Effects of number of layers on thermal behavior and heat generation of Lithium Ion battery

M. Alipour [1], E. Eşen [1], R. Kızılel[2]
1. Department of Chemical and Biological Engineering, Koç University, Istanbul, Turkey
2. Koç University Tüpraş Energy Center, Istanbul, Turkey

Introduction: Lithium ion batteries are promising candidates for electric vehicle (EV) applications due to their properties such as high gravimetric and volumetric energy density, fast charging, and lower material and maintenance costs [1]. However, safety is still a concern for mass production. Uncontrolled temperature elevation due to the self-accelerated exothermic side reactions results in thermal runaway. Furthermore, performance efficiency and cycle life of the lithium ion batteries are greatly affected by the temperature non-uniformity of the cell [2]. Numerous research groups have adopted single-layer cell approach to model the electrochemical and thermal behavior of the Li-ion cells. However, single-layer approach is not sufficient to determine the thermal behavior of high capacity Li-ion batteries. In this study, Li-ion batteries are modeled with multilayer approach and effects of number of layers on thermal characteristics of Li-ion cells are determined precisely. Our study is believed to help development of an efficient thermal management system with a better prediction of potential hot spots on single cells and battery packs.

Computational Method:

- ✓ Using COMSOL Multiphysics, 3D model, coupling electrochemical and heat transfer modules, is developed.
- ✓ Multilayer cells consisting repeating units of positive current collector, positive electrode, separator, negative electrode, and negative current collector are developed (Figure 2).
- ✓ Electrochemical and thermal parameters are obtained by fitting model to experimental data using least square method.
- ✓ Principles of mass transfer, heat transfer, charge transfer, and electrochemical kinetics are used to model electrochemicl-thermal behavior of the 20Ah LiFePO4 battery. The equations are listed in Table 1.

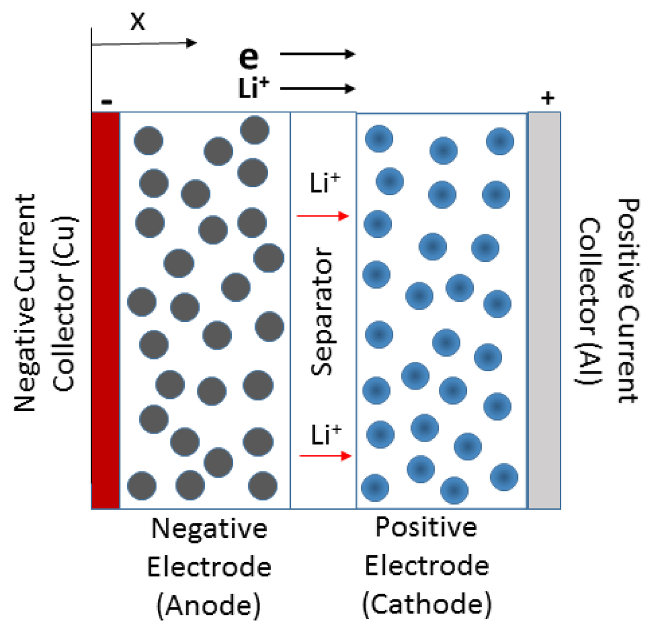


Figure 1. Schematic of 1D lithium ion battery layer

Reactions During Discharge Process:

Anode: LixC6 → 6C + xLi+ + xe-
Cathode: Liy-xFePO4 + xLi+ + xe- → LiyFePO4

Table 1 The Equations used in electrochemical-thermal model

Process	Equation
Material balance, solid phase	$\frac{\partial c_{s,i}}{\partial t} = \frac{D_{s,i}}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_{s,i}}{\partial r}\right)$
Material balance, liquid phase	$\varepsilon_i \frac{\partial c}{\partial t} = D_{l,i}^{eff}\frac{\partial^2 c}{\partial^2 x} + a_i \frac{1+t_+}{F} i_{loc}$
Charge balance, solid phase	$i_s = -\sigma_{s,eff}\nabla\phi_s$
Charge balance, liquid phase	$i_l = -\kappa_{eff}\nabla\phi_l + \left(\frac{2\kappa_{eff}RT}{F}\right)\left(1+\frac{\partial \ln f}{\partial \ln c}\right)\left(1-t^+\right)\nabla \ln c$
Local curent density	$i_{loc} = i_0\left(\exp\left(\frac{\alpha_a F\eta}{RT}\right) - \exp\left(\frac{-\alpha_c F\eta}{RT}\right)\right)$
Exchange current dencity	$i_0 = F(k_c)^{\alpha_a}(k_a)^{\alpha_c}\left(c_{s,\max} - c_{s,sur}\right)^{\alpha_a}\left(c_{s,sur}\right)^{\alpha_c}\left(\frac{c}{c_{ref}}\right)^{\alpha_a}$
Energy balance	$\rho c_p \frac{dT}{dt} - \lambda\frac{\partial^2 T}{\partial x^2} = Q_{rev} + Q_{irrev} + Q_{ohm}$
Reversible entropic heat	$Q_{rev} = a_s i_{loc} T \frac{U_{eq}}{\partial T}$
Irreversible reaction heat	$Q_{irrev} = F a_s i_{loc}(\phi_1 - \phi_2 - U)$
Ohmic heat	$Q_{ohm} = -i_s.\nabla\phi_1 - i_l.\nabla\phi_2$

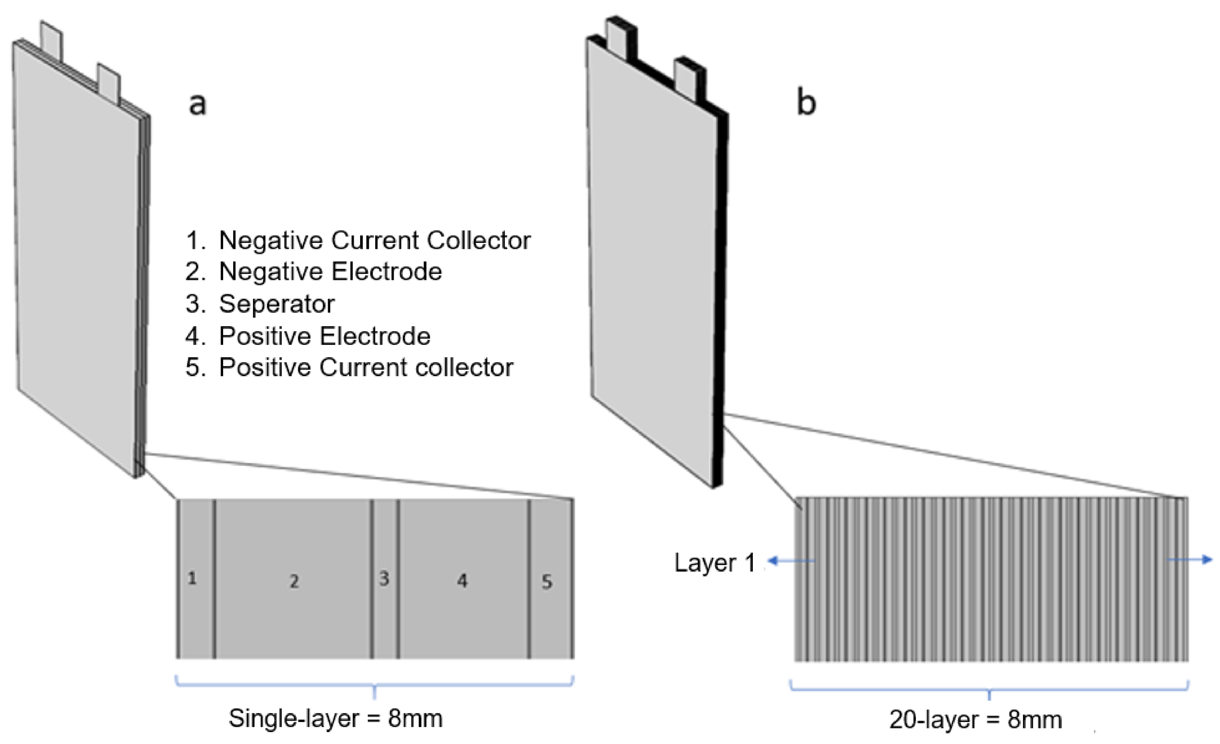


Figure 2. Schematic of (a) single-layer cell and (b) multilayer cell.

Results:

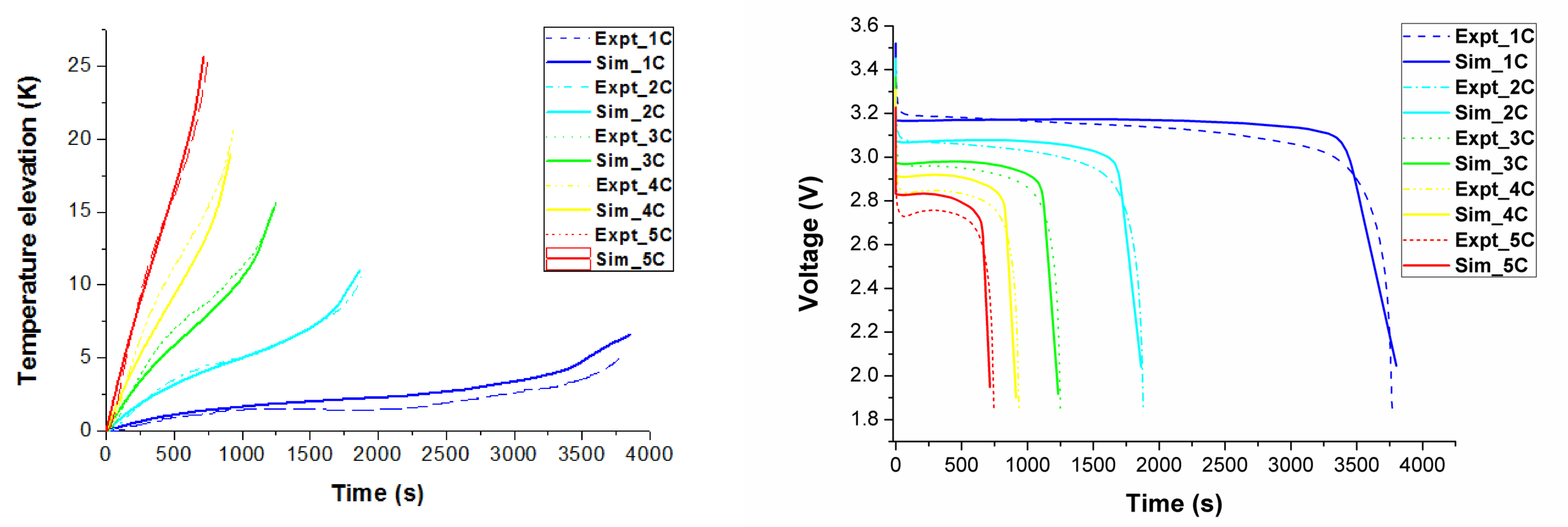


Figure 3. Validation of simulated (a) cell voltage and (b) temperature change at different current rates (Solid: Simulated, Dashed: Experimental).

Multilayer Effects:

- ✓ Compared to single layer approach, multilayer approach shows superior thermal behavior in fitting the experimental data (Figure 4a-b)
- ✓ Uniform surface (Figure 4a) and internal temperature (Figure 5a) profiles of single layer are not consistent with experimental results.
- ✓ Based on Li. etal [3] experimental works, internal temperatures could differ from the surface for as large as 1.1˚C even for a thin laminated cell.

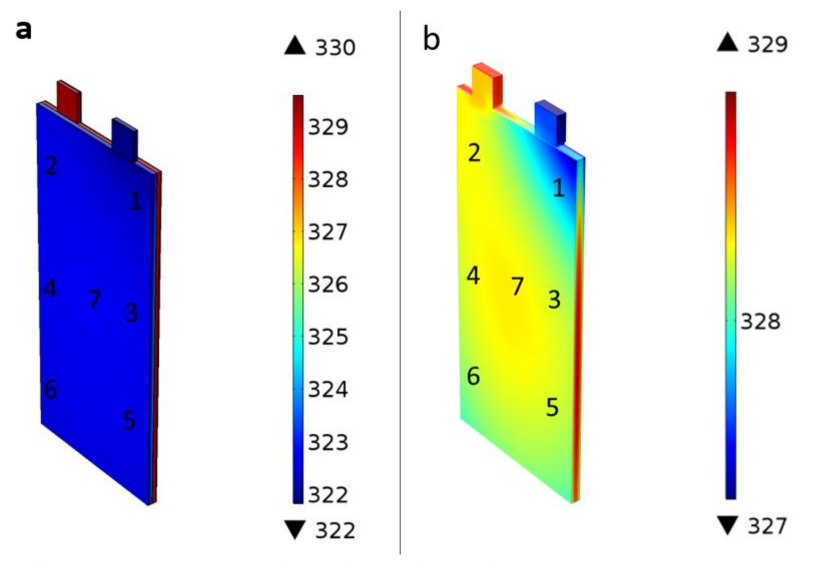


Figure 4. 3-D simulated surface temperature profiles of (a) single-layer and (b) 20-layer cells.

30°C_5C	T1	T2	T3	T4	T5	T6	T7
Experimental T (K)	326.6	328.4	327.7	326.7	327.4	326.1	328.3

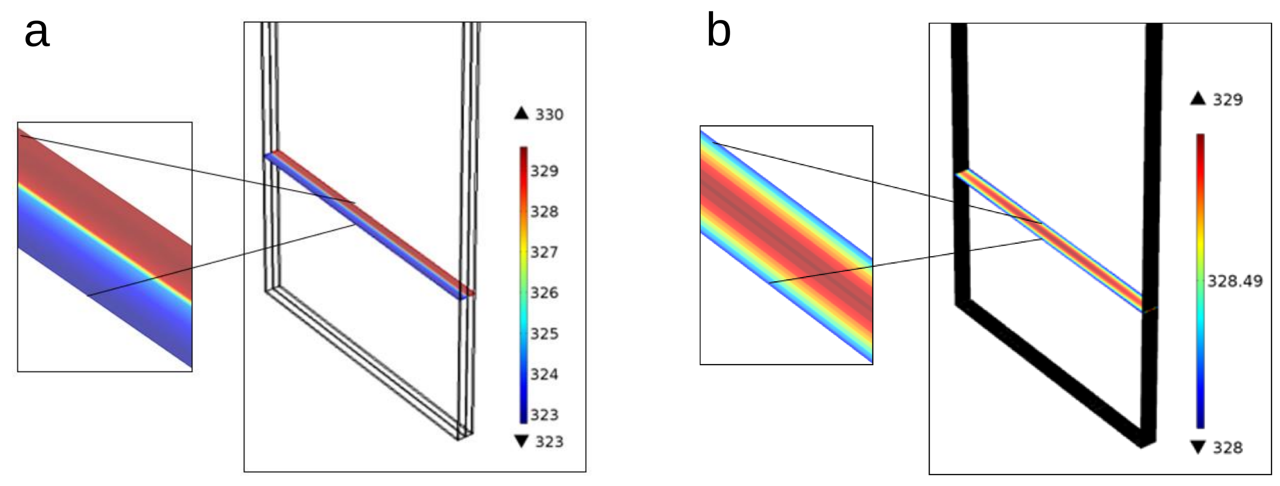


Figure 5. Internal temperature profiles of (a) single-layer cell and (b) 20-layer.

Heat Generation Analysis:

Total Heat Dissipation:
Reversible Entropic Heat
Irreversible Reaction Heat
Ohmic Joule Heat

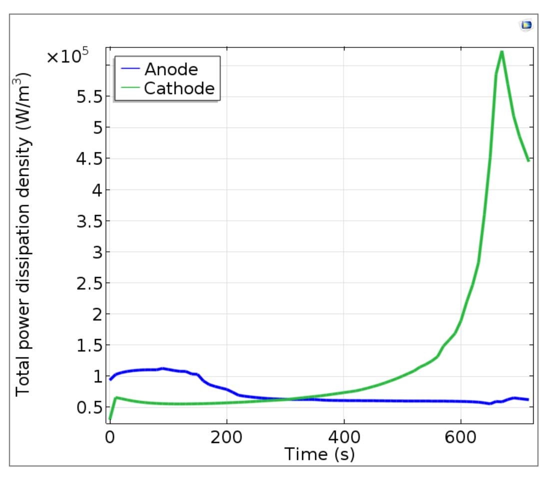
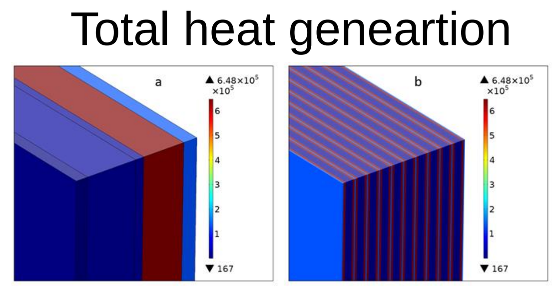


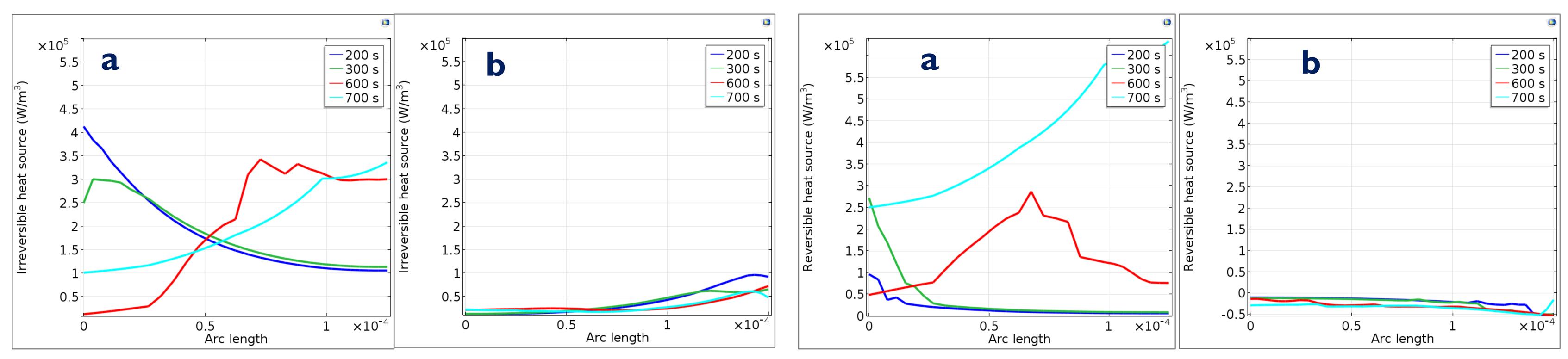
Figure 6. Total Heat Dissipation

Total heat geneartion



(a) Single-layer and (b) 20-layer

- ✓ Depends on amount of avtive material used.
- ✓ Cathod electrode is the main contributer.



Reversible heat generation (a) cathode (b) anode. Irreversible heat generation (a) cathode (b) anode.

Conclusions: Results showed that the single layer approach is not sufficient to model electrochemical and thermal behavior of high capacity Lithium-ion batteries. Inconveniences caused by the single layer approach are corrected in the developed multilayer model. The developed model is applicable to both single cells and battery modules. With a better precision of thermal behavior and heat generation analysis, this study is believed to be promising in development of an efficient thermal management system for high capacity battery packs in electric vehicles (EVs).

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References:

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