TRA445 Advanced battery modelling and control

Tutorial on thermal modelling

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Introduction

In this tutorial, you will extend the SPM by incorporating a lumped thermal model to account for temperature effects in lithium-ion batteries. Temperature plays a crucial role in battery dynamics, influencing parameters such as diffusion coefficients, reaction kinetics, and open-circuit potentials, which can impact battery performance, ageing, and safety. The lumped thermal model assumes a uniform cell temperature and considers heat generation from reversible entropic effects, reaction kinetics, and ohmic losses, while also accounting for heat dissipation through heat transfer by convection. By coupling this thermal model with the SPM, you will observe how temperature variations affect battery dynamics, i.e. concentrations and temperature are coupled. The implementation will involve updating temperature-dependent parameters dynamically and integrating the energy balance equation alongside the electrochemical states. This approach allows for better predictions of battery states and highlights the importance of thermal management in modern energy storage systems.

Part 1: numerical method

Following on from the last tutorial, let's first plot the radial concentration profiles of anode and cathode, respectively.

```
    r1  = linspace(0, para.Rs1, para.Nr_anode+1);
    r3  = linspace(0, para.Rs3, para.Nr_cathode+1);
    for k = 1:2:length(t_sol)
        subplot(2,1,1);
        plot(r1, c_n_all(k,:), 'LineWidth', 5);
        ylabel('c_s (mol/m^3)');
        xlim([0 para.Rs1]);
        ylim([0 para.cs1_max]);
        set(gca, 'XColor', 'k', 'YColor', 'k');

        subplot(2,1,2);
        plot(r3, c_p_all(k,:), 'LineWidth', 5);
        ylabel('c_s (mol/m^3)');
        xlim([0 para.Rs3]);
        ylim([0 para.cs3_max]);
        set(gca, 'XColor', 'k', 'YColor', 'k');
        drawnow;
    end
```

Observe that the concentration at $r = 0$ is not updating. What is wrong?

Well, in our first attempt during the last tutorial to enforce the symmetry condition, i.e.,

$$\frac{\partial c}{\partial r}\Big|_{r=0} = 0$$

we have taken an naive approach in the finite differencing scheme by setting the concentration flux dc/dt to zero. However, this will not update the concentration at r = 0 over time because of the discrete nature of the finite-difference scheme, we need to incorporate the Neumann boundary condition more carefully.

A common approach is to use a ghost node that leverages symmetry. For example, you can start by introducing a ghost node at $r = -\Delta r$.

In a spherically symmetric system, the concentration is even about $r = 0$. Thus,

$$c(-\Delta r) = c(\Delta r).$$

Define:

$$c_0 \equiv c(-\Delta r) = c_2,$$

where c_0 represents the concentration at $r = -\Delta r$ and c_2 at $r = \Delta r$.

Task 1:

1. In the SPM code from the last computer lab, find the line of code that directly sets the time derivative to zero and prevents the node at $r = 0$ from updating.
2. Derive the scheme for the updating of that node. Hint:

$$\frac{dc_i}{dt} = D\left(\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta r^2} + \frac{1}{r_i}\frac{c_{i+1} - c_{i-1}}{\Delta r}\right).$$

Implement this scheme and plot the correct concentration profiles v.s. particle radius.

Part 2: Concentration relaxation

Observe that the surface concentration may exceed the stoichometry limits.

Task 2:

1. Discuss why the surface concentration exceeds the limits and what is it depedent on.
2. Simulate the relaxation and plot the concentration profiles.
3. Calculate the average concentration
4. Compared the average concentrations at the end of 1C and 4C charge, when curoff voltage is set to 4.2V

Part 3: SPM-thermal coupled model

By adding a bulk/lumped thermal model to the single-particle framework, we capture the essential thermal dynamics of the cell without resorting to a full 3D heat conduction and convection model. This approach is suitable when there's no large thermal gradients developed. The inclusion of temperature enables more accurate predictions of battery performance, life, and safety because of the strong dependence of electrochemical processes on temperature.

Task 1: Considering 4 temperature-dependent parameters, i.e. diffusion coefficients and reaction rate constants, write the new parameters based according to the Arrhenius equation (slide 48 of lecture note).

To do this, you need four activation enegies:

```
para.Ea_Ds1 = 35e3;          % Activation energy for anode diffusion [J/mol]
para.Ea_Ds3 = 29e3;          % Activation energy for cathode diffusion [J/
mol]

para.Ea_k1 = 20e3;           % Activation energy for anode reaction rate [J/
mol]
para.Ea_k3 = 58e3;           % Activation energy for cathode reaction rate
[J/mol]
```

Task 2: Couple the temperature dynamics with the concentration dynamics of SPM by calculating dT/dt and include it in the function *spm_ode_system*

$$\rho c_p \frac{dT}{dt} = \dot{q}_{\text{gen}} - \dot{q}_{\text{conv}}$$

In this coupled model, we also consider the OCPs to be temperature-dependent. We start by defining the fitting functions in the reversible heat generation term

```
% Define the fitting coefficients
c1_num = [-16515.05308;38379.18127;-37147.89470;19329.75490;...
        -5812.27813;1004.91101;-91.79326;3.29927;0.00527];
c1_den = [165705.85970;-385821.16070;374577.31520;-195881.64880;...
        59431.30001;-10481.80419;1017.23480;-48.09287;1];
c3_num = [0; 0.61154; -1.36455; 0.92837; -0.19952];
c3_den = [3.04876; -9.82431; 11.47636; -5.66148; 1];

% Create dU/dT(theta) functions
dU1dT = @(x1) 1e-3 * (polyval(c1_num(1:7), x1) ./ polyval(c1_den(1:7),
x1)); %anode
dU3dT = @(x3) 1e-3 * (polyval(c3_num, x3) ./ polyval(c3_den,
x3));           %cathode
```

and a few parameters related to cell geometry and heat transfer by convection:

```
para.Cp     = 750;                  % Heat capacity [J/kg/K]
para.rho    = 1626;                 % Density [kg/m3]

para.height =   65e-3;                % 18650 height [m]
para.diam   =   18e-3;               % 18650 diameter [m]

% Surface area to volume ratio for an 18650 cell [m-1]
para.SA_V   =   4*(1 + para.diam/para.height/2)/para.diam;
% Volume of the cell
para.Vc     =   pi*(para.diam/2)^2*para.height;

% Convective boundary condition
para.h      =   30;         % Convection heat transfer coefficient
[W/m2/K]
para.T_amb  = 25 + 273.15;  % Ambient temperature [K]
```

Hint:

- To include the temperature as a state, one has to expand the initial condition x_0 which was composed of anode and cathode concentrations. Similarly the x in the function *spm_ode_system* also needs to be expanded to include temperature as a state.
- For the reaction term in the heat generation, overpotentials have to be calculated. You have done this already in the function *compute_terminal_voltage*
- The reference temperature is defined as 25 degree celsius at room temperature. You need to convert this to Kelvin in the calculations.

Task 3: Plot temperature v.s. capacity for 1C and 4C. Compare them and discuss the temperation variations.