Effects of the Design and Optimization of Trapezoidal Channels and Baffles (Number and Position) on the Net Power Density of Proton-Exchange Membrane Fuel Cells

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ABSTRACT: The effects of the design and optimization of trapezoidal channels and baffles on the net power density of proton-exchange membrane fuel cells (PEMFCs) are studied. The significant effects of the length of upper and lower sides of the trapezoidal cross section and the number and position of baffles on the net power density of PEMFC have been investigated. It is found that at the same flow rate, changing the effective contact surface between the flow channel and the gas diffusion layer can tremendously improve the current density of fuel cells; moreover, the performance of a PEMFC based on the addition of a baffle can be further improved. The results show that the trapezoidal cross-sectional flow channel with baffles has higher efficiency and better overall performance compared with a basic straight flow channel. In addition, the response surface was used to optimize the trapezoidal cross-sectional flow channel by considering the power loss of output power and the flow rate. The optimal result was obtained with an upper side length of 1.234 mm, a lower side length of 1.8 mm, and a baffle from the entrance at 9.5 mm, increasing the net power density by 4.347%.

1. INTRODUCTION

Environmental and energy issues have always been the obstacles that plagued the sustainable development of society. Nowadays, with the continuous exploitation, excavation, and consumption of fossil energy, energy crisis is looming. Moreover, the problem of environmental pollution caused by the excessive use of fossil energy has become increasingly prominent. Therefore, finding an alternative clean energy to solve environmental and energy problems is high on the agenda. As a new energy technology, fuel cells play a significant role that cannot be ignored. Proton-exchange membrane fuel cells (PEMFCs) have attracted wide attention owing to their low operating temperature, fast start-up speed, and high power density. In order to render fuel cells better operation and performance, it is indispensable to improve their design and optimization.

To obtain the optimal performance of PEMFCs, extensive research studies have been carried out by designing the channel configuration and studying parameters. Bilgili et al. simulated the performance of PEMFCs under different working conditions via setting up obstacles near the exit of the channel. The experimental results indicated that obstacles in the gas flow channel improve concentration distribution along the channel and transfer the reactant gas to the gas diffusion layer (GDL) material, resulting in a higher current density. Ghanbarian et al. added flow channel indentation to cause partial blockage of the flow channel, considering three different indentations (square, semicircular, trapezoidal). It is predicted that the flow will become two-phase when the current density is high, and a sufficient pressure gradient is required so that condensed water is discharged. Alrwashdeh et al. studied the influence of obstacle distribution in the flow channel of PEMFCs on the water distribution during cell operation based on the application of neutron imaging technology. The results showed that additional liquid water condensation increases the airflow resistance. Kang et al. proposed the veinlike flow field and compared it with the serpentine flow field. They found that the veinlike flow field intake power is 3% of that of the serpentine-shaped flow field. Fan et al. introduced two new cathode channel designs, which are multilayer plate channels and integrated multi-layer channels. Frighetto et al. observed that working conditions affect the serpentine flow field of rectangular and trapezoidal cross sections, with trapezoidal being better than rectangular for the faster removal of residual liquid water. Baz et al. designed a new-type serpentine flow field, which improved the cell performance by 22.6%.

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Numerous researchers have used various approaches and evaluation objectives to further optimize the channel’s geometric structure. Heidary et al.11 used the SIMPL algorithm to optimize the partial blockage and complete blockage of the block in the flow channel. It can be inferred that if the number of cathode-side stoppers is 5 and all of them are blocked, the net power will be increased by 30%. Cai et al.16 designed a bionic flow channel through imitating the shape of a cuttlefish fin, using genetic algorithms to optimize the waveform, and compared it with the basic direct flow channel and wavy flow channel. Their research results revealed that the bionic flow channel can increase the output power density by about 2%. Perng et al.17 took advantage of the SIMPLE-C algorithm to find the best cross-sectional shape in the trapezoidal baffle in PEMFCs, which can help increase the net power density of the design by 90% compared with the basic model. Perng et al.18 utilized the SIMPLE-C algorithm to study the effect posed by the number of baffles at the bottom of the cathode and anode channels. The simulation results show that when the number of baffles is 5, the net power is 8% higher than that with no baffles; thus, they used experiments to verify the simulation results but also to measure the net power of the five baffles using electrochemical impedance spectroscopy (EIS). As a result, the total impedance became lower than that of the smooth channel. Seyhan et al.19 used an artificial neural network algorithm to predict the cell performance in a wavy snake-shaped flow field. Considering three aspects—flow rate, amplitude, and temperature—a similar trend with the experimental data can be acquired. The number of experiments can be reduced to a certain extent, and the best operating conditions can be found.

Through the abovementioned research studies, optimizing the flow channel structure can improve the conditions of PEMFCs and boost the transmission capacity of the reactant gas, which is mainly manifested by increasing the electrochemical reaction rate so as to enhance the current density. However, the increase of baffles will inevitably increase the pressure drop in the flow channel. This part of the pressure drop is at the expense of additional power consumption, which is not conducive to improving the performance of PEMFCs. Therefore, the pressure drop also has a non-negligible impact on the overall performance of PEMFCs.21–23 At present, there are a few studies on adding baffles to the trapezoidal cross-sectional flow channel to improve the net power density of PEMFCs. In addition, optimizing the length of the upper and lower sides of the trapezoid can increase the effective contact surface between the reactant gas and the gas diffusion layer, and it is easier to diffuse into the catalytic layer for the oxidation–reduction reaction, thereby increasing the current density. Moreover, the addition of a baffle can further increase the current density. In contrast to the basic straight channel, this trapezoidal cross-sectional flow channel with a baffle is competitive in improving battery performance.16

In this paper, COMSOL Multiphysics constructed a three-dimensional numerical model. The trapezoidal cross-sectional flow channel and baffle influence the overall performance, involving current density and pressure drop; it is investigated while keeping the flow channel section constant. Meanwhile, to validate the effect, comparisons between the trapezoidal cross-sectional flow channel and the basic straight channel are carried out. By optimizing the parameters upper side length and lower side length, the best trapezoidal cross section is obtained. Furthermore, the number and the position of the baffles are considered for the purpose of improving the net power density.

2. DESIGN DESCRIPTION

From Figure 1, it can be seen that the geometrical schematic diagram of a single PEMFC with the trapezoidal cross-sectional channel is demonstrated, while Table 1 shows two parameters: geometrical and operating parameters. A PEMFC is composed of flow channels, GDLs, CLs, and a proton-exchange membrane. The trapezoidal cross-sectional channel is illustrated in Figure 1. From the left of Figure 1, it is evident that the upper side length (L1), the lower side length (L2), and the height (H) are variable parameters.

3. MODEL DEVELOPMENT

3.1. Computational Domain and Model Assumptions.

To evaluate the proposed channel, a three-dimensional PEMFC model that is single-phase, isothermal, and steady-state is constructed.
2.5 In Table 3, there are governing equations including the model are shown in Table 2, which are described in detail electrons and gases.

In order to simplify the model, the following assumptions are made: because of the low relative humidity of inlet

| parameter | value (unit) |
|-----------|-------------|
| channel length ($L_{ia}$) | 20 mm |
| channel width (upper/lower) ($W_{ia}$) | 1.6/1.8 mm |
| channel height ($H_{ia}$) | 0.5882 mm |
| Rib width ($W_{ia}$) | 1 mm |
| GDL thickness ($H_{GDL}$) | 0.3 mm |
| membrane thickness ($H_{mem}$) | 0.108 mm |
| CL thickness ($H_{CL}$) | 0.0129 mm |
| GDL porosity ($ε$) | 0.4 |
| GDL permeability (K) | 1.76 × 10⁻¹¹ m²/s |
| air stoichiometric flow ratio ($ζ_a$) | 0.99 |
| H₂ stoichiometric flow ratio ($ζ_c$) | 3 |
| operating pressure (P) | 1 atm |
| relative humidity of inlet flows (RH) | 100% |
| anode reference exchange current density ($i_{a,ref}$) | 700 A/m² |
| cathode reference exchange current density ($i_{c,ref}$) | 0.007 A/m² |
| oxygen reference concentration ($C_{O_2}^{ref}$) | 56.4 mol/m³ |
| hydrogen reference concentration ($C_{H_2}^{ref}$) | 3.39 mol/m³ |
| reference diffusivity of H₂ in H₂O ($D_{H_2O}^{ref}$) | 9.15 × 10⁻⁵ m²/s |
| reference diffusivity of O₂ in H₂O ($D_{H_2O}^{ref}$) | 2.82 × 10⁻⁵ m²/s |
| reference diffusivity of O₂ in N₂ ($D_{N_2}^{ref}$) | 2.2 × 10⁻⁵ m²/s |
| reference diffusivity of H₂O in N₂ ($D_{H_2O-N_2}^{ref}$) | 2.56 × 10⁻⁵ m²/s |
| equivalent weight of electrolyte in the membrane (EW) | 1100 kg/mol |
| Faraday’s constant (F) | 96 487 C/mol |
| universal gas constant (R) | 8.314 J/mol·K |

“Numerical and experimental investigation of the baffle plate arrangement in the performance of the proton exchange membrane fuel cell. Copyright [2020] [Journal of Power Sources/Xuefeng Wang]. The optimization of channels for a proton exchange membrane fuel cell applying genetic algorithm. Copyright [2017] [International Journal of Heat and Mass Transfer/Xiangbing Zeng].”

developed. The comprehensive influence of the trapezoidal cross-sectional channel on the overall performance of the PEMFC is compared with that of the basic straight channel. As shown in Figure 2, a single fuel cell equipped with a symmetric boundary is used as the computational domain.

In order to simplify the model, the following assumptions are set: because of the low flow rate, the flow in the flow channel is laminar; the water inside the fuel cell is in the vapor phase; the effects of gravity are ignored; GDLs and CLs are deemed to be isotropic and homogeneous; and the PEM is not permeable to electrons and gases.

### 3.2. Governing Equations

The governing equations of the model are shown in Table 2, which are described in detail elsewhere. In Table 3, there are governing equations including several source terms. $D_{ij}^{eff}$ is an effective species diffusion coefficient that can be explained by the Bruggeman equation. It can be expressed in accordance with Berning et al. as follows

$$D_{ij}^{eff} = \epsilon^{1.5} D_{ij}^{eff}(T_0, P_0) \frac{P}{T_0} \frac{T}{T_0}^{1.5}$$

In the membrane water content-governing equation, $λ$ is the water content in the membrane, which is a function of water activity $a$. Furthermore, the electro-osmotic drag coefficient $n_d$, the water diffusivity $D_{w}$, and the ion conductivity $σ_m$ are correlated with $λ$.

$$a = \frac{C_{w}^{ref}RT}{P_{H_2O}^{ref}}$$

$$\lambda = \begin{cases} 0.043 + 17.8a - 39.8a^2 + 36a^3 & 0 < a \leq 1 \\ 14 + 1.4(a - 1) & 1 < a \leq 3 \end{cases}$$

$$n_d = \frac{2.5\lambda}{22}$$

$$D_i = \begin{cases} 3.1 \times 10^{-9} \frac{P_{H_2O}^{ref}}{EW} (e^{i(224) \lambda} - 1) & 0 < \lambda < 3 \\ 4.17 \times 10^{-3} \frac{P_{H_2O}^{ref}}{EW} (1 + 161e^{-8\lambda}) e^{346(1/T)} & 3 \leq \lambda < 17 \end{cases}$$

$$σ_m = (0.5139\lambda - 0.326) \exp \left[ 1268 \left( \frac{1}{303} - \frac{1}{T} \right) \right]$$

Moreover, a simplified agglomeration model was selected to simulate the test, especially the electrochemical reaction that occurred in CLs. The reaction rate $J_i$ is determined by the Butler–Volmer equation. An effective coefficient $η_{agg}$ is defined to modify the rates considering the diffusion resistance. The effective current density $i_{eff}$ can be characterized as follows

$$J_i = f_i \left( \frac{C_{k}}{C_{k}^{ref}} \right)^{\gamma} \left[ \exp \left( \frac{\alpha_i F}{RT} \eta \right) - \exp \left( \frac{\alpha_i F}{RT} \eta \right) \right]$$

$$η_{agg} = \frac{3}{\varphi_L} \left( \frac{1}{\tan h(\varphi_L)} - \frac{1}{\varphi_L} \right)$$

$$\varphi_L = \frac{1}{L_{agg}} \sqrt{\frac{L_j^{eff}}{C_j D_k}}$$

$$J_i^{eff} = η_{agg} i_i$$

$i_i$ represents an anode a or a cathode c, $C_k$ is the reactant concentration, and $k$ represents hydrogen or oxygen.

Figure 2. Computational domain of the PEMFC with different channels.
3.3. Boundary Conditions. Symmetrical boundary conditions are applied on both sides of the entire model. In the meantime, the no-flux conditions are used on the external surface except for the inlets and outlets of the channels. The air inlet adopts the average flow rate condition, and the air outlet uses the pressure condition. The temperature of the entire model is prescriptive and is defined as the operating temperature. Equations 11 and 12 are the average flow rates of the cathode and anode inlets, respectively, which can be calculated as follows

\[
\dot{n}_a = \varepsilon_a \frac{i_{\text{max}}}{2F} \frac{1}{A_m} \frac{RT}{x_{H_2}} \frac{1}{P_{\text{ref}}} A_{\text{ch}} \\
\dot{n}_c = \varepsilon_c \frac{i_{\text{max}}}{4F} \frac{1}{A_m} \frac{RT}{x_{O_2}} \frac{1}{P_{\text{ref}}} A_{\text{ch}}
\]

In these two equations, \(i_{\text{max}}\) is the maximum current density, \(A_m\) is the area of the membrane, \(A_{\text{ch}}\) is the channel cross-sectional area, and \(P_{\text{ref}}\) is the reference pressure.

3.4. Numerical Implementation. Four different sizes of hexahedron element grids are selected in this paper to check the independency of the grids; the numbers are 68 800, 78 432, 88 752, and 103 252. As shown in Figure 3, by setting the operating potential at 0.4 V, the relative error of current density between grid systems with 88 752 and 103 252 elements is limited to less than 0.02%. Consequently, the grid system with 88 752 elements can be adopted for the subsequent simulations because of its sufficient density. The computational grids for the PEMFC with a trapezoidal cross-sectional flow channel are shown in Figure 4. Since the gas diffusion layers, catalytic layer, and membrane are of different thicknesses, mesh densities are increased at varying degrees for improving the calculative accuracy.

3.5. Model Validation. To verify the accuracy of the calculation results, it is essential to contrast the PEMFC polarization curve from the simulation calculation results to the experimental data obtained by Wang et al., as illustrated in Figure 5. The simulation results are consistent with experimental

| Table 2. Governing Equations |
|-------------------------------|
| description | equations | solution zones |
| mass | \(\frac{\partial c}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S_m\) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |
| momentum | \(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau + \mathbf{S}_m\) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |
| energy | \(\frac{\partial h}{\partial t} + \nabla \cdot (\rho h \mathbf{u}) = Q + \mathbf{S}_e\) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |
| gas species | \(\frac{\partial c_i}{\partial t} + \nabla \cdot (\rho c_i \mathbf{u}) = \nabla \cdot (D_i \nabla c_i) + S_{i,m} \) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |
| electronic charge | \(\nabla \cdot (\sigma_{\text{ion}} \mathbf{E}) = \mathbf{S}_{\text{elec}}\) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |
| ionic charge | \(\nabla \cdot (\rho_{\text{ion}} \mathbf{E}) = \mathbf{S}_{\text{ionic}}\) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |
| membrane water content | \(\frac{\partial x_{\text{mem}}}{\partial t} + \nabla \cdot (x_{\text{mem}} \mathbf{u}) = \nabla \cdot (\lambda_x V_{\text{mem}}) + S_{x_{\text{mem}}}\) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |
| liquid water | \(\frac{\partial c_{\text{liq}}}{\partial t} + \nabla \cdot (c_{\text{liq}} \mathbf{u}) = V_{\text{liq}} (\rho_{\text{liq}} D_{\text{liq}} V_{\text{mem}}) + S_{c_{\text{liq}}}\) | anode/cathode channel, anode/cathode GDL, anode/cathode CL |

**Figure 3.** Grid independency test.

**Figure 4.** Computational grids for PEMFC calculation.
results; therefore, there is no doubt that the model can be used for computational optimization.

4. RESULTS AND DISCUSSION

4.1. Comparison of Different Numbers and Positions of Baffles. In this section, the effects of baffles in the trapezoidal cross-sectional flow channel on PEMFC performance are considered. An all-around comparison of baffles (number and position) is affected by the distance between the inlet and outlet, the current density, and the cathode pressure drop. The addition of baffles will inevitably increase the pressure drop that is affected by many parameters. In this paper, we mainly investigate whether the power loss caused by the addition of a baffle can be compensated by the increase in its power—evaluated mainly by the net power density to reach this goal. The height of the baffle in this paper is 20% (0.118 mm) of the height of the trapezoidal one, and the width is 1mm. Different numbers of baffles are arranged at equal intervals, with the number of baffles being 1—5. When the baffle number increases, the trend of current density fluctuates; meanwhile, the pressure drop presents an almost linear upward trend, as shown in Figure 6. The reason is that the concentration of the reactants is continuously decreasing along the flow channel; therefore, the baffle has a prominent effect on the gas and causes more reactants to permeate the GDL. When the number of baffles is 1, the current density is larger but the pressure drop is smaller.

Moreover, to consider the influence of the position of the baffle on PEMFC performance, five positions (2.5, 6, 9.5, 13, and 16.5 mm) based on the oxygen inlet are employed. As shown in Figure 7, various positions of the baffles have different implications for the current density and pressure drop. When the position increases, the current density first increases and then declines; on the contrary, the pressure drop first decreases and then increases. This phenomenon is caused because the concentration of the reactant decreases with the direction of the flow channel. The baffle in the middle has a stronger effect on the gas. The maximum current density is reached when the position is at 9.5 mm. The minimum-pressure drop position is also at 9.5 mm.

4.2. Comparison of Three Types of Channels. PEMFCs with three different flow channels, basic straight flow channel, trapezoidal cross-sectional flow channel, and trapezoidal cross section with baffles, are compared. As depicted in Figure 8, it is distinctly seen that the trapezoidal cross-sectional flow channel with baffles and the trapezoidal cross-sectional flow channel are at the maximum and higher than the basic straight channel; thus, the net power density is also better than that of the basic straight channel.

Figure 9 shows that there are different distributions of current density in the membrane with three different flow channels at 0.4 V. It is clearly observed that the current density in the entrance direction reaches a maximum. The reason is that the reactants are gradually consumed so that the current density gradually decreases along the channel direction. Moreover, the current density in the center of the channel is higher than the current density on both sides of the ribs, which illustrates that the trapezoidal cross-sectional flow channel with baffles can effectively improve the current density distribution in the membrane.

Figure 10 presents the distribution of the hydrogen molar concentration in PEMFCs of three different flow channels at 0.4 V (Figure 11). As shown in Figure 12, the distributions of the
oxygen molar concentration in PEMFCs of three different flow channels at 0.4 V are different. It can be observed that the trapezoidal cross-sectional flow channel has a lower hydrogen concentration at the outlet than the basic straight channel, indicating that more hydrogen in the trapezoidal cross-sectional flow channel participates in the electrochemical reaction. In addition, the concentration range at the entrance of the trapezoidal cross section is significantly smaller than that of the basic straight channel, which shed light on that using the trapezoidal section has a better reaction rate than using the basic straight channel (Figure 13).

Finally, the cathode pressure drop of PEMFCs with three different flow channels can be observed at 0.4 V, as shown in Figure 14. It is shown that the adoption of baffles in the flow channel has implications for the increase of pressure drop. However, the pressure drop of the trapezoidal cross-sectional flow channel is slightly larger than that of the basic straight channel, and when the lower side length increases, more reactant gas enters the GDLs. Furthermore, the pressure on both sides of the ribs of the trapezoidal cross-sectional flow channel is closer to the pressure at the center of the channel, and the mass transfer effect is more obvious.

4.3. Optimization and Discussion of the Trapezoidal Cross-Sectional Flow Channel. The data of the current density from the simulation results mentioned above show that it increases as the length of upper and lower sides increases, and meanwhile, the pressure drop increases as the number of baffles increases. In this section, the response surface is used to optimize these two parameters, so that the best trapezoidal cross section is captured to ensure that the current density is kept large as much as possible and the pressure drop is kept small as much as possible. Furthermore, the current density is further improved while selecting the number of baffles as 1 and the position of the baffle as 9.5 mm.

To evaluate the performance of the PEMFC, the net power density is used as the objective; it can be calculated as follows

$$W_{\text{net}} = iV_{\text{cell}} - \Delta P_{\text{ch}} \frac{v_{\text{cell}}}{A_{\text{ch}}} A_{\text{act}}/\eta$$

In eq 13, $W_{\text{net}}$, $iV_{\text{cell}}$, $\Delta P_{\text{ch}}$, $v_{\text{cell}}$, $A_{\text{ch}}$, $A_{\text{act}}$, and $\eta$ are the fuel cell net power density, current density, potential, cathode pressure drop, cathode inlet velocity, channel area, activation area, and pump efficiency, respectively (the pump efficiency in this study is 70%).

Moreover, several constraints are imposed on the two parameters as follows

$$0.5 \text{ mm} \leq L_1 \leq 1.6 \text{ mm}$$
$$1.2 \text{ mm} \leq L_2 \leq 1.8 \text{ mm}$$

Other parameters are fixed: the operational voltage is 0.4 V and the flow channel area is constantly at 1 mm$^2$, which can guarantee the same flow rate. After 50 generations, the

Figure 8. Polarization curves and net power density of three different flow channels.

Figure 9. Distribution of current density in three different flow channels.

Figure 10. Hydrogen molar concentration of three different flow channels.
optimized results are shown in Figure 13. When the design feasibility of the 25th generation reaches optimum, the length of the upper side $L_1$ is 1.234 mm and the length of the lower side is 1.8 mm; compared with the basic straight channel, the net power density is increased by 4.174%.

According to the optimal results mentioned above, the best parameters are as follows: the upper side length $L_1$ is 1.234 mm,
the lower side length $L_2$ is 1.8 mm, the number of baffles is 1, and the baffle position is 9.5 mm from the entrance. As shown in Figure 14, the performance of the optimal trapezoidal cross-sectional flow channel with baffles and that of the basic flow channel PEMFC are compared. It can be observed that compared with the basic case, the optimal case can produce a larger current density, thereby increasing the net power density. The maximum net power density increases by 4.347% when the potential reaches 0.5 V. Moreover, the pressure drop of the optimal situation is relatively gentle and the fluctuation is slight, but the pressure drop of the overall situation fluctuates greatly. The reason is that these two oblique edges of the trapezoid have the function of a baffle, which can make more reactants enter the GDLs and accelerate the reaction rate.

5. CONCLUSIONS

Here, we investigate the PEMFC with a trapezoidal cross-sectional flow channel and baffles. A three-dimensional numerical model was established, where varying the upper and lower side lengths of the trapezoidal cross section and the number and position of the baffles affects the performance of the PEMFC. The response surface is used to optimize the length of upper and lower sides of the trapezoidal section to obtain the optimal trapezoidal section. The effects of the number and position of the baffles are discussed, and results are compared with those of the basic flow channel. Some important conclusions from simulation results and discussion can be summarized as follows: increasing the length of upper and lower sides of the trapezoid can effectively increase the current density, but the influence of the length of the lower side is relatively greater than that of the length of the upper side; adding baffles on the basis of the trapezoidal cross section can further increase the current density; however, an excessive number of baffles will cause the current density to drop; and compared with the basic flow channel, the larger the contact area between the trapezoidal cross-sectional flow channel and the GDL, the easier the reactants in the flow channel will permeate the GDL, which then increases the fuel utilization and current density. The best performance is obtained when a baffle is from the entrance at 9.5 mm, the upper side length is 1.234 mm, and the lower side length is 1.8 mm. While the potential reaches 0.5 V, the net power density of the optimal case is 4.347% higher than that of the basic case.

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■ NOMENCLATURES

A area (m$^2$)
C molar concentration (mol/m$^3$)
D mass diffusivity (m$^2$/s)
EW equivalent molecular weight of the electrolyte in the membrane (kg/mol)
a water activity
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