Data-driven approaches as a possible means for modeling water transport in gas diffusion layer of fuel cells

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Key Words:
PEFC; GDL; water management; gas diffusion layer; pore networks; machine learning

Adequate water management in polymer electrolyte fuel cells (PEFC) is a key factor for their performance and durability. Liquid water accumulation in either the diffusion media or the gas channel leading device malfunctioning[1]. Strong efforts have been devoted to numerical modeling of liquid water transport in fuel cells with the aim of predicting favorable and unfavorable scenarios. While direct numerical simulation of the behavior of liquid droplets in gas channels using simplified models or even standard CFD tools has been successful [2,3] the analysis of liquid transport in the GDL or microporous layer (MPL) remains a major challenge. Even most recent and sophisticated CFD approaches are incapable of providing results of practical relevance due to the extreme computational cost of the associated simulations[3] . On the other hand, there exist the highly efficient approaches that rely on simplified representation of the physics. Among them, the pore network model (PNM) [4] is one of the most commonly used methods. In the present work we outline the main physical and computational modeling bottlenecks of both the aforementioned CFD and PNM approaches. On the basis of these observations, we outline possible solution strategies that may drastically reduce computational cost of the liquid transport modeling in diffusion media without sacrificing the accuracy in the representation of the involved physical phenomena.

REFERENCES

[1] A. Weber et al. (2014). A critical review of modeling transport phenomena in polymerelectrolyte fuel cells. Journal of The Electrochemical Society, 161(12), F1254.

[2] M. R. Hashemi et al. (2021). Toward droplet dynamics simulation in polymer electrolyte membrane fuel cells: Three-dimensional numerical modeling of confined water droplets with dynamic contact angle and hysteresis. Physics of Fluids, 33(12), 122109.

[3] A. Jarauta and P. Ryzhakov (2018). Challenges in computational modeling of two-phase transport in polymer electrolyte fuel cells flow channels: A review. Archives of Computational Methods in Engineering, 25(4), 1027-1057.

[4] J. Gostick et al. (2016). OpenPNM: a pore network modeling package. Computing in Science & Engineering, 18(4), 60-74.