

Three Dimensional Computations and Experimental Comparisons for a Large-Scale Proton Exchange Membrane Fuel Cell

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Comprehensive experimental validation for a large-scale proton exchange membrane (PEM) fuel cell is performed in this work using the multiphase-mixture (M2) model on a 9.2 million grid-point computational mesh. The predicted fuel cell voltage, high-frequency resistance, as well as current density and temperature distributions all show good agreement with the extensive experimental data under various operating conditions and for two Pt loadings of 0.3 mg/cm² and 0.1 mg/cm². In particular, the present study demonstrates quantitative comparisons of liquid water distribution in the PEM fuel cell with neutron imaging measurements. Such a comprehensive validation against a range of measurements points to the readiness of applying the M2 model to design and develop the next generation of PEM fuel cells and stacks.

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In the past decade, significant advances have been made in polymer electrolyte membrane (PEM) fuel cell technology. However, commercialization of this promising power source for automotive applications is still hindered by high cost and slow, expensive development cycle. Spatially resolved measurements of reaction and transport parameters in a fuel cell, while critical for a basic understanding of the complex electrochemical and transport behaviors, are expensive and difficult, if not impossible to obtain. Modeling and simulation, therefore, play an important role in meeting the increasing demand for details in fuel cell research and development. Additionally, computer simulations have become an increasing part of the discovery and design process for the next generation of highly efficient and compact PEM fuel cells. The latter is epitomized by the advent of 3D fine mesh flow-field deployed in the most recently commercialized fuel cell car, Toyota Mirai.¹

To date, numerous modeling studies have been performed for PEM fuel cells,²⁻²² employing the computational fluid dynamics (CFD) technique to address multi-physics involved in PEM fuel cells under single-phase²⁻⁹ or two-phase¹⁰⁻²² conditions. Several comprehensive and critical reviews have been published on this issue.²³⁻²⁵ However, the majority of prior work is limited to simple geometries such as straight channels, simplified dimensional assumptions such as 1D, 1D + 1D, 2D and 2D + 1D, unrealistic operating conditions such as fully humidified gas feed, or small-scale problems with computational mesh smaller than a million grid-points. While these prior studies helped to understand transport phenomena and reaction occurring in PEM fuel cells, the current challenge facing PEM fuel cell technology is to address real problems arising in development of next generation fuel cells with unprecedented low cost and high durability. Such PEM fuel cells of the future feature a complex 3D flow-field (e.g. the cascade flow-field used in the commercial fuel cell car, Mirai¹), and have auxiliary components, such as coolant channels and inlet/outlet manifolds, so that several million or more mesh elements are minimally needed to build a whole computational domain with sufficient spatial resolution. Although a few large-scale simulations for commercial-size PEM fuel cells have been reported recently,^{26–29} only the single-phase calculations could be handled. For example, the single-phase simulation was presented by Wang and Wang²⁸ for a large-scale PEM fuel cell with 24-channel, 3-pass serpentine flow field. The total mesh number in their study was about 23.5 million. Shimpalee²⁹ also employed the single-phase model to study the dynamic response of a PEM fuel cell during a 20 second cycle using 6.7 million mesh cells. However, these single-phase computations failed to address water flooding and ensuing mass transport loss inherently existing in modern PEM fuel cells under normal operating conditions. Moreover, there has not been

*Electrochemical Society Member. ^zE-mail: cxw31@psu.edu an attempt to validate large-scale simulations against a wide range of experimental measurements including distribution data. Until most recently, experimental validation studies were limited to small-scale calculations. For example, Fink et al.³⁰ and Carnes et al.³¹ performed validation studies on PEM fuel cells with parallel serpentine flow-field, but the computational mesh elements in their works were less than two million and only the current density (CD) distribution was examined.

In this work, a series of 3D computation and experimental validation on a PEM fuel cell used in a U.S. Department of Energy (DOE) project³² is performed using the multiphase-mixture (M2) model. The predicted cell voltage and high-frequency resistance (HFR), current density and temperature distributions, as well as liquid water distribution are compared to the extensive experimental data under various operating conditions and at two platinum (Pt) loadings of 0.3 mg/cm² and 0.1 mg/cm², respectively. The details of the operating conditions and corresponding experimental data can be found on the DOE project website.³²

Numerical Model

This modeling study employed a non-isothermal, fully two-phase model based on the M2 approach.¹² The two-phase flow in both porous components and gas flow channels in PEM fuel cells are taken into account. Equations of mass, momentum, energy, species and charge conservation under either single- or two-phase condition can be summarized as follows:

Continuity equation

$$\nabla \cdot (\rho \vec{u}) = 0 \tag{[1]}$$

Momentum conservation

$$\nabla \cdot \left(\frac{\rho \vec{u} \vec{u}}{\epsilon^2}\right) = -\nabla P + \nabla \cdot (\mu \nabla \vec{u}) + S_u$$
[2]

Energy conservation

$$\nabla \cdot \left(\gamma_T \rho c_p \vec{u} T\right) = \nabla \cdot \left(k^{eff} \nabla T\right) + S_T$$
[3]

Species conservation

$$\nabla \cdot \left(\gamma_C \vec{u} C^i\right) = \nabla \cdot \left(D_g^{i,eff} \nabla C_g^i\right) - \nabla \cdot \left[\left(\frac{mf_l^i}{M^i} - \frac{C_g^i}{\rho_g}\right) \vec{j}_l\right] + S_C^i$$
[4]

Electron conservation

$$0 = \nabla \cdot \left(\sigma_s^{eff} \nabla \Phi_s\right) - j$$
^[5]

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Table I. Physical parameters.^{35–37}

Parameters	Value
Dry membrane density (g cm ⁻³), ρ_e	1.9
EW of dry membrane (g mol ⁻¹), EW	950
Anode Pt loading (mg cm ⁻²)	0.05
Cathode Pt loading (mg cm ⁻²)	0.3/0.1
Anode ionomer carbon weight ratio (I/C)	0.6
Cathode ionomer carbon weight ratio (I/C)	0.95
GDL porosity, ϵ_{GDL}	0.625
MPL porosity, ε_{MPL}	0.5
Carbon fraction in CL, ε_c	0.696
Carbon density (g cm ⁻³), ρ_c	1.95
Volume fraction of ionomer in CL, ϵ_e^{35}	$\varepsilon_e = (I/C)\varepsilon_c \frac{\rho_c}{\rho_e} \left(1 + \frac{M_w \rho_e}{\rho_w EW} \lambda\right)$
Proton conductivity of ionomer (S m ⁻¹), κ^{35}	$\kappa = 22.0 \exp\left(-\frac{E_\kappa}{R} \left(\frac{1}{T} - \frac{1}{353.15}\right)\right) a^{2.24}, \ E_\kappa = 12 \text{kJ/mol}$
Tortuosity of the ionomer phase in the catalyst layer, $\tau_e{}^{35}$	$\tau_e = \begin{cases} 0.0845(\varepsilon_e - 0.04)^{-1.17} & \varepsilon_e < 0.16\\ 1.0 & \varepsilon_e \ge 0.16 \end{cases}$
Water uptake in ionomer, λ^{36}	$\lambda = \begin{cases} \left[1 + 0.2325a^2 \left(\frac{T-303}{30}\right)\right] \left[14.22a^3 - 18.92a^2 + 13.41a\right]a \le 1\\ 8.71 \left[1 + 0.2325 \left(\frac{T-303}{30}\right)\right] (1-s) + (9.22 + 0.181(T-273.15))s \ a > 1 \end{cases}$
Water permeability in membrane (mol m ⁻¹ Pa ⁻¹ s ⁻¹), p_w^{37}	$p_w = 3.2 \times 10^{-11} \exp\left[\frac{E_w}{R} \left(\frac{1}{T} - \frac{1}{363}\right)\right] \exp(3.4a), E_w = 22 \text{kJ/mol}$ $p_{o_2} = p_{dry} \exp(-E_{dry}/RT) + \upsilon_w p_{wet} \exp(-E_{wet}/RT)$
Oxygen permeability in ionomer (mol m ⁻¹ Pa ⁻¹ s ⁻¹), $p_{o_2}^{36}$	$p_{dry} = 0.674 \times 10^{-11}, p_{wet} = 5.05 \times 10^{-11} \text{ mol/(mPas)}$ $E_{dry} = 21.28, E_{wet} = 20.47 \text{ kJ/mol}$
Water volume fraction in ionomer, v_w	$\upsilon_{\rm w} = 18\lambda/(18\lambda + EW/\rho_{\rm e})$
GDL thermal conductivity (W m ⁻¹ K ⁻¹)	0.5
MPL thermal conductivity (W m ⁻¹ K ⁻¹)	0.25
CL thermal conductivity (W m ⁻¹ K ⁻¹)	0.2
Electrical contact resistance (Ω cm ²)	0.012
Coolant specific heat (J g ⁻¹ K ⁻¹)	4.18

Proton conservation

$$0 = \nabla \cdot \left(\kappa_e^{eff} \nabla \Phi_e\right) + j \tag{6}$$

where, ρ , \vec{u} , *P*, *T*, *C*^{*i*}, *j*, Φ_s and Φ_e are the density, superficial fluid velocity vector, pressure, temperature, molar concentration of species *i*, volumetric reaction current, electronic phase potential, and electrolyte phase potential, respectively. For more detail about this model, refer to references.^{12,33} For lower Pt loading (0.1 mg/cm²) simulations, the microscopic transport resistance of oxygen in the cathode catalyst layer (CL) will play an important role in PEM fuel cell performance. We used our recently developed Low-Pt loading model to account for Low-Pt loading effect,³⁴ considering the interfacial transport resistances at ionomer, water film and Pt particle surfaces. The physical parameters relevant to the present study are listed in Table I.

Figure 1 shows the computational geometry and mesh of the modeled PEM fuel cell in this work. This fuel cell includes 11 and 22 zigzag flow channels on the anode and cathode side, respectively. Each side has 12 coolant channels with the arched manifolds near the inlet and outlet. Due to the complex geometry of the gas flow channels and coolant channels, the bipolar plates (BPs) and gas channels, as well as the membrane electrode assembly (MEA) are meshed separately in order to simplify the meshing process and reduce the mesh element number. This results in the non-conformal meshes in both anode and cathode bipolar plates, and in cathode gas diffusion layer (GDL) as shown in Figure 1b. The total number of the mesh elements is about 9.2 million with 95 mesh layers along the through-plane direction of the cell. Details of the geometrical dimensions of the cell are listed in Table II.

The governing Equations 1–6 coupled with the low-Pt loading model for the cathode CL are solved with the commercial CFD software, Fluent 14.5, using SIMPLE algorithm³⁸ and algebraic multigrid (AMG) method.³⁹ User defined functions (UDFs) are added to update the source terms, transport properties, boundary conditions and electrochemical reactions in these equations during calculation. Parallel

computational methodology is used to handle such large-scale simulations on a Linux PC with 24 processors and 32 GB DDR RAM. For a typical two-phase simulation case, several thousand iterations are required to reach convergence with the water imbalance less 2% and species imbalance less than 1%.

Results and Discussion

The present validation studies are performed on 10 cases, including 6 cases with 0.3 mg/cm^2 Pt loading and 4 cases with 0.1 mg/cm^2 Pt loading. These cases have different inlet boundary conditions and operating temperatures. Table III lists the operating conditions, where the Letters B and L in Case No. indicate the cases with 0.3 mg/cm² Pt loading and 0.1 mg/cm² Pt loading, respectively.

Figure 2 shows the contours of the simulated current density (a) and temperature (b) distributions in the membrane, temperature distribution on the cathode bipolar plane (c), as well as water saturation distribution in the cathode gas flow channel (d) and GDL (e) for Case B1 at 1.5A/cm². In Figure 2a, it can be seen that the current density approximately decreases along the cathode flow channels as the oxygen concentration deceasing. The current density distribution patterns closely follow those of the cathode zigzag flowfield, where the area underneath the cathode channel usually has higher local current density due to higher oxygen concentration. Moreover, some regions with much smaller current density exist near the top and bottom edges in the membrane. Near these regions, the gas flow is detoured by the zigzag channels so that the oxygen is difficult to transport there by diffusion. The temperature distribution in the membrane shown in Figure 2b has a matting pattern, because of the different patterns of the zigzag flow channels in anode and cathode sides. On the cathode bipolar plate as shown in Figure 2c, the region above the MEA and near the outlet of the coolant channels has the highest temperature. A region of lower temperature is seen on the right side of the cathode bipolar plat, as caused by the cooling from the anode inlet gas. In Figures 2d and 2e, the water saturation in the cathode gas channel





and GDL increases along the cathode flow direction. Although the anode inlet is almost completely dry in this case, the cathode side still accumulates considerable liquid water through condensation due to the low operating temperature. As seen from Figure 2e, the liquid water saturation rises above 10% in the most part of cathode GDL and becomes higher than 16% near the cathode outlet.

Detailed distributions of the reaction current, temperature and water saturation in the PEM fuel cell shown in Figure 2 are obtained from the 3D computational study with fine mesh. However, it is impossible to obtain these results with such high spatial resolution from the experiments. Usually, the segmented method is used to obtain much coarser distributions of the interested parameters in experimental measurements. According to Reference 32, two 25(length) × 4(width) segmented collectors are used to measure the current density and temperature distributions on anode and cathode bipolar plates, respectively. In order to make direct comparisons, we also divided the simulated results into the same 100 (25×4) segments as in the experiment. In each segment, the simulated values are averaged according to the weight of the mesh area in that segment. Figures 3a and 3b show comparisons of the segmented current density and temperature distributions between the simulation and experiment for Case B2, and Figure 3c shows comparisons of the corresponding 1D profiles along

Table II.	Geometry	parameters	of the	modeled	fuel	cell
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Parameters	Value
Membrane thickness (µm)	18
CCL thickness (µm)	16
ACL thickness (µm)	6
MPL thickness (µm)	30
GDL thickness (µm)	160
Gas channel width (mm)	0.4
Gas channel height (mm)	0.7
Gas channel Length (cm)	18.3
Coolant channel width (mm)	0.7
Coolant channel height (mm)	0.15
Anode land width (mm)	1.5
Cathode land width (mm)	0.5

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			Cathode condition			Anode condition				
Case No.	Loading (mg cm ⁻²)	CD (A cm ⁻²)	Stoich.	Inlet Temp. /Dew point (K)	Inlet Pressure (atm)	Stoich.	Inlet Temp. /Dew point (K)	Inlet Pressure (atm)	Cell Temp. (K)	Coolant Inlet T (K)
B1	0.3	1.5	2	288.21/283.15	1.6	1.5	291.81/173.15	1.01	293	284.85
B2	0.3	1.5	2	309.24/311.27	1.596	1.5	311.81/173.15	1.014	313	304
B3	0.3	1.5	2	329.91/331.06	1.587	1.5	331.69/173.15	1.021	333	323.7
B4	0.3	1.5	2	350.71/350.86	1.602	1.5	351.8/173.15	1.03	353	346.4
B5	0.3	1.5	2	287.98/283.15	1.12	1.5	291.85/173.15	1.51	293	284.37
B6	0.3	1.5	2	310.06/283.15	1.11	1.5	312.98/312.25	1.51	313	306.3
L1	0.1	1.5	2	289.15/283.15	1.68	1.5	293.4/173.15	1.07	293	284.65
L2	0.1	1.5	2	308.51/311.24	1.69	1.5	311.76/173.15	1.08	313	303.19
L3	0.1	1.5	2	328.96/331.06	1.69	1.5	331.45/173.15	1.1	333	323.07
L4	0.1	1.5	2	307.53/283.15	1.24	1.5	311.88/312.32	1.54	313	303.63

Table III. Operating conditions for the validation cases.³²

the cathode flow channels for the same case. It can be seen that the M2 model predictions are in accord with the measured current density and temperature distributions. Moreover, the 1D results successfully capture the trend of current density and temperature variations along the cathode channels. As shown in Figure 3c, the local current density

slightly decreases along the cathode flow channels. In Case B2 with a lower operating temperature of 40°C and higher cathode inlet relative humidity of ~95%, the whole membrane is easily saturated by condensation water, suggesting that the current density profile along the flow direction is controlled by oxygen distribution. Similarly good



(e) Water saturation distribution in cathode GDL

Figure 2. Contours of current density in membrane, temperature in membrane, temperature on cathode BP wall, and saturation in cathode channel and GDL for Case B1 (a) Current density distribution in membrane, (b) Temperature distribution in membrane, (c) Temperature distribution on cathode BP wall, (d) Water saturation distribution in cathode flow channel, (e) Water saturation distribution in cathode GDL.



(c) Current density (I) and temperature (Temp.) distributions along the BP walls

Figure 3. Current density and temperature distributions for case B2 (a) Current density distribution on anode BP wall, (b) Temperature distribution on cathode BP wall, (c) Current density (I) and temperature (Temp.) distributions along the BP walls.



(c) Current density (I) and temperature (Temp.) distributions along the BP walls

Figure 4. Current density and temperature distributions for case B3 (a) Current density distribution on anode BP wall, (b) Temperature distribution on cathode BP wall, (c) Current density (I) and temperature (Temp.) distributions along the BP walls.

agreement of the down-the-channel current density and temperature distributions between model predictions and experiments is achieved in other cases considered, as shown in Figures 4-7 for Case B3, Case B6, Case L3 and Case L4, respectively. Under a higher operating temperature of 60°C as shown in Figure 4, the down-the-channel current density is more non-uniform, showing a lower current density near the cathode outlet than the case of 40°C. This suggests that the higher temperature makes the cell drier, thus resulting in the drier membrane close to the cathode outlet for the much low inlet relative humidity on the anode side. In Case B6, which has the counter-flow of an almost completely dry cathode and a wet anode inlet, the current density shows an obvious peak near the cathode inlet as shown in Figure 5. The increase in current density from the dry cathode inlet originates from gradual wetting of the membrane. However, after the membrane is fully wet, the current density profile starts to be dominated by oxygen concentration which decreases downstream the cathode channel. Near the cathode outlet, the wet cathode stream faces the wet anode inlet, thus further increasing the water saturation along the cathode outlet. As a result, the local current density near the cathode outlet becomes lower than Case B2 at the same operation temperature.

For lower Pt-loading cases shown in Figures 6 and 7, the downthe-channel current density and temperature distributions demonstrate same trend as those at higher Pt loading. Under the same current density loads, the lower Pt cathode hardly impact the macro-scale dis-



Figure 5. Current density and temperature distributions for case B6, (a) Current density distribution on anode BP wall, (b) Temperature distribution on cathode BP wall, (c) Current density (I) and temperature (Temp.) distributions along the BP walls.

tributions of water, reactants and temperature; however it increases the micro-scale transport resistance in the catalyst layer,³⁴ thus decreasing cell voltage. Lower cell voltage in turn means higher waste heat generation rate; as such, the temperature rises in the bipolar plate for lower Pt-loading cases are higher than those in higher Pt-loading cases.

Figure 8 shows the comparisons of the predicted voltage and HFR with the experimental data for all cases with Pt loading of 0.3 mg/cm^2 and 0.1 mg/cm², respectively. The simulations capture the voltage and HFR changes in a wide range of operating conditions for both Pt loadings. Obviously, the cases with lower Pt-loading demonstrate lower cell voltage under the otherwise same operating conditions. The operating temperature also play an important role on cell voltage. In the present work, the cells running at 60°C exhibit the best performance, suggesting an optimal combination of sufficiently wet membrane and hence a low HFR, a low liquid water saturation, and additionally high catalyst and ionomer activities. In addition, good agreement of the voltage and HFR between simulations and experiments is obtained for most cases, while a slightly larger discrepancy in voltage is seen in Case B5 and Case L1. It is worth noting that these two cases both correspond to extreme conditions with output voltage lower than 0.3 V. Under such extreme operating conditions, there is usually large measurement error or uncertainty in the data. On the



(c) Current density (I) and temperature (Temp.) distributions along the BP walls

Figure 6. Current density and temperature distributions for case L3 (a) Current density distribution on anode BP wall, (b) Temperature distribution on cathode BP wall, (c) Current density (I) and temperature (Temp.) distributions along the BP walls.

other hand, the operating temperature in these two cases is relatively low $(20^{\circ}C)$. Under this temperature, the model may underestimate the liquid water saturation. However, the experimental data of the water level under such low temperature is absent at present. Therefore, additional experiments are needed to explain the voltage discrepancy for these cases.

The comparison of the water thickness distribution between simulation and neutron imaging is shown in Figure 9 for Case B2, B3, B4 and B6, respectively. The water thickness in simulations is calculated by

$$t_w = \int s_k \varepsilon_k dx \tag{7}$$

where *s* and ε are the water saturation and porosity in the gas channel, GDL, MPL or CL with the subscript k denoting different components. For the membrane, the product $s_k \ \varepsilon_k$ in Equation 7 is replaced by $\lambda \cdot 18\rho_e$ /EW. The integration is performed across the entire thickness of the cell. It is seen from Figure 9 that the simulated water thickness distribution agrees with the neutron imaging quite well.

The striped pattern of the water thickness distribution is indicative of the rib location distribution of the cathode bipolar plate, where the region under the rib exhibits higher water saturation. The liquid water in the cell decreases gradually as the temperature increases. In Case B2 at 40°C, liquid water nearly spreads through the whole cell,



Figure 7. Current density and temperature distributions for case L4 (a) Current density distribution on anode BP wall, (b) Temperature distribution on cathode BP wall, (c) Current density (I) and temperature (Temp.) distributions along the BP walls.

while the cell has almost no liquid water in Case B4 at 80°C. The liquid water in Case B3 has a better level between Case B2 and Case B4. In addition, although Case B2 and Case B6 work at the same temperature, different water distribution patterns appear due to the different inlet relative humidity conditions. In case B2, the cathode inlet has high relative humidity and the anode inlet is completely dry. The region near the anode inlet therefore has little liquid water. In Case B6, a low relative humidity is employed at the cathode inlet while the anode inlet is much wet, thus resulting in a drier region near the cathode inlet and a higher saturation region near the cathode outlet (or anode inlet). In the present study, the simulations correctly capture the water distribution change with different operating conditions and achieve good agreement with the neutron imaging measurements for water distribution on the cell level. This success demonstrates that the two-phase M2 model is capable to predict water transport and distribution in industrial-scale PEM fuel cells with realistic flow-field geometries.

Conclusions

Large-scale computations of a large-scale PEM fuel cell with parallel zigzag flow-field have been carried out using the multiphasemixture (M2) model. We demonstrate the vast computational capability of M2 model in simulating the comprehensive two-phase



Figure 8. Comparison of voltage and HFR between simulation and measurement for 0.3 mg/cm² Pt loading cases and 0.1 mg/cm² Pt loading cases, respectively (a) 0.3 mg/cm² Pt loading, (b) 0.1 mg/cm² Pt loading.



Figure 9. Comparison of water distribution between simulation and neutron imaging for case B2, B3, B4 and B6 (a) Neutron Imaging, (b) Simulation.

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phenomena in a PEM fuel cell with 9.2 million mesh cells. Ten case studies are performed to examine the validity of these simulations. Reasonable agreement in cell voltage, HFR, and current density and temperature distributions is achieved between simulations and experiments in these cases with various operating conditions under two Pt loadings of 0.3 mg/cm² and 0.1 mg/cm², respectively. In particular, we obtain agreement in predicted and measured liquid water distribution in a practical PEM fuel cell.

While the present work illustrates the two-phase modeling of a PEM fuel cell having 9.2 million mesh cells, larger-scale simulations with more than 30 million mesh cells have also been routinely carried out using the M2 model. In addition, efforts are ongoing to develop a more computationally efficient and robust M2 model. The improved model is expected to simulate PEM fuel cells and stacks with more than 100 million mesh cells on hundreds of computer processors in a few days of calculations. The final goal is to integrate this tool as an efficient and cost-effective means to discover, prototype and optimize the next generation of fuel cells with unprecedented performance, durability, and low cost.

List of Symbols

Specific heat (J kg⁻¹ K⁻¹) $c_p \\ C^i$

- Molar concentration of species $i \pmod{m^{-3}}$
- $D^{i,eff}$ Effective diffusivity of species $i (m^2 s^{-1})$
- Volumetric reaction current density (A m⁻³)
- P Pressure (Pa)
- S Source term in transport equations
- Saturation S
- Т Temperature (K)
- Velocity vector (m s^{-1}) u

Greek

- ε Porosity
- Ionic conductivity (S m⁻¹) к
- Water content in ionomer λ
- Density (kg m^{-3}) ρ
- Electronic conductivity (S m^{-1}) σ

Subscripts/Superscripts

- Ionomer e
- Effective value eff
- Gas g
- Species i
- k Component in cell
- Electronic phase S

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