Co-Simulation Approach for Analyzing Electric-Thermal Interaction Phenomena in Lithium-Ion Battery

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Battery thermal management for electric or hybrid vehicles is crucial to prevent overheating and uneven heating across a battery pack. Thus, this paper provides a reliable and accurate co-simulation approach that can predict the thermal state inside a battery pack by the electrochemical responses of lithium-ion (Li-ion) battery cells. The approach is based on coupling an electric circuit model and a Computational Fluid Dynamics (CFD) model. The effectiveness and validation of the simulation approach are discussed by comparison with the experimental data.

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NOMENCLATURE

α = rate factor
 β = temperature factor
 C_{capacity} = useable capacity (Ah)
 I_B = battery cell current (A)
 V_{OC} = open circuit voltage (V)
 Z_{eq} = equivalent internal impedance (Ω)
 R_O = total Ohmic resistance (Ω)
 R_S = short-term transient resistance (Ω)
 C_S = short-term transient capacitance (F)
 R_L = long-term transient resistance (Ω)
 C_L = long-term transient capacitance (F)
 γ = resistance-correction factor (Ω)
 μ = SOD-correction factor
 ΔE = temperature correction of the potential (V)

1. Introduction

Electric or hybrid vehicles require storage systems with high capacity and high power like battery packs. During charge/discharge behavior of Li-ion batteries, temperature rise and temperature uniformity have a strong influence on the battery pack performance. All the modules in the

battery pack should be operated within the optimum temperature range.^{1,2} For this reason, battery thermal management is crucially important in preventing overheating and uneven heating across a battery pack under realistic operating conditions. In order to design the thermal management system and maintain short design cycles, low cost, and optimal quality, system-level engineers need a simulation approach that can predict the thermal state inside a battery pack prior to fabricating expensive prototypes in early stages of the design process. Many different simulation models for evaluating the thermal performance of a battery cell have been proposed in literature.³⁻¹⁴ The battery thermal models can be generally classified into three categories: physics-based models, electric circuit models and co-simulation battery models.

Detailed physics-based models³⁻⁶ are based on differential equations governing charge transfer or transport in the electrodes and electrolyte. These models have been widely used to study heat generation and temperature distribution within individual cells but are not suitable for thermal simulation of battery modules or packs due to their high computational requirements and the need for specific knowledge of battery model parameters such as cell construction, chemical composition and physical properties. In contrast, electric circuit models⁷⁻¹⁰ are electrical equivalent models capable of representing electrochemical and electrothermal effects for a battery cell by using a combination of voltage sources, resistors, and capacitors. The lumped parameters in the circuit network are extracted from the manufacturer's data or experimental results, based on the assumption that all chemical and physical processes are uniform throughout the entire battery cell. These models have been

extensively used to predict battery behavior on battery control or monitoring of system-levels due to its simple realization and very fast simulation speed. But, circuit models cannot thoroughly examine temperature distribution inside a battery module or pack for thermal management design. On the other hand, CFD can give detailed thermal information considering fluid flow and heat transfer within a battery module or pack to make it possible to design better battery cooling systems. However, it does not support a proper heat generation mechanism by electrochemical reactions in the battery cell. For this reason, a co-simulation approach combining the electric circuit model and the CFD model has been proposed.¹¹⁻¹³

Cold temperature lower than room temperature increases the internal resistance of battery cell and diminishes the capacity of it. In another words, the performance of all battery chemistries drops drastically at low temperature. In addition, battery cells at high discharge rates show the rise of very high internal temperatures. Until now, investigations of low temperature behavior of battery cells have been limited to experimental measurements and observations. For this reason, this paper proposes a reliable and accurate co-simulation approach that can predict the thermal state inside a battery pack under high discharge rates and low temperature conditions. The effectiveness and validation of the simulation approach are also discussed by comparison with the experimental data.

2. Co-Simulation Framework

In this paper, a co-simulation approach is used for the coupling of electric circuit model and CFD model as shown in Fig. 1.¹¹⁻¹³ Fig. 1(a) shows the electric circuit model proposed by Chen.⁸ The circuit model can evaluate battery run time and transient I-V performance, but temperature effects on battery characteristics have not been described in detail. Thus, by adding the definitions of the discharge rate factor, temperature factor and potential-correction term proposed by Gao⁷ into Chen's circuit model, the model can predict the discharge rate and temperature dependences of the capacity, as well as thermal dependence of battery output voltage. However, the model has also shown a minor lack of accuracy under low temperature conditions. Therefore, the purpose of this paper is to propose an enhanced circuit model to improve the accuracy of the prediction.

In the circuit model, all electrochemical and electrothermal processes are approximated as uniform throughout the entire battery cell, and all spatial variations of concentrations, phase distributions and potentials are also ignored.⁷ Thus, the circuit model cannot predict the temperature distribution inside a battery module or pack. Fig. 1(b) depicts CFD model. It does not support a proper heat generation mechanism by an electrochemical reaction in the battery cell. Thus, the CFD requires a heat profile for using as a power source condition in the battery pack simulation. For this reason, the power generated by the circuit model is sent to the CFD model as the heat source profile within each time step of the co-simulation. CFD then determines temperature distribution of a battery cell based on the heat source, and the average temperature is sent back to the circuit model as input to the temperature dependent components of the circuit model.¹¹⁻¹³

Through such processes, the co-simulation approach can evaluate the thermal state inside a battery pack even if the battery discharge rate rapidly increases or decreases, which could happen during real driving conditions.

Fig. 1 Framework of co-simulation approach; (a) Electric circuit model to represent electrochemical response in a battery cell (b) CFD model to calculate the temperature of a battery cell

3. Enhanced Circuit Model

The internal temperature of a battery cell increases faster at low environment temperatures and high discharge rates than in normal operating conditions (1C rate and room temperature). Therefore, we need a reliable and accurate electric circuit model capable of predicting the thermal behavior of a battery cell for the worst operating conditions. However, the existing circuit models have some limitations in that they deviate from the experimental data at low temperatures and at high discharge rates. This paper presents an enhanced circuit model able to obtain more accurate predictions by using additional factors (γ and μ) in the existing circuit model of Fig. 1(a).

3.1 State of Discharge

Chen⁸ has proposed an electric circuit model as shown in Fig. 1(a). The model is composed of the two circuit parts: battery lifetime circuit and voltage-current characteristics circuit. The left part determines either the State of Charge (SOC) or the State of Discharge (SOD) and the runtime of a battery cell according to the given load current (I_B). The function of the capacitor ($C_{capacity}$) is to release electrical energy in the discharge mode and store it in the charge mode. The low self-discharge rate of the Li-ion battery cell has been reported in the literature.¹⁵ From the viewpoint of thermal management design, this study assumes that $C_{capacity}$ depends only on the discharge rate and cell temperature. Consequently, the SOD can be expressed as follows:⁷

$$SOD = \frac{1}{C_{capacity}} \int_0^t \alpha \cdot \beta \cdot I_B dt \text{ or } SOC = 1 - SOD \quad (1)$$

where, α is rate factor and β is temperature factor proposed by Gao.⁷ The rate factor α accounts for the dependence of the SOD on discharge rate and the temperature factor β considers the dependence of the SOD on cell temperature.

3.2 Battery Cell Voltages

The right circuit of Fig. 1(a) describes the relation between the given I_B and the battery terminal voltage (V_B). The output voltage V_B can be calculated by the difference of the battery open circuit voltage (V_{oc}) and the battery equivalent internal impedance (Z_{eq}). Therefore, V_B can be obtained as follows:¹⁰

$$V_B(SOD) = V_{OC}(SOD) - I_B \times Z_{eq}(SOD) \quad (2)$$

where, V_{OC} is the voltage between the battery terminals with no load applied and it depends on the SOD of a battery cell. Each battery cell has different V_{OC} behaviors according to the battery types. This study proposes the following empirical equation:

$$V_{OC}(SOD) = a_1 e^{a_2 \cdot (1-SOD)} + a_3 + a_4 \cdot SOD + a_5 \cdot SOD^2 + a_6 \cdot \delta \cdot SOD^{2.5} + a_7 \cdot SOD^3 \quad (3)$$

where

$$\delta(SOD) = e^{\varepsilon_1 \cdot (1-SOD^3)} \times \cos(\varepsilon_2 \cdot \pi \cdot SOD^2) \quad (4)$$

All coefficients of V_{OC} can be extracted from the least square curve fitting the experimental data.

3.3 Equivalent Internal Impedance

We can generally observe that if the given I_B suddenly cuts off, the output voltage V_B is returned to V_{OC} at a steady state across transient response process due to the cell's internal impedance after a finite time as shown in Fig. 2. The transient response process can be divided into immediate-term, short-term and long-term processes.⁸

The RC network in the right circuit of Fig. 1(a) represents the equivalent internal impedance and it is used to model the transient response process of the battery cell. The impedance consists of a series resistor R_O , and two RC parallel networks composed of R_S , C_S , R_L , and C_L .⁸ R_O denotes the total Ohmic resistance associated with the immediate-term process, which includes terminal resistance and current collector resistance inside a battery cell. R_S and C_S are used to characterize the short-term process of the battery transient response related to charge transfer and double-layer capacitance. R_L and C_L describe the long-term process of the battery transient response in respect to mass transport or diffusion processes.^{8,10}

Normally, the resistance inside a battery cell varies with the cell temperature and SOD. Cold temperatures increase the internal resistance on the battery cells. Conversely, at higher temperatures its resistance decreases due to the activation of the electrochemical reactions, but long exposure to heat reduces battery life. In addition, when a battery cell discharges, the internal resistance increases as its SOC decreases.

For these reasons, system-level designers for thermal management systems should consider the temperature- and SOD- dependencies of the internal resistance. In order to predict the change of internal resistance according to the cell temperature and SOD, the form of each component for the equivalent internal impedance can be expressed by using a resistance-correction factor $\gamma(T)$ and a SOD-correction factor $\mu(T)$ as follows:

$$R_O = \mu_1(T) \cdot e^{\mu_2(T) \cdot (1-SOD)} + b_1 + \mu_3(T) \cdot b_2 \cdot SOD + \gamma(T) \quad (5)$$

$$R_S = \mu_1(T) \cdot e^{\mu_2(T) \cdot (1-SOD)} + c_1 + \mu_3(T) \cdot c_2 \cdot SOD + c_3 \cdot \delta \cdot SOD^{2.5} \quad (6)$$

$$R_L = \mu_1(T) \cdot e^{\mu_2(T) \cdot (1-SOD)} + d_1 + \mu_3(T) \cdot d_2 \cdot SOD + d_3 \cdot \delta \cdot SOD^{2.5} \quad (7)$$

$$C_S = f_1 \cdot e^{f_2 \cdot (1-SOD)} + f_3 + f_4 \cdot SOD + f_5 \cdot \delta \cdot SOD^{2.5} \quad (8)$$

Fig. 2 A typical curve of terminal voltage response under pulsed-current discharge for extraction of the electrical circuit parameters of the proposed battery model

Fig. 3 Determination of the temperature-correction factor $\gamma(T)$

$$C_L = g_1 \cdot e^{g_2 \cdot (1-SOD)} + g_3 + g_4 \cdot SOD + g_5 \cdot \delta \cdot SOD^{2.5} \quad (9)$$

Gao⁷ has proposed a potential correction term $\Delta E(T)$ to compensate for the output voltage drop (ΔV_B) by the change of cell temperatures. According to the same procedures in his paper, a reference temperature curve was chosen as shown in Fig. 3 and at the temperature of 25°C, $\Delta E(25)$ is set to 0. $\Delta E(T)$ will drop at lower temperatures in comparison to the reference curve, while it will rise at higher temperatures. However, this study uses a resistance-correction factor $\gamma(T)$ ($=\Delta E(T)/I_B$) in Eq. (5) instead of $\Delta E(T)$ to consider the heat power source with the change of cell internal resistance causing voltage rise or voltage drop. In Fig. 3, the dot-dashed line is the curve that is predicted by both the resistance-correction factor $\gamma(T)$ and temperature factor $\beta(T)$. However, it is shown that there is a difference in the values between the experimental data of the dotted line and the prediction by the two factors. Consequently, this work suggests the use of the SOD-correction factor $\mu(T)$ to improve the accuracy of the circuit model. As SOD increases, $\mu(T)$ can reflect the resistance increments except the variation of internal resistance by γ .

4. Extraction of Circuit Parameters

The tests were carried out by using a 20 Ah lithium titanate cell with 1.5 - 2.7 V operating in order to evaluate the effectiveness and accuracy of the proposed circuit model. An electronic load was used to discharge

Fig. 4 Configuration of battery cell test equipments

Fig. 5 Output voltage curve with pulse discharge currents

the battery cell as shown in Fig. 4. Two multi-meters were utilized to measure the cell terminal voltage and the load current. Five thermocouples for measuring the average of cell temperature were installed on the surface of the battery cell and one thermocouple was also set to measure the ambient temperature of the cell as denoted in Fig. 4. A temperature chamber was used to investigate the performance of the battery cell at high/low ambient temperatures. From the battery tester, the terminal output voltages, discharge currents and cell temperatures were simultaneously monitored.

The basic parameters of μ , γ , a , b , c , d , f , g and δ in Eqs. (5)-(9) were determined from nonlinear least squares curve fitting the experimental data by pulse discharge currents with interval of 5 % SOD and rest time of 90 seconds for 0.98 discharge rate (C-rate). The tests were also carried out under the ambient temperature of approximately 25°C. Fig. 5 shows the terminal voltage measurement for the pulse discharge currents. The RC network parameters can be then derived by the following equations:¹⁰

$$R_O(SOD) = \frac{V_1 - V_0}{I_B} \quad (10)$$

$$V_B(t) = I_B \cdot \left\{ R_S \cdot (1 - e^{-t/(R_S \cdot C_S)}) + R_L \cdot (1 - e^{-t/(R_L \cdot C_L)}) \right\} + V_1 \quad (11)$$

where V_0 and V_1 are depicted in Fig. 2. In Eq. (11), the terminal output voltage V_B becomes the open circuit voltage V_{OC} of Eq. (3) at each SOD as illustrated in Fig. 2, when $t \rightarrow \infty$. After a rest time of approximately 400 seconds, it can be confirmed that the terminal output voltage V_B is equal to the open circuit voltage V_{OC} . All parameters of the battery model are represented in Table 1. Fig. 6 shows the fitted curves and the data points for all parameters of the Li-ion battery cell.

Three factors (α , β , γ) in Eqs. (1) and (5) can be determined through

Table 1 Battery model parameters for the Li-ion cell at ambient temperature of approximately 25°C

μ_1	2	c_2	0.2	f_4	4700	a_2	-147
μ_2	-37	c_3	6.10E-08	f_5	1.50E-03	a_3	2.6205
μ_3	1	d_1	0.33	g_1	-55000	a_4	-1.1316
ε_1	18	d_2	0.22	g_2	-16	a_5	1.137
ε_2	6.2	d_3	2.60E-07	g_3	111000	a_6	-7.00E-09
b_1	0.76	f_1	-12300	g_4	-49000	a_7	-0.5737
b_2	0.1	f_2	-16	g_5	8.50E-03	γ	0
c_1	0.31	f_3	18300	a_1	-0.42	-	-

Fig. 6 Extracted parameters of the Li-ion battery at room temperature

Fig. 7 Determination of the SOD-correction factor for discharge curve procedures in Ref. 7. The reference curve was chosen as 1 C-rate (20 A) at the ambient temperature of 25°C as shown in Fig. 3. The rate factor α and temperature factor β on the SOD of battery cell can be obtained as follows:

$$\alpha(I_B) = 0.9225 - 0.0004457 \cdot (I_B) + 0.02876 \cdot \ln(I_B) \quad (12)$$

$$\beta(T) = 0.000049 \cdot T^2 - 0.00615 \cdot T + 1.129 - 0.00507 \cdot e^{0.05 \cdot (35-T)} \quad (13)$$

where, the variable T in the temperature factor $\beta(T)$ means the ambient temperature of the battery cell. In the reference curve, $\alpha(20)$ and $\beta(25)$ have values of 1.

The resistance-correction factor $\gamma(T)$ related to a potential correction term $\Delta E(T)$ in Ref. 7 is also calculated as follows:

$$\gamma(T) = 0.001307 - 0.000091 \cdot T + 0.000002 \cdot T^2 - 1.75 \cdot 10^{-8} \cdot T^3 \quad (14)$$

In this paper, the value of $\gamma(T)$ is determined from the average cell temperature calculated by the CFD.

As stated previously, this study suggests the use of the SOD-correction factor $\mu(T)$. The authors determined the numerical values of the parameters of μ_1 , μ_2 , and μ_3 that make Eqs. (5)-(7) which give the best fit to experimental data for discharge curves under various temperature conditions as a function of SOD. The terminal voltage predicted by those methods is shown in Fig. 7. It has a good match with the experimental data. The SOD-correction factor is obtained as follows:

$$\mu_1(T_a) = 0.0000069 \cdot T_a^3 - 0.000811 \cdot T_a^2 + 0.0559 \cdot T_a - 0.00203 \quad (15)$$

$$\mu_2(T_a) = -0.0000203 \cdot T_a^3 + 0.00265 \cdot T_a^2 - 0.114243 \cdot T_a + 3.5186 \quad (16)$$

$$\mu_3(T_a) = -0.0003242 \cdot T_a^3 + 0.033955 \cdot T_a^2 - 0.556 \cdot T_a - 39.2598 \quad (17)$$

where $\mu_1(25)$, $\mu_2(25)$ and $\mu_3(25)$ for the reference curve are equal to the values in Table 1. The variable T_a in SOD-correction factor $\mu(T_a)$ also means the ambient temperature of the battery cell.

5. Validation of Co-Simulation Approach

Simulations and tests are carried out to validate the enhanced co-

Fig. 8 CFD mesh of battery cell and plastic support

Table 2 Material properties for CFD analysis

Material	Density (kg/m ³)	Specific heat (J/kg-K)	Thermal conductivity (W/m-K)	Viscosity (kg/m-s)
Battery cell	1957.1	901.961	0.5	-
Plastic support	1250	1300	0.35	-
Air (25°C)	Ideal-Gas (1.184)	1006.43	0.0242	1.79E-05

simulation approach for a single battery cell as well as a 12-cell battery module under various operating conditions, especially at low temperatures and high C-rates.

5.1 Co-Simulation of Single Battery Cell

The CFD model for a single battery cell was used for verifying the reliability and accuracy of the co-simulation approach. Fig. 8 shows the CFD model used for it. The mesh was created using hexahedral elements. The material properties for the battery cell, plastic support, and air are summarized in Table 2. In the simulations, solid material properties were assumed to be constant, ignoring changes that occur with increasing temperature. As the input power source profile of CFD model, heat generation at each time step determined from the circuit model was applied to the cell, and that heat power in the cell was modeled to be uniformly distributed. Natural convection open boundary conditions were specified to the exterior of the CFD model except for the bottom surface. Under these boundary conditions, the authors examined the responses of cell temperatures and terminal output voltages based on the buoyancy-driven natural convection flow of air inside the block enclosure.

Fig. 9 shows the response curves of Li-ion battery cell for the discharge of 1 C-rate at ambient temperatures of -21, 0 and 25°C. The co-simulation results were highly consistent with the experimental data. The level of consistency between the experimental data and simulation results demonstrates the reliability and accuracy of the co-simulation approach.

Fig. 10 shows that simulation results are compared to the experimental data in order to verify the accuracy and validity of the proposed co-simulation approach at high discharge rates (2.5 and 3 C-rates). Fig. 11 represents the simulated and measured results for a pulse current discharge scenario composed of high discharge currents to evaluate the nonlinear transient responses and runtimes of battery cell.

In addition, Fig. 12 compares the terminal voltage response obtained from simulation with experimental data for constant pulse current discharge with the rest time of 90 seconds and 2 C-rate. Very satisfactory

Fig. 9 Simulation and experimental data for various levels of ambient temperatures at 1 C-rate

Fig. 10 Terminal voltage and cell temperature for high discharge rates (3 C and 2.5 C) at room temperature

Fig. 11 Comparison between simulation results and experimental data for pulse current discharge scenario

Fig. 12 Comparison between co-simulation results and experimental data for 40 A pulse discharge current

Fig. 13 Experimental setup for air cooling of battery module

agreements have been obtained as shown in the Figs. 10-12.

From the verification above, it can be stated that the proposed co-simulation approach with enhanced circuit model and CFD model is reliable and accurate in detecting the terminal voltages and cell temperatures under various C-rates and temperature conditions, particularly at low temperatures and high C-rates.

5.2 Co-Simulation of Battery Module

Under air cooling conditions in two different cases for a battery module, forced convection flow tests are carried out in order to compare with corresponding co-simulation results to verify the effectiveness and the reliability of the proposed approach. Fig. 13 shows the air cooling system for a module assembled with 12-cell battery connected in 2 parallel rows of 6 series (2P6S). The module has a nominal voltage of 13.8 V, cut-off voltage of 9.0 V and capacity of 40 Ah. The air is drawn by a 12 V blower installed at a connection position between the inlet duct and the transition duct as illustrated in Figs. 13-14. The transition duct was designed and fabricated according to AMCA standards.¹⁶ The air is vented through the outlet hole after having passed through the test chamber. The blower has two settings with medium and high speeds as represented in Table 3. The forced convection flow tests were conducted for the two settings of the blower, based on 100 A discharge current and each temperature condition in Table 3. The six thermocouples were attached on surfaces of the battery cells as depicted in Fig. 14. The temperature responses of the thermal probes were obtained from the tests.

Fig. 14 CFD model and 12-cell circuit model for co-simulation of battery module

Table 3 Battery module flow characteristics

Blower setting	Voltage (V)	Current (A)	RPM	Air Flow rate (m ³ /s)	Inlet velocity (m/s)	Inlet temp (°C)
Medium	5.17	1.73	1400	0.01709	6.045	29
High	9.11	3.516	2800	0.02601	9.2	28.7

Fig. 15 Temperature distributions of battery module at 97% SOD in a discharge process for two blower RPMs

Co-simulations for the two test cases were also performed. Fig. 14 plots a temperature dependent 12-cell circuit model and CFD model for the co-simulations. The circuit model consists of 2 parallel rows and they are connected in 6 series to a load current I_M . The inlet velocities for the co-simulations are listed in Table 3.

The sectional views in Fig. 15 show the simulated battery module temperatures at 97 % SOD in a discharge process for two settings of the blower. The surfaces of the cells have lower temperature distribution than inner regions of the cells as a result of the air cooling. Moreover, it also shows that the cell surfaces cooled by the middle RPM blower represent higher temperature distribution than those by the high RPM

Fig. 16 Comparison of simulation and test results according to the blower speeds on the temperature responses at thermal probes; (a) Middle speed (b) High speed

blower. Fig. 16 represents the temperature variations measured at the six thermocouples from simulations and tests for air cooling conditions. In addition, it also depicts the variations of output voltages along with

temperatures during the full discharge process. From the comparison, the co-simulation results for the two blower RPMs are in good agreement with those gathered by tests at each time step. These results show that the proposed co-simulation approach can accurately capture the temperature variations of each cell for the battery module.

6. Conclusions

The purpose of this study is to propose a reliable and accurate co-simulation approach that can predict the thermal state inside a battery pack by electrochemical response of lithium-ion (Li-ion) battery cells in order to design a thermal management systems and maintain short design cycles, low cost and better quality.

This study demonstrated that the proposed co-simulation approach with enhanced circuit model and CFD model is reliable and accurate in detecting the terminal voltages and cell temperatures of a single battery cell at low temperatures and high discharge rates.

These findings also showed that the co-simulation approach can accurately capture the temperature variations of each cell for the battery module.

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