know about HF and LF models?

- structure of HF and LF, i.e. ODE, PDE, etc.
- model respond in a simple (unphysical) case, e.g. constant current.
- XXXX