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Process for lumping parameters to enable nondestructive parameter estimation for lithium-ion physics-based models

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Introduction

- A model is **nonidentifiable** if at least two distinct parameter sets produce same input/output function
- The physics-based **Doyle–Fuller–Newman (DFN)** lithium-ion cell **model is nonidentifiable** in this sense
- If we wish to estimate parameters from current/voltage data, **we must reformulate the DFN model**

Original DFN Model Equations

- Describes: (1–2) charge and mass conservation in solid; (3–4) charge and mass conservation in electrolyte; (5) reaction kinetics

(1)
$$\frac{\partial}{\partial x}\sigma^{\mathrm{r}}_{\mathrm{eff}}\frac{\partial}{\partial x}\phi^{\mathrm{r}}_{\mathrm{s}} = a^{\mathrm{r}}_{\mathrm{s}}Fj^{\mathrm{r}}$$

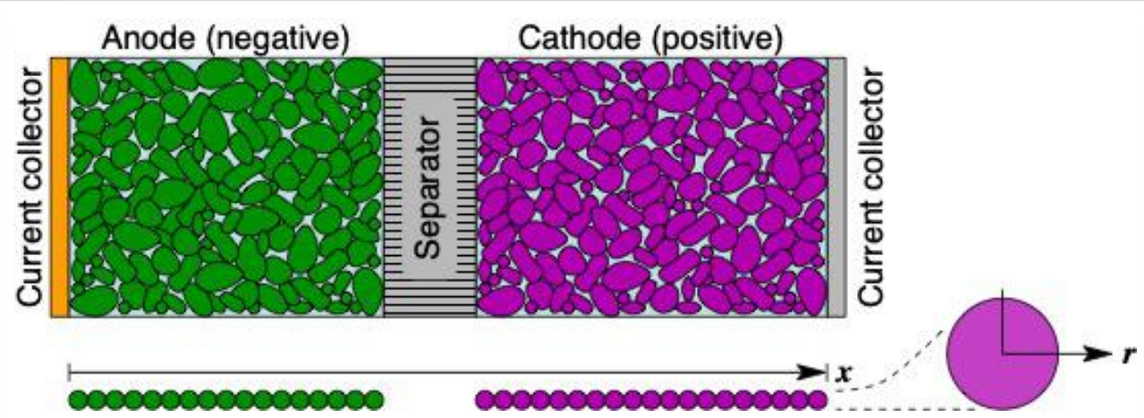
(2)
$$\frac{\partial c^{\mathrm{r}}_{\mathrm{s}}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D^{\mathrm{r}}_{\mathrm{s}}r^2\frac{\partial c_{\mathrm{s}}}{\partial r}\right)$$

(3)
$$\frac{\partial}{\partial x}\left(\kappa^{\mathrm{r}}_{\mathrm{eff}}\frac{\partial}{\partial x}\phi^{\mathrm{r}}_{\mathrm{e}} + \kappa_D\frac{\partial \ln c^{\mathrm{r}}_{\mathrm{e}}}{\partial x}\right) + a^{\mathrm{r}}_{\mathrm{s}}Fj^{\mathrm{r}} = 0$$
$$\kappa^{\mathrm{r}}_{D} = \frac{2RT\kappa^{\mathrm{r}}_{\mathrm{eff}}\left(t^0_+ - 1\right)}{F}\left(1 + \frac{\partial \ln f_{\pm}}{\partial \ln c_{\mathrm{e}}}\right)$$

(4)
$$\frac{\partial(\varepsilon^{\mathrm{r}}_{\mathrm{e}}c^{\mathrm{r}}_{\mathrm{e}})}{\partial t} = \frac{\partial}{\partial x}D^{\mathrm{r}}_{\mathrm{e,eff}}\frac{\partial}{\partial x}c^{\mathrm{r}}_{\mathrm{e}} + a^{\mathrm{r}}_{\mathrm{s}}(1-t^0_+)j^{\mathrm{r}}$$

(5)
$$j^{\mathrm{r}} = j^{\mathrm{r}}_0\left\{\exp\left(\frac{(1-\alpha^{\mathrm{r}})F}{RT}\eta^{\mathrm{r}}\right) - \exp\left(\frac{-\alpha^{\mathrm{r}}F}{RT}\eta^{\mathrm{r}}\right)\right\}$$
$$j^{\mathrm{r}}_0 = k^{\mathrm{r}}_{\mathrm{norm},0}\left(\left(\frac{c^{\mathrm{r}}_{\mathrm{e}}}{c^{\mathrm{r}}_{\mathrm{e},0}}\right)\left(1-\frac{c^{\mathrm{r}}_{\mathrm{s,e}}}{c^{\mathrm{r}}_{\mathrm{s,max}}}\right)\right)^{1-\alpha^{\mathrm{r}}}\left(\frac{c^{\mathrm{r}}_{\mathrm{s,e}}}{c^{\mathrm{r}}_{\mathrm{s,max}}}\right)^{\alpha^{\mathrm{r}}}$$
$$\eta^{\mathrm{r}} = \phi^{\mathrm{r}}_{\mathrm{s}} - \phi^{\mathrm{r}}_{\mathrm{e}} - U^{\mathrm{r}}_{\mathrm{ocp}}(c^{\mathrm{r}}_{\mathrm{s,e}}/c^{\mathrm{r}}_{\mathrm{s,max}}) - FR^{\mathrm{r}}_{\mathrm{f}}j^{\mathrm{r}}$$

DFN Model Geometry



Example Nonidentifiable Model

- Consider Ohm's law: $V = IR$ or $V = I/(\sigma L)$
- In first form, if we collect several (V, I), we can estimate the value of R ▶ ***identifiable***
- In second form, we cannot independently estimate values of σ and L ▶ ***nonidentifiable***
- Must lump intensive parameter σ with dimensional parameter L to make identifiable

Process

- We use the following process to convert the DFN model to a lumped-parameter model (LPM):

Normalize equation length dimensions → Create pseudo-dimensionless variables → Lump together parameters that appear as groups → Recast equations using more convenient names

Lumped Parameter Models

- Final LPM can predict **voltage**, **internal potentials**, and scaled versions of other **electrochemical variables**
- Specifically, variables ϕ_S and ϕ_e are unchanged; concentrations are normalized: $\theta_s = c_s/c_{s,max}$ and $\theta_e = c_e/c_{e,0}$; fluxes are scaled: $\dot{n} = a_s ALj$
- All dimensions are eliminated, and lumped parameters have different forms; e.g., $\bar{\sigma} = \sigma_{\mathrm{eff}}A/L$
- Final form of LPM shown to the right, where numbered equations correspond to those in original DFN model
- **36 parameters ▶ 23 identifiable parameters**

(1)
$$\bar{\sigma}^{\mathrm{r}}\frac{\partial^2\phi^{\mathrm{r}}_{\mathrm{s}}}{\partial\tilde{x}^2} = F\dot{n}^{\mathrm{r}}$$

(2)
$$\frac{\partial\theta^{\mathrm{r}}_{\mathrm{s}}}{\partial t} = \frac{1}{\tilde{r}^2}\frac{\partial}{\partial\tilde{r}}\left(\bar{D}^{\mathrm{r}}_{\mathrm{s}}\tilde{r}^2\frac{\partial\theta^{\mathrm{r}}_{\mathrm{s}}}{\partial\tilde{r}}\right)$$

(3)
$$\frac{\partial}{\partial\tilde{x}}\left(\bar{\kappa}^{\mathrm{r}}\left(\frac{\partial}{\partial\tilde{x}}\phi^{\mathrm{r}}_{\mathrm{e}} + \bar{\kappa}_D T\frac{\partial\ln(\theta^{\mathrm{r}}_{\mathrm{e}})}{\partial\tilde{x}}\right)\right) + F\dot{n}^{\mathrm{r}} = 0$$

(4)
$$\bar{n}^{\mathrm{r}}_{\mathrm{e}}\frac{\partial\theta^{\mathrm{r}}_{\mathrm{e}}}{\partial t} = \bar{\psi}\frac{\partial}{\partial\tilde{x}}\bar{\kappa}^{\mathrm{r}}\frac{\partial}{\partial\tilde{x}}\theta^{\mathrm{r}}_{\mathrm{e}} + \dot{n}^{\mathrm{r}}$$

(5)
$$\dot{n}^{\mathrm{r}} = \dot{n}^{\mathrm{r}}_0\left(\exp\left(\frac{(1-\alpha^{\mathrm{r}})F}{RT}\eta^{\mathrm{r}}\right) - \exp\left(\frac{-\alpha^{\mathrm{r}}F}{RT}\eta^{\mathrm{r}}\right)\right)$$
$$\dot{n}^{\mathrm{r}}_0 = \bar{k}^{\mathrm{r}}_0(\theta^{\mathrm{r}}_{\mathrm{e}})^{1-\alpha^{\mathrm{r}}}(1-\theta^{\mathrm{r}}_{\mathrm{ss}})^{1-\alpha^{\mathrm{r}}}(\theta^{\mathrm{r}}_{\mathrm{ss}})^{\alpha^{\mathrm{r}}}$$
$$\eta^{\mathrm{r}} = \phi^{\mathrm{r}}_{\mathrm{s}} - \phi^{\mathrm{r}}_{\mathrm{e}} - U^{\mathrm{r}}_{\mathrm{ocp}}(\theta^{\mathrm{r}}_{\mathrm{ss}}) - F\bar{R}^{\mathrm{r}}_{\mathrm{f}}\dot{n}^{\mathrm{r}}$$

Summary

- It is **mathematically impossible** to estimate parameters of DFN model uniquely without cell teardown
- However, **all final LPM parameters can be estimated from current/voltage data** only, as shown in a series of papers we have published; please email the authors for references to those articles