A Dual-Scale Modeling Framework for Predicting Platinum Degradation in Polymer Electrolyte Fuel Cells

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Fuel cell vehicles (FCVs) offer a promising solution to reducing carbon emissions from consumer vehicles and slowing down global warming. With significant progress made in the past decade, FCVs are now being commercialized by car manufacturers and are increasingly being used in heavy-duty applications [1].

Within the transportation applications, the fuel cell stacks are exposed to a high number of potential cycles, which makes the low durability of fuel cell components, particularly the platinum catalyst, a significant limitation for proton exchange membrane (PEM) fuel cells. Several experimental studies have investigated the stability of Pt, a commonly used catalyst in PEM fuel cells. These studies have revealed that Pt can dissolve, causing morphological changes in the catalyst and reducing its activity in oxygen reduction. This degradation process is considered the primary cause of reduced performance and durability in fuel cells. Ongoing research is focused on developing new models and methods to improve the understanding and analysis of Pt catalyst degradation in PEM fuel cells [3-6].

To ensure optimal performance and durability of polymer electrolyte fuel cells, it has become increasingly necessary to develop robust degradation models that can accurately predict the fuel cell's lifespan during field operation. These models are also essential for implementing an effective control strategy that can maintain the performance of the fuel cell for longer time in model predictive control paradigm.

This study presents a novel dual-scale modeling framework that includes a multi-physics model and a catalyst degradation model for PEM fuel cells. The multi-physics model is used to determine the internal state of the fuel cell, such as cell voltage, relative humidity, and proton concentration, under various operating conditions, while the degradation model for Pt/C catalyst is proposed considering various factors affecting platinum particle size distribution, including platinum oxidation, dissolution, redeposition, detachment, and agglomeration. By coupling the two models, microscopic degradation and macroscopic performance and operations are linked. It is thus possible to estimate the amount of platinum loss and predict the degradation performance of the catalyst with arbitrary time varying operating conditions. It is therefore possible to further conduct an optimal control using the proposed model to mitigate the catalyst degradation.

REFERENCES

[1] M. de las N. Camacho, D. Jurburg, and M. Tanco, "Hydrogen fuel cell heavy-duty trucks: Review of main research topics," *Int. J. Hydrog. Energy*, vol. 47, no. 68, pp. 29505–29525, Aug. 2022, doi: 10.1016/j.ijhydene.2022.06.271.

[2] P. Ren, P. Pei, Y. Li, Z. Wu, D. Chen, and S. Huang, "Degradation mechanisms of proton exchange membrane fuel cell under typical automotive operating conditions," *Prog. Energy Combust. Sci.*, vol. 80, p. 100859, Sep. 2020, doi: 10.1016/j.pecs.2020.100859.

[3] R. M. Darling and J. P. Meyers, "Mathematical Model of Platinum Movement in PEM Fuel Cells," *J. Electrochem. Soc.*, vol. 152, no. 1, p. A242, Dec. 2004, doi: 10.1149/1.1836156.

[4] A. Kneer and N. Wagner, "A Semi-Empirical Catalyst Degradation Model Based on Voltage Cycling under Automotive Operating Conditions in PEM Fuel Cells," *J. Electrochem. Soc.*, vol. 166, no. 2, p. F120, Jan. 2019, doi: 10.1149/2.0641902jes.

[5] W. Bi and T. F. Fuller, "Modeling of PEM fuel cell Pt/C catalyst degradation," *J. Power Sources*, vol. 178, no. 1, pp. 188–196, Mar. 2008, doi: 10.1016/j.jpowsour.2007.12.007.

[6] L. Kim, C. G. Chung, Y. W. Sung, and J. S. Chung, "Dissolution and migration of platinum after long-term operation of a polymer electrolyte fuel cell under various conditions," *J. Power Sources*, vol. 183, no. 2, pp. 524–532, Sep. 2008, doi: 10.1016/j.jpowsour.2008.05.062.