Popular science summary

Green energy is important in making electricity while keeping the planet clean. One terrific way to do this is with a proton exchange membrane fuel cell. It makes electricity using hydrogen and oxygen gas, and the only leftovers are water and heat without pollution. Imagine it like a high-tech sandwich, with layers of different sponge-like ”bread” (called porous structures) in the middle, and each layer is filled with tiny pores of various sizes. The two sides are flanked by plates with grooves (small channels). Hydrogen and oxygen separately enter through channels in the two plates, pass through the tiny connecting pores, and reach the central area. There, a special reaction occurs, producing water and energy to power cars, houses, and more!

While water is naturally made in the fuel cell, it also presents a significant challenge. Since fuel cells work at warm but not very hot temperatures (around 60–80 °C), most of the water stays as a liquid. The water needs to be removed so the fuel cell can keep working smoothly. Think of it like breathing through a straw: if there is too much water inside, the air cannot get through, and one will struggle to breathe. In the same way, if water gets stuck inside the tiny pores and channels of the fuel cell, it blocks the hydrogen and oxygen from getting where they need to go. This makes the fuel cell work less efficiently or even completely stop working. Thus, controlling the water inside the fuel cell is crucial to keep it running well for a long time.

Understanding the movement of water and gases inside fuel cells could provide better guidance for managing water. But, it is not straightforward to observe internal fluid flow directly because the fuel cells have a closed and opaque structure. Advanced image scanning techniques are utilized to visualize water movement, much like using X-rays or nuclear magnetic resonance to reveal internal structures in the human body. However, these methods are expensive, difficult to access, and not flexible enough for many studies. As a result, computer-based numerical simulations have emerged as a viable alternative. These models provide a three-dimensional representation of velocity, pressure, and water content over time, offering insights that are otherwise difficult to obtain experimentally.

Even though significant improvements have been made in studying how water and air move in fuel cells, there are still many unanswered questions. One of the ongoing debates is: Should the inside walls of fuel cell channels repel water (hydrophobic) or attract it (hydrophilic) to work better? Another challenge is that many simulations study different parts of the fuel cell separately, such as the gas channels or one of the sponge-like porous layers made of stacked tiny fibers (hence the fibrous layer). Few studies have examined how these two layers work together, making it harder to understand how water flows between them. Another research gap involves the role of fiber

structure within the fibrous porous layer. The effects of fiber shape, such as thickness and curvature, on the overall pore structure and water transport remain underexplored. Furthermore, defining how water enters the simulation space is not standardized. Different models use varying inlet designs, ranging from local to global water inputs or single-hole versus multi-hole configurations. The impact of these choices on simulation accuracy is not yet fully understood.

To address these limitations, this thesis employs a popular numerical model, the volume of fluid model, in an open-source simulation framework to examine water-gas transport in a porous layer and channel assembly. This model can simulate how water and gases move while maintaining a clear boundary between them, ensuring their natural separation, also known as immiscibility. A new method for reconstructing the fibrous porous layer has been developed, mimicking the stacking of cylindrical spaghetti in a bowl to create pore spaces. The findings reveal that hydrophobic channel surfaces initially enhance water removal but may gradually develop a hydrophilic property over time, affecting long-term performance. The study also shows that increasing fiber diameter reduces water accumulation in the porous layer but leads to greater accumulation in the gas channel, requiring a balance in drainage design. Additionally, fiber curvature has a significant impact on water movement. Higher curvature increases the number of small pores, which slows down water transport and causes water to remain trapped for longer periods. It is like water in a dense sponge with tiny pores, moving slowly, while in a loose sponge with larger pores, it can flow easily.

Another important discovery is that the randomness of fiber influences simulation outcomes. Even when porous layers have nearly identical porosity (pore space) and dimensional size, differences in fiber arrangement during stacking led to variations in water behavior. In particular, straight-fiber porous domains exhibited inconsistent water distribution, while curved-fiber porous domains had more uniform saturation patterns. This suggests that running multiple simulations with different random fiber arrangements is crucial for obtaining reliable predictions, a factor that has been frequently overlooked in previous studies. Furthermore, the results indicate that the water inlet configuration has a significant influence on drainage patterns. To ensure more accurate assessments of porous layer performance, a global inlet design is recommended for thorough evaluation of water transport.

This thesis makes two significant contributions to the field. First, it introduces a novel method for reconstructing fibrous porous structures, incorporating fiber characteristics to provide a more realistic model for studying the internal fluid transport. Second, the simulation results provide more profound insights into two-phase flow behavior, enabling future studies to enhance fuel cell design and develop more efficient water management strategies for proton exchange membrane fuel cells.