

Optimization in Fuel Cell Catalyst Layer Composition

Jayanth Kolli

Independent Researcher, USA

ABSTRACT

Catalyst layers are essential in fuel cells and their performances are determined by the ability to enhance reaction rates, proton transport and diffusion of the gases involved. This review first presents fundamental approaches for modifying the catalyst layer such as decreasing the content of Pt, controlling the distribution of the ionomer, and discussing Pt-alternatives. Studying the problem, special attention is paid to increasing the efficiency of mass transport and introducing non-Noble metals, as well as the possible advantages of DPG in proton and mass transport improvement. Improvements which should be sought in the future include the continued development of cheaper materials, application of real time control strategies, and substitution of the traditional ionomers. In the overall goal of enhancing the functionality of the fuel cells besides making them affordable.

Keyword: Fuel cell, catalyst layer, platinum loading, ionomer distribution, non-noble metals, proton transport, fuel cell optimization.

INTRODUCTION

Fuel cell is an electrochemical converter that converts the chemical energy into electrical energy that has high efficiency and less pollution. The most important one of them is the so called catalyst layer which is a thin composite layer where some important reactions takes place, namely the ORR and the HOR.

One has therefore noted that the composition of the catalyst layer must be improved to increase the productivity, performance as well as the cost affordability of fuel cells. This has to do with the optimization of such elements as Pt-based catalysts, ionomers and carbon substrates in relation to reaction rates, proton transport and diffusion of gases. Also, elimination of the dependency on expensive metals and optimizing the dispersion of materials are critical to increase the scale of fuel cell technology economically.

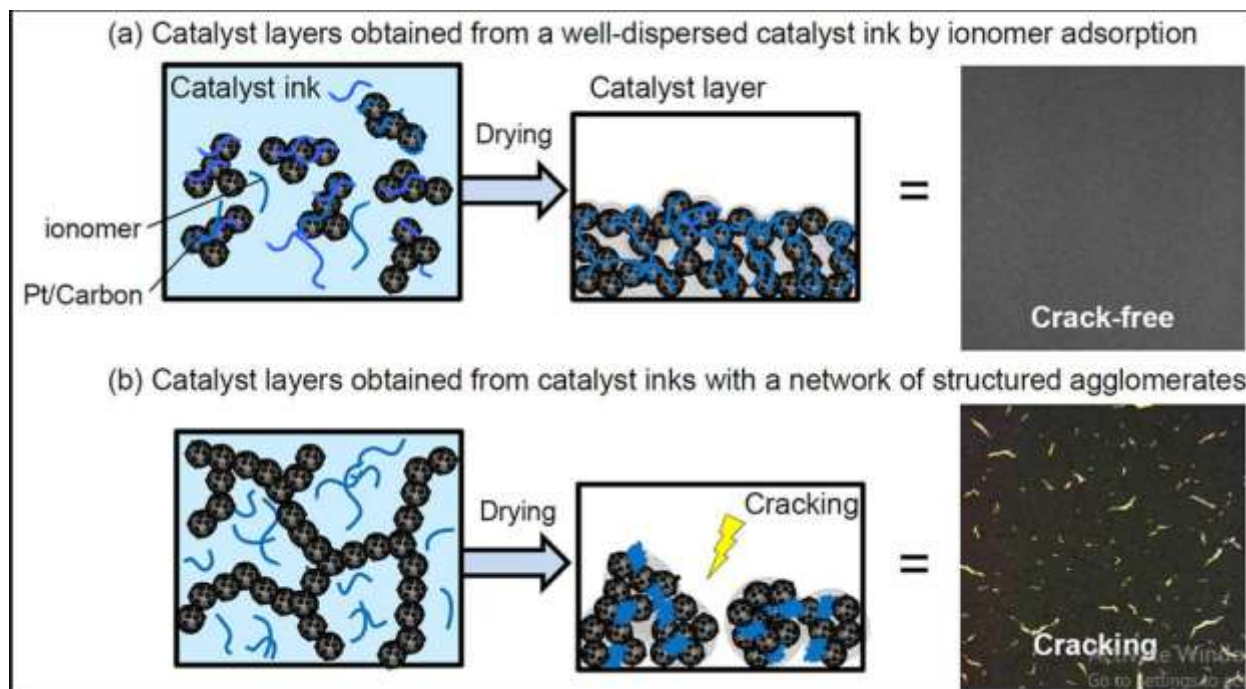
Such a complex relationship between these factors underlines the need to undertake a systematic approach to the selection and design of the catalyst layer to achieve a high overall performance and simultaneously address related performance and sustainability issues hindering the development of cleaner energy systems.

LITERATURE REVIEW

Fuel cell catalyst layer optimization techniques

According to Ohma *et al.* 2011, to boost the penetration of the FCVs, further reduction in the cost of fuel cell systems is paramount and of paramount significance is the Pt loading in CLs. Reduction of Pt loading in the MEA of PEMFCs needs improvement in mass transport and an efficient catalyst so as to make Pt productive and efficient.

In this work, we review the analytical and computational methods of lowering the Pt loading based on the CL microstructure and its relation to interfacial mass transport properties (Ohma *et al.* 2011). Based on these experiments, a fundamental CL model using experimental data has been constructed to simulate the I–V performance and to evaluate effects of decreased Pt loading.

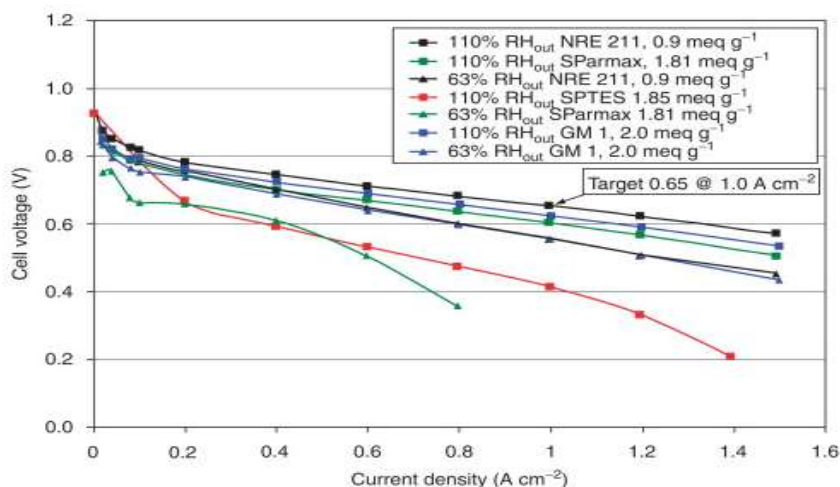


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Figure 1: Fuel Cell Catalyst Layer

Composition effects on fuel cell performance

According to Pinto *et al.* 2011, In this investigation, we analyze the effect of the external load on the continuous performance of MFCs and also optimize the practical performance of MFCs in real time based on a perturbation/observation algorithm. The MFCs fed with acetate were operated at external resistance greater than, lower than, or equal to the internal resistance. Supplementation of external resistance further promoted maximum power density, higher Coulombic efficiency and minimized methane generation (Pinto *et al.* 2011). The efficiency of the algorithm was demonstrated during a 40 day trial with simulated wastewater where it gained an average coulombic efficiency of 29 percent. The results point to the need for real-time resistance optimization to enhance MFC efficiency and sustainable operation performance.

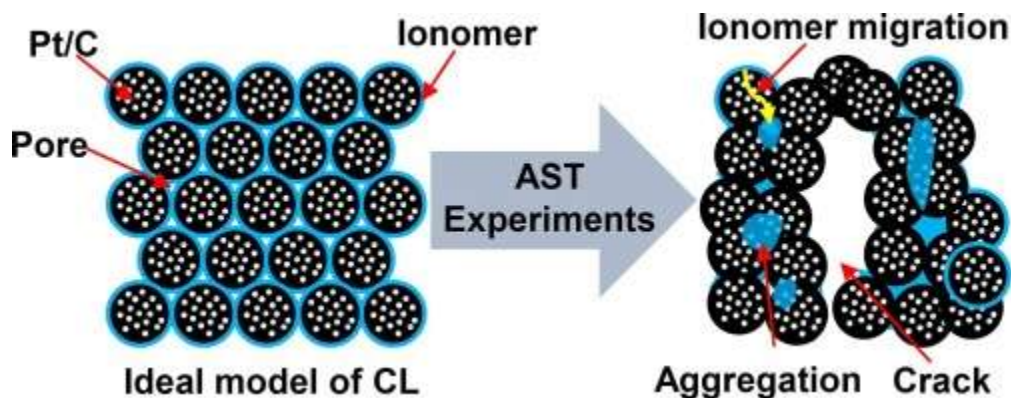


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Figure 2: Fuel Cell Performance

Ionomer content in fuel cell catalysts

According to Doo *et al.* 2018, Public interest has been driven by the need to develop better polymer electrolyte membrane fuel cells with better ionomer distribution in the catalyst layers or CLs. The current work focuses on the extent of tunable ionomer distribution across the dispersion media of DPG or Water solutions. Molecular dynamic simulations and dynamic light scattering reveal that the amount of DPG has an exponential decrease in ionomer aggregate size because of the higher binding constants between DPG and Nafion ionomers (Doo *et al.* 2018). The highest power performance is obtained at 50 wt percentage DPG which effectively mediates proton and mass transfer. The ionomer aggregates which have close proximity to the Pt/C aggregate size cool the catalyst to form a connected network that provides high porosity and improved CL performance regardless of feed humidity.

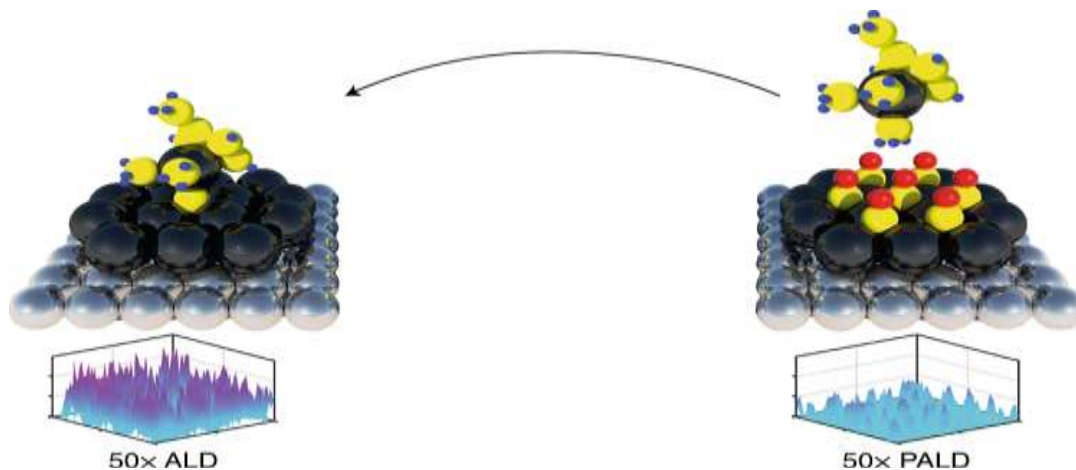


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Figure 3: Ionomer content in Cell Catalyst

Platinum catalyst efficiency in fuel cells

According to Morozan *et al.* 2011, Cathode limiting current density associated with oxygen reduction reaction or ORR is a critical aspect of PEMFC because it affects water generation and fuel cell efficiency. Due to the high cost and rarity of platinum or Pt the development of other ORR catalysts has become relevant. This paper presents a discussion of ORR catalysts with special emphasis on their categorization, working principles, reactivity and efficiency (Morozan *et al.* 2011). It also extends from conventional Pt-based catalysts to those in non-noble metal as well as bio-inspired categories, as well as revealing great improvement achieved in the ORR catalysis. They all call for an enhanced cost and resource efficiency and an increase in the performance and durability of PEMFCs.

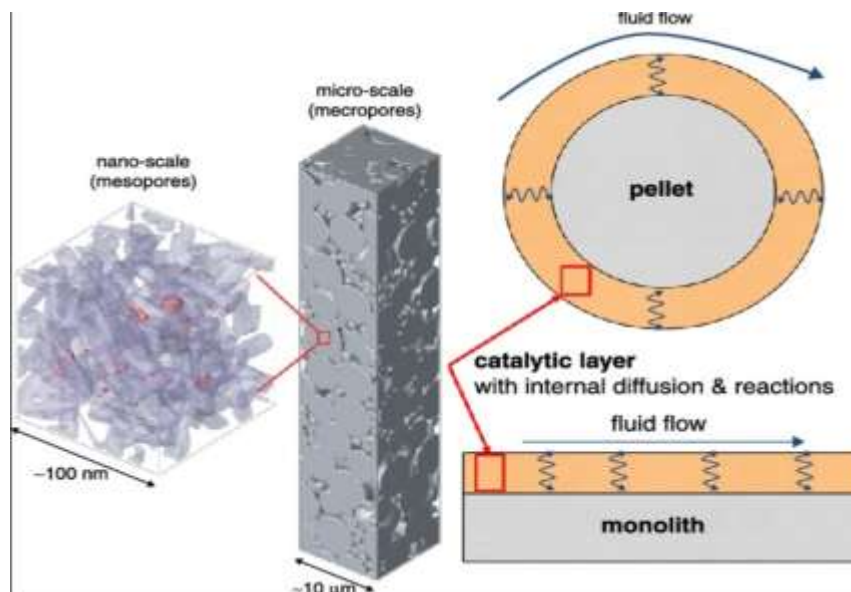


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Figure 4: Platinum Catalyst for Fuel Cells

Gas transport in catalyst layer design

According to Holdcroft, 2014, In PEM fuel cell technology, the polymeric ionomer serves a double role as a proton and water transporting membrane and as an adhesive binding the catalyst particles in the catalyst layer. In this work, some fundamental features of catalyst layer ionomers are reviewed with respect to their characteristics in catalyst inks that form the microstructure of the catalyst layer (Holdcroft, 2014). They also review the important properties determining the next generation ionomer designs and the issues arising from the switch from PFSA ionomers to hydrocarbon-based systems. Knowledge of these interactions and properties is crucial for future improvement of PEM fuel cells based on the criteria of efficiency, durability, and cost.



(Source: <https://ars.els-cdn.com/content/>)

Figure 5: Understanding the gas transport in porous catalyst layers

Methods

Catalyst layer composition in fuel cells is a complex problem, which requires the consideration of different approaches presented in the current work. The research method to use in secondary research is deductive approach derived from interpretivism philosophy. This approach starts with existing theories or frameworks for the design of the catalyst layer (Zamel, 2016). From there, this makes various assumptions to identify possible ways of improvement within a qualitatively designed system.

The secondary type of data is collected through reviewing scientific journals, magazines, patents, and databases of pertinent fuel cell technologies. Sources of peer reviewed Journals, conference proceedings and technical reviews which offered information about previous studies on catalyst material selection, ionomer integration and performance. These documents are scrutinized to extract patterns, trends and gaps which define the current state of practice.

Secondary data analysis is then done in order to aggregate the collected data to enable a more viable comparison of one method to another. Methods including thematic analysis are applied in order to find out key issues, for instance, the variation in efficiency due to platinum loading vs the job done by carbon supports in endurance (Khajeh-Hosseini-Dalasm^{et al.} 2012). It makes it valuable to comprehend the general trends when it comes to specific outcomes and indicates how these results might be used to create recommendations. This produces efficient and affordable investigations into optimization of the catalyst layer composition in fuel cells.

RESULTS

Improving catalyst layers or CLs at the fuel cells is a fundamental issue that may progress the fuel cell area. The following is a summary of some of the following results highlighted from the reviewed literature below.

Reduction of Platinum (Pt) Loading

Ohma *et al.* 2011, discussed that decreasing the Pt loading in the membrane electrode assembly or MEA is fundamental to bring down costs without losing efficiency in proton exchange membrane fuel cells or PEMFCs. The major requirements for the optimisation of such conversions were identified as better mass transport and the efficiency of the use of catalysts (Secanell *et al.* 2011). Overall, the multitechnique experimental and numerical analysis showed the dependence of the CL microstructure on the interfacial mass transport parameters. By incorporating experimental data, a CL model was established to predict I-V performance successfully meaning high performance could be attained with minimal Pt loading.

Composition Effects in Microbial Fuel Cells (MFCs)

Pinto *et al.* (2011) highlighted the role of external resistance in optimizing MFC performance. Real-time resistance adjustment using a perturbation/observation algorithm improved power density, Coulombic efficiency, and reduced methane production. A 40-day test with synthetic wastewater confirmed the algorithm's effectiveness, achieving a 29 percent Coulombic efficiency. These findings underscore the need for dynamic resistance optimization for sustainable and efficient MFC operation.

Ionomer Distribution and Performance

In their work, Doo *et al.* (2018) proved that distribution of ionomers in CLs affected by DPG content is significant for PEMFC performance. It was also observed from the molecular dynamics analysis that with the increment of DPG ionomer aggregate size was established to be small hence evenly distributed. Maximum performance was noticed at 50 wt percentage of DPG where the transport of the proton and the mass was favorable. When considering the Ionomer Pt/C aggregate size distribution, the catalyst structure formed a highly porous continuum which did not depend either on the feed humidity and therefore improved performance.

Platinum Alternatives in ORR Catalysis

Moroza *et al.* (2011) surveyed the development of ORR electrocatalysts, with special emphasis on the use of Pt substitutes. It was also the year that non-noble metal and bio inspired catalysts demonstrated promising progress in the increased efficiency of catalysis, as well as, sustainable utilization and longevity of the catalysts themselves. These alternatives relate to the difficulties arising from Pt scarcity and high cost whilst enabling a high level of PEMFC performance.

Gas Transport and Ionomer Role

Transport media and structural binders Both the requirements were met by polymeric ionomers as discussed by Holdcroft (2014). Information on CT ionomer behavior and CL microstructure was used to specify the properties of the ionomer for next generation catalyst inks (Zhang *et al.* 2015). Switching from PFSA to hydrocarbon based ionomers has its own problems but at the same time holds numerous potentialities to cut cost and increase efficiency.

These results give an avenue for augmenting the catalogue of fuel cell efficiency complemented by the catalyst layer, materials, and procedures.

DISCUSSION

The studies under review focus on the key issues regarding the CLs which should be considered for improving the fuel cell performance. One of the primary challenges remains cutting the platinum loading in the prototype proton exchange membrane fuel cells PEMFCs while maintaining high efficiency as was reported by Ohma *et al.* (2011). This creates the need to enhance the mass transport of species as well as the efficiency of the catalyst being used. Recent trends revealing models with experimental data on I-V performance predicts that minimal Pt loading will also give high efficiency (Khajeh-Hosseini-Dalasm *et al.* 2010).

In an article by Pinto *et al.*, 2011 the authors show that external resistance needs to be properly managed in microbial fuel cells to get enhanced power density, Coulombic efficiency and sustainability of the system. In addition, working on controlling the distribution of the ionomer with the help of dipropylene glycol or DPG improves the future protons and mass transportation in PEMFCs at the peak concentration of about 50 wt percentage of DPG. Furthermore, Moroza *et al.* (2011) reveal non-Pt group metal and bio derived ORR catalysts that have potential to replace Pt due to its rarity. Holdcroft (2014) specifically discusses how ionomers function in PEMFCs and suggests that replacing them with hydrocarbon systems could make the fuel cell more economical (Hwang *et al.* 2011). In combination, these works indicate that improvements in catalyst materials, optimization techniques, and ionomer synthesis are critical for fuel cell technology development.

Future Directions

Based on the research presented in the previous sections, more strategies for the optimization of the fuel cell catalyst layer should aim at minimizing the quantities of the platinum, as this increases cost and is also a scarce material. Extension of work should be done on new generation non-Pt based catalysts and bio-mimetically derived materials. Also, more studies aimed at the distribution of ionomer and its influence on proton or mass transport, especially in utilizing such materials as dipropylene glycol or DPG for the applications (Marquis and Coppens, 2013). The overall performance should be improved by real-time operational strategies that include resistance optimization in microbial fuel cells or MFCs. As well, the shifts from the PFSA to the hydrocarbon-based ionomers will provide a direction for development of more cost effective and superior fuel cell technologies in the future.

CONCLUSION

Here mainly conclude that optimization of the fuel cell catalyst layers remains important for enhancing future generation of fuel cells to mainly achieve higher efficiency at lower level of costs. Some of them are reduction of Pt loading by mainly using non-precious types of metals and ionomer type optimization for mainly improved types of protons along with mass transport. New generation types of catalysts along with ionomer types of materials including bio-inspired and hydrocarbon based systems present ways forward to problems of cost and performance. Future work in these directions accompanied by real time operation research is very critical to improve the overall performance, efficiency along with cost effective solutions in fuel cells. These specific types of goals will go a very long way within helping push the overall rate of deployment of cleaner types of energy systems.

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