# Thermo-Electrochemical Level-Set Topology Optimization of a Heat Exchanger for Lithium-Ion Batteries for eVTOL vehicles

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#### Abstract

Developing electric vertical take-off and landing vehicles (eVTOL) that can meet the demanding power and energy requirements entails significant challenges, one of which is due to the weight of the battery packs. To address this challenge, optimization techniques can be employed to achieve lightweight designs while satisfying thermal criteria. In this study, we focus on optimizing a battery heat exchanger housing a highenergy-density cylindrical cell using the level-set topology optimization method. To accurately account for heat generation from battery electrochemistry, we utilize both a high-fidelity, the Doyle Fuller Newman

#### 2 Topology Optimization of Battery Heat Exchanger

(DFN) model, and a low-fidelity electrochemical model, the Single Particle Model (SPM), which are compared to experimental results for an eVTOL flight profile. The heat generated by the battery is incorporated as a source term in an unsteady heat conduction finite element model, forming the basis of the optimization process. Our objective is to minimize the integrated thermal compliance over time while satisfying a volume constraint, employing the level-set method. The SPM proves competent in predicting the voltage profile but underestimates the temperature increase. On the other hand, the DFN model accurately predicts both the temperature increase and the voltage profile, making it suitable for the thermal analysis of cells in eVTOL vehicles. Surprisingly, steady-state optimization turns out to be sufficient to generate optimized topologies that perform similarly to transient cases for the case investigated but at a reduced cost. By integrating electrochemical modeling, level-set topology optimization, and heat transfer analysis, our study contributes to the development of lightweight and thermally efficient battery heat exchangers for eVTOL vehicles, which can be extended to battery packs. Importantly, the presented methodology is versatile and can be applied to different battery chemistries, form factors, and power profiles.

**Keywords:** eVTOL, lithium-ion battery, thermal optimization, electrochemical modeling, transient optimization, level-set topology optimization

# Highlights

- Two physics-based electrochemical models for eVTOL flights to predict voltage profile and temperature increase are investigated and compared with experimental data
- A new thermo-electrochemical level-set topology optimization methodology reusable and extendable for electric vehicles is proposed
- Transient and steady-state heat conduction models for topology optimization in the context of eVTOL flight profiles are compared

# 1 Introduction

The aerospace sector is undergoing a significant transformation due to the electrification of aircraft and the emergence of urban air mobility (UAM) concepts [1, 2]. Among the solutions for UAM, Electric Vertical Take-Off and Landing (eVTOL) vehicles have garnered attention. These vehicles offer a potential solution for alleviating ground traffic congestion and providing a safe, environmentally friendly alternative to conventional individual transportation [3]. As a result, eVTOL vehicles hold the promise of revolutionizing transportation systems in urban areas.

Despite the promising prospects of UAM, its development is accompanied by a range of challenges. Key concerns that the technology currently faces include ensuring safety standards, reducing noise emissions in urban and suburban areas, and enhancing the power and energy density at the battery pack level [4, 5]. Addressing the battery challenge can be approached from two angles: enhancing battery technology at the cell level, such as through advancements in all-solid-state batteries [6], or exploring improvements in the battery containment module, the latter of which is the focus of the present study.

A popular design method to optimize parts and reduce their mass while fulfilling a set of requirements is topology optimization (TO). Since its introduction at the end of the eighties [7], TO has become increasingly popular and has been applied in numerous applications [8]. For instance, the optimization of the components of battery packs such as the cooling plate has been investigated. In [9], the authors discussed the optimization of two-dimensional cold plates based on a fluid flow model coupled to a thermal model. TO has also been recently used to design entire battery packs with temperature and stress constraints [10]. The presented methodology relies on the level-set method and investigated steady-state two-dimensional examples where the heat generation from the cells was assumed to be fixed and was not related to the behavior of the cells. The level-set topology optimization has also been used to optimize load-carrying battery packs while considering fluid flow, structural, and thermal requirements [11]. The thermal load was again considered to be given constant.

In this work, we extend the previous studies by introducing a threedimensional transient topology optimization of a battery heat exchanger based on physics-derived electrochemical models coupled to a heat transfer model. By doing so our aim is to investigate the dynamic effects associated with future eVTOL flights in optimization. Additionally, the utilization of electrochemical models provides valuable information regarding cell response, enabling battery chemistry selection, state of health prediction, and battery optimization. Two models, the Doyle Fuller Newman (DFN) model and the Single Particle Model (SPM), are investigated and compared to experiments for constant discharge cases, and a power profile for an eVTOL vehicle for the first cycle such that battery degradation is not considered for this work. Furthermore, these models can be used *a priori*, resulting in savings in cost and time and the development of the thermo-electrochemical model also represents a step toward creating digital twins for battery packs.

The remainder of the paper is structured as follows: In Section 2, we introduce the electrochemical models and compare them to constant discharge cases. Section 3 describes the transient thermal model. Next, in Section 4, we present the level-set method and the optimization formulation. Finally, we demonstrate the effectiveness of our proposed methodology through numerical examples in Section 5 where we compare the optimized topologies obtained with the two electrochemical models and with steady-state cases. We conclude our findings in Section 6.

# 2 Electrochemical models

## 2.1 Doyle-Fuller-Newman model

The Doyle-Fuller-Newman (DFN) model is a continuum model for porous electrodes applied to batteries and was developed in the seminal work by Newman and collaborators [12-14]. Specifically in this work, we are interested in lithium-ion cells. The DFN model is a physics-based model describing the electrochemistry behavior of a cell based on the molar conservation of lithium and electronic and electrostatic charge conservation in the system. The model is solved for the lithium-ion concentrations, electric potentials, current densities, and molar fluxes. It is assumed that the particles are spherical and that the ions transport is mainly unidirectional such that only the effects from one current collector to another are considered where the current collectors are not included in the model. Hence, the model is effectively a one-dimensional model with coordinate x with a pseudo-second dimension for the solid phase diffusion in the active material with coordinate r along the radius of a particle. For this reason, The model is sometimes referred to as a Pseudo-2-Dimensional (P2D) model. The conservation equations in the x-coordinate and r-coordinate are coupled with the description of the intercalation phenomena at the electrode/electrolyte interface with the Butler-Volmer equation. A representation of the model is presented in Fig. 1.



Fig. 1: Schematic of the battery model

The governing equations of the DFN model are the following:

- 1. Solid state lithium-ion diffusion in the active material with Fickian diffusion
- 2. Concentrated electrolyte theory for mass transport in the electrolyte
- 3. Conservation of charge in the active material based on Ohm's law
- 4. Conservation of charge in the electrolyte based on MacInnes' equation which is a modified Ohm's law to account for the gradient of concentration in the electrolyte
- 5. Coupling of the mass and molar conservation at the macroscale and in the pseudo-second dimension with the Butler-Volmer equation which describes the intercalation on the surface of the active particles

More details are given in Appendix A. Throughout the paper, the subscript k is used to indicate the subdomain considered where n, sep, and p correspond to the anode, separator, and cathode domains respectively. The three domains are defined as

$$\Omega_n = \{ x \mid x \in [0, L_n) \}$$

$$\tag{1}$$

$$\Omega_{sep} = \{ x \mid x \in [L_n, L_n + L_{sep}) \}$$

$$\tag{2}$$

$$\Omega_p = \{ x \mid x \in [L_n + L_{sep}, L] \}$$
(3)

where  $L_n$ ,  $L_{sep}$ , and  $L_p$  are the thicknesses of the anode, separator, and cathode respectively, and L is the overall thickness. In addition, there is a domain  $\Omega_r$ corresponding to a spherical particle of active material at each location along x such that

$$\Omega_{r,k} = \{ r_k \mid r_k \in [0, R_k] \}, k \in \{n, p\}$$
(4)

where  $R_k$  is the radius of the particle in an electrode. As mentioned before, the model is solved for the electric potentials  $\phi$ , the molar fluxes N, the current densities i, and the lithium-ion concentrations c. The variables in each region are

 $\phi_{e,k}, c_{e,k}, i_{e,k}, N_{e,k}, \qquad x \in \Omega_k, \quad k \in \{n, sep, p\}$ (5)

$$\phi_{s,k}, i_{s,k} \qquad \qquad x \in \Omega_k, \quad k \in \{n, p\} \tag{6}$$

$$c_{s,k}, N_{s,k} \qquad r_k \in \Omega_{r,k}, \quad k \in \{n, p\}$$

$$\tag{7}$$

The subscript e and s denote the electrolyte and solid phase respectively. Table A.1 summarizes the dimensionless form of the DFN and is given as part of the Appendix A. The model is also described in great details in [15–19].

#### 2.2 Single-Particle Model

The DFN model is computationally intensive, solving nonlinear partial differential equations. To alleviate the computational burden the Single Particle Model (SPM) offers a simplified alternative [15, 16]. The SPM reduces complexity by disregarding electrolyte properties and simplifying transport phenomena. In the SPM, rather than modeling each individual point within the electrode, the focus shifts to a single representative particle. This assumption implies that all particles behave the same way. To derive the SPM from the DFN model, several assumptions are made:

- Charge transfer occurs uniformly across the surface of each active material particle, where intercalation takes place.
- The solid phase within the electrode is assumed to possess high electrical conductivity, resulting in a uniform local volumetric current density through the electrode's thickness.
- Solid phase diffusion dynamics are governed by concentration gradients induced by pore-wall flux density at the particle surfaces. This flux is driven by a constant averaged electrochemical reaction rate.
- The SPM considers instantaneous charge transport between electrodes through the electrolyte. This assumption is based on the fact that electrolytic diffusion occurs significantly faster than solid diffusion.

The last point of the SPM assumptions implies that mass transport in the electrolyte is neglected, resulting in a zero gradient of concentration in the electrolyte. This means that the dynamics of the electrolyte are assumed to have little influence on the behavior of the cell. As a consequence, the Ohmic heating, denoted as  $Q_{Ohm}$ , from the electrolyte is neglected in the SPM. Note that the heat generated by the current collectors due to Ohmic heating is also neglected. Instead, only heat generation from the electrochemical reactions,  $Q_{Reaction}$ , and due to entropic changes,  $Q_{Entropic}$ , are considered. While this simplification reduces the computational cost, it can result in inaccurate predictions for high discharge rates [18]. However, the SPM can provide valuable insight into the overall behavior of the cell and trends in variables of interest. Therefore, it can serve as a low-fidelity model for optimization at the module level. The dimensionless form of the SPM is given in Appendix B. For more information regarding the SPM and its derivation, we refer to [15, 16]. Both the SPM and DFN models are solved using the finite volume method [20] which is appropriate for the conservation laws. The electrochemical models are implemented using the open-source Python library dedicated to battery modeling PyBaMM [21].

# 2.3 Experimental validation of the electrochemical models

To meet the power, capacity, and therefore energy requirements for our considered eVOTL aircraft, we choose state-of-the-art commercially available lithium-ion cylindrical cells (LG Chem, INR21700M50LT) that possess a high nominal capacity of 5000 mAh and are capable of high current discharge 14.4 A. To be conservative, the minimum capacity of 4850 mAh is used throughout this work to compute the C-rates. This limits the maximum C-rate to 2.97 C. We consider this cell to be theoretically best suited for eVTOL applications due to its cell chemistry, where the NMC811 cathode possesses the highest specific capacity of the stable layered oxides (> 200 mAh/g). This chemistry has been extensively studied and used in electric vehicles and proposed for eVOTL applications [4]. In addition, the 21700 cylindrical form factor enables a high energy density for commercially available lithium-ion cells of 260 Wh/kg. The 21700 form factor provides a good compromise between specific capacity and safety since the heat generated is not significantly different compared to 18650 [22, 23]. This cell configuration was chosen as an ideal candidate for our aircraft.

To validate the electrochemical models, preliminary simulations and experiments were conducted to capture discharge behavior under constant current discharge conditions and a more complex discharge profile is investigated in Section 5.2. lithium-ion cells were cycled under ambient conditions using highcurrent channels (Arbin Instruments). The cells were charged under 0.1 C (0.485 A) until 4.2 V, then held at 4.2 V until a leakage current of 50 mA was reached. This was done to ensure cells reached 100 % SOC (state of charge). The cells were then subsequently discharged at either slow, medium, or fast rates. The slow discharge rate of 0.1 C was used to capture the initial voltage drop without having to consider kinetic limitations. The medium discharge rate of 0.5 C (2.425 A) and the high discharge rate of 1 C (4.85 A) were tested to better emulate discharge rates experienced during flight, which will be further discussed in Section 5.2. The parameters for this cell's electrochemistry were taken from [24]. The parameters were adjusted to consider calendar aging by modifying the solid electrolyte interface (SEI) thickness and resistivity. The results for the rates with low and high-fidelity electrochemical models are presented in Fig. 2.

## 3 Thermal model

The governing equation for the thermal model is

$$\nabla \cdot (\kappa \nabla T) + Q = \rho c_p \frac{\partial T}{\partial t} \tag{8}$$

where  $\kappa$  is the thermal conductivity, T is the temperature, Q is the volumetric heat generation rate,  $\rho$  is the material density,  $c_p$  is the specific heat, and tis the time. The heat source term accounts for the Ohmic heating  $Q_{Ohm}$  due to resistance in the solid and in the electrolyte, irreversible heating  $Q_{Reaction}$ due to the electrochemical reactions, and reversible heating  $Q_{Entropic}$  due to the entropic changes defined as

$$Q_{Ohm} = \begin{cases} -\left(i_{s,k}\frac{\partial\phi_{s,k}}{\partial x} + i_{e,k}\frac{\partial\phi_{e,k}}{\partial x}\right) & k = n, p\\ -i_{e,sep}\frac{\partial\phi_{e,sep}}{\partial x} & k = sep \end{cases} \qquad \qquad k \in \{n, sep, p\}$$
$$Q_{Reaction} = a_k J_k \eta_k \qquad \qquad k \in \{n, p\}$$



Fig. 2: Voltage profiles as a function of time for different constant discharge rates

$$Q_{Entropic} = a_k J_k T \frac{\partial U_{oc,k}}{\partial T} \bigg|_{T = T_{ref}} \qquad \qquad k \in \{n, p\} \qquad (9)$$

where  $a_k$  is the electrode surface area density,  $J_k$  is the interfacial current density,  $\eta_k$  is the overpotential,  $U_{oc,k}$  is the open circuit potential, and  $T_{ref}$  is the reference temperature. The total heat generation Q is defined as the sum of the different heat generation, i.e.,  $Q = Q_{Ohm} + Q_{Reaction} + Q_{Entropic}$ . The following boundary conditions are considered for the thermal problem.

$$T = T_b \text{ on } \Gamma_T$$
  
-(\kappa \nabla T) \cdot n = q\_N \text{ on } \Gamma\_N  
(\kappa \nabla T) \cdot n = 0 \text{ on } \Gamma\_A (10)

 $T_b$  is a prescribed temperature,  $q_N$  is a prescribed heat flux, and  $\Gamma_T$ ,  $\Gamma_N$ , and  $\Gamma_A$  correspond to the surfaces associated with prescribed temperature boundary condition, prescribed flux boundary condition, and adiabatic boundary conditions respectively. The thermal model is solved using the finite element method [25]. Let  $\mathcal{V}$  and  $\mathcal{S}$  be the space of test functions and the set of trial functions, respectively such that

$$\mathcal{V} = \{ v(x) \mid x \in \Omega, v \in \mathcal{H}^1(\Omega), v = 0 \text{ on } \Gamma_T \}$$
$$\mathcal{S} = \{ u(x,t) \mid x \in \Omega, t > 0, u \in \mathcal{H}^1(\Omega), u = T_b \text{ on } \Gamma_T \}$$
(11)

The weak form of the unsteady thermal model with heat generation due to the electrochemical behavior of a lithium-ion battery is,

Given 
$$Q, \kappa, q_n, \rho, c_p$$
 find  $u \in S$  such that  $\forall v \in V$ 

$$\int_{\Omega} Qv \, d\Omega - \int_{\Omega} \kappa \nabla v \cdot \nabla u \, d\Omega - \int_{\Gamma_N} v q_N \, d\Gamma_N = \int_{\Omega} \rho c_p \dot{u} v \, d\Omega \tag{12}$$

We apply the finite difference method with an implicit backward Euler scheme for the time discretization which is unconditionally stable such that

$$\dot{u}_n = \frac{u_n - u_{n-1}}{\Delta t} \tag{13}$$

where n is the time index and  $\Delta t$  is the time step. So, finally, we have the following

$$\int_{\Omega} Q_n v \, d\Omega - \int_{\Omega} \kappa \nabla v \cdot \nabla u_n \, d\Omega - \int_{\Gamma_N} v q_N \, d\Gamma_N = \int_{\Omega} \rho c_p \frac{u_n - u_{n-1}}{\Delta t} v \, d\Omega \quad (14)$$

The weak form is approximated using the standard Galerkin approximation with linear shape functions. The thermal model is implemented using FEniCS [26, 27] which is an open-source finite element package for solving partial differential equations. It has been chosen because of its ease of implementation of the weak form and for its efficiency. In addition, FEniCS has a Python interface which allows for easy communication with PyBaMM.

To summarize, a given power profile is passed to the electrochemical model as an input to compute the heat generation from the cells. The volumetric heat generation is then fed into the transient thermal model which is solved for the temperature distribution. A sensitivity analysis is then carried out to solve the design optimization problem and update the battery pack until convergence. More details regarding the optimization method are given in Section 4. The optimization workflow is presented in Fig. 3.



Fig. 3: Optimization workflow

## 4 Level-set topology optimization

## 4.1 Level-set method

The level-set method (LSM) was originally developed in the context of front propagation [28]. It then became a popular method for topology optimization for its ability to clearly define the interfaces between the different regions of the design domain [29]. Indeed, the topology is unambiguously defined throughout the optimization history and no additional filtering is necessary in order to obtain a physical optimized part. An implicit function  $\phi(x)$  is used to describe the design in the domain. This function is usually initialized as a signeddistance function and is such that

$$\begin{cases} \phi(x) \ge 0, x \in \Omega\\ \phi(x) = 0, x \in \Gamma\\ \phi(x) < 0, x \notin \Omega \end{cases}$$
(15)

where  $\Omega$  is the solid domain and  $\Gamma$  is the boundary. The following Hamilton-Jacobi equation, so-called the level-set equation, is used to update the boundary at each iteration.

$$\frac{\partial\phi(x)}{\partial t} + |\nabla\phi(x)|V_n(x)| = 0$$
(16)

where t is the fictitious time and  $V_n$  is the normal design velocity. In its discretized form used for the numerical implementation with an explicit forward

Euler scheme, it reads,

$$\phi_i^{k+1} = \phi_i^k - \Delta t |\nabla \phi_i^k| V_{n,i} \tag{17}$$

where k is the current iteration number, i is a point in the domain, and  $\Delta t$  is the fictitious time-step. The design velocities are determined by solving a sub-optimization problem. The solution to that problem is a combination of the shape sensitivities and the problem is solved for the boundary movement at each boundary point [30]. The spatial gradient of the level-set function, i.e.,  $|\nabla \phi_i^k|$ , is computed with the Hamilton-Jacobi weighted essentially non-oscillatory (HJ-WENO) scheme [31]. An Eulerian grid, i.e., a fixed grid, is used to mesh the domain. Thus, as the boundary is updated, the zero level-set partially cuts finite elements and the element's effective properties must be computed. The effective thermal conductivity of each element is defined as follows,

$$\kappa_e = (\gamma_{min}(1 - \gamma_e) + \gamma_e) \kappa \tag{18}$$

where  $\kappa_e$  is the effective thermal conductivity,  $\gamma_e$  is element density which corresponds to the fraction of the volume of the element cut by the level set function,  $\kappa$  is the thermal conductivity of the solid phase, and  $\gamma_{min}$  is a small value used for numerical stability, typically  $1 \times 10^{-6}$  to  $1 \times 10^{-9}$ . The quantity  $\rho c_p$  is interpolated in the same way.

#### 4.2 Optimization problem formulation

One of the main concerns about lithium-ion batteries for electric vehicles is safety [32]. In particular, thermal runaway has been a major concern as it led to various electric-powered systems ranging from phones to electric vehicles catching fire or exploding [33]. It is one of the common failure mechanisms of batteries and mitigating strategies is an active research topic [34-36]. Thermal runaway is the phenomenon associated with an uncontrollable self-sustaining heating state. Indeed, once some abuse conditions are met, chemical exothermic reactions start leading to additional exothermic reactions in a positive feedback loop until failure. Several abuse scenarios include mechanical impact or overheating, e.g., due to overcharging/overdischarging the cell or a failure in external cooling. The external cooling is the primary concern in this work. The objective for the optimization problem is to minimize the integral of thermal compliance due to the heat source over the analysis time. This objective corresponds to thermal energy due to heat generation from the cells stored in the module over time. Thermal compliance, C, is defined for a steady-state problem as

$$C = \mathbf{Q}^T \mathbf{T} \tag{19}$$

where  $\mathbf{Q}$  and  $\mathbf{T}$  are the vectors of thermal loads and nodal temperature respectively. This objective is commonly used in thermal optimization problems, e.g., [37, 38]. To evaluate the objective over time, thermal compliance is computed at each time step and the values are summed using the trapezoidal rule. Additionally, the mass of the batteries and the associated packs is one of the design constraints to the development of eVTOL vehicles. Indeed, the mass of the battery system is  $\approx 20 - 25\%$  of the gross weight in the case of an eVTOL while the mass of the fuel represents only  $\approx 2.5-5\%$  in the case of a traditional VTOL vehicle [39]. Moreover, the energy density of a lithium-ion battery is only one-hundredth of the energy density of aviation fuel [40, 41]. Thus, it is essential to save as much mass as possible to save energy in order to increase the mission range of eVTOL aircraft. For this reason, a volume constraint is included in the optimization formulation to obtain a lightweight design. In a discrete form and for a transient problem the optimization problem reads

$$\begin{array}{ll} \underset{\Omega}{\text{minimize}} & \frac{\Delta t}{2} \left( \mathbf{Q}_{t_1}^T \mathbf{T}_{t_1} + 2 \sum_{t_i=2\Delta t}^{t_f - \Delta t} \mathbf{Q}_{t_i}^T \mathbf{T}_{t_i} + \mathbf{Q}_{t_f}^T \mathbf{T}_{t_f} \right) \\ \text{subject to} & V - \chi V_0 \le 0 \\ & \mathbf{R}_i(\boldsymbol{\gamma}, \mathbf{T}(\boldsymbol{\gamma})) = \mathbf{0} \end{array} \tag{20}$$

where  $V_0$  is the volume of the entire design domain,  $\chi$  is the prescribed volume fraction,  $\mathbf{R}_i$  is the residual of Eq. 14 at  $t_i$  with the index  $i \geq 1$ , V is the volume of the optimized topology,  $t_0$  is the initial time, and  $t_f$  is the final time. In addition, let

$$\langle \boldsymbol{a} \rangle \triangleq \frac{\Delta t}{2} \left( \mathbf{a}_{t_1} + 2 \sum_{t_i = \Delta t}^{t_f - \Delta t} \mathbf{a}_{t_i} + \mathbf{a}_{t_f} \right)$$
(21)

Finally, the optimization problem in a concise form is:

$$\begin{array}{ll} \underset{\Omega}{\text{minimize}} & J = \left\langle \mathbf{Q}^{T} \mathbf{T} \right\rangle \\ \text{subject to} & V - \chi V_{0} \leq 0 \\ & \mathbf{R}_{i}(\boldsymbol{\gamma}, \mathbf{T}(\boldsymbol{\gamma})) = \mathbf{0} \end{array}$$
(22)

The design variables for the level-set method are the boundary points movement. Thus, the sensitivity of the objective function J with respect to a boundary movement z at a point j must be computed. This quantity is denoted  $\frac{dJ}{dz_j}$ . First, the sensitivities with respect to the element density  $\gamma_e$  are computed at the centroid of each element using semi-symbolic automatic differentiation via the open-source package dolfin adjoint [42] which yields  $\frac{dJ}{d\gamma_e}$ . Then, the sensitivities at each discretized boundary point j with respect to a boundary movement are computed via a least squares interpolation scheme [43].

## 5 Numerical examples

## 5.1 Material properties and problem setup

Aluminium is chosen for the pack material and the LGM50 cell introduced in section 2.3 is considered. The electrochemical properties of the cell are taken from [24]. The thermal properties of the cell and of aluminium are summarized in Table 1 where the pack material and the cell are considered isotropic and transversely isotropic, respectively.

Property	Aluminium	LGM50 21700	
Thermal conductivity $\kappa$ [W.m <sup>-1</sup> .K <sup>-1</sup> ] Volumetric heat capacity $\rho c_p$ [J.m <sup>-3</sup> .K <sup>-1</sup> ]	237.0 2,457,000	$\begin{array}{c} 1.164^1 \ / \ 23.1^2 \\ 1.767,574^3 \end{array}$	

 Table 1: Material thermal properties

<sup>1</sup>Thermal conductivity in the transverse direction [44, 45]

<sup>2</sup>Thermal conductivity in the longitudinal direction [44, 45]

<sup>3</sup>The effective specific heat is computed as  $\rho c_{p,eff} = \left(\sum_{k}^{n,sep,p} \rho_k c_{p,k} L_k\right) / L[18]$ 

For the analysis, a cell is studied within the surrounding aluminium. Cooling of the cell occurs at both the top and the bottom. Consequently, film boundary conditions are applied for the thermal analysis on these surfaces, with a heat transfer coefficient of 5 W.m<sup>-2</sup>.K<sup>-1</sup> and an ambient temperature of 298.15 K. The heat generation, derived from the electrochemical model, is assumed to be uniformly distributed throughout the cell. The geometry of the system and the thermal boundary conditions are depicted in Fig. 4a and Fig. 4b, respectively. Accounting for symmetry, only one-eighth of the cell is modeled.

## 5.2 Power profile

We evaluate the power profiles of a flight path and specifications from [39] considering the lift+cruise configuration. Given the power requirement, the percentage of power required for each flight segment, and the flight segment duration, we can estimate the energy requirement. Power requirements can be calculated using the following equations [39],

$$P_{cr} = GTOM \frac{g}{\eta_{cr}} \frac{V_{cr}}{(L/D)_{cruise}}$$
$$P_{cl} = GTOM \frac{g}{\eta_{cl}} \left( ROC + \frac{V_{climb}}{(L/D)_{climb}} \right)$$
(23)

where  $P_{cr}$  and  $P_{cl}$  are the power required during the cruise and the climb segment, respectively. Power is a function of aerodynamic parameters like lift-to-drag ratio L/D, velocity V, and gross takeoff mass GTOM which is taken as



Fig. 4: Geometry of the cell with pack material and boundary conditions for the thermal analysis, wherever the boundary conditions are not specified adiabatic boundary conditions are used

4268.3 kg assuming a payload of 6 passengers. Climb power,  $P_{cl}$  is a function of the rate of climb ROC, the gravity acceleration g, and electric motors efficiency  $\eta$ . The details for calculations are shown in Table 2, where the trip duration, distance, and energy requirement are calculated at the battery pack level.

Segment	$1^a$	$2^b$	$3^c$	$4^d$	$5^e$	$6^f$	$7^c$	$8^b$
Duration [s]	15	30	10	264	1002	10	30	30
Distance [mi]	-	-	-	7.4	35.8	-	-	-
% Max. power <sup><math>g</math></sup>	10	100	100	63	60	100	100	100
Power [kW]	46.8	829	829	525	282	829	829	829
Energy [kWh]	0.19	6.91	2.30	38.3	78.6	2.30	6.91	6.91

 Table 2: Details for the power profile computation

<sup>a</sup>Taxi with cruise rotor

 $^b50~{\rm ft}$  vertical climb/descent at 100 ft/min

<sup>c</sup>Transition/Hover

 $^d \text{Climb}$  to 3950 ft with ROC=900 ft/min,  $V_{climb}=101.3$  mph,  $\eta_{cl}=0.79,$  and  $(L/D)_{climb}=8.5$ 

<sup>e</sup>Cruise for 35.8 miles with  $V_{cruise} = 128.6$  mph,  $\eta_{cr} = 0.87$ , and  $(L/D)_{cruise} = 9.8$ 

 $^{f}$ Descent back to 50 ft above ground level

 $^g{\rm Max.}$  cruise power is 468 kW with 1 rotor of 468 kW and max. lift power is 829 kW with 8 rotors of 103.6 kW each

To size the battery pack and hence the flight profile and C-rates requirements, the maximum depth of discharge of 80 % is used to preserve the health of the battery. We obtain that the energy of the battery pack is 179 kWh. Note that we do not account for reserve in this analysis. Using the expected weight

fraction of the battery to be 20 % of the total aircraft, this results in a battery pack possessing an energy density of 233 Wh.kg<sup>-1</sup>, with the target cell gravimetric energy density being 300 Wh.kg<sup>-1</sup> (assuming a cell-to-pack efficiency of 75 %). The estimated energy density of the battery pack indicates that cell energy density (300 Wh.kg<sup>-1</sup>) is beyond the current state-of-the-art battery chemistries available commercially. The voltage for the mission is chosen to be 800 V from the motor attributes discussed in [39]. The nominal voltage of the 21700 cells allows the determination of the required cells in series to meet the voltage requirements. With a system voltage of 800 V, the battery pack capacity of 223 Ah is obtained, where 45 cells in parallel were assumed for this vehicle. Knowing the power requirement, duration, and the current, C-rate can be calculated since the power is the product of the current and the voltage and the C-rate is the current divided by the battery pack capacity which was estimated to be 223 Ah.

Table 3 summarizes these results for the entire battery pack and the expected power profile. This computation led to C-rates greater than 1.7 C which cannot be tested in the experimental facility available for this work due to safety. Thus, the C-rate was kept at a maximum of 1.7 C (1 C = 4.85 A), and the power profile was adjusted such that the cell could complete the power profile as shown in Table 3. The scaled power profile was used for the experiments and the electrochemical models, i.e., DFN and SPM.

Phase	Duration [s]	Calculated C-rate [C]	Adjusted C-rate [C]	Current [A]
Taxi	15	0.2	0.2	0.78
Takeoff	40	4.4	1.7	8.4
Climb	264	3.0	1.5	7.2
Cruise	1002	1.6	0.9	4.5
Landing	70	4.4	1.7	8.4

 Table 3: Power profile used for this work

It is noted that for the eVTOL flight profiles, the C-rate and power requirements during the takeoff and landing phases are high. These flight segments pose the most significant challenge for the current state-of-the-art battery technology and will be the focus of the primary investigation for optimization in this work. Thus, only the heat generated during the landing segment is considered for transient thermal optimization.

#### 5.3 Cell response to power profile

The surface temperature increase and terminal voltage are measured experimentally on a pristine LGM50 21700 cell using the power profile described in Section 5.2. The experiment is done three times and a new LGM50 21700 cell is used for each experiment. The voltage profile and the temperature increase from the experiments are compared to the voltage and temperature increase of the electrochemical models in Fig. 5. The voltage and temperature increase after the flight, when the cell is at rest, is also shown.

Although some variability is observed, both the SPM and DFN models effectively represent the experimental voltage profiles reasonably closely. The absolute relative error used for the terminal voltage comparison is defined as the absolute difference between the results from the physics-based models and the experimental data divided by the experimental data. The absolute relative error for the voltage profile is shown in Fig. 5b. The highest peak error in Fig. 5b corresponds to the transition from the cruise to the landing phase. The other peaks with a relative error greater than 5 % also correspond to transitions from one flight segment to another. This is most likely due to a slight discrepancy between the data acquisition rate and the time in the electrochemical models. Indeed, the duration at a given discharge rate associated with each segment has some uncertainties when measured experimentally. For example, when subtracting the model from the experimental results, a few data points from the experiments might still be in the cruise segment while the computational model had entered the landing segment. Except for these uncertainties in the transitions, the relative error for both electrochemical models is less than 5 % as shown in Fig. 5b.

The absolute temperature difference between the experimental and computational data is shown in Fig. 5d where it is seen that the DFN model reasonably approximates the surface temperature increase with a maximum error of 2.5 K. The SPM significantly underestimates the temperature rise due to neglecting electrolyte behavior with the maximum error of up to 8 K or an absolute relative error of about 41 %. This is expected since it has been shown for pouch cells that an electrolyte correction is needed to account for mass and electrostatic contributions to the total voltage loss and the total heat generated [18]. The SPM does not account for any Ohmic heating from the electrolyte, and the reaction-based heating is approximated using an averaged particle size. Consequently, the SPM generates less heat, particularly during high C-rate segments like takeoff and landing, leading to a significant underprediction of the cell surface temperature. Nevertheless, if only the terminal voltage is required, such as for testing different flight profiles and determining if the voltage cut-off is reached, the SPM offers meaningful results, especially in the case of low to moderate C-rates (0-1.5 C). Notably, the computational time of the SPM for the studied power profile is only 1.2 seconds on a typical laptop, while the DFN model applied to the same power profile requires over 11 minutes on the same laptop.

## 5.4 Topology optimization results

#### 5.4.1 Single particle model vs Doyle-Fuller-Newman model

For the first example of optimization, four target volume constraint values are considered: 45% ( $\chi = 0.45$ ), 50% ( $\chi = 0.50$ ), 55% ( $\chi = 0.55$ ), and 60% ( $\chi = 0.60$ ). The structure is discretized with 30x30x70 hexahedral linear finite



Fig. 5: Cell response to power profile

elements and optimized for thermal compliance integrated over the landing segment. The volumetric heat generated by the battery during the landing phase is calculated using the DFN and the SPM models and the heat generation during the complete flight is shown in Fig 6.



**Fig. 6**: Volumetric heat generation as a function of time for the power profile considered

The eight optimized topologies obtained with the heat generation from each electrochemical model with symmetry and with the four different volume fractions are shown in Fig. 7. For the volume fraction  $\chi = 0.45$  shown in Fig. 7a and Fig. 7e, there is no apparent difference between the design optimized using the SPM and DFN models. For  $\chi = 0.50$ , the main difference between the two model results is the size of the groove near the top half of the cell in Fig. 7b and Fig. 7f. For the results with higher volume fractions shown in Fig. 7c, Fig. 7g, Fig. 7d, and Fig. 7h, the major distinction is the shape of the bulges nearer the bottom.

To quantify the impact of these features, i.e., the grooves and the bulges, on the performance of the heat exchanger, the optimized designs are further analyzed. To maintain consistency, the optimized results from both models are analyzed with the finite element method for the same heat loads obtained from the higher fidelity model (DFN in Fig. 6).

In Fig. 8, the temperature distribution within the optimized battery exchanger is presented at the last time step, i.e. the step with maximum temperature distribution. The optimized shape is shown by the outline within the whole design domain. For a given volume fraction, the temperature distribution within the exchanger optimized with SPM loading is similar to its DFN counterparts. In Fig. 9, validation results for shapes obtained from both power profiles are compared together. For a given volume fraction, an average difference of 0.006 K is observed between the maximum temperature in the geometries optimized for SPM and DFN loading. Hence it can be concluded that the optimization results for loading obtained from SPM, a lower-fidelity battery model are comparable to the results obtained from the DFN power profile in terms of thermal performance, even with the apparent design differences.

Note that higher volume fraction constraints enable better heat dissipation effects but at the cost of utilizing more material which will directly affect the gravimetric and volumetric energy density of the battery pack. With a volume



(a) DFN ;  $\chi = 0.45$  (b) DFN ;  $\chi = 0.50$  (c) DFN ;  $\chi = 0.55$  (d) DFN ;  $\chi = 0.60$ 



(e) SPM ;  $\chi = 0.45$  (f) SPM ;  $\chi = 0.50$  (g) SPM ;  $\chi = 0.55$  (h) SPM ;  $\chi = 0.60$ **Fig. 7**: Topology optimization results of the battery exchanger for four volume fractions ( $\chi$ ) and two electrochemical models (DFN, SPM)

fraction of 45 %, a 14 % reduction of gravimetric energy density is estimated compared to the cell alone, from 260 Wh/kg to 224 Wh/kg. With the higher volume fraction constraint of 55 %, the impact is nearly doubled with a 30 % reduction, reducing the gravimetric energy density to 185 Wh/kg. These are important considerations when implementing heat exchangers into the battery pack/module design. Coman *et al.* [46] and Darcy [47] designed and tested battery modules with a gravimetric energy density of around 190 Wh/kg with a cell-to-module mass factor of  $\approx$  1.4. The gravimetric energy densities obtained with the topologically optimized heat exchangers show an 18 % improvement for the case with a 45 % volume fraction. However, the wiring and battery management system are not modeled and should also be considered for actual pack designs.



Fig. 8: Temperature distribution of the optimized battery exchanger for four volume fractions ( $\chi$ ) and two electrochemical models (DFN, SPM) at the final time step, max(T) denotes the maximum nodal temperature

#### 5.4.2 Comparison to steady-state optimization

To evaluate the significance of utilizing an unsteady diffusion model for optimization, a steady-state topology optimization scenario is studied. In this case, the time-dependent temperature term is eliminated from the weak form given



**Fig. 9**: Temperature distribution at the convection boundary conditions of the battery exchanger optimized for DFN and SPM at the final time step

in Eq. 14, resulting in the following weak form.

$$\int_{\Omega} Q_n v \, d\Omega - \int_{\Omega} \kappa \nabla v \cdot \nabla u_n \, d\Omega - \int_{\Gamma_N} v q_N \, d\Gamma_N = 0 \tag{24}$$

The objective of the steady state optimization is to minimize the thermal compliance, i.e.,  $J = \mathbf{Q}^T \mathbf{T}$ . The volumetric heat generation is taken as the maximum heat generation during flight predicted by the DFN model. The optimized topologies obtained for the steady-state cases for the same target volume fraction as in Section 5.4.1, that is 45% ( $\chi = 0.45$ ), 50% ( $\chi = 0.50$ ), 55% ( $\chi = 0.55$ ), and 60% ( $\chi = 0.60$ ), are shown in Fig. 10. Expanding conduction paths from the middle of the cell to the top of the cell are observed. The grooves and bulges seen in Fig. 7 for transient optimizations are not visible in the designs from the steady state optimization.

To assess the computational costs, we present the average computational cost per optimization iteration for each case in Table 4. Remarkably, a transient optimization iteration over the landing phase costs roughly 30 times more than the steady-state optimization.

In addition, the thermal behavior of the optimized structures obtained with the steady-state optimization, Fig. 10, is compared to the results from the previous section, Fig. 7. The optimized designs are analyzed with the finite element method and subjected to the heat loads obtained from the DFN



Fig. 10: Steady-state topology optimization results of the battery exchanger for four volume fractions ( $\chi$ )

Target volume fraction	Optimized for	Average wall time per optimization iteration [s]
	DFN	371.5
$\chi = 0.45$	SPM	375.2
	Steady-state	13.40
	DFN	364.1
$\chi = 0.50$	SPM	374.9
	Steady-state	12.11
	DFN	368.2
$\chi = 0.55$	SPM	360.3
	Steady-state	11.62
	DFN	369.5
$\chi = 0.60$	SPM	367.1
	Steady-state	11.84

 Table 4: Comparison of the computational time for all cases

model in Fig. 6. In Fig. 11, the temperature distributions on the film boundary are shown. An average difference of 0.02 K is observed in the maximum temperature between the designs obtained from DFN or steady-state loading.

In Fig. 12, a comparison of the thermal compliance integrated over time,  $J = \langle \mathbf{Q}^T \mathbf{T} \rangle = \int_t \mathbf{Q}^T \mathbf{T} dt$  is given. Thermal compliance here is obtained only for the landing segment which was used for the transient optimizations. The differences in total compliances of optimized geometries obtained from three different loading conditions are negligible even if the geometrical differences are noticeable. However, for the higher target volume fractions of 55 % and 60 %, where enough material is available to manifest more features that can optimize the objective, we see lower values of thermal compliance in structures optimized for DFN loading. For a target volume fraction of 60 %, the thermal compliance is 0.65 W.K.s less for the design optimized for DFN as compared to the design optimized for steady-state.



Fig. 11: Temperature distribution at the convection boundary conditions of the battery exchanger optimized for DFN and steady-state at the final time step

The maximum temperatures at each time step for the 12 optimization cases, i.e., the 4 target volume fractions and steady-state, DFN, and SPM, are shown in Fig. 13. The maximum temperature at each time step for the battery without a heat exchanger is also shown for reference. The steady-state optimization proves to be sufficient for the cases investigated here, as it yields optimized topologies that perform similarly, in terms of maximum temperature and temporally integrated thermal compliance, to the structures obtained through optimization considering the transient loading over landing, at a fraction of the computational cost. The transient effects appear to be secondary as the heat is continuously conducted out of the domain for an extended period, which is the case for the power profile of a flight mission. Hence, for power profiles resembling the one we examined, which are divided into a few segments with constant current, steady-state heat conduction optimization proves to be a viable and more computationally efficient choice. Nevertheless, the heat generation as a function of time as predicted by the electrochemical models allows for a comprehensive post-optimization analysis and evaluation of the optimized topologies throughout the entire flight.



Fig. 12: Compliance integrated over the landing phase for all optimized heat exchangers



Fig. 13: Maximum temperature as a function of time for all cases considered, the maximum temperature for the battery without heat exchanger is shown for reference

# 6 Conclusions

We have introduced a transient thermo-electrochemical topology optimization formulation for designing a heat exchanger dedicated to lithium-ion batteries in an eVTOL vehicle. We explored and evaluated two electrochemical models, namely the DFN and SPM models, which are based on the fundamental physics. These models were utilized to predict the voltage profile and the volumetric heat generation rate for a given flight profile. We compared the performance of the two electrochemical models with the experimental data obtained from constant discharge rates and a scaled flight profile. Both models showed reasonably good agreement for the voltage profile, with the SPM model offering an efficient alternative, being up to two orders of magnitude faster than the DFN model for the cases investigated. However, in terms of predicting the cell temperature increase, the DFN model demonstrated accuracy with the maximum error of 2.5 K for the profile studied, making it suitable for thermal analyses of lithium-ion batteries in the context of eVTOL flight profiles and for validating batteries' heat exchangers. On the other hand, the SPM model failed to accurately capture the temperature increase with a relative error of around 41 % at the peak temperature although still managed to represent the overall trend.

The level-set topology optimization is used as a design tool and the temperature distribution is computed using a transient heat conduction finite element model. We conducted numerical simulations focusing on a cell and its surrounding material, considering natural convection for cooling. We analyzed the influence of two different electrochemical models and compared optimized topologies obtained with transient and steady-state heat conduction models to a reference case without a heat exchanger over the entire flight. Notably, the steady-state heat conduction optimization resulted in topologies with thermal performance comparable to the transient examples, i.e., less than 1 % difference in terms of both maximum temperature and thermal compliance for a given target volume fraction, but at a lower computational cost, on average more than 30 times faster for the cases investigated.

In future work, we plan to explore battery pack configurations and examine the interplay between the individual cells. Additionally, note that in practice, battery degradation should be considered for repeated power profiles and that the material properties would change as a function of age [48, 49]. We intend to investigate cooling strategies for battery packs and analyze the impact of repeated flights on cell degradation.

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## Declarations

Not applicable.

# Appendix A - Details on the Doyle Fuller Newman model

#### Molar conservation

Throughout the Appendices, the notations introduced in Section 2 are used. Fick's law of diffusion describes the transient diffusion process from a higher concentration to a lower concentration in an electrode particle. In spherical coordinates, Fick's first and second laws are given as follows:

$$N_{s,k} = -D_{s,k} \frac{\partial c_{s,k}}{\partial r_k} \qquad \qquad k \in \{n,p\}$$
(A.1)

$$\frac{\partial c_{s,k}}{\partial t} = -\frac{1}{r_k^2} \frac{\partial}{\partial r_k} \left( r_k^2 N_{s,k} \right) \qquad \qquad k \in \{n,p\}$$
(A.2)

where  $D_{s,k}$  is the diffusivity of lithium ions in a particle. As for the boundary conditions, there is no molar flux at the center due to symmetry, and lithium intercalation takes place at the surface such that:

$$N_{s,k}|_{r_k=0} = 0 k \in \{n, p\} (A.3)$$

$$N_{s,k}|_{r_k=R_k} = \frac{J_k}{a_k F} \qquad \qquad k \in \{n, p\} \tag{A.4}$$

where F is Faraday's constant and  $J_k$  is the interfacial current density from the charge transferred to the electrolyte at the macroscale, and  $a_k$  is the active surface area per unit volume. In the electrolyte, the molar conservation of lithium can be described as follows:

$$\epsilon_k \frac{\partial c_{e,k}}{\partial t} = \frac{\partial N_{e,k}}{\partial x} + \frac{1}{F} \frac{\partial i_{e,k}}{\partial x} \qquad \qquad k \in \{n, sep, p\}$$
(A.5)

$$N_{e,k} = \epsilon_k^{bk} D_{e,k} \frac{\partial c_{e,k}}{\partial x} + \frac{t^+}{F} i_{e,k} \qquad k \in \{n, sep, p\}$$
(A.6)

where  $\epsilon_k$  is the volume fraction of electrolyte,  $D_{e,k}$  is the diffusivity of lithiumion in the electrolyte which is a function of  $c_{e,k}$  such that  $D_{e,k} \equiv D_{e,k}(c_{e,k})$ ,  $t^+$ is the cation transference number which is the fraction of the current being carried by the cation, i.e, by the positively charged ion, and bk is the Bruggeman coefficient usually taken as 1.5 for porous structures such as a lithium-ion battery. For consistency, continuity of flux and concentration is imposed between the different domains:

$$N_{e,n}|_{x=L_n} = N_{e,sep}|_{x=L_n} \qquad N_{e,sep}|_{x=L_n+L_{sep}} = N_{e,p}|_{x=L_n+L_{sep}}$$

$$c_{e,n}|_{x=L_n} = c_{e,sep}|_{x=L_n} \qquad c_{e,sep}|_{x=L_n+L_{sep}} = c_{e,p}|_{x=L_n+L_{sep}} \qquad (A.7)$$

Additionally, there is no flux at the current collectors:

$$N_{e,n}|_{x=0} = 0 N_{e,p}|_{x=L} = 0 (A.8)$$

#### Charge conservation

The interfacial current density  $J_k$  considers the total charge transfer due to intercalation kinetics at a location x and acts as a source term for current densities in the electrolyte and electrode where the active material is present:

$$\frac{\partial i_{e,k}}{\partial x} = -\frac{\partial i_{s,k}}{\partial x} = \begin{cases} J_k, & k = n, p\\ 0, & k = sep \end{cases} \qquad k \in \{n, sep, p\}$$
(A.9)

The current densities are computed using Ohm's law for solid material (Eq A.10) and MacInnes' equation (Eq A.11) for the electrolyte which relates the current density to the electric potential and electrolyte concentration in the following fashion

$$i_{s,k} = -\sigma_k \frac{\partial \phi_{s,k}}{\partial x} \qquad \qquad k \in \{n, p\} \quad (A.10)$$

$$i_{e,k} = \epsilon_k^{bk} \zeta_e \left[ -\frac{\partial \phi_{e,k}}{\partial x} + 2(1-t^+) \frac{R_g T}{F} \frac{\partial \log c_{e,k}}{\partial x} \right] \quad k \in \{n, sep, p\}$$
(A.11)

where  $\zeta_e$  is a reference electric conductivity of the electrolyte,  $\sigma_k$  is the electric conductivity of the electrode material,  $R_g$  is the universal gas constant, and T is the temperature. Again, continuity is imposed between the different domains and there is no current density in the electrode at the anode/separator and separator/cathode boundaries such that

$$i_{e,n}|_{x=L_n} = i_{e,sep}|_{x=L_n} \qquad i_{e,sep}|_{x=L_n+L_{sep}} = i_{e,p}|_{x=L_n+L_{sep}} \phi_{e,n}|_{x=L_n} = \phi_{e,sep}|_{x=L_n} \qquad \phi_{e,sep}|_{x=L_n+L_{sep}} = \phi_{e,p}|_{x=L_n+L_{sep}} i_{s,n}|_{x=L_n} = 0 \qquad \qquad i_{s,p}|_{x=L_n+L_{sep}} = 0$$
(A.12)

Additionally, the current  $i_{app}$  is applied at the current collectors to the active material where the electrolyte current density is zero which gives four additional boundary conditions

$$i_{s,n}|_{x=0} = i_{app} i_{s,p}|_{x=L} = i_{app} i_{e,n}|_{x=0} = 0 i_{e,p}|_{x=L} = 0 (A.13)$$

Note that because of continuity and charge conservation, we have the following relationships

$$i_{s,k} + i_{e,k} = i_{app} \qquad \qquad k \in \{n, p\}$$
$$i_{e,sep} = i_{app} \qquad \qquad (A.14)$$

The terminal voltage V is defined as the potential difference between the two current collectors where the reference potential is  $\phi_{s,n}|_{x=0} = 0$ 

$$V = \phi_{s,p}|_{x=L} - \phi_{s,n}|_{x=0} = \phi_{s,p}|_{x=L}$$
(A.15)

#### Intercalation kinetics

The Butler-Volmer equation describes the intercalation kinetics of lithium. This reaction couples the macroscale and microscale and is as follows

$$J_k = J_{k,0} \sinh\left(\frac{F}{2R_g T}\eta_k\right) \qquad \qquad k \in \{n,p\} \qquad (A.16)$$

where  $J_{k,0}$  is the exchange current density and  $\eta_k$  is the overpotential which are defined as

$$J_{k,0} = \mu_k (c_{s,k} c_{e,k})^{1/2} (c_{s,k}^{max} - c_{s,k}|_{r_k = R_k})^{1/2} \qquad k \in \{n, p\}$$
  
$$\eta_k = \phi_{s,k} - \phi_{e,k} - U_{oc,k} \qquad \qquad k \in \{n, p\}$$
(A.17)

where  $\mu_k$  is the reaction rate,  $c_{s,k}^{max}$  is the maximum lithium-ion concentration in the active material, and  $U_{oc,k}$  is the open circuit potential which is a function of  $c_{s,k}|_{r_k=R_k}$  fitted from experimental values.

#### Initial conditions and dimensionless quantities

The DFN model is transient. Consequently, initial conditions at t = 0 are given as

$$c_{s,k} = c_{s,k}^{0}, \qquad k \in \{n, p\}$$

$$c_{e,k} = c_{e,k}^{0}, \qquad k \in \{n, sep, p\}$$

$$\phi_{s,k} = \begin{cases} 0, & k = n \\ U_{oc,p}^{0} - U_{oc,n}^{0}, & k = p \end{cases}$$

$$k \in \{n, p\}$$

$$\phi_{e,k} = -U_{oc,n}^{0} \qquad k \in \{n, sep, p\}$$

$$U_{oc,k} = U_{oc,k}^{0} \qquad k \in \{n, p\}$$
(A.18)

The other quantities are initially set to zero. The equations are implemented in a dimensionless form where a dimensionless quantity a is denoted  $\tilde{a}$ . The parameters are non-dimensionalized considering the geometry of the cell, discharge timescale, diffusion timescale, and reaction timescale following the methodology presented in [15]. The dimensionless DFN model is summarized in Table A.1 where  $C_e$  is the ratio of electrolyte transport timescale to discharge timescale,  $C_k$  is the ratio of solid diffusion timescale to discharge timescale,  $\zeta_e = (R_g T/F)/(I_{ref}L/\zeta_{e,ref})$  where subscript ref denotes reference quantities, and  $\mathcal{T}_e$  is the ratio of a reference electrolyte concentration to the maximum concentration in a negative particle. More details regarding the DFN model can be found in the literature, see for instance [16–19].

Description	Governing equation	k
Molar conservation	$\mathcal{C}_k rac{\partial  ilde{c}_{s,k}}{\partial  ilde{t}} = rac{1}{ ilde{r}_k^2} rac{\partial}{\partial  ilde{r}_k} \left(  ilde{r}_k^2 rac{\partial  ilde{c}_{s,k}}{\partial  ilde{r}_k}  ight)$	$\{n,p\}$
	$\epsilon_k \mathcal{C}_e \mathcal{T}_e rac{\partial  ilde{c}_{e,k}}{\partial  ilde{t}} = -\mathcal{T}_e rac{\partial  ilde{N}_{e,k}}{\partial x} + \mathcal{C}_e rac{\partial  ilde{h}_{e,k}}{\partial  ilde{x}}$	$\{n, sep, p\}$
	$\tilde{N}_{e,k} = -\epsilon_k^{bk} \tilde{D}_{e,k} \frac{\partial \tilde{c}_{e,k}}{\partial \tilde{x}} + \frac{t^+ \mathcal{C}_e}{\mathcal{T}_e} \tilde{i}_{e,k}$	$\{n, sep, p\}$
Charge conservation	$\frac{\partial \tilde{i}_{e,k}}{\partial x} = -\frac{\partial \tilde{i}_{s,k}}{\partial \tilde{x}} = \begin{cases} \tilde{J}_k, & k = n, p \\ 0, & k = sep \end{cases}$	$\{n, sep, p\}$
	$\tilde{i}_{e,k} = \epsilon_k^{bk} \hat{\zeta}_e \zeta_e \left[ -\frac{\partial \tilde{\phi}_{e,k}}{\partial \tilde{x}} + 2(1-t^+) \frac{\partial \log \tilde{c}_{e,k}}{\partial \tilde{x}} \right]$	$\{n, sep, p\}$
	$ ilde{i}_{s,k} = - ilde{\sigma}_k rac{\partial  ilde{\phi}_{s,k}}{\partial  ilde{x}}$	$\{n,p\}$
Intercalation kinetic	$ ilde{J}_k = 2 ilde{J}_{k,0} \sinh\left(rac{ ilde{\eta}_k}{2} ight)$	$\{n,p\}$

Table A.1: Dimensionless equations of the DFN model

# Appendix B - Single Particle Model equations

The dimensionless equations of the SPM are summarized in Table B.1 where  $\tilde{a}_k$  is the product of the representative particle radius and surface area density, and  $\mathcal{T}_k = c_{k,max}/c_{n,max}$ .

Table B.1: Dimensionless equations of the SPM

Description	Governing equation	k
Molar conservation	$\mathcal{C}_k \frac{\partial \tilde{c}_{s,k}}{\partial \tilde{t}} = rac{1}{\tilde{r}_k^2} rac{\partial}{\partial \tilde{r}_k} \left( \tilde{r}_k^2 rac{\partial \tilde{c}_{s,k}}{\partial \tilde{r}_k}  ight)$	$\{n,p\}$
	$-\frac{\mathcal{T}_k}{\mathcal{C}_k} \frac{\partial \tilde{c}_{s,k}}{\partial \tilde{r}_k} _{\tilde{r}_k=1} = \begin{cases} \frac{\imath_{app}}{\tilde{L}_n \tilde{a}_n} & k=n\\ -\frac{\imath_{app}}{\tilde{L}_p \tilde{a}_p} & k=p \end{cases}$	$\{n,p\}$

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