SIMULATION OF LITHIUM-ION CONCENTRATION PROFILES IN SEPARATOR AND CATHODE OF LITHIUM-ION BATTERY USING THETA FORMULATION UNDER FINITE DIFFERENCE METHOD

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ABSTRACT

This research focuses on the material balance equation governing the lithium-ion concentration in an electrolyte/solution phase of a lithium-ion battery. The main objective of this research is to obtain the solution for this governing equation in order to simulate the concentration profile of a lithium-ion battery during discharge process. The second objective of this research is to study the behavior of these lithium-ion concentrations in the electrolyte/solution phase of a lithium-ion battery under various conditions. In order to achieve the second objective of this study, various simulations of lithium-ion concentrations in the electrolyte/solution phase of a lithium-ion battery were performed. Several difference parameter values of discharge current (*I*), electrode porosity (ε), discharge time (τ) and combination of separator/cathode thicknesses (L_s/L_c) were used to simulate the behavior of lithium-ion in the battery system.

The material balance equation governing the lithium-ion concentration in the electrolyte/solution phase of a lithium-ion battery for separator is defined as

$$\frac{\partial(c)}{\partial t} = \nabla \cdot (D \nabla c) - \frac{i_2 \cdot \nabla t_+^0}{z_+ v_+ F}$$

and for cathode is defined as

$$\varepsilon \frac{\partial(c)}{\partial t} = \nabla \cdot (\varepsilon D_{eff} \nabla c) - \frac{i_2 \cdot \nabla t_+^0}{z_+ v_+ F} + \frac{a j_n (1 - t_+^0)}{v_+}$$

These equations are solved using the Theta formulation from Finite Difference Method (FDM) based on the relevant initial and boundary conditions. Three schemes are considered from this Theta formulation, which are explicit scheme $(\alpha = 0)$, implicit scheme $(\alpha = 1)$ and Crank Nicolson scheme $(\alpha = 0.5)$. The coding for all three schemes are done using Wolfram MATHEMATICA 8 software and were solved.

The significant *t*-test is used to prove that the profiles of lithium-ion concentration calculated from this work are in good agreement with the published analytical results within 95% confidence interval. The Root Mean Square Error (RMSE) and Mean Absolute Error (MAE) are used to evaluate the effectiveness and accuracy of the profiles of lithium-ion concentration calculated from this work compared to the published work. Computational time needed by Wolfram Mathematica 8 software to solve the equation is also recorded to identify the fastest scheme based on the same style of computer coding from Theta formulation.

ABSTRAK

Kajian ini memberi tumpuan pada persamaan imbangan bahan yang mempengaruhi kepekatan ion litium di dalam elektrolit/fasa larutan bateri ion litium. Tujuan utama dari kajian ini adalah untuk mendapatkan penyelesaian bagi persamaan imbangan bahan ini bagi membolehkan dilakukan simulasi profil kepekatan bateri litium-ion semasa proses nyahcas. Tujuan kedua dari kajian ini adalah untuk mempelajari perilaku kepekatan ion litium dalam elektrolit/fasa larutan bateri litium-ion di bawah pelbagai keadaan. Bagi mencapai tujuan kedua kajian ini, pelbagai simulasi kepekatan ion litium dalam elektrolit/fasa larutan bateri litium-ion telah dijalankan. Beberapa nilai parameter yang berbeza seperti arus nyahcas (I), keporosan elektrod (ε), masa nyahcas (τ) dan kombinasi ketebalan pemisah/katod (L_s/L_c) telah digunakan untuk mensimulasi perilaku ion litium di dalam sistem bateri.

Persamaan imbangan bahan yang mempengaruhi kepekatan ion litium di dalam fasa elektrolit/larutan bateri litium-ion untuk pemisah ditakrifkan sebagai

$$\frac{\partial(c)}{\partial t} = \nabla \cdot \left(D \nabla c\right) - \frac{i_2 \cdot \nabla t_+^0}{z_+ v_+ F}$$

dan untuk katod sebagai

$$\varepsilon \frac{\partial(c)}{\partial t} = \nabla \cdot \left(\varepsilon D_{eff} \nabla c\right) - \frac{i_2 \cdot \nabla t_+^0}{z_+ v_+ F} + \frac{a j_n \left(1 - t_+^0\right)}{v_+}$$

Persamaan imbangan bahan ini diselesaikan dengan formulasi Theta dari Kaedah Beza Terhingga berdasarkan nilai awal dan nilai sempadan yang relevan. Tiga skim dipertimbangkan dalam formulasi Theta iaitu skim eksplisit $(\alpha = 0)$, skim implisit $(\alpha = 1)$ dan skim Crank Nicolson $(\alpha = 0.5)$. Pengatucaraan komputer untuk ketiga-tiga skim ini dibuat mengunakan perisian Wolfram MATHEMATICA 8 dan diselesaikan.

Ujian signifikan-t digunakan untuk membuktikan bahawa profil kepekatan ion litium yang dikira dari kajian ini adalah menepati keputusan analitik yang pernah diterbitkan bagi 95% julat kesahihan. Ralat Bagi Punca Kuasa Dua Min dan Ralat Mutlak Min digunakan untuk menilai keberkesanan dan ketepatan profil kepekatan ion litium yang didapati dari kajian ini dibandingkan dengan hasil kerja analitik yang pernah diterbitkan. Masa pengkomputeran yang diperlukan oleh perisian Wolfram Mathematica 8 untuk menyelesaikan persamaan imbangan bahan ini juga direkodkan untuk mengenalpasti skim penyelesaian terpantas berdasarkan gaya pengaturcaraan yang sama dari formulasi Theta.

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A. Paper published

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LIST OF SYMBOLS

a	specific interfacial area (cm^{-1})
c_i	concentration of species *i* (mol/dm^3)
c_T	total concentration
D	diffusion coefficient (cm^2/s)
f_{+-}	mean molar activity coefficient of the electrolyte
F	Faraday's constant (96487 C/cq)
I	superficial current density (mA/cm^2)
j_n	pore wall flux of lithium-ion across interface ($mol/m^2/s$)
K_{ij}	friction coefficients (or interaction coefficients)
m	molality
n	number of electrons transferred in electrode reaction
N_i	diffusive flux of species *i* ($mol/cm^2/s$)
R	universal gas constant (8.3143 J/mol/K)
t	time (seconds)
t_+^0	transference number of lithium-ion
T	temperature (K)
v_i	*velocity of species i*
x	distance along x-axis (μm)
y	dimensionless distance
z_i	ionic valence of the charged species *i*.

Greek letters

ε	porosity
δ	thickness
$\wp$	diffusion coefficient of the electrolyte based on a thermodynamic driving force
ϑ	dimensionless concentration
τ	dimensionless time
μ_i	electrochemical potential of species *i*
γ_{+-}	mean molal activity coefficient

Subscripts/Superscripts

A	anode
C	cathode
S	separator
0	initial condition
2	electrolyte/solution phase

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