SIMULATION OF PERFORMANCE OF A DIRECT MIXED ALCOHOL FUEL CELL

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Abstract

Most of all direct alcohol fuel cell models have been developed for handling only pure fuel, either methanol or ethanol. These models cannot be employed to describe the behavior of the cell fed with mixed alcohol (methanol/ethanol) solution. The model becomes more complicated when one has to consider the oxidation of various liquid fuels. In this study, the model of direct mixed alcohol fuel cell was developed a using rate expression derived from the multistep heterogeneous reaction mechanism including adsorption of intermediate species and dual site surface electrochemical reaction. The model was therefore constructed using MATLAB software to calculate all polarizations including activation, ohmic and mass transport losses. The simulation results showed that the major loss in direct mixed alcohol fuel cell was due to activation and mass transport resistance. The fast drop of cell performance as ethanol was mixed into the fuel was caused by the competitive adsorption of ethanol on Pt surface with methanol resulting in the reduction of methanol surface coverage. The kinetic parameters estimated from the case of pure alcohol solution can be used to predict the behavior of the cell fed with mixed alcohol. By comparing with the in-house experimental data, a relatively good agreement between the simulated and experimental data was achieved.

Keywords: Activation Loss/ Ohmic Loss/ Concentration Loss/ Direct Alcohol Fuel Cell/ Direct Mixed Alcohol Fuel Cell (Methanol/Ethanol)/ MATLAB

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บทคัดย่อ

การพัฒนารูปแบบจำลองเซลล์เชื้อเพลิงแบบแอลกอออฮอล์โดยตรง ในปัจจุบันเป็นรูปแบบจำลองสำหรับเชื้อเพลิงแอลกอฮอล์บริสุทธิ์ กล่าวคือเป็นของสารละลายเมธานอล หรือเป็นของสารละลายเอธานอลเพียงอย่างเดียว แต่ยังไม่มีรูปแบบจำลองที่ใช้อธิบายพฤติกรรมของเซลล์เชื้อเพลิงที่ใช้สารละลายผสมระหว่างเมธานอลกับเอธานอลเป็นเชื้อเพลิง ดังนั้นงานวิจัยนี้จึงได้พัฒนารูปแบบจำลองสำหรับเซลล์เชื้อเพลิงแอลกอฮอล์ผสม โดยใช้นิยามจลนพลศาสตร์ที่แสดงถึงขั้นตอนการเกิดปฏิกิริยาที่พื้นผิวตัวเร่งปฏิกิริยาอันได้แก่ การดูดซับและการเกิดปฏิกิริยาที่พื้นผิวแบบด้านว่องไวคู่ โดยใช้โปรแกรม MATLAB ในการสร้างรูปแบบจำลองพฤติกรรมของเซลล์เชื้อเพลิง โดยพิจารณาการสูญเสียค่าความต่างศักย์ของเซลล์เชื้อเพลิงเกิดจาก 3 สาเหตุหลักคือ การสูญเสียอันเนื่องจากพลังงานกระตุ้น การสูญเสียแบบโอห์มมิก และการสูญเสียอันเนื่องจากการส่งถ่ายมวลสาร ผลลัพธ์ที่ได้จากรูปแบบจำลองแสดงให้เห็นว่า การสูญเสียหลักเกิดจากพลังงานกระตุ้นและการส่งถ่ายมวลสาร และการลดลงอย่างรวดเร็วของความต่างศักย์ของเซลล์เมื่อมีการผสมเอธานอลเข้าไปในเชื้อเพลิงเมธานอลเกิดจากการที่เอธานอลเข้าไปแย่งดูดซับบนตัวเร่งแพลตินัม แล้วทำให้เมธานอลที่ครอบครองพื้นผิวว่องไวมีค่าลดลง จากการเปรียบทียบผลการคำนวณกับผลการทดลองที่ค่าอัตราส่วนผสมต่างๆ ของแอลกอฮอล์ผสม พบว่ารูปแบบจำลองสามารถทำนายเส้นกราฟโพลาไรเซชั่นของเซลล์เชื้อเพลิงได้ดีไม่ว่าจะเป็นกรณีที่ใช้เชื้อเพลิงเมธานอลบริสุทธิ์ เอธานอลบริสุทธิ์ หรือสารละลายผสมเมธานอล/เอธานอล

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A.2 Effect of anode catalyst Pt-Ru on fed with 1M methanol and 1M ethanol 73

LIST OF SYMBOLS

E_{thermo}	Thermodynamically predicted fuel cell voltage output (V)
η_{act}	Activation loss (V)
η_{Ohmic}	Ohmic loss (V)
η_{conc}	Concentration loss (V)
j	Current density (A/cm^2)
F	Faraday's constant (C/mol)
r	Reaction rate (mol/cm^2s)
c_R^*	Reactant concentration at the catalyst layer (mol/ml)
c_P^*	Product concentration at the catalyst layer (mol/ml)
j_o	Exchange current density (A/cm^2)
α	Transfer coefficient
σ	Conductivity of Nafion
D^{eff}	Effective reactant diffusivity
j_L	Limiting current density (A/cm^2)
θ_M	Surface coverage of methanol
θ_{CO}	Surface coverage of carbon monoxide
k_i	Kinetic rate constant of reaction I (mol/cm^2s)
C_M	Methanol concentration at the catalyst layer (mol/ml)
θ_{CH3CHO}	Surface coverage of acetaldehyde
β_i	Transfer coefficient of reaction i
θ_{OH}	Surface coverage of hydroxide
n	Number of electron transferred during electrooxidation
j_{EtOH}	Current density of ethanol (A/cm^2)
j_{MeOH}	Current density of methanol (A/cm^2)
λ	Membrane hydration of Nafion
t_m	Membrane thickness(cm)
R_t	Overall resistance
R_{ionic}	Ionic or membrane resistance
R_{elec}	Electronic resistance
J_{diff}	Diffusion flux of reactants to catalyst layer (mol/cm^2s)
δ	Thickness of the diffusion layer (cm)
E^{OCV}	Open circuit voltage (V)