Numerical Investigation of the Effects of Interfacial Contact Resistance in PEM Fuel Cells with Coated Metal Bipolar Plates

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Aim

Fuel cells have emerged as promising next-generation electrochemical energy converters due to their high power density and low emissions, making them attractive for transportation and stationary energy applications (S. Wang et al., 2017) .In particular, replacing conventional internal combustion engines with fuel cells is expected to play a crucial role in transitioning to sustainable energy systems [(Qasem & Abdulrahman, 2024).

Fuel cells comprise various components, including the bipolar plate and membrane electrode assembly. Due to its crucial role in efficient thermal and electrical management, as well as ensuring proper gas distribution and mechanical stability, the bipolar plate is one of the most important components of the system (Xiong et al., 2021).

Graphite, traditionally used as a bipolar plate material, requires a significant volume to achieve adequate mechanical strength, which limits its application in compact fuel cell designs such as automotive systems. To address this challenge, metal bipolar plates offer superior mechanical properties, allowing more fuel cell units to be integrated within the same volume. However, metal bipolar plates suffer from poor corrosion resistance, requiring protective coatings to enhance their durability. These coatings not only provide benefits in terms of corrosion resistance but also have an impact on interfacial contact resistance (ICR) (Xiong et al., 2021).

ICR is an electrical resistance that occurs at the interface between two contacting surfaces in a fuel cell, such as between the bipolar plate and the gas diffusion layer (GDL). It arises due to surface roughness, material properties, and contact pressure (Lædre et al., 2022). Additionally, each coated metal bipolar plate has a different ICR value, which affects the overall performance and efficiency of the fuel cell (Leng et al., 2020).

It has been observed that the ICR of coatings is not typically included in simulations of metal bipolar plate PEM fuel cells. In this study, The numerical model was first validated using data from an experimental study, and then ICR values of three widely used coatings were obtained from the literature and incorporated into the study. The results were presented comparatively.

Material and Method

This study uses Ansys Fluent PEM [6] modules to analyse the effect of ICR on PEM fuel cell performance. Different coating materials are considered, and their influence on interfacial resistance is examined through numerical simulations. The model incorporates key electrochemical and transport phenomena within the fuel cell structure. The numerical model, which has also been used in experimental studies in the literature (L. Wang et al.,

2003) , was utilized in this study to examine the effect of coatings on ICR. The numerical model is presented in Figure 1.

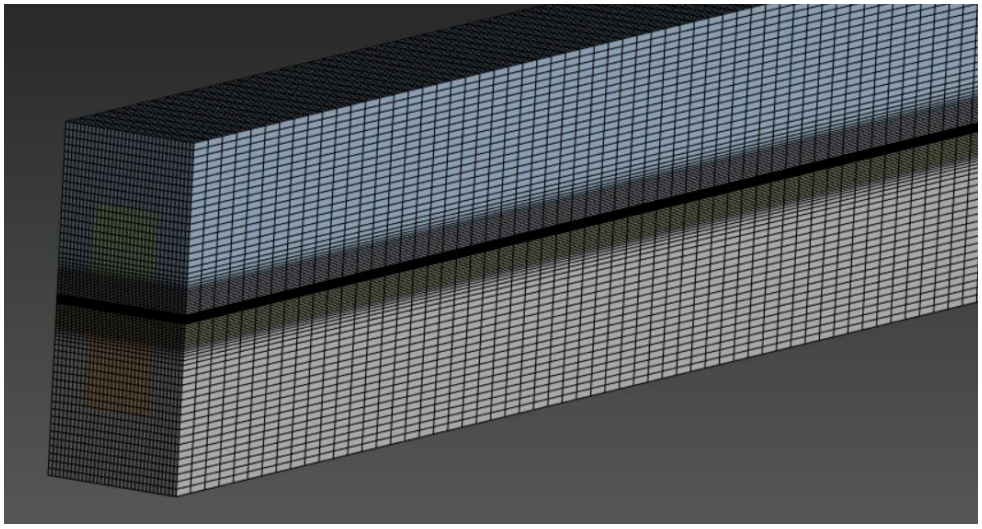


Figure 1. Mesh Structure of PEM Fuel Cell

The numerical model presented in Figure 1 was meshed using Ansys Meshing (Fluent, A. N. S. Y. S. (2011). Ansys Fluent Theory (2011). The mesh parameters were configured in accordance with the low skewness and high orthogonality values recommended in the literature (Choopanya et al., 2016.). A skewness value of 0 and an orthogonality quality value of 1 were achieved, ensuring the accuracy of the numerical study (Choopanya et al., 2016).

Parameters for numerical study were obtained from the literature study used for validation (L. Wang et al., 2003.). Additionally, the diffusivity values of H_2, O_2, and H_2O reference diffusivity (m^2/s) and Equivalent weight of membrane (kg/kmol) were taken from a study that included the numerical analysis of the uncoated model (Chen et al., 2021). Parameters used in the analyses are presented in Table 1.

Table 1. Parameters used in the PEM fuel cell simulation (Chen et al., 2021; L. Wang et al., 2003)

Parameters	Value	Ref
Operating temperature (K)	343	(L. Wang et al., 2003)
Operating pressure (atm)	2,7	(L. Wang et al., 2003)
GDL porosity	0,4	(L. Wang et al., 2003)
CL porosity	0,4	(L. Wang et al., 2003)
Anode exchange coefficient	0,5	(L. Wang et al., 2003)
Cathode exchange coefficient	2	(L. Wang et al., 2003)
H_2 reference diffusivity (m^2/s)	1.10×10^{-4}	(Chen et al., 2021)
O_2 reference diffusivity (m^2/s)	3.23×10^{-5}	(Chen et al., 2021)
H_2O reference diffusivity (m^2/s)	7.35×10^{-5}	(Chen et al., 2021)
H_2O reference concentration(mol/m^3)	56,4	(L. Wang et al., 2003)
O_2 reference concentration (mol/m^3)	3,39	(L. Wang et al., 2003)
Equivalent weight of membrane (kg/kmol)	1100	(Chen et al., 2021)

The numerical analyses were conducted at 343 K and 2.7 atm pressure, in accordance with the experimental study used for validation. The current density-voltage curve reflects the general electrochemical behavior of the fuel cell and serves as a fundamental tool for validation, enabling a direct comparison between the numerical and experimental performance (Energy S, 2011) Through numerical analyses, current and voltage values were obtained, and the corresponding current density values at different voltage levels were compared with experimental data from the literature (L. Wang et al., 2003.) and presented.

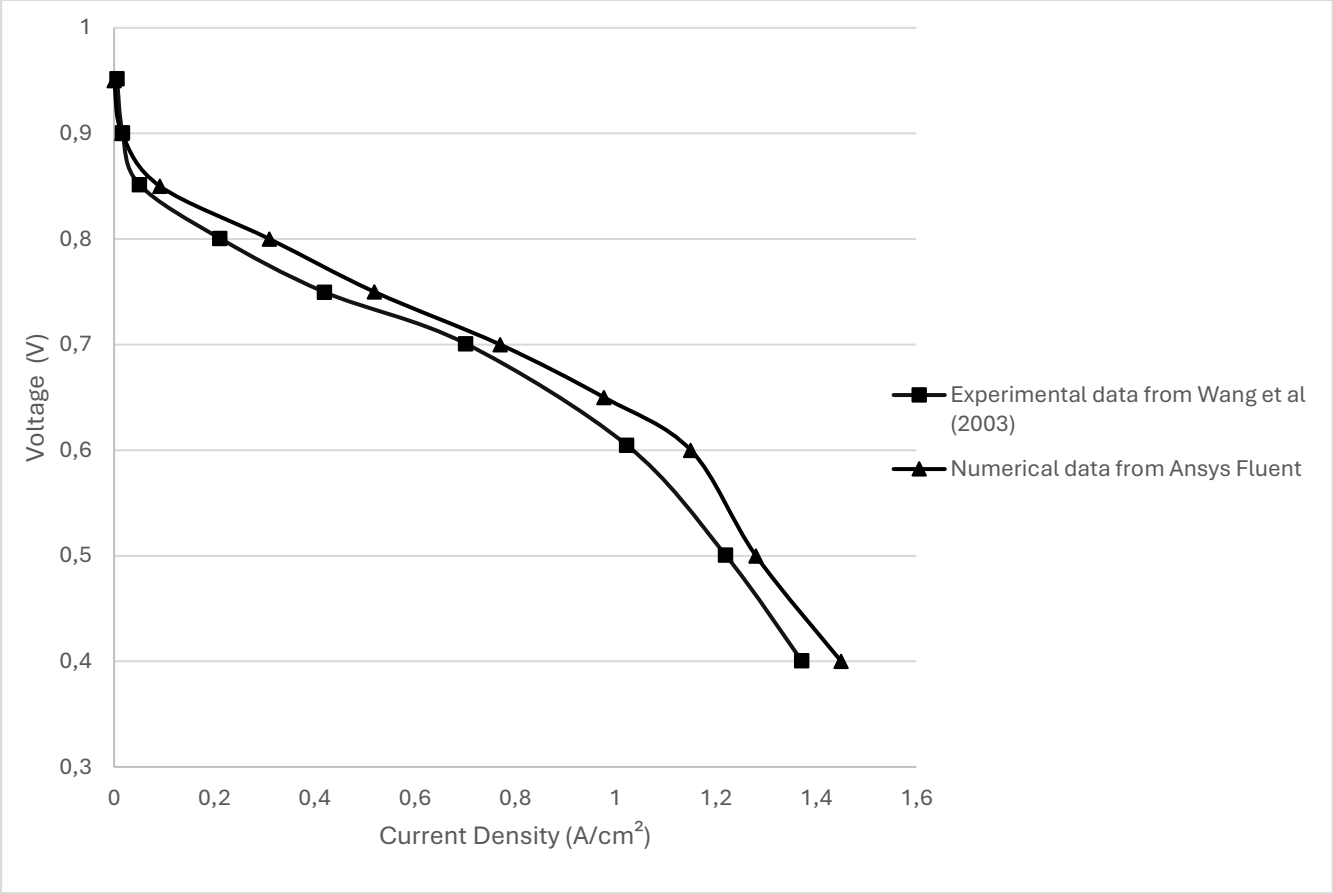


Figure 2. Validation using Data from Experimental Studies

When examining Figure 2, the analyses were validated with a maximum error of 10% within the operating range of fuel cells, which is between 0.5 V and 0.65 V (Qasem & Abdulrahman, 2024) Using the validated numerical model, ICR definitions were assigned to Using the validated numerical model, ICR definitions were assigned to the interfaces between the bipolar plate and the GDL at surfaces A, B, C, and D, as shown in Figure 3, to investigate the effects of coatings

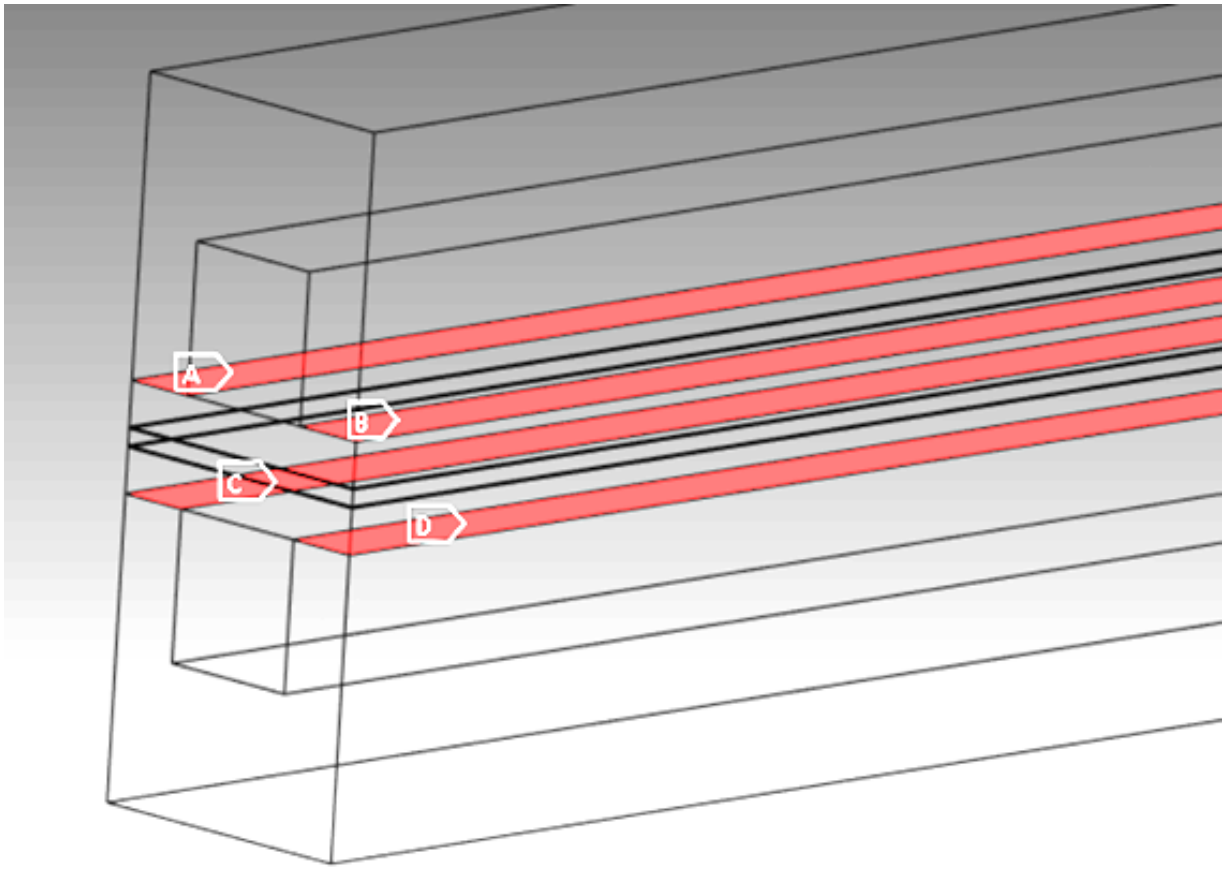


Figure 3. Interfacial Contact Resistance between GDL and Bipolar Plate.

(ICR) assigned to the surfaces shown in Figure 3 vary depending on the coating material. The coating materials used in the literature are CrN (Chromium Nitride), TiN (Titanium Nitride), and Ti/TiN (Titanium/Titanium Nitride), and the corresponding contact resistance values are presented in Table 2.

Table 2. ICR values of coatings used in metal bipolar plates (Haghighat Ghahfarokhi et al., 2016; Jannat et al., 2019; Lee et al., 2013)

Metal Material	Coating	ICR ($m\Omega \cdot cm^2$)	References
SS316L	CrN	23	(Lee et al., 2013.)
SS316L	TiN	7,41	(Haghighat Ghahfarokhi et al., 2016)
SS316L	Ti\TiN	11	(Jannat et al., 2019.)

ICR of different coatings presented in Table 2 were defined on PEM module. The results of the numerical analyses are presented in the Findings section.

Findings

As shown in Figure 4, variations in ICR caused by different coating materials influence fuel cell performance. In this study, numerical analyses were conducted to examine how current density varies at a constant voltage level depending on the ICR of the coating material.

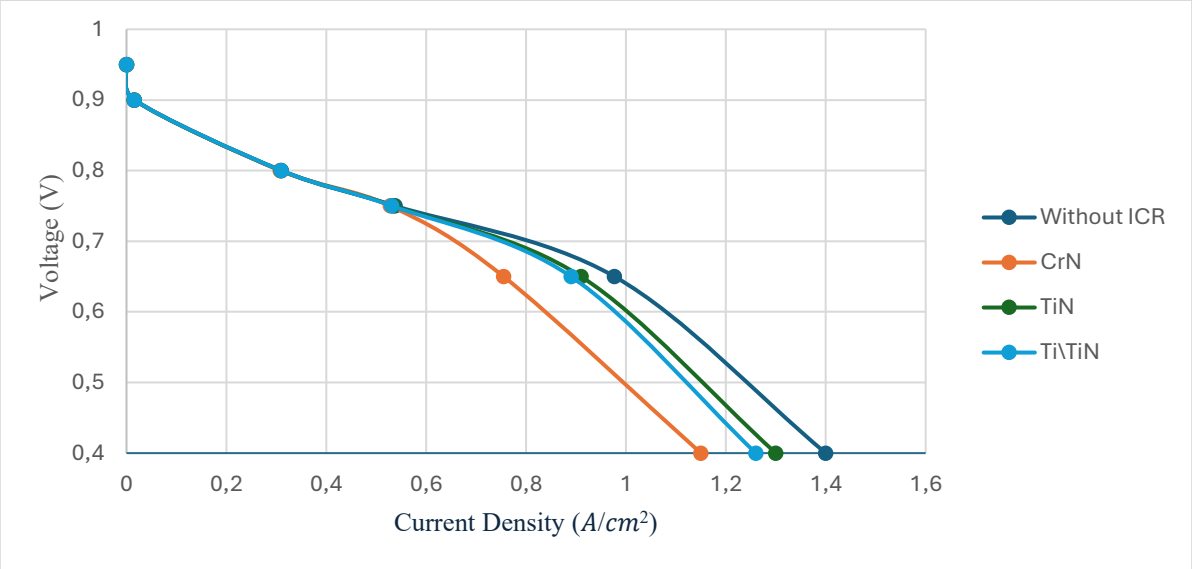


Figure 4. Effect of Electrical Contact Resistance on the Voltage-Current Density Curve

Figure 4 shows that the ICR of the coatings significantly affects the fuel cell performance. The current density per unit voltage has considerably decreased compared to the case without contact resistance. Consequently, this has led to a significant reduction in the power density per unit area of the single-cell PEM fuel cell.

At an operating voltage of 0.65 V, the current density is 0.97 A/cm² without contact resistance. However, with the application of a CrN coating, it decreases to 0.82 A/cm², while Ti/TiN and TiN coatings result in reductions to 0.89 A/cm² and 0.91 A/cm², respectively.

In the absence of ICR the power density was determined to be 0.63 W/cm² at an operating voltage of 0.65 V. However, due to ICR of the CrN coating, the power density decreased to 0.49 W/cm², while for the Ti\TiN and TiN coatings, it was observed to decrease to 0.57 W/cm² and 0.59 W/cm², respectively. This indicates that the CrN coating has an effect of 24.62%, while the Ti\TiN and TiN coatings have effects of 12.31% and 9.23%, respectively. Additionally, it is noted that the impact of ICR becomes more evident at lower voltage levels (0.4 V - 0.6 V).

Conclusion

The conclusions of this study emphasize the significant impact of ICR on coated metal bipolar plates in fuel cells, affirming that the effect of coatings on ICR should not be neglected, as observed in previous simulation studies. As the voltage decreases, the impact of ICR becomes more pronounced, and its influence on the system becomes increasingly significant. For CrN coating at 0.65 V, there is a 15.46% decrease in current density and a 24% decrease in power density. For TiN and Ti/TiN coatings, current density decreases by 6.19% and 8.25%, while

power density decreases by 9.23% and 12.31%, respectively. Furthermore, the results indicate that the influence of the TiN coating is lower compared to the other two coating types, suggesting that TiN is currently the most suitable coating for metal bipolar plate fuel cells.

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