# Supplementary Material for "Mitigating Electrochemical Degradation in Optimal Vehicle-to-Grid Dispatch via Digital Twin"

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## I. Existing SEI Thickness for Battery SEI Growth

Figures 1(a)–(d) respectively plot the $(S_i^t, I_i^t, \Delta\theta_i^t)$-spaces under $\theta_i^t = 0\,[\text{nm}]$, $\theta_i^t = 20\,[\text{nm}]$, $\theta_i^t = 40\,[\text{nm}]$, and $\theta_i^t = 80\,[\text{nm}]$, using the same scale for all axes. Intuitively, $\theta\theta_i^t$ has a slight shape variation under different $\theta_i^t$. Thus, existing SEI thickness $\theta_i^t$ [nm] can be negligible in the SEI growth $\Delta\theta_i^t$ per charge-discharge cycle.

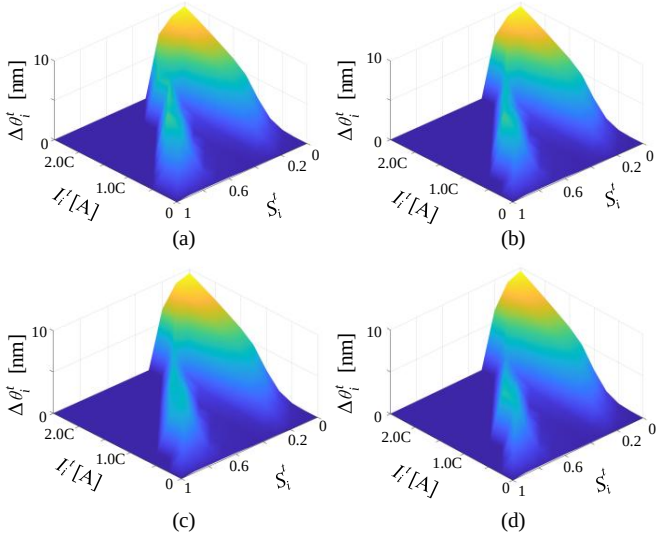


Fig. 1. PDE-based SEI growth surface $\Delta\theta_i^t$: (a) $\theta_i^t = 0\,[\text{nm}]$; (b) $\theta_i^t = 20\,[\text{nm}]$; (c) $\theta_i^t = 40\,[\text{nm}]$; (d) $\theta_i^t = 80\,[\text{nm}]$;

## II. Derivation of Second-order Conic Constraint

We reformulate the constraint $\gamma_i^{t+1} \geqslant (z_{i,N_I}^{t+1})^2$ with $f = (\gamma_i^{t+1} + 1)^2$ and $g = (\gamma_i^{t+1} - 1)^2 + (2z_{i,N_I}^{t+1})^2$, yielding

$$f - g = 4\gamma_i^{t+1} - 4(z_{i,N_I}^{t+1})^2 \geqslant 0, \tag{II-1}$$

Rearranging this inequality (II-1), we express

$$(\gamma_i^{t+1} + 1)^2 \geqslant (\gamma_i^{t+1} - 1)^2 + (2z_{i,N_I}^{t+1})^2, \tag{II-2}$$

This is equivalent to the standard second-order conic constraint

$$\left\|\gamma_i^{t+1} + 1\right\|_2^2 \geqslant \left\|(\gamma_i^{t+1} - 1,\ 2z_{i,N_I}^{t+1})^{\mathrm{T}}\right\|_2^2. \tag{II-3}$$

## III. Battery Cell Parameter Values

In this study, we suppose each EV consists of 21700-type battery cells with the capacity of 80 kWh. Each EV battery pack has 96 cells in series and 46 cells in parallel (96S46P), giving it a total of 4416 cells. Each battery cell capacity $I_{b,i} = 5\,\text{Ah}$, nominal voltage $v_{\text{flat},i} = 3.65\,\text{V}$ with the operating voltage ranging from 2.5 V to 4.2 V, and current rate $C_{r,i}^t \in [0, \overline{C}_{r,i}]$, where the EV aggregator selects $\overline{C}_{r,i} = 2.5$ to avoid sharp charge-discharge cycling. For a battery cell, $\overline{p}_i \approx 3.65 \cdot 0.005 \cdot 2.5 \approx 0.046\,\text{kW}$. The ambient temperature is 28°C. Other parameters for electrochemical kinetics are given in Table I.

## IV. Existing Battery Aging Formulations

We revisit the existing linear and nonlinear battery aging methods in [2] and [5]. The linear battery degradation cost $F_i^t$ is defined for each charging and discharging cycle at time period $t$ until the required state of charge (SoC) in the last time period $t = N_t$, i.e., $S_i^{N_t} = \overline{S}$, yielding

$$F_i^t = C_i \frac{\kappa_i}{100}\left(-\frac{1}{\eta_v} p_{d,i}^t \theta t + \overline{S} - S_i^0\right) \tag{IV-4}$$

where $\kappa_i = 1$ denotes the slope of the linear approximation of the EV $i$'s battery life as a function of cycles. $C_i = 1$ represents the purchase cost of the EV $i$'s battery divided by its useful capacity [\$/Ah]. $S_{0,i}$ is the initial SOC value.

The nonlinear battery degradation cost $G_i^t$ is an approximation function with respect to depth of discharge by $1 - S_i^t$ and cell current $I_i^t$ (denoted in C-rate) based on the experimental data [5]. We have

$$G_i^t = \frac{1}{f_c(I_i^t) \cdot f_d(S_i^t)}, \tag{IV-5}$$

where $f_c$ and $f_d$ respectively represent battery life loss under different DoDs and cell currents.

$$f_d = \begin{cases} 4000, & \text{if } S_i^t > 0.95 \\ 946.1 \cdot (1 - S_i^t)^{-1.079}, & \text{if } S_i^t \leqslant 0.95 \end{cases} \tag{IV-6a}$$

$$f_c = \begin{cases} 4, & \text{if } I_i^t < 0.2 \\ 1.041 \cdot (I_i^t)^{-0.445}, & \text{if } 0.2 \leqslant I_i^t \leqslant 2.5 \end{cases} \tag{IV-6b}$$

Subsequently, we express

$$G_i^t = \begin{cases} 0.6 \cdot 10^{-4}, & \text{if } S_i^t > 0.95,\ I_i^t < 0.2 \\ 0.2 \cdot 10^{-3} \cdot (I_i^t)^{0.445}, & \text{if } S_i^t > 0.95,\ 0.2 \leqslant I_i^t \leqslant 2.5 \\ 0.2 \cdot 10^{-3} \cdot (1 - S_i^t)^{1.079}, & \text{if } S_i^t \leqslant 0.95,\ I_i^t < 0.2 \\ 10^{-3} \cdot (1 - S_i^t)^{1.079} \cdot (I_i^t)^{0.445}, & \text{if } S_i^t \leqslant 0.95,\ 0.2 \leqslant I_i^t \leqslant 2.5 \end{cases} \tag{IV-7a}$$

## V. Comparison of Resulting Degradation

We further compare the electrochemical degradation costs between the nonlinear method [5] and the ICNNs-based formulation (2b)–(2d) under a random set of 66 SoC values. We normalize the electrochemical degradation costs in a continuous range $[0, 1]$ and present their solutions on the normalized PDE-based degradation surface $\Delta\theta_1^{t+1}$ in Fig. 2. This figure shows that blue square markers by the ICNNs-based approach are closer to the PDE-based degradation surface than the yellow circle markers. As compared, the 84.8% and 19.7% of markers have only with less than 1% error for the ICNNs-based and the nonlinear degradation cost methods, respectively. And the ICNNs-based electrochemical degradation cost method has less than 2% error across the domain, and is thus accurate for the optimal V2G model.

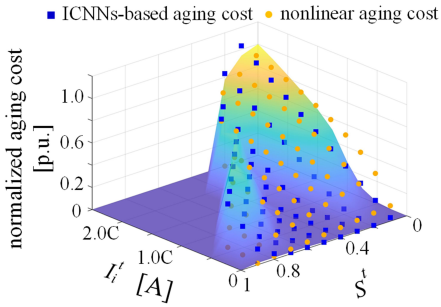


Fig. 2. Comparison between nonlinear and ICNNs-based degradation costs.

TABLE I
Parameters for Electrochemical Kinetics

| Parameter | Negative electrode | Separator | Positive electrode |
|---|---|---|---|
| electrode plate area ($m^2$) | 0.163 | 0.163 | 0.163 |
| electrode thickness ($m$) | $78 \cdot 10^{-6}$ | $20 \cdot 10^{-6}$ | $45 \cdot 10^{-6}$ |
| $Li^+$ diffusion coefficient ($m^2/s$) | $3.9 \cdot 10^{-5}$ | - | $1.8 \cdot 10^{-8}$ |
| active electrode volume fraction (%) | 0.6 | - | 0.6 |
| electrolyte phase volume fraction (%) | 0.3 | - | 0.3 |
| max solid phase concentration ($mol/m^3$) | 31507 | - | 49000 |
| particle radius ($m$) | $6 \cdot 10^{-6}$ | - | $5 \cdot 10^{-6}$ |
| reaction rate efficiency ($A/m^2$) | $9.77 \cdot 10^{-2}$ | - | $1.19 \cdot 10^{-2}$ |
| exchange current density of side reaction ($A/m^2$) | 10 | - | 10 |
| initial electrolyte concentration ($mol/m^3$) | $1.25 \cdot 10^4$ | $1.25 \cdot 10^4$ | $1.25 \cdot 10^4$ |
| Binder volume fraction(%) | 0.1 | - | 0.1 |
| Separator volume fraction(%) | - | 0.4 | - |
| Thickness of current collectors ($m$) | $10 \cdot 10^{-6}$ | - | $10 \cdot 10^{-6}$ |