Inadequecy Representation in Models of Supercapacitor Batteries

Part II: updates on inadequacy formulation

Danial Faghihi

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

PECOS Inadequecy Meeting
Wednesday Fab 17, 2017

Summary of Models and QoI

High Fidelity (1D) model

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

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

Low Fidelity (0D) model

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

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

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

Quantity of Interest

Potential drop across the system (electrode)

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

Model Inadequacy - Version I

Inadequacy representation

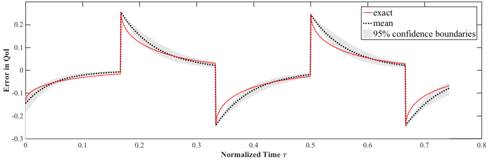
Auxiliary Stochastic ODE:

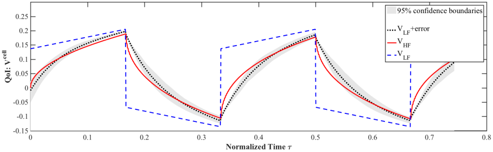
$$\frac{\partial \epsilon}{\partial \tau} = -\lambda \epsilon + \alpha \frac{\partial I}{\partial \tau}$$

where λ is a stochastic process with following time evolution:

$$\frac{\partial \lambda}{\partial \tau} = -c(\lambda - \lambda_{mean}) + \beta \frac{\partial W}{\partial \tau}$$

where $W(\tau)$ is a Wiener process.





- The ODE accounts for some of hidden features of HF i.e. the term $\lambda\epsilon$ takes care of the Kernel $\mathcal{K}$ and the term $\alpha \dfrac{\partial I}{\partial \tau}$ accounts for discontinuity of I.
- It needs to be trained by HF data i.e. calibrating parameters of inadequacy representation $(\alpha, \beta, c, \lambda_{mean})$.

Model Inadequacy - Version I

Problems with deterministic part of the current ODE

- It does not capture the short time behavior after sudden change in current.
- It does not account for a wide range of current frequency.

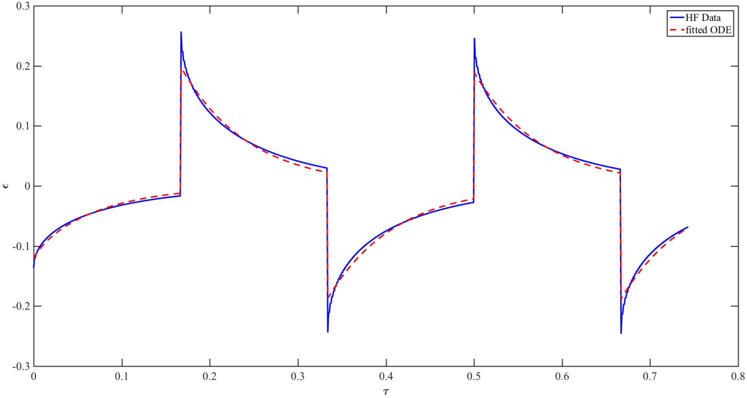


Figure: Step change current.

Model Inadequacy - Version I

Sinusoidal current:

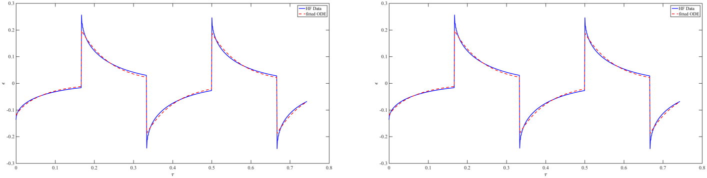


Figure: (a) $I = \sin(50\tau)$. (b) $I = \sin(10\tau)$

Sinusoidal current:

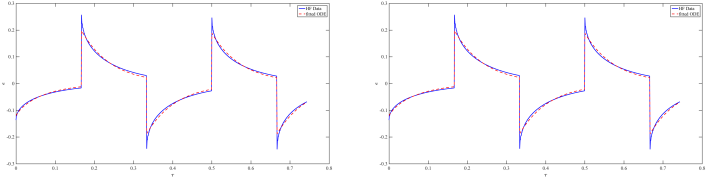


Figure: (a) $I = \sin(50\tau)$. (b) $I = \sin(10\tau)$

Closer look at behavior of over potential:

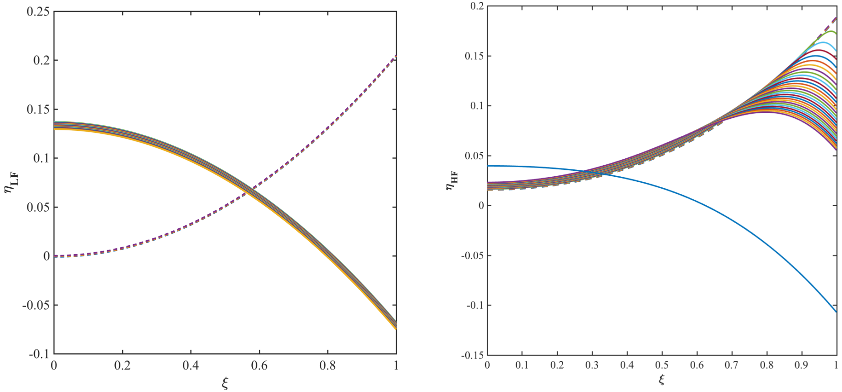


Figure: Step change current when sign of current changes.

Closer look at behavior of over potential:

Stokes's first problem with Neumann boundary condition

on the board ...

Model Inadequacy - Version II

- when current step changes, at the boundary and short time $\eta_{HF} \propto \sqrt{\tau}$.
- since η_{LF} changes rapidly at the boundary, one can conclude $\epsilon \propto \sqrt{\tau}$
- from $\epsilon \propto \sqrt{\tau}$ one can infere $\dfrac{d\epsilon}{d\tau} \propto \dfrac{1}{\sqrt{\tau}}$

From above consideration, we postulated a possible inadequacy representation for short time after step change as:

$$\frac{\partial \epsilon}{\partial \tau} = -\frac{\lambda}{\sqrt{\tau - T(\tau)}} + \alpha \frac{\partial I}{\partial \tau},$$

where $T(\tau) = \tau_{jump}$ in case of step change current. **plot on the board**

Does this form works for long time also?

Model Inadequacy - Version II

Test Problem:

$$\text{option1}: \quad \frac{\partial \epsilon}{\partial \tau} = -\frac{\lambda}{\sqrt{\tau - T(\tau)}} + \alpha \frac{\partial I}{\partial \tau}$$

$$\text{option2}: \quad \frac{\partial \epsilon}{\partial \tau} = -\frac{\lambda \epsilon}{\sqrt{\tau - T(\tau)}} + \alpha \frac{\partial I}{\partial \tau}$$

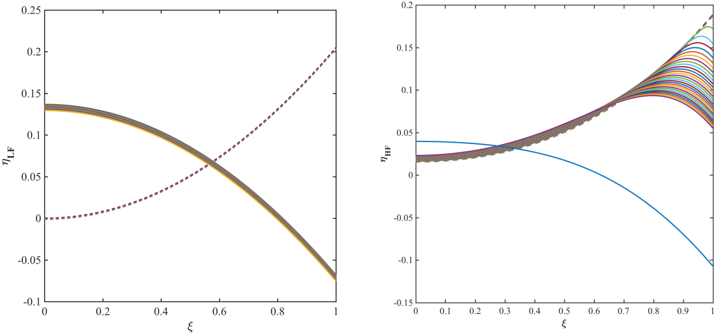


Figure: (a) change in current with time; (b) two inadequacy options calibrated with

Model Inadequacy - Version II

Inadequacy representation (v.2)

Auxiliary Stochastic ODE:

$$\frac{\partial \epsilon}{\partial \tau} = -\frac{\lambda \epsilon}{\sqrt{\tau - T(\tau)}} + \alpha \frac{\partial I}{\partial \tau}$$

where λ and α are parameters of inadequacy representation.

What is a general form for $T(\tau) \propto I(\tau)$?

- $T(\tau)$ should be consistent with what we expect in step changes current.
- In sinusoidal current it seems $T(\tau)$ should take care of lagging time between HF and LF model.

From above consideration, we postulated a possible evolution equation for $T(\tau)$ as:

$$\frac{\partial T}{\partial \tau} = (\tau - T(\tau)) \left| \frac{\partial I}{\partial \tau} \right|$$