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学 位 論 文 題 名

Two Phase Flow Simulation in a Polymer Electrolyte Membrane Fuel Cell Channel Using the Lattice Boltzmann Method

(格子ボルツマン法によるPEM形燃料電池におけるセパレータ流路内二相流の数値解析研究)

学位論文内容の要旨

Polymer electrolyte membrane (PEM) fuel cells, which convert the chemical energy stored in hydrogen fuel directly and efficiently to electrical energy with water as the only byproduct, have the potential to reduce our energy use, pollutant emissions, and dependence on fossil fuels. The proper operation of a PEM Fuel cell is guaranteed only if proper water management is achieved. Performance depends on water transport mechanisms in each cell. In particular, the liquid water transport is strongly affected by the air flow-water (vapor or liquid droplets) interaction at the interface between the porous electrode and the gas flow channel. On the other hand, the water management is only practically achievable through indirect control of the inlet flows properties, i.e. (flow rate, humidity, pressure, and temperature) and gas channel wettability and channel-shape design.

In this work, challenge was made to establish a computational model which enables to analyze the main water transport mechanisms through the PEM Fuel Cell gas-channel. A two-phase flow scheme using the Lattice Boltzmann method (LBM), with large density difference, was developed. The LBM is a powerful technique for simulating transport and fluid flows involving interfacial dynamics and complex geometries. It is based on first principles and considers flows to be composed of a collection of pseudo-particles residing on the nodes of an underlying lattice structure. However, there were problems with the applicability of the simulation results, e.g. there remained the issue of non conservation of the mass of liquid water. Improvements to the calculation process, the formulations for the Successive Over Relaxation (SOR) method, the derivation method of density with steep gradients, and other refinements, were made for stable and reliable simulations of two-phase flows with large density differences.

Using the LBM with large density difference scheme, we developed a model which links the water flow inside the gas channel to the PEM fuel cell performance and the water-air interaction in the cathode channel. First, the basic characteristics of a liquid water droplet placed on the gas channel, having contact with the Gas Diffusion Layer (GDL), and moving under a Poiseuille like flow are determined. It was shown that, after a certain time step, the droplet keeps moving at a constant velocity and the pressure drop of air flow reaches a steady value. These two parameters, the droplet velocity called ''droplet terminal velocity'' and the pressure drop, were used to evaluate the effect of other conditions on the droplet behavior. It is important for the best fuel cell performance to drain water efficiently. So, we introduced a new dimensionless parameter ''pumping efficiency'', which combines the droplet terminal velocity, pressure drop, droplet mass, and air flow rate. The higher is the pumping efficiency, the better is water droplet removal with less pump work and so a better fuel cell

performance.

One of the important effects on the droplet behavior is its location. We compared the two cases; the first one is when the droplet is initially placed at the center of the gas channel and having contact with the GDL and the second one corresponded to the same conditions, but the droplet is initially placed at the corner of the channel. The results showed a large difference scale of droplet terminal velocity due to the higher contact wall resistance and the fact that the droplet at corner was far from the Poiseuille flow mainstream (center of the channel where the velocity is the highest). In the corner case, droplet is decelerated and the pumping efficiency was minimal.

Another parameter which affects the drainage performance is the channel geometry, such as the gas channel height. Thus, simulations were done for various channels heights having the same width and air flow rates conditions. In these special cases, the droplet is decelerated and the pressure drop is significantly changed for shallower channels. Even though the pumping efficiency for deeper channels is high, the GDL surface covered by water was more important, which will prevent the gas diffusion. But, as far as the attaching behavior is considered, the shallower channels are superior in term of performance and droplet velocity removal. This is due to the fact that for shallower channels the pumping efficiency is less affected when the droplet attaches to the wall.

This model also studied the effect of channel wettability on the drain performance. The wettability effect is considered by an index function of the solid wall. We compared the cases of hydrophobic and hydrophilic channel walls for the same GDL surface wettability condition (hydrophobic). In the hydrophobic condition, the droplet terminal velocity and pumping efficiency are higher. Another important result was that for the same conditions, in a shallower gas channel the droplet is able to maintain a relatively high velocity and the pumping efficiency is less affected by the wettability.

Finally, a set of numerical simulations for a complex gas channel geometries i.e. rectangular, triangular and trapezoidal channels were conducted for both conditions; same channel cross-section and same channel width. The results showed that the optimum gas channel design was the rectangular channel, which always gave the best results for pumping efficiency. The optimum gas channel design was about 0.5 mm height and 1.0 mm width. This design gave the best pumping efficiency and was able to maintain relatively high droplet velocity which will result in a high ''drainage speed''.

In conclusion, this work presents a basic understanding for the liquid water droplet behavior in a single PEM fuel cell gas channel and elucidates the effect of important parameters on the fuel cell performance from the drainage point of view. This paper provides the basic work for the extension to more complex and larger scale fuel cell simulation.

学位論文審査の要旨

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固体高分子形燃料電池は次世代自動車や家庭用のコジェネレーションとして期待されており、様々な研究開発がなされている。それらの課題のひとつとして、燃料電池内で生成する水と反応ガスの流動制御がある。すなわち、広い運転条件において燃料電池内で発生する水を円滑に排出する一方、電解質膜の含水量を適度に保つような装置構造を明らかにすることが、システムの簡素化と効率の向上を図る上で求められている。燃料電池の水管理問題の一つとして、ガス流路内の凝縮水挙動がある。一般に表面性状や濡れ性に敏感な微小流路内の凝縮水挙動を実験的に明らかにすることは難しく、実験的な報告はほとんどない。本研究においても実験的な観察を試みたが信頼できる結果を得るには至らなかった。そこで本研究では電池内の複雑な凝縮水挙動を数値計算で表現するための手法をまず開発し、次にそれを用いて凝縮水排出に有効なガス流路の形状を明らかにすることを試みた。

濡れ性影響を考慮しながら複雑な形状内の気液二相流をシミュレートする有効な手法として格子ボルツマン (LBM) 法を用いることとした。しかし、通常の LBM 法は密度比の小さな二相流計算に用いられるものが多く、凝縮水と空気のように 1000 倍程度の密度比の系に対してそのまま適用することは適切とはいえない。そこで、本研究ではこうした高密度比条件においても精度良い計算が出来るように、稲室らの計算手法をベースに、Successive Over Relaxation (SOR) 法や壁面近傍のポテンシャル勾配の設定法に改良を加え、安定した計算が行えるようにした。また、密度勾配の急な気液界面では質量の保存性が保たれなくなる場合が多く発生したので、この改良を行った。こうした修正を加えたモデルを用いて流動液滴前後の接触角や液滴内部の流速を解析した結果、ほぼ妥当な計算が成されていることを確認した。

次に本計算手法を用いて燃料電池ガス流路内の凝縮水液滴の排出特性に及ぼす流路高さおよび気体流速の影響について解析を行った。排出特性を評価する指標として、液滴流速や圧力損失に加えてポンプ効率を新たに定義した。このポンプ効率は摩擦係数の逆数に相当する無次元量であり、少ないコンプレッサー仕事で多量の凝縮水を排出し得る能力を表している。計算の結果、凝縮水が流路中央にある場合と流路角部にある場合では、液滴流速やポンプ効率が大きく異なるほか、液滴が側壁や上壁面に接触した場合にもそれらが顕著に変化する様子を定量的に示すことができた。また、それらを総合した広い条件でバランスよく液滴を排出できる最適な流路高さは約 0.5mm 程度

であることを示した。一方、壁面の濡れ性を変え、凝縮水形状の特徴を比較した結果、疎水性のガス拡散層に比べて流路壁面の濡れ性を親水性とする事によって液滴を壁面側に引き寄せることができ、その結果、ガス拡散層表面の凝縮水カバー面積を少なくし得ることが示された。

最後に、矩形に加えて台形や三角形断面を有する流路形状について、凝縮水の排出性の比較を行った。その結果、ガス流路における液滴位置や壁面の濡れ性の如何にかかわらず、矩形形状のものが液滴排出速度、ポンプ効率および拡散層表面の凝縮水カバー面積の点で有利であることが示された。

以上、本研究により実験の困難な燃料電池における微小ガス流路内の凝縮水排出挙動を解析可能な数値計算法を提案したほか、最適な流路形状条件を明らかにすることが出来た。こうした知見は燃料電池の効率を改善するための電池構造設計を行う上で有用である。また本解析法はさらに複雑な微細繊維構造に対しても適用可能であり、未解明な燃料電池ガス拡散層内の凝縮水挙動の解明に対しても有用になるものと考えられる。

これを要するに、著者は、固体高分子形燃料電池の凝縮水管理に必要な基礎的な知見を得たものであり、エネルギー工学の発展に対して貢献するところ大なるものがある。よって著者は, 北海道大学博士 (工学) の学位を授与される資格あるものと認める。