Electrochemical Cell Modeling

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This code regenerates results from 'Electrochemistry Based Battery Modeling For Prognostics' by Matthew Daigle and Chinmay S Kulkarni.

Battery Voltage 'V' (an algebraic equation) is given by,

$$V = V_{U,p} - V_{U,n} - V_o{}' - V_{\eta,p}{}' - V_{\eta,n}{}'$$

Where,

$$V_{U,i} = \text{Equilibrium Potential given by Nernst Equation affected by Concentration Overpotential and Redlich} - \text{Kister activity correction}$$

$$V_o = \text{Ohmic Potential including electrodes, electrolyte and current collector}$$

$$V_{\eta,i} = \text{Surface Overpotential given by Butler} - \text{Volmer Equation and caused due to charge transfer resistance and SEI kinetics}$$

By formula,

$$V_{U,i} = U_{0,i} + \frac{\mathrm{RT}}{\mathrm{nF}} \ln \frac{(1 - x_{s,i})}{x_{s,i}} + V_{\mathrm{INT},i}$$

$$V_{\mathrm{INT},i} = \frac{1}{\mathrm{nF}} \left(\sum_{k=0}^{N_i} A_{i,k} \left((2x_i - 1)^{(k+1)} - \frac{(2x_i k(1 - x_i))}{(2x_i - 1)^{1-k}} \right) \right)$$

$$V_0 = i * R_0$$

$$V_0{}' = \frac{(V_0 - V_0{}')}{t_0}$$

$$V_{\eta,i}{}' = \frac{(V_{\eta,i} - V_{\eta,i}{}')}{t_{\eta,i}}$$

```
% Battery Parameters
clear all;
qmax=1.32E+04;
R=      8.314;
T=      292;
F=      96487;
n=      1;
D=      7.00E+06;
t0=     10;
alpha=  0.5;
R0=     0.085;
Sp=     2.00E-04;
kp=     2.00E+04;
vsp=    2.00E-06;
vbp=    2.00E-05;
tnp=    9.00E+01;
Sn=     2.00E-04;
kn=     2.00E+04;
vsn=    2.00E-06;
vbn=    2.00E-05;
tnn=    9.00E+01;

U0p=4.03;
Ap=[-33642.23;
    0.11;
    23506.89;
    -74679.26;
    14359.34;
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    307849.79;
    85053.13;
    -1075148.06;
    2173.62;
    991586.68;
    283423.47;
    -163020.34;
    -470297.35;];
U0n=0.01;
An=[86.19];

% Calculate Voltages (Vup, Vun, Vo, Vnp, Vnn)
ii=1; xp=0.4;xn=1-xp;
for t=0:1*60:10000*60 % time in seconds
    qtransfer=i*t;
    xp=0.4+qtransfer/qmax;
    xn=1-xp;
    result=0;

    for k=1:13
        temp=Ap(k)*((2*xp-1)^(k-1+1)-((2*xp*(k-1)*(1-xp)/(2*xp-1)^(1-(k-1)))));
        result=result+temp;
    end

    VINTp=1/(n*F)*result;
    VINTn=1/(n*F)*An*((2*xn-1)^(1));

    Vup(ii)=U0p+(R*T)/(n*F)*log((1-xp)/xp)+VINTp; %#ok<*SAGROW>
    Vun(ii)=U0n+(R*T)/(n*F)*log((1-xn)/xn)+VINTn;

    % Discharge Current
    if (t<=10*60)
        i=6;
    elseif (t>10*60) && (t<=20*60)
        i=5;
    elseif (t>20*60) && (t<=30*60)
        i=4;
    elseif (t>30*60) && (t<=40*60)
        i=3;
    elseif (t>40*60)&&(t<=50*60)
        i=2;
    elseif t>50*60
        i=1;
    end
    current(ii)=i; %to plot current

    %Ohmic Overpotential (Depends on current only)
    Vo=i*R0;

    %Surface Overpotential (dependent on current and Mole Fraction (SOC))
    Jp=i/Sp;Jn=i/Sn;% Current density
    Jp0=kp*(1-xp)^alpha*(xp)^(1-alpha);% Exchange current density
    Jn0=kn*(1-xn)^alpha*(xn)^(1-alpha);

    Vnp(ii)=R*T/(F*alpha)*asinh(Jp/(2*Jp0));
    Vnn(ii)=R*T/(F*alpha)*asinh(Jn/(2*Jn0));

    if xp>=0.99
        break
    end
    ii=ii+1;
```

```
end
Vup(end)=[];Vun(end)=[];
Vnp(end)=[];Vnn(end)=[];

%Cell output voltage (V)
V=Vup-Vun-Vo-Vnp-Vnn;

%Make plots

subplot(2,1,1);
plot(current,'LineWidth',2,'Color','r');
title ('Discharge Current Vs Time');
ylabel('Current (A)');
xlabel('Time, t (min)');
ylim([0 8])
grid on

subplot(2,1,2);
v1=Vup;
plot(v1,'*'); hold on
v2=Vup-Vun;
plot(v2,'*');
v3=Vup-Vun-Vo;
plot(v3,'*');
v4=Vup-Vun-Vo-Vnp-Vnn;
plot(v4,'*');hold off

ylim([2.4 4.4]);
legend('v1=Vup','v2=Vup-Vun','v3=Vup-Vun-Vo','v4=Vup-Vun-Vo-Vnp-Vnn','Location',"best");
title('Cell Voltage Vs Time, SOC: 1 to 0, xp= 0.4 to 1')
ylabel('Voltage, V (V)')
xlabel('Time, t (min)')
grid on
```