

論文 / 著書情報
Article / Book Information

題目(和文)	
Title(English)	Modeling Reaction Kinetics and its Bridging to Transport Phenomena in a PEM Fuel Cell Under Contamination
著者(和文)	SAIFULHASMADY
Author(English)	Hasmady Saiful
出典(和文)	学位:博士(工学), 学位授与機関:東京工業大学, 報告番号:甲第9771号, 授与年月日:2015年3月26日, 学位の種別:課程博士, 審査員:伏信 一慶,佐藤 勲,花村 克悟,齊藤 卓志,野崎 智洋
Citation(English)	Degree:., Conferring organization: Tokyo Institute of Technology, Report number:甲第9771号, Conferred date:2015/3/26, Degree Type:Course doctor, Examiner:,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	要約
Type(English)	Outline

論文要約
(THESIS OUTLINE)

Title: Modeling Reaction Kinetics and its Bridging to Transport Phenomena in a PEM Fuel Cell Under Contamination
Year: 2014
Author: Saiful Hasmady
Dept. of Mechanical and Control Engineering,
Tokyo Institute of Technology.
Advisor: Assoc. Prof. Dr. Kazuyoshi Fushinobu
Dept. of Mechanical and Control Engineering,
Tokyo Institute of Technology.

Dissertation Outline:

This dissertation is structured to contain five chapters detailing the contents of this research work. The chapters are, in their written order, is described briefly as follows:

Chapter 1 outlines the research background, from the motivation of using PEM fuel cell (PEMFC) as a promising energy solution for the future, the science behind it, and the issues and challenges associated with its operation and global usage proliferation. The issues are narrowed down into two major topics, which are thermal and water management, and catalyst contamination, which form the subject of this dissertation work itself.

Chapter 2 describes the intensive modeling and experimental work associated with elucidating thermal and water management issue within the limits of dissimilar spatial scales of kinetics and transport phenomena. First, a detailed description of macro-scale conservation equations of mass, momentum, liquid water saturation, charges and energy is done. This is followed by the kinetics model development at the anode and cathode electrocatalysts, by considering elementary reaction steps instead of the overall reaction. Via adsorption-desorption kinetics and singling out the rate-determining step, the reaction rate and overpotential relationship is obtained. An effort is done to bridge the dissimilar scales of transport phenomena and electrochemical kinetics using a heterogeneous isotherm. Later, the construction of an experimental cell with the capability of assessing a typical PEMFC performance with a set operating parameters by a polarization curve, and measuring the temperature distribution in-situ via infrared thermography is made. The kinetics model is validated with polarization curves, and the bridging with transport phenomena is validated with in-situ infrared thermograms. Discussions on the results are done mainly on the multi-dimensional distribution of the kinetics and transport variables, and their role in assessing thermal and water management in the cell.

Chapter 3 extends the kinetics model in the previous chapter to include the effect of carbon monoxide (CO) contamination at the anode electrocatalyst. Explanation on how CO molecules is modeled to enter the cell pre-mixed with humidified hydrogen analogous to a reformat fuel feed, and competitively adsorbed on the active Pt sites is made. Then the bridging to macro-scale two-phase conservation equations in transport phenomena is described through Langmuir-Freundlich isotherm taking into account

heterogeneity in binding site energetics in the rough electrocatalyst surface. The effects of varying bulk CO concentration and cell temperature towards the severity of performance loss are discussed alongside validation of the model with experimental data published in the literature.

Chapter 4 describes the extension of the modeling work in the previous chapter by using another type of contaminant, namely sulfur dioxide (SO₂). Description on modeling work with respect to the kinetics of the anode and cathode electrocatalyst under weakly-adsorbed SO₂ is made, and the bridging in scale with macro-scale conservation equations is explained. The results are discussed primarily on the effects of varying bulk SO₂ concentration in the reactant feed, to which validation work is done with published literature data. Discussions on the contribution of weakly-adsorbed SO₂ to the overall loss in performance due to SO₂ contamination is subsequently made.

Chapter 5 summarizes the important conclusions in the research work contained in this dissertation. The chapter also proposes future work that can be done to address unresolved issues, minimize assumptions, and expand its usage limits.

In addition to the above, the dissertation also contains an **Appendix A** describes calculation procedure of three important transport properties used in this work for gas mixtures; dynamic viscosity, diffusion coefficient, and thermal conductivity.