A dual-scale modelling framework for predicting catalyst degradation in Polymer Electrolyte Fuel Cells

Walid Touil[1, 2], Zhongliang Li[1], Rachid Outbib[2], Samir Jemei[1], Daniel Hissel[1,3]

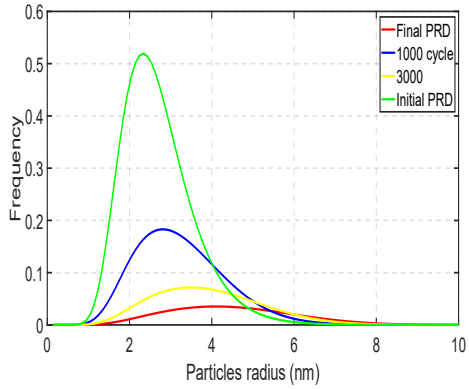
[1]Univ. de Franche-Comté, UTBM, CNRS, FEMTO-ST, FCLAB, Belfort, France
[2]Aix-Marseille Univ., CNRS, LIS, Marseille, France
[3]Institut Universitaire de France

The durability of fuel cell components, especially the platinum catalyst, remains a significant limitation for proton exchange membrane (PEM) fuel cells used in transportation applications. Developing robust degradation models that can predict the fuel cell's lifespan during field operation is crucial to maintaining optimal performance and durability.

In the pursuit of advancing our understanding and prediction of Pt catalyst degradation in PEM fuel cells, continuous research efforts are dedicated to the development of new models and methods to analyze and mitigate the catalyst degradation. There are currently three main categories of models used to study Pt catalyst degradation in PEM fuel cells. The first is the bi-model degradation model, which focuses solely on the dissolution redeposition process and lacks a distribution component [1]. The second is the particle radius distribution (PRD) model, which provides a more comprehensive description by considering four main degradation mechanisms: dissolution, redeposition, agglomeration, and detachment [2]. However, the PRD models have not yet been connected to fuel cell system dynamic models which limits their use for online use. The third category consists of empirical models [3], which do not explicitly define the impact of degradation on the catalyst and are often studied in conjunction with multi-physics models. In our research, we aim to leverage the strengths of each approach and establish a connection between the detailed degradations of the catalyst and the multi-physics models.

This study proposes a dual-scale modeling framework that includes a multi- physics model and a catalyst degradation model in PRD modelling category for PEM fuel cells. The multi-physics model determines the internal state of the fuel cell, while the degradation model for Pt/C catalyst considers various factors affecting platinum particle size distribution (figure 1). By coupling the two models, it is possible to estimate platinum loss, predict catalyst degradation performance under arbitrary operating conditions, and conduct optimal control to mitigate degradation.

a)



b)

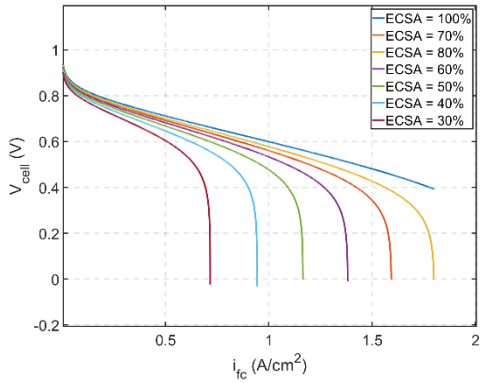


Figure 1. a) PRD evolution, b) Polarisation curves

[1] W. Bi and T. F. Fuller, "Modeling of pem fuel cell pt/c catalyst degradation," Journal of Power Sources, vol. 178, no. 1, pp. 188–196,2008.
[2] S. G. Rinaldo, W. Lee, J. Stumper, and M. Eikerling, "Catalyst degradation: nanoparticle population dynamics and kinetic processes," ECSTransactions, vol. 50, no. 2, p. 1505, 2013.
[3] A. Kneer and N. Wagner, "A semi-empirical catalyst degradation model based on voltage cycling under automotive operating conditions in pem fuel cells," Journal of The Electrochemical Society, vol. 166, no. 2, p. F120, 2019.

*author to whom correspondence should be addressed: *zhongliang.li@univ-fcomte.fr*