Design optimization of lithium-ion battery using hybrid electric vehicle simulation model

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Abstract
As electric vehicle (EV) and hybrid electric vehicle (HEV) have been developed, the importance of research and development of lithium-ion battery is on the rise in automobile industry. However, the design method for lithium-ion battery using physical experiment requires expensive cost and much time. Therefore, computational simulation of the battery was introduced to reduce the cost and development-time. In this paper, optimum design of the battery is suggested by using optimization techniques and HEV lithium-ion simulation. We carry out analysis of variance to select the important parameters as design variables. By using these design variables, we build kriging surrogate model for total energy of the battery and define the optimization problem. Finally, we perform the optimization to obtain the maximum energy of lithium-ion battery within mass constraint.

Keywords: Design Optimization, Lithium-ion Battery, Simulation Model, Hybrid Electric Vehicles, Analysis of Variance, Kriging surrogate model

1 Introduction
Due to the depletion of fossil fuel and tightening environmental regulation, electric vehicle (EV) and hybrid electric vehicle (HEV) have been developed and nowadays lithium-ion battery is widely used for these vehicles for several advantages. Low volumetric mass density and high energy density of lithium-ion battery are suitable for vehicles in terms of fuel efficiency. Memory effect of lithium-ion battery is also suitable for vehicles which need frequent charging and discharging. However, design of lithium-ion battery traditionally depends on intuition of designer or experimental results. Some researchers about optimization of lithium-ion battery are performed recently. However, in this optimization process, it is difficult to reduce calculation time and cost. Some researchers use simplified battery models¹ or reduce the number of design variables to overcome the difficulties.

In this paper, accuracy and cost reduction are achieved by employing accurate battery model, screening technique and surrogate model. To maximize energy of the battery within mass constraint, optimization is performed by applying these techniques and the optimized lithium-ion battery is verified using HEV simulation.

2 HEV simulation model
In this research, we use power-split HEV simulation model made by MapleSim software as in Figure 1. The model consists of 70-cell Li-ion battery pack, 4-cylinder 1.8L gasoline IC engine, 50kW electrical motor/generator, a power-
Table 1: Governing equation of state variables in electrodes.

<table>
<thead>
<tr>
<th>State variable</th>
<th>Governing equation</th>
</tr>
</thead>
</table>
| $c$            | $\frac{\partial c}{\partial t} - \nabla \cdot (c \mathbf{D})$ 
$1 - \frac{d}{d \ln c} \frac{\partial}{\partial t} c + \frac{\partial}{\partial t} i_2 = \frac{i}{x} \cdot \mathbf{F} - \frac{\partial c}{\partial t} + \frac{\partial c}{\partial t} = \frac{\partial}{\partial t} t_2 - \frac{t_2}{x} \cdot \mathbf{F}$ |
| $c_s$          | $\frac{\partial c_s}{\partial t} - \nabla \cdot (c_s \mathbf{D})$ 
$1 - \frac{d}{d \ln c} \frac{\partial}{\partial t} c_s - \frac{i}{x} \cdot \mathbf{F} = \frac{\partial c_s}{\partial t} - \frac{\partial c_s}{\partial t} = \frac{\partial}{\partial t} t_s - \frac{t_s}{x} \cdot \mathbf{F}$ |
| $i_{in}$       | $\nabla \cdot \left( \frac{\partial}{\partial t} i_{in} - i_{in} \right) = \exp \left( \frac{\alpha_i F (\phi_i - \phi_e - U)}{RT} \right) - \exp \left( \frac{-\alpha_i F (\phi_i - \phi_e - U)}{RT} \right)$ |
| $\phi_2$       | $\nabla \phi - \frac{i_2}{\kappa} \frac{2kT}{F} \left[ \frac{1}{x} \cdot \mathbf{F} \right] \left( \frac{\partial c}{\partial t} + \frac{\partial c}{\partial t} \right)$ |
| $\phi_1$       | $1 - i_{in} = -\sigma D_i$ |

controller, an inverter, a power split device, 14 degree of freedom chassis with differential gearbox, etc.

The input of this model is driving cycle. There are 4 outputs of this model such as state of charge (SOC), voltage and current of the battery and mileage of the vehicle. When the simulation starts, velocity information of driving cycle is sent to the power control component. The power control component calculates power requirement of motor and engine, sending the information to motor and engine component. Using this power requirement information, engine component operates IC engine and sends power to power split device. In this power split device, the power is distributed. Some of the power is transferred to the generator to recharge battery and the rest of the power combined with the power of the motor drive vehicle.

[2,3]

Figure 1: Power-split HEV simulation model

2.1 Numerical model of lithium-ion battery

Generally, there are two types of Li-ion battery modelling technique. One is equivalent circuit model, the other is electrochemical model. Equivalent circuit battery model represents battery behaviour as electrical circuit. This model simplifies the cell behaviour as an ohmically limited system, which is simple and easy to create and simulate. However, since this equivalent circuit battery model is accurate only for narrow range of current, new equivalent circuit has to be developed as battery parameters are changed.

The electrochemical battery model, by contrast, can consider wide range of applied current and many configuration parameters can be changed. In this paper, we employ the electrochemical battery model because of the effect of change of battery parameters. This electrochemical battery models are derived from the porous electrode and concentrated solution theories proposed by Newman and Doyle [4,5]. They describe charge/discharge and species transport in the solid and liquid phases as a simplified 1D spatial cell structure. This 1D battery model considers only one axis’ dynamic, neglecting other two axis’ dynamics. The solution theory is used to examine the energy and power capacity of cell with respect to parameters. This model uses governing equation which is derived from the electric behaviours between electrode and separator [6]. The governing equation is as shown in table 1. In this governing equation, five state variables are computed in the cell model, ion concentration in electrolyte and in solid phase, interfacial reaction rate, and potentials in liquid phase and solid phase.

Figure 2: Anatomy of lithium-ion cell

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In this research, we employ the 1D electrochemical battery models. We apply the galvanostatic discharge profile as input of the battery cell model and extract two outputs. One is voltage and the other is SOC. Using this output, we derive the total energy of battery cell that one needs to perform optimization. Analysis of variance due to its orthogonality. 3 experiments needed to perform analysis of variance such as F-ratio, p-value and contribution ratio. Contribution ratio is ratio between variation of performance due to its orthogonality. 3-level orthogonal array is chosen as design of experiment to consider nonlinear property of performance and analyse the main effect of each design variable standing for global sensitivity. A few criteria exist to determine importance of design variables for improving the performance such as F-ratio, p-value and contribution ratio. Contribution ratio is used as criterion to select significant design variables.

### 3.1 ANOVA procedure

In order to perform ANOVA effectively and efficiently, an appropriate design of experiment is needed. Orthogonal array is the most famous design experiment to select sample points. Orthogonal array provides least number of experiments needed to perform analysis of variance. Also, this 1D electrochemical battery model has 29 parameters. Among these parameters, we select 9 parameters for analysis of variance. The information of parameters is listed in Table 2.

### Table 2: Parameters of the battery for analysis of variance

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Lower bound</th>
<th>Current value</th>
<th>Upper bound</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_n$</td>
<td>Porosity of anode</td>
<td>0.45</td>
<td>0.485</td>
<td>0.6</td>
<td></td>
</tr>
<tr>
<td>$e_p$</td>
<td>Porosity of cathode</td>
<td>0.2</td>
<td>0.358</td>
<td>0.42</td>
<td></td>
</tr>
<tr>
<td>$e_s$</td>
<td>Porosity of separator</td>
<td>0.6</td>
<td>0.724</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Electronic conductivity of electrode</td>
<td>1</td>
<td>100</td>
<td>100</td>
<td>$S/m$</td>
</tr>
<tr>
<td>$L_n$</td>
<td>Thickness of anode</td>
<td>72e-6</td>
<td>80e-6</td>
<td>88e-6</td>
<td>$m$</td>
</tr>
<tr>
<td>$L_p$</td>
<td>Thickness of cathode</td>
<td>72e-6</td>
<td>80e-6</td>
<td>88e-6</td>
<td>$m$</td>
</tr>
<tr>
<td>$L_s$</td>
<td>Thickness of separator</td>
<td>22.5e-6</td>
<td>25e-6</td>
<td>27.5e-6</td>
<td>$m$</td>
</tr>
<tr>
<td>$\phi_n$</td>
<td>Volume fraction of fillers of anode</td>
<td>0.01</td>
<td>0.0326</td>
<td>0.08</td>
<td></td>
</tr>
<tr>
<td>$\phi_s$</td>
<td>Volume fraction of fillers of cathode</td>
<td>0.01</td>
<td>0.025</td>
<td>0.08</td>
<td></td>
</tr>
</tbody>
</table>

Also, this 1D electrochemical battery model has 29 parameters. Among these parameters, we select 9 parameters for analysis of variance. The information of parameters is listed in Table 2.

### Table 3: Analysis of variance results

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Contribution ratio (%)</th>
<th>F-ratio</th>
<th>P-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_n$</td>
<td>60.4</td>
<td>270.4</td>
<td>4.5E-08</td>
</tr>
<tr>
<td>$e_p$</td>
<td>3.8</td>
<td>17.0</td>
<td>0.001</td>
</tr>
<tr>
<td>$e_s$</td>
<td>0.7</td>
<td>3.3</td>
<td>0.1</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>0.5</td>
<td>2.1</td>
<td>0.2</td>
</tr>
<tr>
<td>$L_n$</td>
<td>17.9</td>
<td>80.2</td>
<td>5.1E-06</td>
</tr>
<tr>
<td>$L_p$</td>
<td>1.8</td>
<td>8.1</td>
<td>0.01</td>
</tr>
<tr>
<td>$L_s$</td>
<td>0.3</td>
<td>1.2</td>
<td>0.4</td>
</tr>
<tr>
<td>$\phi_n$</td>
<td>13.4</td>
<td>60.1</td>
<td>1.5E-05</td>
</tr>
<tr>
<td>$\phi_s$</td>
<td>0.3</td>
<td>1.5</td>
<td>0.3</td>
</tr>
</tbody>
</table>

3. Analysis of variance for lithium-ion battery

Optimization procedure becomes more expensive and difficult as number of variables increases. Screening technique provides more important variables to improve the performance of a system. Thus screening technique is adopted when too many variables are involved in the design and number of design variables is needed to be reduced to perform optimization. Analysis of variance (ANOVA), one of screening techniques, is a collection of statistical models used to analyse the differences between group means and their associated statistics such as variation among and between groups.
3.2 ANOVA results and selection of design variables

The main effect of each parameter to the performance is represented in the Table 3. The most dominant design variables are $e_n$ and $L_n$ whose contribution ratios are 60.4 % and 17.9% respectively. The contribution ratios of $\phi_n$ and $e_p$ are 13.4% and 3.8% which are also verified to be significant. Therefore, $e_n$, $e_p$, $L_n$ and $\phi_n$ are determined as design variables for optimization.

4 Optimum design formulation for lithium-ion battery

In this section, we formulate and solve design optimization of lithium-ion battery problem to maximize the performance of battery with mass constraint.

4.1 Optimum design formulation

Using selected 4 design variables, we make kriging surrogate model[8] based on 75 optimal Latin hypercube design (OLHD) sample points[9,10]. Accuracy of the kriging surrogate model is validated by root mean square error (RMSE). The RMSE value is 0.46%. Using this kriging surrogate model, we formulate the design optimization problem for maximizing total energy of battery subject to mass constraint, as follows:

Maximize $E_{\text{tot}}$

s.t. $x^T\text{mass} \leq \text{mass}_{\text{current}}$

where $x$ mean the design variables mass$_{\text{current}}$ means mass of current design.

<table>
<thead>
<tr>
<th>Description</th>
<th>Current design</th>
<th>Optimum design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1$ Porosity of anode</td>
<td>0.485</td>
<td>0.45</td>
</tr>
<tr>
<td>$x_2$ Porosity of cathode</td>
<td>0.385</td>
<td>0.4213</td>
</tr>
<tr>
<td>$x_3$ Thickness of anode[m]</td>
<td>80e-6</td>
<td>85.085e-6</td>
</tr>
<tr>
<td>$x_4$ Volume fraction of filler of anode</td>
<td>0.0326</td>
<td>0.0318</td>
</tr>
</tbody>
</table>

Con mass 1 (Active)

Obj Energy 1 1.0512. (5.12%↑)

SOC Final SOC 0.7104 0.7144

4.2 Results

Results of optimization are shown as Table 4.

The objective function and mass constraint are represented by normalized value. Design variable $x_1$ goes to lower boundary and mass is same as current design mass. Objective function is increased by 5.12%.

Using these optimum design variables, we simulate the HEV simulation model using HWFET (Highway Fuel Economy Test) cycle. Final value of SOC is increased from 0.7104 to 0.7144.

Figure 3: State of charge of HEV simulation using HWFET driving cycle

5 Conclusion

In this research, we performed HEV simulation model using electrochemical lithium-ion battery model and using this HEV simulation we carried out design optimization of lithium-ion battery. Through this design optimization, we derive high performance battery design.

1) Analysis of variance to select the most influential parameters as design variables are performed and 4 parameters are selected as design variables.

2) Using HEV simulation and design of experiment based surrogate model, optimization of lithium-ion battery is performed.

3) Through the optimization process, 5.12% of battery performance is increased under the same mass and the battery performance is confirmed using driving cycle.

References


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