

Heat generation breakdown of Lithium-ion Batteries

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Introduction: The thermal behavior of lithium ion batteries could be investigated by efficient simulation method. Here, we developed an electrochemical-lumped thermal analytical model to analyze the thermal response and heat breakdown of a pouch LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂ battery (3Ah) under fast-discharging conditions at 7C(environment temperature:20°C). The key parameters of the proposed model (such as diffusion coefficient and reaction rate constant) possess the temperature dependent Arrhenius behavior while temperature is relevant to heat generation, heat conduction, and convective heat dissipation. Based on the method of integral transformation, the state estimation algorithm is able to rapidly recover the model states of current, voltage and temperature. The theoretical solution is tested to be highly accurate through comparison of numerical solution results and experimental data. As a consequence, our simulation model can scientifically and precisely calculate the heat generation and temperature distribution of lithium ion batteries. The model is based on Batteries and Batteries, Lithium-Ion Module of COMSOL Multiphysics.

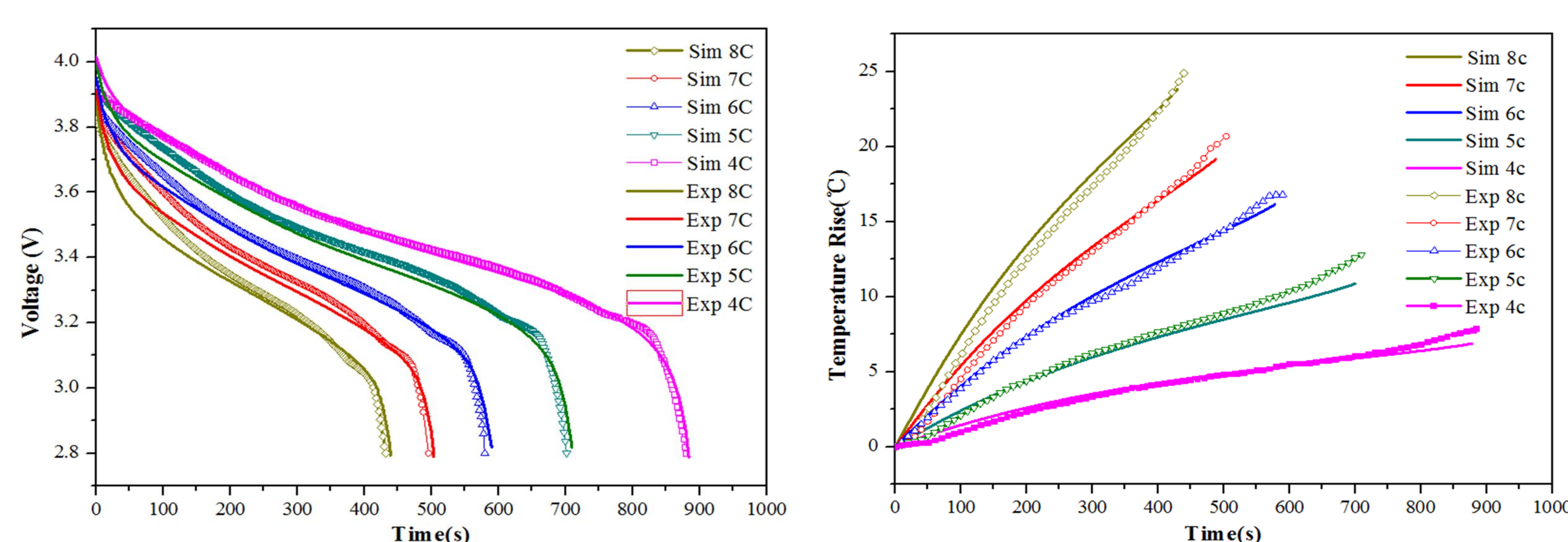


Figure 1. Charge curve fitting at different rates(Left) and Temperature curve fitting at different rates(right)

Modeling:

The Electrochemical-Lumped thermal model considered here consists of the 1D electrochemical model coupled to a bulk thermal model. The electrochemical model describes the transport of lithium ion, reaction kinetics, thermodynamics and heat generation at the electrode level while the bulk thermal model describes the evolution of cell temperature. The electrochemical and thermal models are coupled together through the potential-dependent and concentration-dependent heat generation rate and the temperature-dependent physical and chemical properties of the 1D model. A common approach assumes Arrhenius' law temperature dependency given by:

$$\varphi = \varphi^{ref} * \exp\left(\frac{E_a}{R} \left(\frac{1}{T^{ref}} - \frac{1}{T}\right)\right)$$

where φ denotes the parameter considered and φ^{ref} is the value of this parameter at T^{ref} . E_a is activation energy(kJ/mol). R is Gas constant(J/mol/K)

•The 1D electrochemical model is coupled to a lumped thermal model described by the following energy balance equation:

$$A\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (Ak\nabla T) + Ap_{ohm} + AP_0 + Ap_{rax}$$

$$p_{ohm} = \delta_{eff} \left(\frac{\partial \varphi_s}{\partial x}\right)^2 + k_{eff} \left(\frac{\partial \varphi_l}{\partial x}\right)^2 + \frac{2k_{eff}RT}{F} (1-t^+) \frac{\partial c_l}{\partial x} \frac{d\varphi}{dx} \frac{1}{c_l}$$

$$p_{rax} = FJ(\varphi_s - \varphi_l - U)$$

$$P_0 = h(T_{ext} - T)$$

where A : the surface of cell(m²); ρ : the cell density(kg/m³), C_p : the specific heat capacity(J/Kg/k), T_{ext} is environment temp.(K), J is Volumetric reaction rate(A/m³); F :Faraday's constant(C/mol), φ_s :solid-phase electric potential(V); φ_l :electrolyte-phase electric potential(V); U : equilibrium potential(V); c_l : electrolyte concentration(mol/m³); δ_{eff} : electron conductivity(s/m); k_{eff} : ionic conductivity(s/m); h : Convective heat transfer coefficient(W/m²*K); P_{ohm} : ohmic heating(J); P_{rax} : reaction heat(J); P_0 : Convective heat(J).

Results:

Fig.1. shows an excellent agreement between the analytical results and experimental measurements. Fig.2 shows temperature distribution and comparison between the simulation and experimental. The comparison shows that even the model is accurate enough to calculate heat breakdown. As illustrated by Fig.3, heat consist of cathode(47.1%),anode(42.4%) separator(10.3%) and the Al and Cu is negligible. The cathode main contribution to the global heat generation rate arises from the ohm resistance heat generation followed by the ohmic heat generation(P_{ohm}), the reaction heat generation (P_{rax}). The cell design can improve, reduce the heat source, fall of temperature to manage the better battery. When we know that every part of the heat generated by the battery.

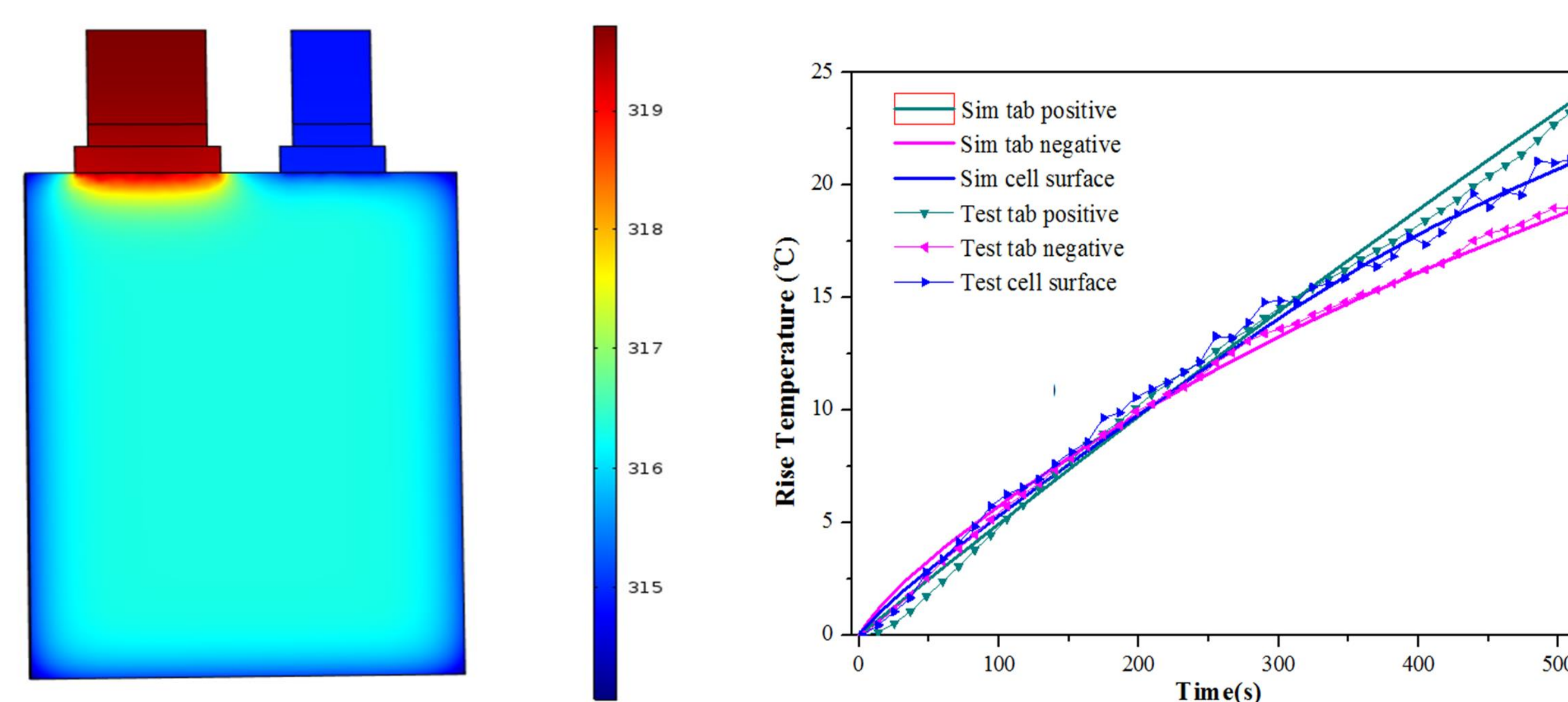
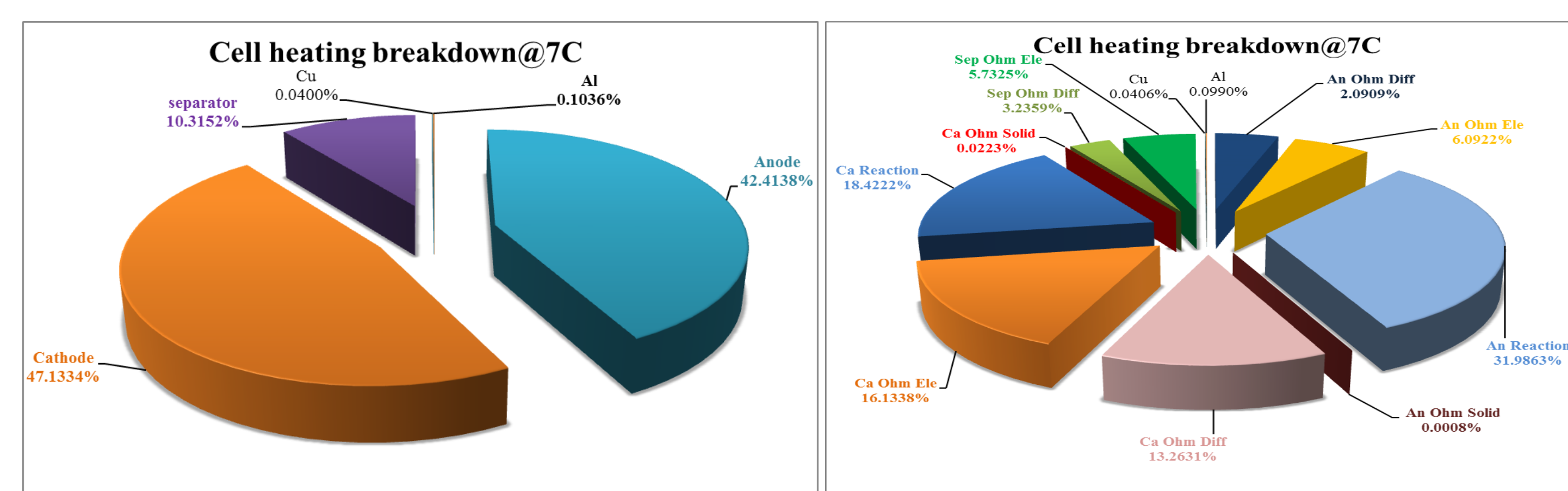


Figure 2. Temperature distribution 8C rate on ZY surface and Comparison of simulation and test sample



•Figure 3.Heat contribution of different components (Left) and (Ca=Cathode; An=Anode; Sep=Separator; Cu= Cu current collector; Al= Al current collector; Ohm Diff= Ohmic heat in liquid phase; Ohm Ele= heat from Li⁺ migration in liquid phase; Ohm Solid= Ohmic heat by solid phase; Reaction=Reaction heat)

Conclusions:

A coupled, Electrochemical-Lumped thermal modeling study for cell heat breakdown based on the local heat generation method has been presented. The model incorporates the reaction and ohmic heat in the matrix and solution phases. The temperature coefficients of the various transport and kinetic parameters are accounted for using Arrhenius-type relationships based on the literature data. The results are matching with the experimental results with good accuracy. The study could be used to further build models for thermal management and heat generating analysis of the battery available in the market.

References:

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