Lithium-Ion Battery Models and Thermal Coupling in LS-DYNA®

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Abstract

We have developed two Lithium-ion battery models in LS-DYNA®: i) a single insertion lithium metal model, and ii) a dual insertion composite model. Our models are intended to assist users in tackling problems ranging from the fundamental battery cell physics to very complex situations such as thermal management (TM) of electric vehicle (EV), and eventually, battery-structure-interaction (BSI) problems. The battery models in LS-DYNA® are based on the following multiphysics aspects: 1) thermodynamics, 2) kinetics, and 3) transport. In thermodynamics, the role of electrochemical potential, which is the driving force in the concentrated solution will be discussed, and an example will be provided as to how to set up the open-circuit potential card in the keyword input. Detailed presentation of Bulter-Volmer kinetics illustrates how to correctly evaluate the surface overpotential at the interface between electrode and electrolyte, and also the pore-wall flux from the insertion materials in compsite electrodes. In addition, comprehensive keyword set up for the transport properties in both aqueous and polymer electrolyte will be provided, including the concentrated material transport theory. For the thermal treatment of the battery model, we have coupled with existing thermal solver and structure solver and thus, we will present a keyword example showing how to simulate a thermal problem in a battery cell stack, module and pack in the practical scaled-up EV application. Finally, we will provide the future development plan to handle more complex problems confronting the battery related industries by using BSI solver in LS-DYNA®.

1 Introduction

Lithium batteries have been the subject of many studies including thermal treatment because of their high theoretical energy densities, fewer environmental issues on disposal process, and less toxic than lead acid cells. An increasing demand for the development of high energy density, power density, and long-life cycle is required for portable electronics, especially mobile phones, and EV including hybrid electric vehicles (HEV). The use of modeling and simulation in the design of batteries is indispensable since once validated experimentally, it can be used to optimizing design parameters, filttering unnecessary factors out, and identifying the optimal operating performance for the final designs. In addition, mathematical modeling allows the designer to explore a wide variety of system parameters with a minimum expenditure of time and materials. Howver, the ability of the battery model depends on the knowledge of the experimental data that are input to the model. For example, if much of the transport and thermodynamic data needed in the model are unknown, then it is unlikely that the model will give good results, especially when extrapolating outside the ranges of explored behavior.

Recently, we. have developed lithium-ion battery models in LS-DYNA®. Our models are based on the thermodynics, kinetics, and concentrated solution transport theories in poros composite electrodes called a single insertion lithium metal model and a dual insertion composite model. These LS-DYNA® models are intended to assist users in tackling problems ranging from the fundamental battery cell physics to very complex situations such as thermal management (TM) of EV, and internal response of the battery via battery-structure-interaction models. To this end, we have designed detailed keywords for the electrodes, electrolytes, transport material properties, and even thermal couplings for such applications

2 Battery Models

The models that we develop here are intended to be sufficiently general to apply to many of the different specific systems that allow user's various applications. Thus, based on Doyle's studies [1-2], our models consist of two main classes of lithium cells: a single insertion reaction with a solid lithium on the other electrode, and a cell using two different insertion reactions, the so-called dual lithium-ion insertion cell or "rocking-ehair" cell as shown in figure 1. The negative electrode on the left is either a solid lithium foil or an insertion-type electrode, respectivley while the positive electrode, on the right, is in both cases an insertion-type electrode. All of the insertion electrodes are configured as porous electrodes. The electrolyte is assumed to consist of a single salt in a single solvent in both cases with

the concentrated solution theory. In both models, the cell can be theoretically divided into three regions: the negative electrode, separator, and positive electrode.
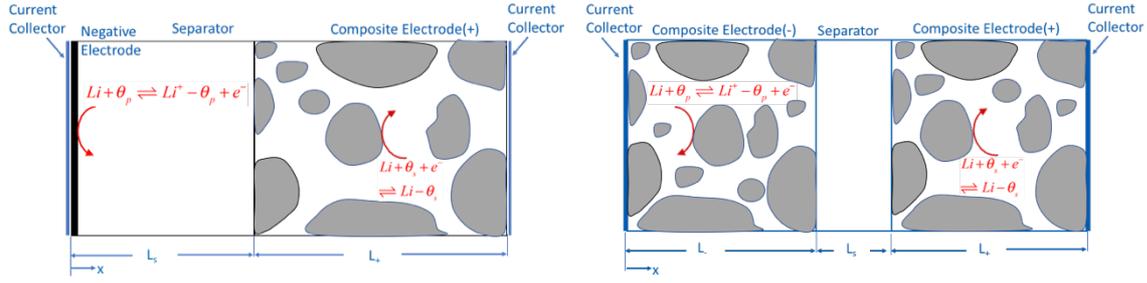
Fig. 1: Lithium insertion cells. (a) a single insertion cell, and (b) a dual insertion cell

2.1 Electrochemical equations

Transport in the separator is modelled with concentrated solution theory, assuimg a binary electrolyte and solvent. A material balance and potential in solution are given as,

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{v}_0) = \nabla \cdot \left\{ D(c) \left[1 - \frac{d \ln c_0}{d \ln c} \right] \nabla c \right\} - \frac{\mathbf{i}_2 \cdot \nabla t_+^0}{z_+ \nu_+ F}$$

(2)

$$\nabla \Phi = -\frac{\mathbf{i}}{\kappa(c)} + \frac{2RT}{F} \left[1 + \frac{d \ln f_\pm}{d \ln c} \right] (1 - t_+^0) \nabla \ln c$$

(3)

The corresponding sets of equations in the composite electrode are,

$$\varepsilon \frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{v}_0) = \nabla \cdot \left\{ \varepsilon D(c) \left[1 - \frac{d \ln c_0}{d \ln c} \right] \nabla c \right\} - \frac{\mathbf{i}_2 \cdot \nabla t_+^0}{z_+ \nu_+ F} + \frac{a j_n (1 - t_+^0)}{\nu_+}$$

(4)

For the potential in solution and particle electrode,

$$\nabla \Phi_2 = -\frac{\mathbf{i}_2}{\kappa_{eff}(c)} + \frac{2RT}{F} \left[1 + \frac{d \ln f_\pm}{d \ln c} \right] (1 - t_+^0) \nabla \ln c$$

(5a)

$$\nabla \Phi_1 = -\frac{\mathbf{i}_1}{\sigma_{eff}(c)}$$

(5b)

Here subscript 1 stands for electrode and 2 for solution. For a single electrode reaction of the form is given as,

$$\sum_k s_k M_k^z \qquad ne^-$$

(6)

The pore wall flux from the solid electrode can be equal to the divergence of the current density in the solution phase.

$$a j_{+n} = -\frac{s_+}{nF} \nabla \mathbf{i}_2$$

(7)

In the above equations, c is the lithium ion concentration, D is the diffusion coefficient, I is the current density, t is the transport number, k is the conductivity in electrolyte, e is the volume fraction, jn is the pore wall flux at $r=R_s$. More details on the governing variables can refer in keyword manuals.

2.2 Solid electrode equations

The kinetics equation in the interface between the electrodes and electrolytes is Bulter-Volmer equation.

$$\frac{\partial c_s}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_s r^2 \frac{\partial c_s}{\partial r}\right)$$

(8)

With the boundary conditions as,

$$\left.\frac{\partial c_s}{\partial r}\right|_{r=0} \text{ and } \left.-D_s\frac{\partial c_s}{\partial r}\right|_{r=R} = -j_{+n}$$

2.3 Kinetics equations

The kinetics equation in the interface between the electrodes and electrolytes is Bulter-Volmer equation.

$$I = Fj_n = i_{0,k}\left\{\exp\left(\frac{\alpha_{a,k}F\eta_{s,k}}{RT}\right) - \exp\left(-\frac{\alpha_{c,k}F\eta_{s,k}}{RT}\right)\right\}$$

(9)

where, the over potential is given as,

$$\eta_{s,k} = \Phi_1 - \Phi_2 - U_k$$

(10)

2.4 Themal equations

The general governing equation in thermal solver is the heat conduction equation and is given as,

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(k\nabla T) + \langle q \rangle$$

(11)

where ρ is density, c_p the specific heat, T temperature, and t time, respectively. $\langle q \rangle$ is the average heat generation in each cell.

3 Keywords

The keywords related for the cell battery models:

*BATTERY_ECHEM_CONTROL_SOLVER
*BATTERY_ECHEM_PART
*BATTERY_ECHEM_MAT_ANODE
*BATTERY_ECHEM_MAT_CATHODE
*BATTERY_ECHEM_MAT_ELECTROLYTE
*BATTERY_ECHEM_THERMAL

The keywords related for the thermal solver in LS-DYNA®:

*CONTROL_THERMAL_SOLVER
*CONTROL_THERMAL_TIMESTEP
INITIAL_TEMPERATURE_*option
BOUNDARY_TEMPERATURE_*option
*MAT_THERMAL_BATTERY

4 Preliminary results

Fig. 2 shows a) the cell potential as function of utilization of cathode material for galvanostatic chargeing. b) concentration profiles in a single cell insertion model through cell domain for 2 hours, and c) the temperature profiles as function of time for discharge of a 144 cell-stack for about 3 hours, with a heat generation calculated from isothermal cell model and the convective heat transfer boundary condition in 1D unsteady thermal solver.

a)   b)   c)
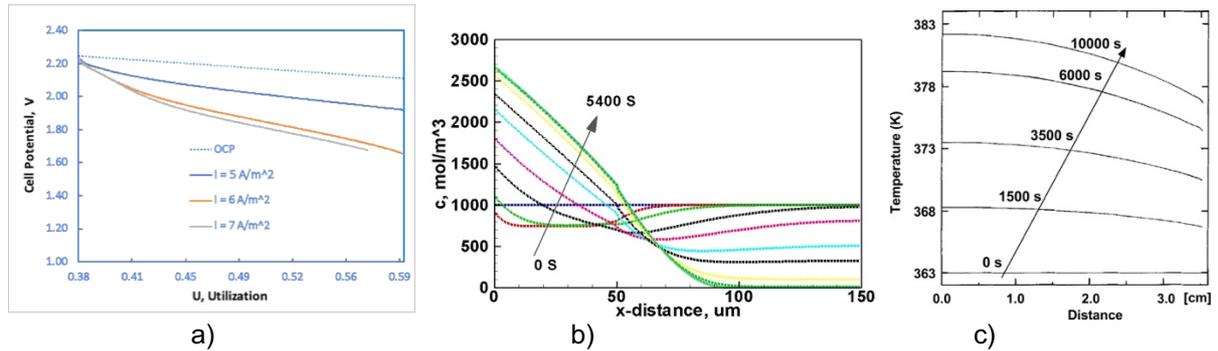
Fig2: Preliminary results: a) Cell potential vs the utilization of the active material in composite electrode, b) concentration profiles as function of time, and c) temperature profiles as a function of time for the sample EV battery.

5 Summary

We have developed Lithium-ion battery models in LS-DYNA®. The current models are coupled with existing thermal and structure solver in LS-DYNA®. With these battery models, users will be able to simulate their battery model and to be assisted to tackle design problems from the starting to final processes in the area of the EV, HEV, even portable electronics. Nothe that battery models in LS-DYNA® are based on the thure multiphysics: 1) thermodynamics, 2) kinetics, and 3) charged ion transport in conjuction with detailed keyword descriptions For the thermal treatment, we demonstrated how to couple with existing thermal and FEM solver. Thereore, it is strongly believed that the current developed model will help for users to design and simulate theris problems.

6 Reference

[1] Doyle, M., Fuller, T. F., and Newman, J., "Modeling of Galvanostatic Charge and Discharge of the Lithium/Polymer/Insertion Cell", J. Electrochem. Soc., Vol. 140, No. 6, 1993, pp1526-1533.
[2] Fuller, T. F.,Doyle, M., and Newman, J., "Simulation and Optimization of the Dual Lithium Ion Insertion Cell", J. Electrochem. Soc., Vol. 141, No. 1, 1994, pp1-10.