Inadequecy Representation in Models of Supercapacitor Batteries

Part II: updates on inadequacy formulation

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PECOS Inadequecy Meeting
Wednesday Fab 17, 2017

Summary of Models and QoI

High Fidelity (1D) model

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

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

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

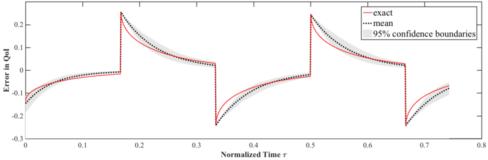
Auxiliary Stochastic ODE:

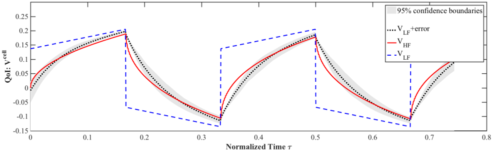
$$\frac{\partial \epsilon}{\partial \tau} = -\lambda \epsilon + \alpha \frac{\partial I}{\partial \tau}$$

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.

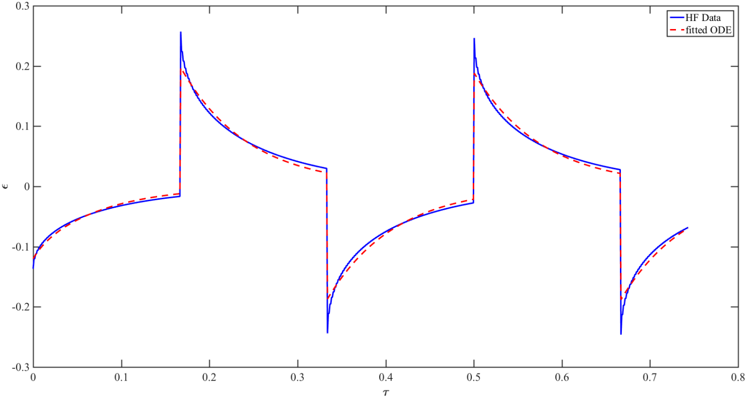
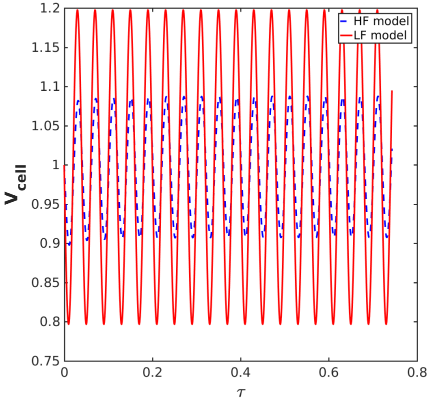


Figure : Step change current.

Model Inadequacy - Version I

Sinusoidal current:



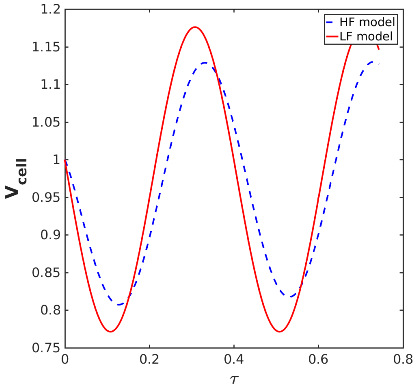


Figure : (a) $I = \sin(50\pi\tau)$. (b) $I = \sin(5\pi\tau)$

Sinusoidal current:

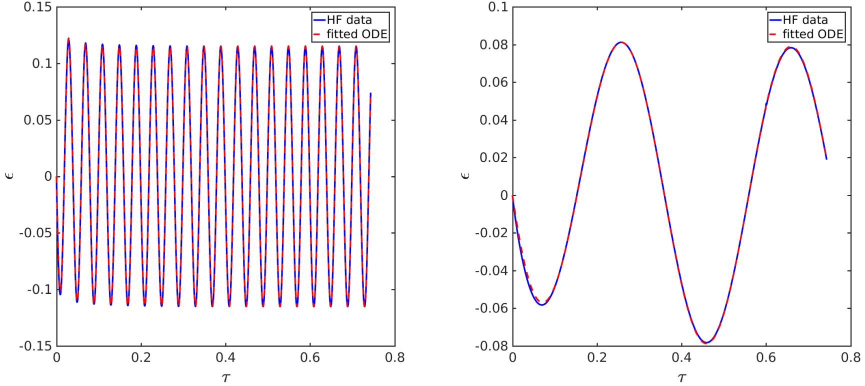


Figure : (a) $I = \sin(50\pi\tau)$. Calibrated parameters: $c =$56.9962, $\lambda_{mean} =$28.0998, $\alpha =$0.2822; (b) $I = \sin(5\pi\tau)$ Calibrated parameters: $c =$1834.5, $\lambda_{mean} =$11.8, $\alpha =$0.2395

Closer look at behavior of over potential:

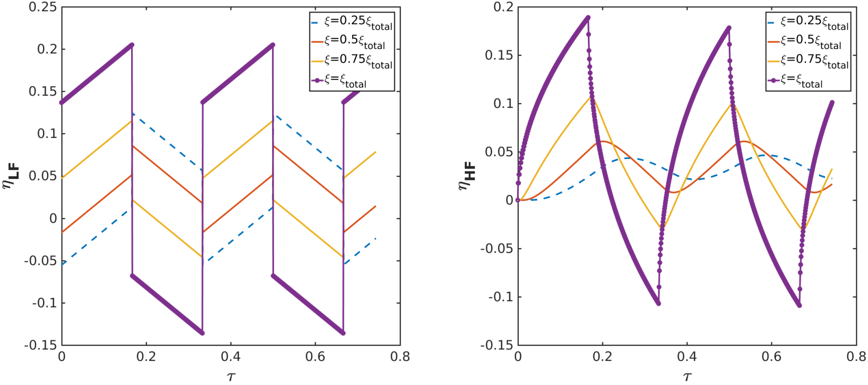


Figure : Step change current.

Closer look at behavior of over potential:

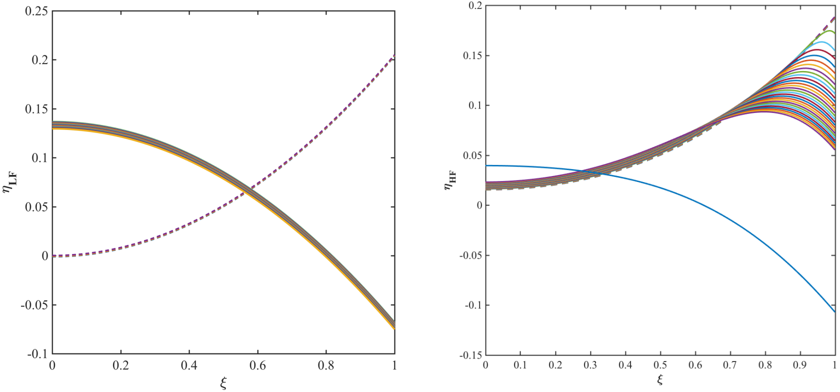


Figure : Step change current when sign of current changes.

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:

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

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

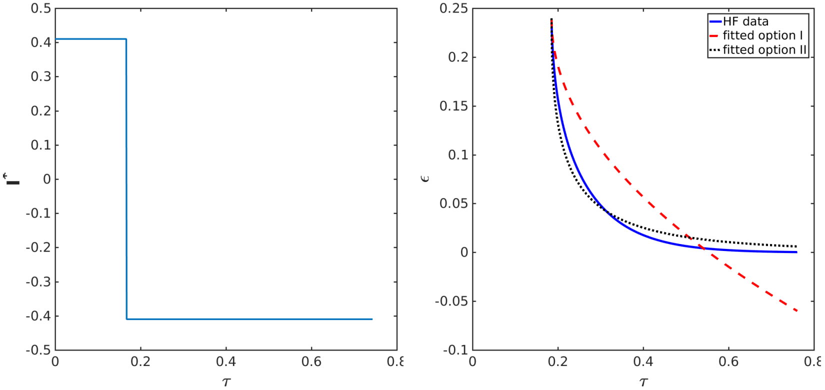


Figure : (a) change in current with time; (b) two inadequacy options calibrated with HF data.

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 $T(\tau) \propto I(\tau)$?

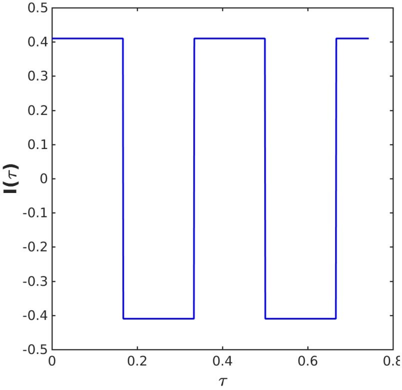
- $T(\tau)$ should be consistent with what we expect in step changes current.
- In sinusoidal current it seems $T(\tau)$ should take care of lagging time between HF and LF model.

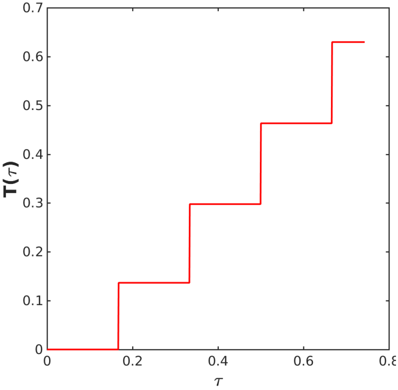
From above consideration, we postulated a possible evolution equation for $T(\tau)$ as:

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

Model Inadequacy - Version II

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





Model Inadequacy - Version II

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