

Thermal Modelling of a Cylindrical 2.3Ah LiFePO4 Battery

We would like to calculate the temperature in the Li-ion battery as a function of time. The parabolic equation describing heat transfer is

$$\rho C \frac{\partial u}{\partial t} - \nabla \cdot (k \nabla u) = q,$$

where ρ , C , and k are the density, specific heat, and thermal conductivity of the material, respectively, u is the temperature, and q is the heat generated in the battery.

Since the problem is axisymmetric, it is convenient to write this equation in a cylindrical coordinate system.

$$\rho C \frac{\partial u}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(kr \frac{\partial u}{\partial r} \right) - \frac{1}{r^2} \frac{\partial}{\partial \theta} \left(k \frac{\partial u}{\partial \theta} \right) - \frac{\partial}{\partial z} \left(k \frac{\partial u}{\partial z} \right) = q,$$

where r , θ , and z are the three coordinate variables of the cylindrical system. Because the problem is axisymmetric, $\partial u / \partial \theta = 0$ and after multiplying by r the equation can be rewritten as

$$r \rho C \frac{\partial u}{\partial t} - \frac{\partial}{\partial r} \left(kr \frac{\partial u}{\partial r} \right) - \frac{\partial}{\partial z} \left(kr \frac{\partial u}{\partial z} \right) = r q.$$

The equation can be converted to the form supported by PDE Toolbox if r is defined as y and z is defined as x . Rewriting the above equation gives

$$\rho C y \frac{\partial u}{\partial t} - \nabla \cdot (ky \nabla u) = qy.$$

The boundary conditions contain Dirichlet type, where the temperature on the boundary is specified, or Neumann type where the heat flux is specified. The generalized Neumann boundary condition equation is

$$\vec{n} \cdot (k \nabla u) + qu = g$$

The equation can be rewritten as temperature expression

$$\vec{n} \cdot (k \nabla T) + qT = g$$

Convection and radiation heat transfer have been applied on surface of battery and zero heat flux (zero Neumann boundary) has been applied on axial-symmetry in this study using generalized Neumann boundary condition equation.

Optimized parameters have been used to obtain results.

Simulation results have been compared with experimental results in this study.

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experimental power data (W) is used in this study calls @expfcoef function mfile

```
addpath( 'functions' );

clearvars -global -except rad* leng* irad* lengActive* thickAlu* thickGas* vol*
clear;
clc;
close all;
load('HeatPower.mat')
load TempDataMaccor
load TempDataPCB
```

Geometry Properties

```
global rad leng irad radActive lengActive thickAlu thickGas vol HeatPowerExp mymodel Ta mesh

rad = 1.3e-2; % battery radius meter(m)
thickAlu = 0.4e-3; % thickness of aluminum case (m)
irad = 1.65e-3; % inner tube's radius (m)
radActive = rad - 1*thickAlu; % active material's radius (m)
leng = 6.5e-2; % length of battery (m)
thickGas = 0.005; % thickness of gas insulator (m)
lengActive = leng - 2*(thickAlu+thickGas); % active material's length (m)
vol = pi*lengActive*(radActive^2 - irad^2); % active volume (m^3)
```

Experimental Plots

```

HeatPower1(:,1) = HeatPower(43000:51000,1) - HeatPower(43000,1); % Measurement time
HeatPower1(:,2) = HeatPower(43000:51000,2); % Power = I * eta

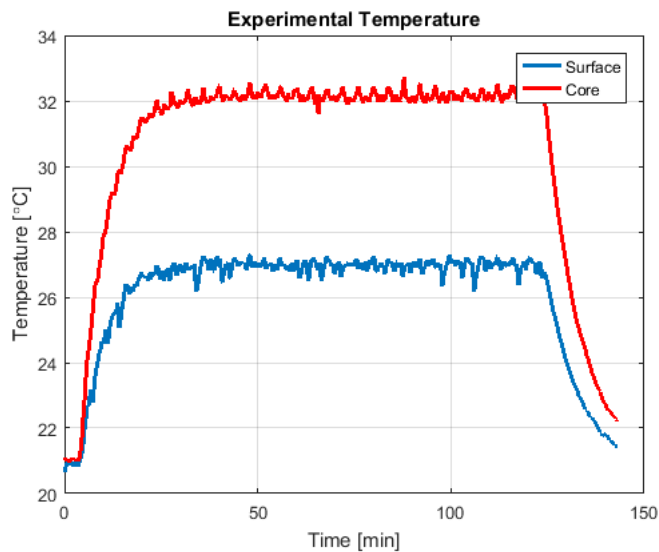
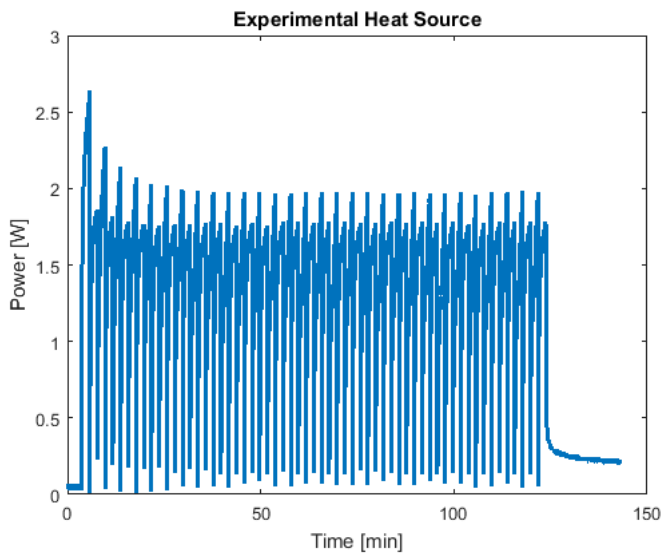
HeatPowerExp = HeatPower1;

figure;
plot( HeatPowerExp(:,1)./60 , HeatPowerExp(:,2) , 'LineWidth' , 2 );
xlabel('Time [min]');
ylabel('Power [W]');
title('Experimental Heat Source')

TempSurf = TempDataMaccor(43000:51000,3);
TempCore = TempDataMaccor(43000:51000,2);

figure;
plot( HeatPowerExp(:,1)./60 , TempSurf , ...
      HeatPowerExp(:,1)./60 , TempCore , 'r' , 'LineWidth' , 2 );
xlabel('Time [min]');
ylabel('Temperature [\textcircled{C}]');
title('Experimental Temperature');
legend( 'Surface' , 'Core' );
grid on

```



Create The PDE Model

```

mymodel = createpde; % for 1 equation

P1 = [2,8,...
      thickAlu, (leng-thickAlu), (leng-thickAlu), leng-(thickAlu+thickGas), leng-(thickAlu+thickGas), (thickAlu+thickGas), (thickAlu+thickGas), thickAlu,...
      0, 0, (rad-thickAlu), (rad-thickAlu), irad, irad, (rad-thickAlu), (rad-thickAlu)];

R2 = [3, 4, 0, leng, leng, 0, 0, 0, rad, rad]; % aluminum case
R2 = [R2,zeros(1,length(P1) - length(R2))];

R3 = [3, 4, (thickAlu+thickGas), leng-(thickAlu+thickGas), leng-(thickAlu+thickGas), (thickAlu+thickGas), irad, irad, (rad-thickAlu), (rad-thickAlu)];
R3 = [R3,zeros(1,length(P1) - length(R3))]; % active domain

gdm = [P1;R2;R3]';

```

```

sf = '(P1+R2+R3)';
ns = char('P1','R2','R3');
ns = ns';
[d1,bt] = decsg(gdm,sf,ns);
geometryFromEdges(mymodel,d1);

% [d12,bt2] = csgdel(d1,bt); % remove subdomain

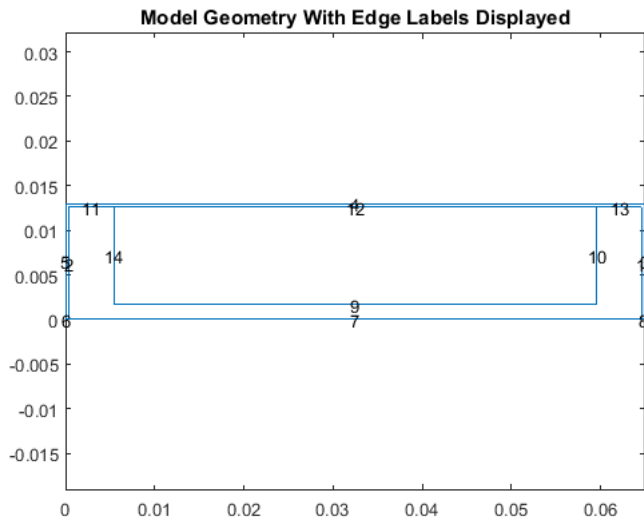
```

Geometry of Battery

```

figure;
pdegplot(mymodel,'edgeLabels','on');
title('Model Geometry With Edge Labels Displayed');
axis equal;

```

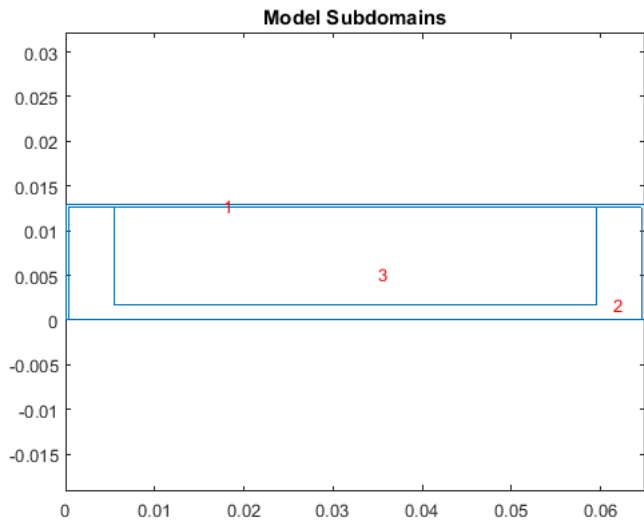


Subdomains Plot

```

figure;
pdegplot(mymodel,'SubdomainLabels','on');
title('Model Subdomains');
axis equal;

```

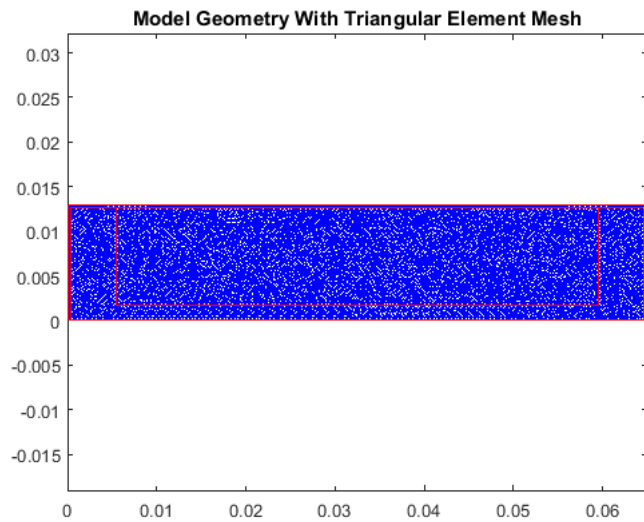


Generate Mesh

```

hmax = 0.0004; % control mesh density
mesh = generateMesh(mymodel,'Hmax',hmax,'GeometricOrder','linear','Jiggle','on');
figure;
pdeplot(mymodel);
title('Model Geometry With Triangular Element Mesh');
axis equal;

```



Material Properties

```
% Active(positive electrode + separator + negative electrode) material
kActive = 0.5548; % W/m*K % thermal conductivity of active metal
CpActive = 958; % J/kg*K % heat capacity of active material
rhoActive = 2000; % kg/m^3 % density of active material

% Aluminum
kAlu = 238; % W/m*K % thermal conductivity of aluminum %1.7602;
CpAlu = 903; % J/kg*K % heat capacity of aluminum
rhoAlu = 1500; % kg/m^3 % density of aluminum

% Assumed gas(air) in tubes
kGas = 0.025; % W/m*K % thermal conductivity of gas
CpGas = 1.005; % J/kg*K % heat capacity of gas
rhoGas = 1.205; % kg/m^3 % density of gas
```

System Constants

```
kelvin = 273.15;
Ta = 20 + kelvin; % ambient temperature (K)
hCoef = 20; % heat transfer coefficient (W/m^2/K)
emissivity = 0.65; % emissivity coefficient for radiation heat transfer
stefanBoltzmann = 5.67e-8; % stefan-boltzmann constant
```

Insert Optimized Values

```
load x5.mat;

p.ini = x5;
```

Specify Coefficients

```
m = 0; % common coefficient for all domains
a = 0; % common coefficient for all domains

cActive = @(region,~) p.ini(1) * region.y; % 'c' coefficient for active domain
dActive = @(region,~) p.ini(3) * p.ini(2) * region.y; % 'd' coefficient for active domain

cAlu = @(region,~) p.ini(4) * region.y; % 'c' coefficient for aluminum case
dAlu = @(region,~) p.ini(6) * p.ini(5) * region.y; % 'd' coefficient for aluminum case

cGas = @(region,~) p.ini(7) * region.y; % 'c' coefficient for air
dGas = @(region,~) p.ini(9) * p.ini(8) * region.y; % 'd' coefficient for air

% Call heat source function
f = @expfcoef;

% Specify Coefficient for each subdomain
specifyCoefficients(mymodel, 'm', m, 'd', dAlu, 'c', cAlu, 'a', a, 'f', 0, 'face', 1);
specifyCoefficients(mymodel, 'm', m, 'd', dGas, 'c', cGas, 'a', a, 'f', 0, 'face', 2);
specifyCoefficients(mymodel, 'm', m, 'd', dActive, 'c', cActive, 'a', a, 'f', f, 'face', 3);
```

Boundary Conditions

```
gb = @(region,state) region.y .* ( p.ini(10) * Ta + stefanBoltzmann * p.ini(11) * Ta^4 );
qb = @(region,state) region.y .* ( p.ini(10) + stefanBoltzmann * p.ini(11) * state.u.^3 );

% Apply boundary condition on edges for cooling
applyBoundaryCondition(mymodel, 'Edge', 6, 'g', 0, 'q', 0);
applyBoundaryCondition(mymodel, 'Edge', 7, 'g', 0, 'q', 0);
applyBoundaryCondition(mymodel, 'Edge', 8, 'g', 0, 'q', 0);
applyBoundaryCondition(mymodel, 'Edge', 3, 'g', gb, 'q', qb);
```

```
applyBoundaryCondition(mymodel,'Edge',4,'g','gb','q',qb);
applyBoundaryCondition(mymodel,'Edge',5,'g','gb','q',qb);
```

Unsteady State Condition

```
tlist = HeatPowerExp(:,1);
T0 = 21 + kelvin; % initial temperature

% Set initial conditions
setInitialConditions(mymodel, T0);

% Set solver options
mymodel.SolverOptions.AbsoluteTolerance = 1e-8;
mymodel.SolverOptions.RelativeTolerance = 1e-4;
mymodel.SolverOptions.ResidualTolerance = 1e-5;
mymodel.SolverOptions.MaxIterations = 100;
mymodel.SolverOptions.MinStep = 1e-6;

% Simulate model
result = solvepde(mymodel, tlist);

% Get dependent variable result (temperature)
u = result.NodalSolution;
```

Result and Plot

```
% Get a node near the specific point using helper function
getClosestNode = @(p,x,y) min((p(1,:) - x).^2 + (p(2,:) - y).^2);

% Call this function to get a node
[~,nid] = getClosestNode( mesh.Nodes, leng/2, 0 );

% Core Temperature Node
[~,nid1] = getClosestNode( mesh.Nodes, leng/2, 0 );

% Surface Temperature Node
[~,nid4] = getClosestNode( mesh.Nodes, leng/2, rad );

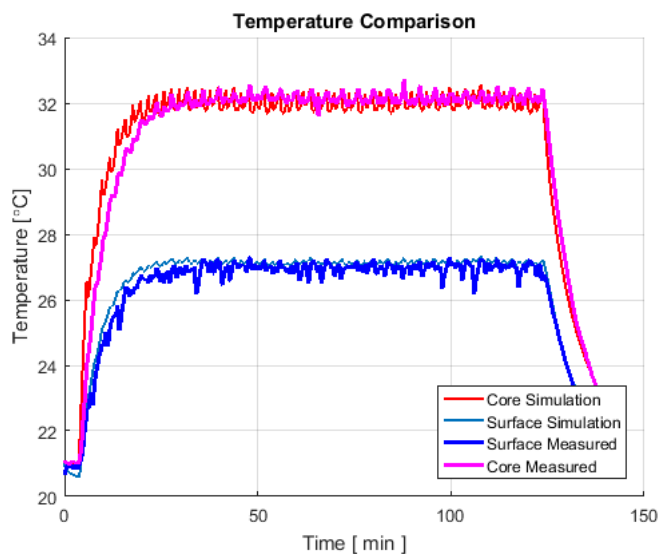
% Plot of temperature comparisons at different locations

% Core & Surface Temperature of Simulation
TempCoreSim = u(nid1,:) - kelvin;
TempSurfSim = u(nid4,:) - kelvin;

figure;
hold on;

plot(tlist./60, TempCoreSim, 'r', 'LineWidth',1.5);
plot(tlist./60, TempSurfSim, 'LineWidth', 1.5);
plot( HeatPowerExp(:,1)./60, TempSurf, 'b', ...
      HeatPowerExp(:,1)./60, TempCore, 'm', 'LineWidth', 2 );

xlabel('Time [ min ]');
ylabel('Temperature [\textcircled{C}]');
title('Temperature Comparison');
legend( 'Core Simulation', 'Surface Simulation', 'Surface Measured', 'Core Measured', 'Location', 'SouthEast' );
grid on;
```



Error Analysis

```
% Absolute Difference of Measured and Simulation Temperature
diffCore = abs(TempCore' - TempCoreSim);
diffSurf = abs(TempSurf' - TempSurfSim);

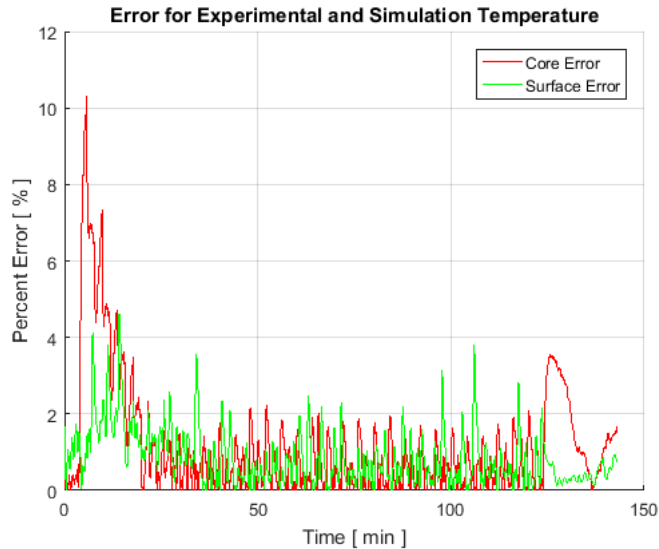
% Percent Error
```

```

errorCore = (diffCore./TempCoreSim)*100;
errorSurf = (diffSurf./TempSurfSim)*100;

figure;
hold on;
plot(tlist./60, errorCore,'r', 'LineWidth', 1);
plot(tlist./60, errorSurf,'g', 'LineWidth', 1);
xlabel('Time [ min ]');
ylabel('Percent Error [ % ]');
legend('Core Error', 'Surface Error');
title('Error for Experimental and Simulation Temperature');
grid on;

```



Two plots are useful in understanding the results from this transient analysis. The first is a plot of the maximum heating and temperature during the simulation. The second is a plot of the temperature at core in the battery

```

% Get Maximum Temperature
maxT = max(u') - kelvin;

s = figure;
s.Position = [1 1 2 1].*s.Position;

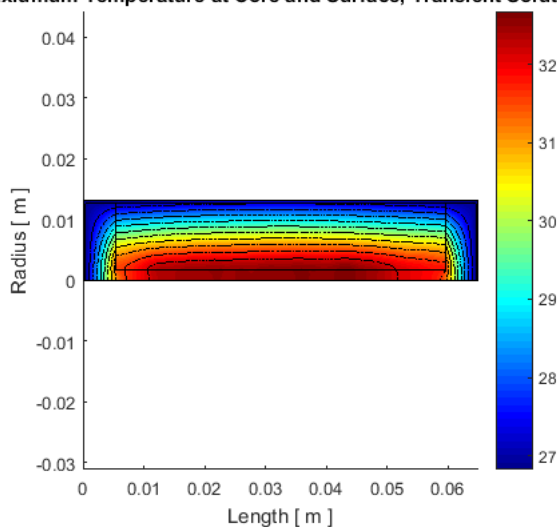
subplot(1,2,1);
pdeplot(mymodel,'xydata',maxT,'contour','on','colormap','jet');
title('Maximum Temperature at Core and Surface, Transient Solution');
xlabel('Length [ m ]');
ylabel('Radius [ m ]');
axis equal;

subplot(1,2,2);
plot(tlist./60, (u(nid,:)-kelvin),'LineWidth', 1.5)
title('Temperature Changes at Core as a Function of Time');
xlabel('Time [ min ]');
ylabel('Temperature [ \circ C ]');
grid on;

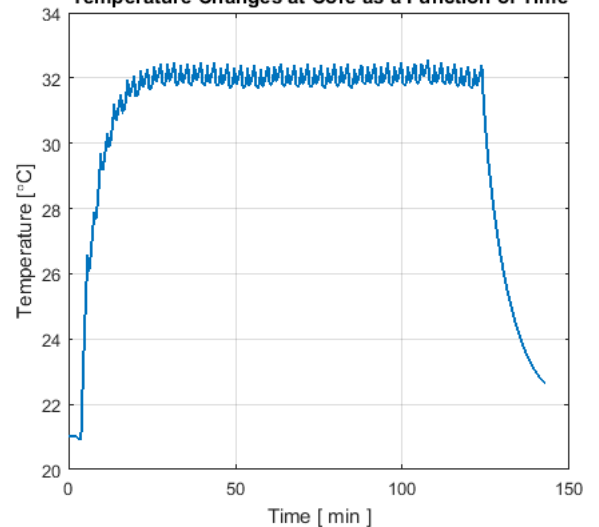
% The two plots are shown side-by-side in the figure below

```

Maximum Temperature at Core and Surface, Transient Solution



Temperature Changes at Core as a Function of Time



```
% model report on command window  
mymodel.SolverOptions.ReportStatistics = 'on'
```

```
mymodel =
```

```
PDEModel with properties:
```

```
    PDESystemSize: 1  
    IsTimeDependent: 1  
        Geometry: [1x1 AnalyticGeometry]  
EquationCoefficients: [1x1 CoefficientAssignmentRecords]  
    BoundaryConditions: [1x6 BoundaryCondition]  
    InitialConditions: [1x1 InitialConditionsRecords]  
        Mesh: [1x1 FEMesh]  
    SolverOptions: [1x1 PDESolverOptions]
```

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