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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

MODELING REACTION KINETICS AND ITS BRIDGING TO TRANSPORT PHENOMENA IN A PEM FUEL CELL UNDER CONTAMINATION

Proton exchange membrane fuel cell (PEMFC) is a promising energy converter due to its prospect for future energy sustainability. However, there are still many issues pertaining to the performance of the cell, namely the issues related to the thermal and water management during operation at low humidification of the reactants, and platinum (Pt) electrocatalyst contamination originated from the reactant feeds. In the former, operating the cell at high temperature is desired as it increases the rate of heterogeneous surface reaction at the electrocatalyst, thus reducing the loss associated with the intrinsic activation polarization of the electrodes. However, such an operation is highly undesirable at low relative humidity, as high temperature will dry the membrane faster thus impeding the ion transport from anode to cathode. For the latter, presence of even minute concentrations of carbon monoxide (CO) in the anode reformate feed, as well as sulfur dioxide (SO2) in the cathode environmental air feed is enough to poison the Pt electrocatalyst causing substantial performance loss.

This research work is therefore done under the motivation to elucidate the intricate coupling between the dissimilar-scaled electrochemical reaction kinetics, thermal energy and two-phase water transport phenomena in an operating cell. This research work also aims to develop a theoretical based method in predicting the severity of PEMFC performance loss due to electrocatalyst contamination towards mitigation purposes. Both aspects will involve in part rigorous investigation on the inter-connected behavior of the kinetics and transport variables in PEMFC through experimental and theoretical analysis. With that in mind, the research work is divided into three phases. The details in these three phases are reported in three separate chapters contained in this dissertation.

The first phase is reported in Chapter 2, and is about developing an elementary heterogeneous reaction kinetics model in micro-scale to be sequentially bridged to two-phase transport phenomena in macro-scale in a normal PEMFC. The reaction rate in both electrodes is modeled as a function of surface coverage of participating adsorbates and overpotential of the rate-determining step. The bridged model solves for the three-dimensional distribution of most of the kinetics and transport variables in a PEMFC, and is validated using a specially constructed cell that allows for in-situ temperature measurement. Excellent agreement is found in the kinetics results through comparison with the experimental polarization curves at 80 and 90°C, implying applicability of the model. The predicted temperature distribution inside the cell also shows good agreement with in-situ measurement results. Having a distinct distribution in temperature affects the non-equilibrium rate of evaporation and condensation in the porous medium. Results also reveal very low magnitude of liquid phase water saturation in the anode porous media even at high humidity due to evaporation, and high rate of liquid water buildup under the ribs at cathode due to condensation.

The second phase, reported in Chapter 3, extended the work in first phase to include CO contamination to the anode electrocatalyst, and predicts the loss in potential experienced by the cell. The model results are validated with experimental data procured from two different research groups, to which excellent agreement is found. The competitive Langmuir-Freundlich isotherm used in this work is found to be more suitable for rough heterogeneous surfaces physically found in PEMFC catalysts as compared to the extensively used Langmuir isotherm. The results also reveal that the region under the ribs at anode catalyst layer registered higher magnitude of current density due to blockage from CO-ad under channel. The anode catalyst layer also shows an increase in local temperature comparable to the cathode catalyst layer that can aggravate dehydration of the membrane, which in turn may affect its durability in long-term operation.

The third phase is reported in Chapter 4, and is about extending the model once more to include SO2 contamination to both electrodes, and assess the damage to the cell performance. This too, is compared with experimental data from literature, which confirms that though the model successfully predicted higher potential loss with higher bulk SO2 concentration in the reactant feed, inclusion of only weakly adsorbed SO2 will under-predict the exact potential loss experienced by the electrodes. Results also show operating PEMFC at higher temperature reduces SO2-ad coverage for both electrodes due to higher kinetics of hydrogen oxidation reaction and oxygen reduction reaction, which is also the possible reason why the model predicts reduced SO2-ad coverage at cathode by operating the cell at higher relative humidity. Model results also reveal lower SO2-ad coverage at cathode at higher reactant stoichiometry due to increased amount of O2 transported to the catalyst layer. Strongly adsorbed sulfur containing species must be adopted into the future model in order to better predict the severity of degradation of the cell due to SO2 contamination.

(779 words)

備考 ： 論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。
Note : Thesis Summary should be submitted in either a copy of 2000 Japanese Characters and 300 Words (English) or 1copy of 800 Words (English).