Supplementary Materials

I. Benchmark P2D-T Model

The pseudo-two-dimensional (P2D) model of lithium-ion (Li-ion) batteries was established based on the porous electrode theory and the concentrated solution theory [1]–[3]. It has a sandwich-like structure with three domains, including the positive electrode (pos), the negative electrodes (neg), and the separator (sep) in between. The lithium ions are stored in a number of assumed particles in the solid phase of the electrode, and the transport of the lithium ions during charge/discharge would cause the variation of the Li-ion concentrations in the particles as well as in the electrolyte. The P2D model describes the cell behaviors in the horizontal axis (x-direction) on the macro scale as well as the pseudo radial axis (r-direction) on the micro scale. This results in a 1-D P2D model. The model consists of a set of tightly coupled and highly nonlinear partial differential algebraic equations (PDAEs), i.e.

For the positive electrode, the negative electrode, and the separator:

$$\frac{\partial c_e(x,t)}{\partial t} = \frac{1}{\varepsilon_e}\frac{\partial}{\partial x}\left(D_{\text{eff}}\frac{\partial c_e(x,t)}{\partial x}\right) + \frac{t_a^0}{F\varepsilon_e}\frac{\partial i_e(x,t)}{\partial x} \tag{1}$$

$$\frac{\partial \Phi_e(x,t)}{\partial x} = -\frac{i_e(x,t)}{\kappa_{\text{eff}}} + \frac{2R_gT(x,t)t_a^0}{F}\frac{\partial \ln c_e(x,t)}{\partial x} \tag{2}$$

$$\frac{\partial i_e(x,t)}{\partial x} = a_s F j_I(x,t) \tag{3}$$

For the positive electrode and the negative electrode:

$$\frac{\partial c_s(x,r,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_s r^2 \frac{\partial c_s(x,r,t)}{\partial r}\right) \tag{4}$$

$$\frac{\partial \Phi_s(x,t)}{\partial x} = -\frac{i_s(x,t)}{\sigma_{\text{eff}}} \tag{5}$$

$$\frac{\partial i_s(x,t)}{\partial x} = -a_s F j_I(x,t) \tag{6}$$

$$j_I(x,t) = \frac{2i_0(x,t)}{F}\sinh\left(\frac{F\eta_s(x,t)}{2R_gT(x,t)}\right) \tag{7}$$

$$i_0(x,t) = Fk_0\sqrt{c_e(x,t)(c_{s,\max} - c_{\text{ss}}(x,t))c_{\text{ss}}(x,t)} \tag{8}$$

$$\eta_s(x,t) = \Phi_s(x,t) - \Phi_e(x,t) - U_{\text{ss}}(x,t) - Fr_f(x,t)j_I(x,t) \tag{9}$$

$$U_{\text{ss}}(x,t) = U_{\text{ss}}^* + \left.\frac{\partial U}{\partial T}\right|_{T^*}(T(x,t) - T^*) \tag{10}$$

In the separator, the ionic molar flux $j_I(x,t)$ in (3) is considered zero. The equilibrium potential U_{ss}^* in (10) is a function of the normalized solid-phase surface concentration, i.e. $U_{\text{ss}}^* = f_{\text{OCP},i}(c_{\text{ss}}/c_{s,\max})$, where the function $f_{\text{OCP},i}(\cdot)$ used in this paper is given by

For the positive electrode:

$$f_{\text{OCP},i}(\theta) = f_{\text{OCP}}^{\text{pos}}(\theta) = \frac{-4.656 + 88.669\theta^2 - 401.119\theta^4 + 342.909\theta^6 - 462.471\theta^8 + 433.434\theta^{10}}{-1 + 18.933\theta^2 - 79.532\theta^4 + 37.311\theta^6 - 73.083\theta^8 + 95.96\theta^{10}} \tag{11}$$

For the negative electrode:

$$\begin{aligned} f_{\text{OCP},i}(\theta) = f_{\text{OCP}}^{\text{neg}}(\theta) &= 0.7222 + 0.1387\theta + 0.029\theta^{0.5} - 0.0172\theta^{-1} + 0.0019\theta^{-1.5} \\ &+ 0.2808\exp(0.9 - 15\theta) - 0.7984\exp(0.4465\theta - 0.4108) \end{aligned} \tag{12}$$

The terminal voltage is calculated by

$$V_{\text{bat}}(t) = \Phi_s(x,t)|_{x=0} - \Phi_s(x,t)|_{x=L^{\text{tot}}} + r_{\text{col}} i_{\text{app}}(t) \tag{13}$$

where $x = 0$ is the position at the current collector of the positive electrode, and $x = L^{\text{tot}} = L^{\text{pos}} + L^{\text{sep}} + L^{\text{neg}}$ refers to the position at the current collector of the negative electrode. The applied current density $i_{\text{app}}(t)$ is specified in the boundary conditions as the input variable of the model at the terminals of the two electrodes. The model can be solved if the boundary conditions and the initial conditions are given. See [4], [5] for detail. Note that in the original P2D model, the local temperature $T(x,t)$ is usually considered constant at all location. This isothermal condition can be extended with the description of the heat transfer and generation process along the x-axis, resulting in a distributed electrochemical-thermal coupled model. However, with the derivation presented in Section II, a simplified lumped heat transfer model is obtained and used in this paper, i.e.

$$C_T \frac{dT(t)}{dt} = \frac{T_{\text{amb}} - T(t)}{R_T} + A \int_0^{L^{\text{tot}}} q_T(x,t) dx \tag{14}$$

where the local heat source $q_T(x,t)$ is calculated as

$$\begin{aligned} q_T(x,t) = & \overbrace{\sigma_{\text{eff}} \left(\frac{\partial \Phi_s(x,t)}{\partial x} \right)^2 + \kappa_{\text{eff}} \frac{\partial \Phi_e(x,t)}{\partial x} \left(\frac{\partial \Phi_e(x,t)}{\partial x} + \frac{2R_g T(t) t_a^0}{F} \frac{\partial \ln c_e(x,t)}{\partial x} \right)}^{\text{Ohmic heat}} \\ & + \overbrace{F a_s j_I(x,t) \eta_s(x,t)}^{\text{Reactive heat}} + \overbrace{F a_s j_I(x,t) T(t) \left. \frac{\partial U}{\partial T} \right|_{T^*}}^{\text{Reversible heat}} \end{aligned} \tag{15}$$

The model (1)-(15) is referred to as the benchmark P2D-T model. The physical meanings of the symbols in the P2D-T model are given in the Nomenclature. Note that the parameters ε_e, σ_{eff}, $c_{s,\max}$, ρ, and c_p are constant but different for different domains, while parameters D_{eff}, D_s, κ_{eff}, k_0 are usually concentration- and/or temperature-dependent. The values and expressions of the parameters used in this paper are obtained from [5].

II. Development of a Lumped Heat Transfer Model

The distributed heat transfer model is obtained from [4], [5]

$$\rho c_p \frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T(x,t)}{\partial x} \right) + q_T(x,t) \tag{16}$$

with boundary conditions

$$\lambda \frac{\partial T(x,t)}{\partial x} \bigg|_{x=0} = h(T(x,t) - T_{\text{amb}})|_{x=0} \tag{17a}$$

$$\lambda \frac{\partial T(x,t)}{\partial x} \bigg|_{x=L^{\text{tot}}} = h(T_{\text{amb}} - T(x,t))|_{x=L^{\text{tot}}} \tag{17b}$$

Integrating (16) from $x = 0$ to $x = L^{\text{tot}}$ yields

$$\int_0^{L^{\text{tot}}} \rho c_p \frac{\partial T(x,t)}{\partial t} dx = \left(\lambda \frac{\partial T(x,t)}{\partial x} \right) \bigg|_0^{L^{\text{tot}}} + \int_0^{L^{\text{tot}}} q_T(x,t) dx \tag{18}$$

With the consideration that the gradient of temperature along the battery thickness is very small, we have

$$\frac{\partial T(x,t)}{\partial t} = \frac{dT(t)}{dt} \tag{19}$$

Substituting (17) and (19) into (18) gives

$$\left(\int_0^{L^{\text{tot}}} \rho c_p dx \right) \frac{dT(t)}{dt} = 2h \left(T_{\text{amb}} - T(t) \right) + \int_0^{L^{\text{tot}}} q_T(x,t) dx \tag{20}$$

Let $C_T = A \int_0^{L^{\text{tot}}} \rho c_p dx = A \left(L^{\text{pos}} \rho^{\text{pos}} c_p^{\text{pos}} + L^{\text{sep}} \rho^{\text{sep}} c_p^{\text{sep}} + L^{\text{neg}} \rho^{\text{neg}} c_p^{\text{neg}} \right)$, $R_T = \frac{1}{2hA}$, (20) can be rewritten as (14).

TABLE I
NOMENCLATURE

Symbol	Physical Meanings	Unit
Φ_s	solid-phase potential	V
Φ_e	electrolyte potential	V
i_s	solid-phase current density	$\mathrm{A{\cdot}m^{-2}}$
i_e	electrolyte current density	$\mathrm{A{\cdot}m^{-2}}$
c_s	solid-phase concentration	$\mathrm{mol{\cdot}m^{-3}}$
$c_{s,\max}$	theoretical maximum solid-phase concentration	$\mathrm{mol{\cdot}m^{-3}}$
c_{ss}	surface concentration of solid-particle	$\mathrm{mol{\cdot}m^{-3}}$
c_e	electrolyte concentration	$\mathrm{mol{\cdot}m^{-3}}$
j_I	intercalation molar flux	$\mathrm{mol{\cdot}m^{-2}{\cdot}s^{-1}}$
i_0	exchange current density	$\mathrm{A{\cdot}m^{-2}}$
η_s	activation overpotential	V
U_{ss}	equilibrium potential of the electrode	V
U^*_{ss}	equilibrium potential at the reference temperature	V
D_s	solid-phase diffusion coefficient	$\mathrm{m^2{\cdot}s^{-1}}$
D_{eff}	effective electrolyte diffusion coefficient	$\mathrm{m^2{\cdot}s^{-1}}$
a_s	specific surface area of electrode (=$3\varepsilon_s/R_p$)	$\mathrm{m^{-1}}$
ε_s	volume fraction of the solid phase	-
ε_e	porosity or volume fraction of the electrolyte	-
σ_{eff}	effective solid-phase conductivity	$\mathrm{S{\cdot}m^{-1}}$
κ_{eff}	effective electrolyte conductivity	$\mathrm{S{\cdot}m^{-1}}$
k_0	reaction rate constant	$\mathrm{A{\cdot}m^{2.5}mol^{-1.5}}$
L	thickness	m
ρ	density	$\mathrm{kg{\cdot}m^{-3}}$
c_p	specific heat	$\mathrm{J{\cdot}kg^{-1}{\cdot}K^{-1}}$
h	heat transfer coefficient	$\mathrm{W{\cdot}m^{-2}{\cdot}K^{-1}}$
λ	thermal conductivity	$\mathrm{W{\cdot}m^{-1}{\cdot}K^{-2}}$
r_f	SEI film resistance	$\Omega{\cdot}\mathrm{m^2}$
r_{col}	resistance of the current collector	$\Omega{\cdot}\mathrm{m^2}$
F	Faraday constant	$\mathrm{s{\cdot}A{\cdot}mol^{-1}}$
T	temperature	K
T_{amb}	ambient temperature	K
q_T	heat flux density	$\mathrm{W{\cdot}m^{-3}}$
R_g	universal gas constant	$\mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$
t_a^0	transference number	-
A	electrode plate area	$\mathrm{m^2}$

III. Physics-Based Equivalent Circuit Model With Thermal Dynamics (PB-ECM-T)

The PB-ECM-T developed in the paper is summarized as the continuous-time linear time-varying state-space system (21), i.e.

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \tag{21a}$$

$$\mathbf{z}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t) \tag{21b}$$

The detail expressions of the matrices are provided in the following three sub-sections. The order of Padé approximation for the solid phase model is $M = 1$. Note that the subscript $m \times n$ of a matrix indicates that the dimension of the matrix is m by n.

A. State Matrix and Output Matrix

$$\mathbf{A} = \begin{bmatrix}
\mathbf{B}_1\mathbf{R}_1^{-1}\mathbf{E}_1 & \mathbf{0}_{N^{\mathrm{pos}}\times N^{\mathrm{neg}}} & \mathbf{B}_1\mathbf{R}_1^{-1}\mathbf{E}_1 & \mathbf{0}_{N^{\mathrm{pos}}\times N^{\mathrm{sep}}} & \mathbf{0}_{N^{\mathrm{pos}}\times N^{\mathrm{neg}}} & \mathbf{0}_{N^{\mathrm{pos}}\times 1} \\
\mathbf{0}_{N^{\mathrm{neg}}\times N^{\mathrm{pos}}} & -\mathbf{B}_2\mathbf{R}_2^{-1}\mathbf{E}_2 & \mathbf{0}_{N^{\mathrm{neg}}\times N^{\mathrm{pos}}} & \mathbf{0}_{N^{\mathrm{neg}}\times N^{\mathrm{sep}}} & -\mathbf{B}_2\mathbf{R}_2^{-1}\mathbf{E}_2 & \mathbf{0}_{N^{\mathrm{neg}}\times 1} \\
\mathbf{B}_3\mathbf{R}_1^{-1}\mathbf{E}_1 & \mathbf{0}_{N^{\mathrm{pos}}\times N^{\mathrm{neg}}} & \mathbf{A}_1 + \mathbf{B}_3\mathbf{R}_1^{-1}\mathbf{E}_1 & \mathbf{A}_2 & \mathbf{0}_{N^{\mathrm{pos}}\times N^{\mathrm{neg}}} & \mathbf{0}_{N^{\mathrm{pos}}\times 1} \\
\mathbf{0}_{N^{\mathrm{sep}}\times N^{\mathrm{pos}}} & \mathbf{0}_{N^{\mathrm{sep}}\times N^{\mathrm{neg}}} & \mathbf{A}_3 & \mathbf{A}_4 & \mathbf{A}_5 & \mathbf{0}_{N^{\mathrm{sep}}\times 1} \\
\mathbf{0}_{N^{\mathrm{neg}}\times N^{\mathrm{pos}}} & -\mathbf{B}_4\mathbf{R}_2^{-1}\mathbf{E}_2 & \mathbf{0}_{N^{\mathrm{neg}}\times N^{\mathrm{pos}}} & \mathbf{A}_6 & \mathbf{A}_7 - \mathbf{B}_4\mathbf{R}_2^{-1}\mathbf{E}_2 & \mathbf{0}_{N^{\mathrm{neg}}\times 1} \\
\mathbf{0}_{1\times N^{\mathrm{pos}}} & \mathbf{0}_{1\times N^{\mathrm{neg}}} & \mathbf{0}_{1\times N^{\mathrm{pos}}} & \mathbf{0}_{1\times N^{\mathrm{sep}}} & \mathbf{0}_{1\times N^{\mathrm{neg}}} & \mathbf{A}_T
\end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix}
\mathbf{B}_1\mathbf{R}_1^{-1}\mathbf{R}_3 \\
-\mathbf{B}_2\mathbf{R}_2^{-1}\mathbf{R}_4 \\
\mathbf{B}_3\mathbf{R}_1^{-1}\mathbf{R}_3 \\
\mathbf{0}_{N^{\mathrm{sep}}\times 1} \\
-\mathbf{B}_4\mathbf{R}_2^{-1}\mathbf{R}_4 \\
\mathbf{0}_{1\times 1}
\end{bmatrix}_{(N^{\mathrm{pos}}+N^{\mathrm{neg}}+N+1)\times 1}$$

where

$$\mathbf{R}_1 = \begin{bmatrix} R_{\Sigma,1} + R_{\text{se},1.5} & -R_{\Sigma,2} & 0 & \dots & 0 & 0 \\ R_{\text{se},2.5} & R_{\Sigma,2} + R_{\text{se},2.5} & -R_{\Sigma,3} & \dots & 0 & 0 \\ R_{\text{se},3.5} & R_{\text{se},3.5} & R_{\Sigma,3} + R_{\text{se},3.5} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ R_{\text{se},N^{\text{pos}}-0.5} & R_{\text{se},N^{\text{pos}}-0.5} & R_{\text{se},N^{\text{pos}}-0.5} & \dots & R_{\Sigma,N^{\text{pos}}-1} + R_{\text{se},N^{\text{pos}}-0.5} & -R_{\Sigma,N^{\text{pos}}} \\ 1 & 1 & 1 & \dots & 1 & 1 \end{bmatrix}_{N^{\text{pos}} \times N^{\text{pos}}}$$

$$\mathbf{R}_2 = \begin{bmatrix} R_{\Sigma,N^{\text{pos}}+N^{\text{sep}}+1} + R_{\text{se},N^{\text{pos}}+N^{\text{sep}}+1.5} & -R_{\Sigma,N^{\text{pos}}+N^{\text{sep}}+2} & 0 & \dots & 0 & 0 \\ R_{\text{se},N^{\text{pos}}+N^{\text{sep}}+2.5} & R_{\Sigma,N^{\text{pos}}+N^{\text{sep}}+2} + R_{\text{se},N^{\text{pos}}+N^{\text{sep}}+2.5} & -R_{\Sigma,N^{\text{pos}}+N^{\text{sep}}+3} & \dots & 0 & 0 \\ R_{\text{se},N^{\text{pos}}+N^{\text{sep}}+3.5} & R_{\text{se},N^{\text{pos}}+N^{\text{sep}}+3.5} & R_{\Sigma,N^{\text{pos}}+N^{\text{sep}}+3} + R_{\text{se},N^{\text{pos}}+N^{\text{sep}}+3.5} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ R_{\text{se},N-0.5} & R_{\text{se},N-0.5} & R_{\text{se},N-0.5} & \dots & R_{\Sigma,N-1} + R_{\text{se},N-0.5} & -R_{\Sigma,N} \\ 1 & 1 & 1 & \dots & 1 & 1 \end{bmatrix}_{N^{\text{neg}} \times N^{\text{neg}}}$$

$$\mathbf{R}_3 = \begin{bmatrix} R_{s,1.5} \\ R_{s,2.5} \\ \vdots \\ R_{s,N^{\text{pos}}-0.5} \\ 1 \end{bmatrix}_{N^{\text{pos}} \times 1} \qquad \mathbf{R}_4 = \begin{bmatrix} R_{e,N^{\text{pos}}+N^{\text{sep}}+1.5} \\ R_{e,N^{\text{pos}}+N^{\text{sep}}+2.5} \\ \vdots \\ R_{e,N-0.5} \\ 1 \end{bmatrix}_{N^{\text{neg}} \times 1}$$

$$\mathbf{E}_1 = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 \\ 0 & 0 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{bmatrix}_{N^{\text{pos}} \times N^{\text{pos}}} \qquad \mathbf{E}_2 = \begin{bmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -1 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{bmatrix}_{N^{\text{neg}} \times N^{\text{neg}}}$$

$$\begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 & \mathbf{0} \\ \mathbf{A}_3 & \mathbf{A}_4 & \mathbf{A}_5 \\ \mathbf{0} & \mathbf{A}_6 & \mathbf{A}_7 \end{bmatrix} = \begin{bmatrix} -F_{1,1} & F_{1,1} & 0 & \cdots & 0 & 0 \\ F_{1,2} & -(F_{1,2}+F_{2,2}) & F_{2,2} & \cdots & 0 & 0 \\ 0 & F_{2,3} & -(F_{2,3}+F_{3,3}) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -(F_{N-2,N-1}+F_{N-1,N-1}) & F_{N-1,N-1} \\ 0 & 0 & 0 & \cdots & F_{N-1,N} & -F_{N-1,N} \end{bmatrix}_{N \times N}$$

$$\mathbf{B}_1 = \text{diag}(\frac{1}{C_{s,1}}, \frac{1}{C_{s,2}}, \cdots, \frac{1}{C_{s,N^{\text{pos}}}}), \mathbf{B}_2 = \text{diag}(\frac{1}{C_{s,N^{\text{pos}}+N^{\text{sep}}+1}}, \frac{1}{C_{s,N^{\text{pos}}+N^{\text{sep}}+2}}, \cdots, \frac{1}{C_{s,N}}),$$
$$\mathbf{B}_3 = \text{diag}(\frac{1}{C_{d,1}}, \frac{1}{C_{d,2}}, \cdots, \frac{1}{C_{d,N^{\text{pos}}}}), \mathbf{B}_4 = \text{diag}(\frac{1}{C_{d,N^{\text{pos}}+N^{\text{sep}}+1}}, \frac{1}{C_{d,N^{\text{pos}}+N^{\text{sep}}+2}}, \cdots, \frac{1}{C_{d,N}})$$

$$\mathbf{A}_T = -\frac{1}{R_T C_T} + \frac{1}{T(t)} \left(\frac{T_{\text{amb}}}{R_T} + \sum_{i=1}^{N} Q_{T,i}(t) \right)$$

$$F_{i,j} := 1/(R_{d,i+0.5} C_{d,j})$$

$$R_{\text{se},i+0.5} := R_{s,i+0.5} + R_{e,i+0.5}$$

$$R_{\Sigma,i} := R_{\eta,i} + R_{f,i}$$

B. Output Matrix and Direct Feedthrough Matrix

$$\mathbf{C} = \begin{bmatrix} \mathbf{K}_1\mathbf{R}_1^{-1}\mathbf{E}_1 + \mathbf{M}_1 & \mathbf{K}_2\mathbf{R}_2^{-1}\mathbf{E}_2 - \mathbf{M}_2 & \mathbf{K}_1\mathbf{R}_1^{-1}\mathbf{E}_1 + \mathbf{M}_1 & \mathbf{0}_{N\times 1} & \mathbf{K}_2\mathbf{R}_2^{-1}\mathbf{E}_2 - \mathbf{M}_2 & \mathbf{0}_{1\times 1} \end{bmatrix}_{1\times(N^{\text{pos}}+N^{\text{neg}}+N+1)}$$

$$\mathbf{D} = \left(r_{\text{col}}/A + R_{e,\text{sep}} + \mathbf{K}_1\mathbf{R}_1^{-1}\mathbf{R}_3 + \mathbf{K}_2\mathbf{R}_2^{-1}\mathbf{R}_4\right)_{1\times 1}$$

where

$$\mathbf{K}_1 = \begin{bmatrix} \sum_{i=1}^{N^{\text{pos}}} R_{e,i+0.5} + R_{\Sigma,1} & \sum_{i=2}^{N^{\text{pos}}} R_{e,i+0.5} & \dots & R_{e,N^{\text{pos}}-0.5} + R_{e,N^{\text{pos}}+0.5} & R_{e,N^{\text{pos}}+0.5} \end{bmatrix}_{1\times N^{\text{pos}}}$$

$$\mathbf{K}_2 = \begin{bmatrix} R_{e,N^{\text{pos}}+N^{\text{sep}}+0.5} & R_{e,N^{\text{pos}}+N^{\text{sep}}+0.5} + R_{e,N^{\text{pos}}+N^{\text{sep}}+1.5} & \dots & \sum_{i=N^{\text{pos}}+N^{\text{sep}}}^{N-2} R_{e,i+0.5} & \sum_{i=N^{\text{pos}}+N^{\text{sep}}}^{N-1} R_{e,i+0.5} + R_{\Sigma,N} \end{bmatrix}_{1\times N^{\text{neg}}}$$

$$\mathbf{M}_1 = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \end{bmatrix}_{1\times N^{\text{pos}}},\ \mathbf{M}_2 = \begin{bmatrix} 0 & 0 & 0 & \dots & 1 \end{bmatrix}_{1\times N^{\text{neg}}},\ R_{e,\text{sep}} = \sum_{i=N^{\text{pos}}+1}^{N^{\text{pos}}+N^{\text{sep}}-1} R_{e,i+0.5}$$

C. Expression of Circuit Parameters as Functions of Electrochemical Parameters and States

See Table II on the next page.

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TABLE II
EXPRESSIONS OF CIRCUIT COMPONENTS OF PB-ECM-T

Symbol	Expressions
$C_{s,i}$	$\dfrac{Al_iF\varepsilon_{s,i}c_{s,\max,i}}{-f'_{\mathrm{OCP},i}(c_{s,\mathrm{avg},i}/c_{s,\max,i})}$
$C_{2,i}$	$\frac{3}{7}C_{s,i}$
$R_{s,i+0.5}$	$\frac{0.5}{A}\left(\frac{l_i}{\sigma_{\mathrm{eff},i}}+\frac{l_{i+1}}{\sigma_{\mathrm{eff},i+1}}\right)$
$R_{e,i+0.5}$	$\frac{0.5}{A}\left(\frac{l_i}{\kappa_i}+\frac{l_{i+1}}{\kappa_{i+1}}\right)$
$R_{d,i+0.5}$	$\frac{0.5\Upsilon t_a^0}{AF}\left(\frac{l_iT_i}{D_{\mathrm{eff},i}}+\frac{l_{i+1}T_{i+1}}{D_{\mathrm{eff},i+1}}\right)\frac{1}{c_{e,i}}\varsigma$
	where
	$\varsigma=\begin{cases}\dfrac{\frac{V_{e,i+1}}{\Upsilon T_{i+1}}-\frac{V_{e,i}}{\Upsilon T_i}}{\exp\left(\frac{V_{e,i+1}}{\Upsilon T_{i+1}}-\frac{V_{e,i}}{\Upsilon T_i}\right)-1}, & \frac{V_{e,i+1}}{T_{i+1}}\neq\frac{V_{e,i}}{T_i}\\ 1, & \frac{V_{e,i+1}}{T_{i+1}}=\frac{V_{e,i}}{T_i}\end{cases}$
	$\Upsilon=\frac{2R_gt_a^0}{F}$
$C_{d,i}$	$\frac{Al_iF\varepsilon_{e,i}c_{e,i}}{t_a^0\Upsilon T_i}$
$R_{\eta,i}$	$\frac{1}{Al_ia_{s,i}}\frac{R_gT_i}{F^2k_{0,i}c_{s,\max,i}}\frac{1}{\sqrt{c_{e,i}\hat{\theta}_{\mathrm{ss},i}(1-\hat{\theta}_{\mathrm{ss},i})}}\xi$
	where
	$\hat{\theta}_{\mathrm{ss},i}=\frac{c_{s,\mathrm{avg},i}}{c_{s,\max,i}}$
	$\xi=\begin{cases}\frac{\sinh^{-1}(\hat{\tau}_i)}{\hat{\tau}_i}, & \hat{\tau}_i\neq0\\ 1, & \hat{\tau}_i=0\end{cases}$
	$\hat{\tau}_i=\frac{\hat{I}_{I,i}}{Fl_i}\frac{1}{2a_{s,i}i_{0,i}}$
	$\hat{I}_{I,i}=\begin{cases}\frac{3}{N^{\mathrm{pos}}}\left(\frac{2i-1}{2N^{\mathrm{pos}}}\right)^2I_{\mathrm{app}}, & i\in\mathcal{S}^{\mathrm{pos}}\\ -\frac{3}{N^{\mathrm{neg}}}\left(\frac{4N-2N^{\mathrm{neg}}-2i+1}{2N^{\mathrm{neg}}}\right)^2I_{\mathrm{app}}, & i\in\mathcal{S}^{\mathrm{neg}}\end{cases}$
$R_{f,i}$	$\frac{r_{f,i}}{Al_ia_{s,i}}$
$C_{T,i}$	$A\left(L^{\mathrm{pos}}\rho^{\mathrm{pos}}c_p^{\mathrm{pos}}+L^{\mathrm{sep}}\rho^{\mathrm{sep}}c_p^{\mathrm{sep}}+L^{\mathrm{neg}}\rho^{\mathrm{neg}}c_p^{\mathrm{neg}}\right)$
$R_{T,i}$	$\frac{1}{2hA}$