Effect of a cell undergoing thermal runaway on the temperature of an adjacent cell

Group 9

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Governing Equation

In Cartesian Coordinates :

$$\rho\, c_{\mathrm{p}} \frac{\partial T}{\partial t}(\mathbf{x}, t) = \kappa \Delta T(\mathbf{x}, t) + Q_{\mathrm{gen}}(\mathbf{x}, t)$$

In Polar Coordinates :

$$\frac{\partial(\rho_{\mathrm{batt}} c_{\mathrm{p,batt}} T)}{\partial t} - \left(\frac{1}{r}\frac{\partial}{\partial r}\left(\kappa_{\mathrm{T,rad,batt}}\, r \frac{\partial T}{\partial r}\right) + \kappa_{\mathrm{T,z,batt}} \frac{\partial^2 T}{\partial z^2}\right) = Q_{\mathrm{gen}}$$

Boundary and Initial Conditions

In Cartesian Coordinates :

$$T(\mathbf{x},0) = T_0(\mathbf{x}),\ \forall \mathbf{x} \in \overline{\Omega},$$
$$\mathbf{n} \cdot (\kappa \nabla T) = -h(T - T_{\text{env}}) - \epsilon\sigma(T^4 - T_{\text{env}}^4),\ \forall \mathbf{x} \in \partial\Omega.$$

In Polar Coordinates :

$$T(r,z,0)=T_0$$

$$k\frac{\partial T}{\partial r} = -h(T - T_{env}) + \epsilon\sigma(T^4 - T_{env}^4)$$

Governing equations

Governing Equations for Modeling Thermal Runaway :

$$mc_p \frac{dT}{dt} = I^2 R_{in} + q_{exotherm}$$

Initial Condition :

$$T(0) = T_{env} = 293K$$

The $q_{exotherm}$ depends on the temperature of the cell.

Governing Equations for Modeling the Neighbouring Cell :

$$mc_p \frac{dS}{dt} = KA(\frac{T - S}{l}) + \sigma A(T^4 - S^4)$$

Initial Condition :

$$S(0) = T_{env} = 293K$$

Modeling thermal runaway

SEI film decomposition reaction

$$k_{\mathrm{SEI}}(T, c_{\mathrm{SEI}}) = A_{\mathrm{SEI}} \cdot \exp\left(-\frac{E_{a,\mathrm{SEI}}}{RT}\right) \cdot c_{\mathrm{SEI}}^{m_{\mathrm{SEI}}}$$

$$Q_{\mathrm{SEI}} = H_{\mathrm{SEI}} \cdot W_c \cdot k_{\mathrm{SEI}}$$

$$\frac{dc_{\mathrm{SEI}}}{dt} = -k_{\mathrm{SEI}}$$

Negative-Electrolyte reaction

$$k_{\mathrm{ne}}(T, c_{\mathrm{ne}}) = A_{\mathrm{ne}} \cdot \exp\left(-\frac{E_{\mathrm{a,ne}}}{RT}\right) \cdot c_{\mathrm{ne}}^{m_{\mathrm{ne}}} \cdot \exp\left(-\frac{t_{\mathrm{SEI}}}{t_{\mathrm{SEI,ref}}}\right)$$

$$\frac{dc_{\mathrm{ne}}}{dt} = -k_{\mathrm{ne}}$$

Positive-Electrolyte reaction

$$k_{\mathrm{pe}}(T, \alpha) = A_{\mathrm{pe}} \cdot \alpha^{m_{\mathrm{pe,1}}} (1-\alpha)^{m_{\mathrm{pe,2}}} \cdot \exp\left(-\frac{E_{\mathrm{a,pe}}}{RT}\right)$$

$$\frac{d\alpha}{dt} = k_{\mathrm{pe}}$$

Electrolyte decomposition reaction

$$k_{\mathrm{e}}(T, c_{\mathrm{e}}) = A_{\mathrm{pe}} \cdot c_{\mathrm{e}}^{m_{\mathrm{e}}} \cdot \exp\left(-\frac{E_{\mathrm{a,e}}}{RT}\right)$$

$$\frac{dc_{\mathrm{e}}}{dt} = -k_{\mathrm{e}}$$

Modelling Arrhenius equations

```
for i=1:nt
    if T(i)<378
        q=0;
    elseif T(i)>=378&&T(i)<393
        k1=(a1*c1*exp(-e1/(R*T(i))));
        q=w1*k1*h1;
        c1=c1+(-k1)*dt;
        if c1<0
            c1=0;
  elseif T(i)>=393&&T(i)<443
      k1=(a1*c1*exp(-e1/(R*T(i))));
      q1=w1*k1*h1;
      k2=(a2*c2*exp(-e2/(R*T(i))));
      q2=w2*k2*h2;
      q=q1+q2;
      c1=c1-k1*dt;
      c2=c2-k2*dt;
      if c1<0
          c1=0;
      end
      if c2<0
          c2=0;
      end
```

```
elseif T(i)>=443&&T(i)<473
    k1=(a1*c1*exp(-e1/(R*T(i))));
    q1=w1*k1*h1;
    k2=(a2*c2*exp(-e2/(R*T(i))));
    q2=w2*k2*h2;
    k3=(a3*c3*(1-c3)*exp(-e3/(R*T(i))));
    q3=w3*k3*h3;
    q=q1+q2+q3;
    c1=c1-k1*dt;
    c2=c2-k2*dt;
    c3=c3-k3*dt;
    if c1<0
        c1=0;
    end
    if c2<0
        c2=0;
    end
    if c3<0
        c3=0;
    end
```

```
else
    k1=(a1*c1*exp(-e1/(R*T(i))));
    q1=w1*k1*h1;
    k2=(a2*c2*exp(-e2/(R*T(i))));
    q2=w2*k2*h2;
    k3=(a3*c3*(1-c3)*exp(-e3/(R*T(i))));
    q3=w3*k3*h3;
    k4=(a4*c4*exp(-e4/(R*T(i))));
    q4=w4*k4*h4;
    q=q1+q2+q3+q4-(dt/(p*c))*(((I^2)*r)/(pi*81*4225*10^(-9)));
    c1=c1-k1*dt;
    c2=c2-k2*dt;
    c3=c3-k3*dt;
    c4=c4-k4*dt;
    if c1<0
        c1=0;
    end
    if c2<0
        c2=0;
    end
    if c3<0
        c3=0;
    end
    if c4<0
        c4=0;
    end
end
```

The constants for these equations are referred from the reference:

Modeling thermal runaway- Discretization

Discretized Temporal points for battery undergoing thermal runaway

```
T(i+1)=T(i)+(dt/(p*c))*(((I^2)*r)/(pi*81*4225*10^(-9))+(q)-((sigma/0.009)*(T(i)^4-T0^4))-h*(T(i)-T0));
```

Discretized temporal points for the neighboring cells

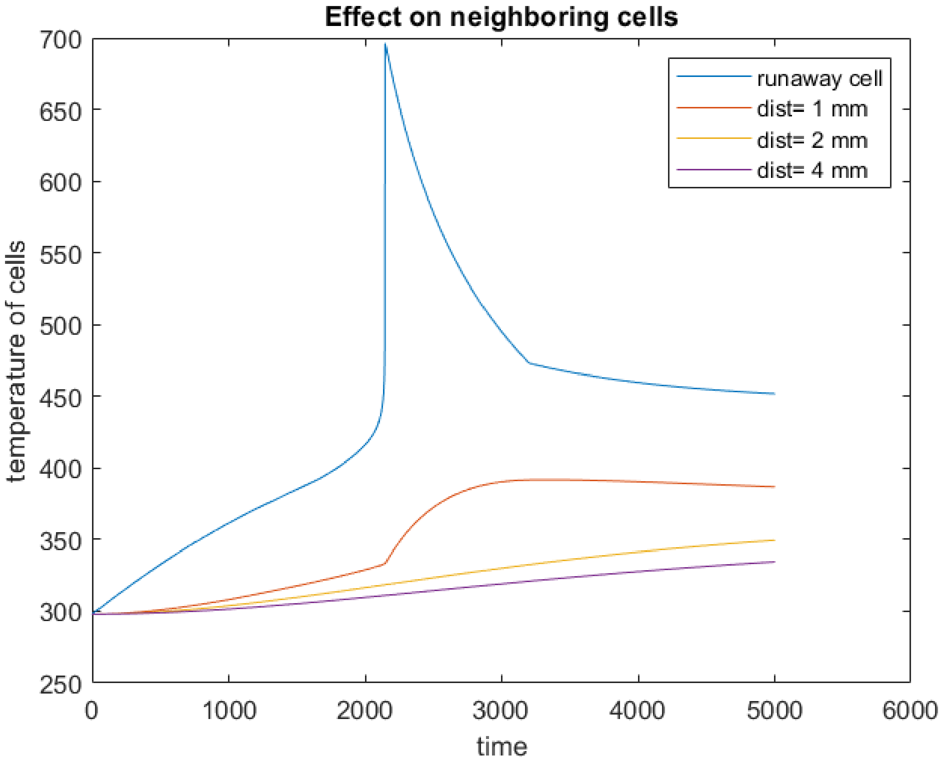
```
S(i+1)=S(i)+(dt*k/(c*p*l))*(T(i)-S(i))+(dt*sigma/(p*c*0.009))*(0.125*(T(i)^4-S(i)^4)-(S(i)^4-T0^4));
```

2D discretized equations

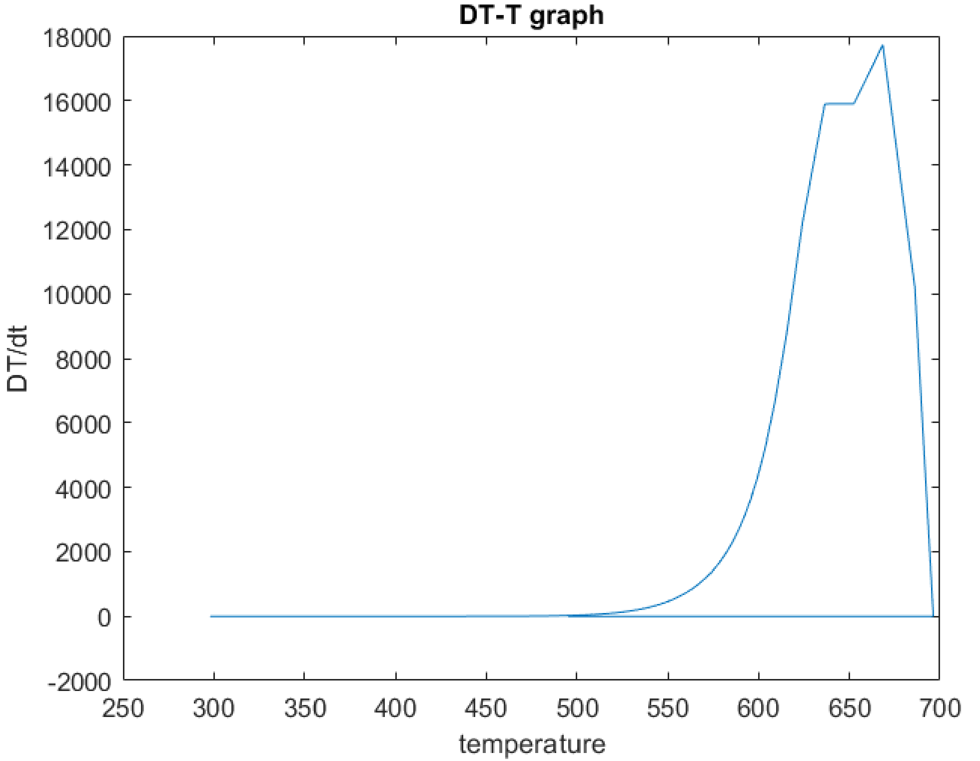
```
%interior points
for j=2:nx-1
  for k=2:ny-1
      F(j,k)=T(j,k)+(dt/(rho*cp))*((kr*(T(j+1,k)-2*T(j,k)+T(j-1,k))/(dx^2))+(kr*(T(j,k+1)-2*T(j,k)+T(j,k-1))/(dy^2)));
  end
end

%right boundary
for j=1:ny
  F(nx,j)=F(nx-1,j)-(dx/kr)*(h*(F(nx-1,j)-To)+((sigma)*(F(nx-1,j)^4-To^4)));
end
%left boundary
for j=1:ny
   F(1,j)=F(2,j)+(dx*lx/kr)*(q+i_eng)*0.5;
end
```

Results

Variation of temperature w.r.t time with different cell distances

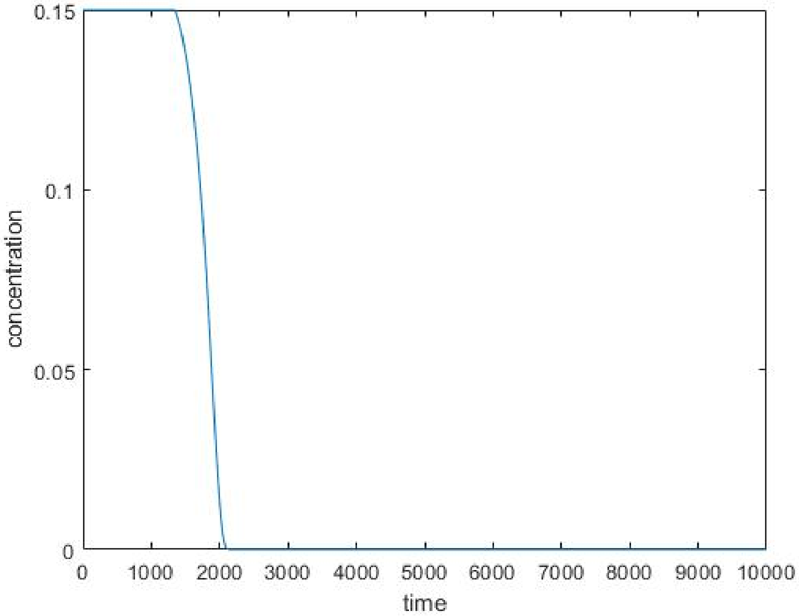


Rate of change of temperature to temperature for the cell undergoing runaway



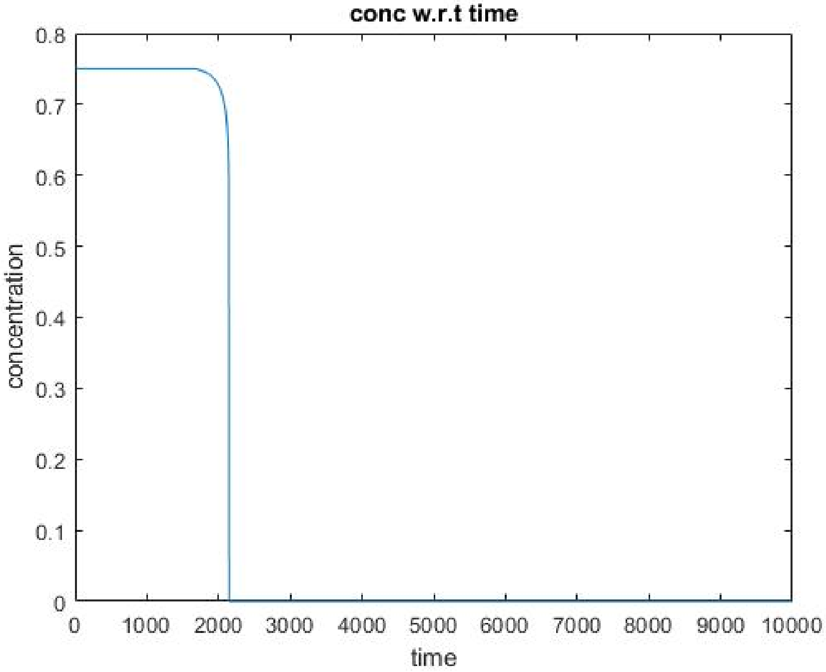
Variations of concentrations for reactions during thermal runaway

SEI decomposition reaction



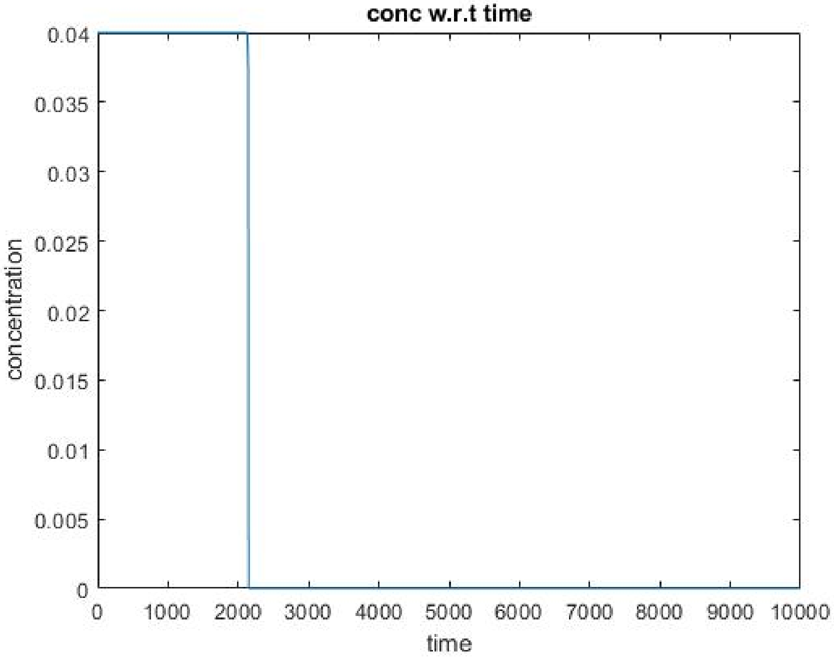
Variations of concentrations w.r.t for reactions during thermal runaway

Negative-Solvent reaction



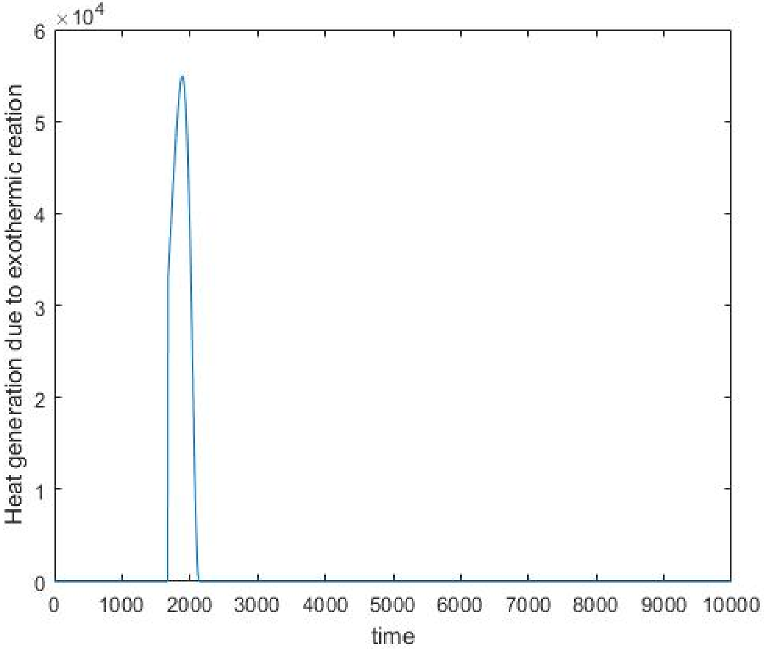
Variations of concentrations w.r.t time for reactions during thermal runaway

Positive Solvent reaction



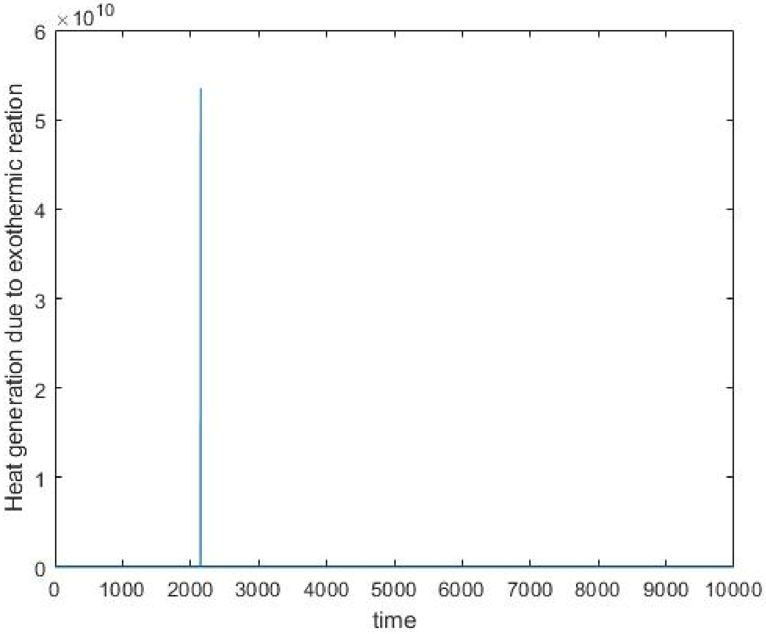
Heat Generation w.r.t time

SEI decomposition reaction



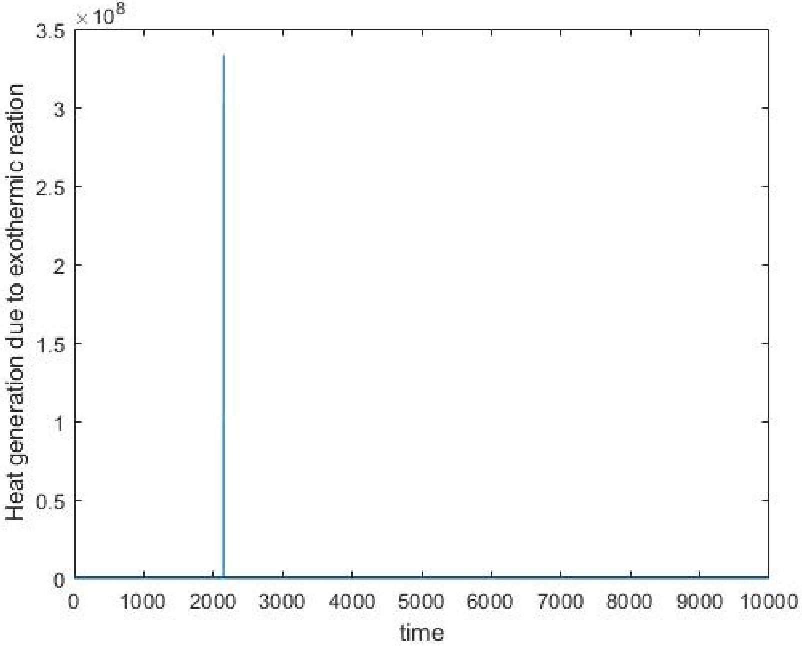
Heat Generation w.r.t time

Negative-Solvent reaction



Heat Generation w.r.t time

Positive Solvent reaction



References

- Modeling and Simulation of the Thermal Runaway in Cylindrical 18650 Lithium-Ion Batteries : Andreas Melcher* , Carlos Ziebert, Magnus Rohde, Boxia Lei, Hans Jürgen Seifert
- Experimental Analysis of Thermal Runaway and Propagation in Lithium-Ion Battery Modules : Carlos F. Lopez, Judith A. Jeevarajan, and Partha P. Mukherjee

Thank you