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Short communication

A simplified method for solving anisotropic transport phenomena in PEM fuel cells

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Abstract

A simplified isotropic numerical treatment for solving the anisotropic electron transport phenomenon in PEM fuel cells has been proposed. In order to maintain appropriate lateral current distribution, the in-plane electronic conductivity in the catalyst and gas diffusion layers is utilized, while an extra contact resistance is added between the gas diffusion layer (GDL) and the current-collecting land to compensate the reduced through-plane electronic resistance. This simplified method is also applicable for solving the anisotropic heat transfer phenomenon in PEM fuel cells, and it improves numerical convergence and stability in three-dimensional large-scale simulations.

Keywords: PEM fuel cell; Anisotropic transport phenomenon; Electron transport; Heat transfer; Numerical efficiency

1. Introduction

Significant progress in numerical modeling and simulation of PEM fuel cells has been made in the past several years, and many three-dimensional multi-physics models, which closely integrate transport phenomena with electrochemical kinetics, have been developed [1–4]. Comprehensive reviews can also be found in the open literature [5–7].

In recent studies of Meng and Wang [8,9], the electron transport phenomenon in PEM fuel cells has been addressed. It was concluded that by solving the electron transport equation in the catalyst layers, the gas diffusion layers (GDL), and the current-collecting plates on both anode and cathode sides, it enabled further capabilities in modeling PEM fuel cells, including direct incorporation of the contact resistances between the membrane electrode assembly (MEA) and GDL, and between GDL and the current-collecting land. However, in these studies, the electron transport process in the catalyst layer and GDL was assumed to be isotropic, but in reality, the GDL material is highly anisotropic; for example, the GDL electronic conductivity in the through-plane direction is 300–500 $S\,m^{-1}$, while it is 3000–5000 $S\,m^{-1}$ in the in-plane direction, showing an order of magnitude difference. As examined by Meng and Wang [8], different values of the electronic conductivity could result in large difference in the lateral electronic resistance, and as a result, very different current density distributions. Therefore, in PEM fuel cell modeling, the anisotropic property of the GDL material must be taken into account properly.

In theory, there is little difficulty in considering the anisotropic transport phenomenon, but in numerical calculations, an order of magnitude difference in the electronic conductivity in the anisotropic GDL material could cause significant difficulty in terms of numerical convergence and stability, especially in numerical implementation of a PEM fuel cell model into the commercial CFD packages, i.e. Star-CD and Fluent, through their user-coding capabilities.

In this technical note, a simplified method for solving the anisotropic electron transport phenomenon in a PEM fuel cell is proposed and evaluated. Further extension of this method for solving the anisotropic heat transfer phenomenon is discussed as well.

2. Theoretical analysis and result discussion

We will first analyze the effects of anisotropic electronic conductivities on the current distribution and cell performance. As presented in Meng and Wang [8], the equivalent lateral electronic

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resistance can be expressed as

$$R_l = \frac{w^2}{2\sigma_s t}, \quad (1)$$

where the parameters, w and t, represent the half-channel width and GDL thickness, respectively, and σ_s the electronic conductivity. Based on Eq. (1), the lateral resistance in a typical GDL with a half width of 500 μm and a thickness of 300 μm can be calculated as

$$R_{l,1} = \frac{(500\,\mu\text{m})^2}{2 \times 5000\,(\text{S m}^{-1}) \times 300\,\mu\text{m}} = 0.83\,\text{m}\Omega\,\text{cm}^2. \quad (2)$$

If we calculate the lateral electronic resistance using the through-plane electronic conductivity of 500 S m^{-1}, we will get

$$R_{l,2} = \frac{(500\,\mu\text{m})^2}{2 \times 500\,(\text{S m}^{-1}) \times 300\,\mu\text{m}} = 8.33\,\text{m}\Omega\,\text{cm}^2. \quad (3)$$

In a numerical model assuming isotropic GDL properties, as detailed in Meng and Wang [8,9], the effect of the two different lateral electronic resistances on current distribution is clearly illustrated in Fig. 1. In the present calculation, a single-channel PEM fuel cell has been simulated, and the cell geometry and other relevant physicochemical parameters are presented in Meng and Wang [8,9]. The x-coordinate is in the through-membrane direction, y along-the-channel direction, z the lateral direction. As can be seen in Fig. 1, current distributions in the lateral direction are completely different in the two cases. Variations of the lateral currents in the middle of the cell length from the two cases are further compared in Fig. 2. In this figure, the lateral variation of the solid line is dictated by oxygen supply, as it is in the same trend as that without solving the electron transport, as shown in Meng and Wang [8]. In contrast, the lateral variation of the dashed line is mainly determined by the lateral electronic resistance.

Based on the numerical results, in order to maintain a correct current distribution in the lateral direction, the in-plane electronic conductivity of the GDL material must be used in a numerical model of PEM fuel cell assuming isotropic electron transport. However, in this method, the electronic resistance in the through-plane direction becomes incorrect. Next, we will examine the electronic resistance in the through-plane direction. As presented in Meng and Wang [8], it can be expressed as

$$R_{tp} = \frac{t}{\sigma_s}. \quad (4)$$

Therefore, a typical resistance in the through-plane direction is

$$R_{tp,1} = \frac{300\,\mu\text{m}}{500\,\text{S m}^{-1}} = 6\,\text{m}\Omega\,\text{cm}^2. \quad (5)$$

In an isotropic treatment using the in-plane electronic conductivity to maintain proper lateral current distribution, as discussed earlier, the electronic resistance in the through-plane direction becomes

$$R_{tp,2} = \frac{300\,\mu\text{m}}{5000\,\text{S m}^{-1}} = 0.6\,\text{m}\Omega\,\text{cm}^2. \quad (6)$$

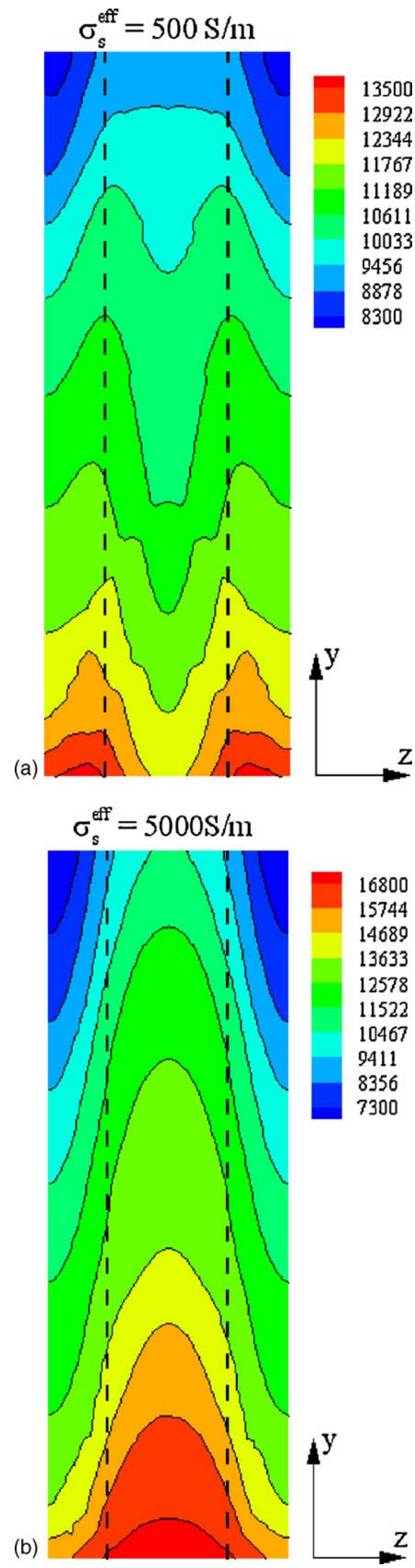

Fig. 1. Current distribution in the middle of the membrane, (a) using the through-plane electronic conductivity of 500 S m^{-1}, and (b) using the in-plane electronic conductivity of 5000 S m^{-1}.

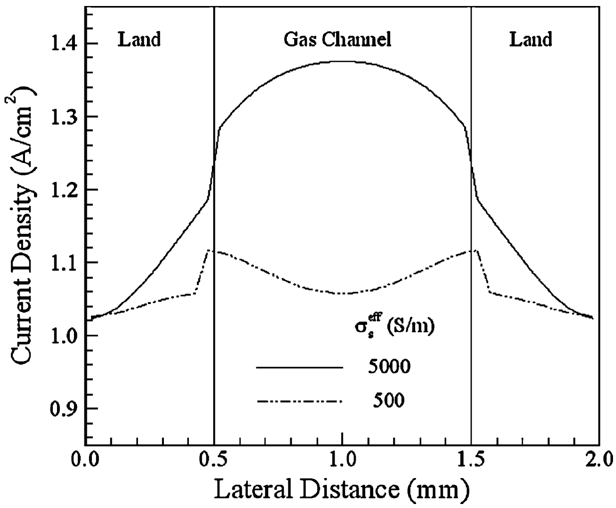

Fig. 2. Variation of current density in the lateral direction in the mid-cell length.

This electronic resistance is thus reduced by 5.4 mΩ cm^2. The reduced electronic resistance is defined as R_r,

$$R_r = R_{tp,1} - R_{tp,2}. \tag{7}$$

Since the electronic resistance in the through-plane direction significantly influences cell performance, the reduced resistance must be compensated in the isotropic treatment using the in-plane electronic conductivity. In anisotropic calculations, since the lateral electronic resistance is very small, as calculated in Eq. (2), the overall effect of the electronic resistance is predominantly one-dimensional, in the through-plane direction. The through-plane electronic resistance will mainly affect cell performance and the along-channel current variation, not the lateral current distribution. Therefore, a simplified method can be established by adding the reduced resistance to the contact resistance. In this treatment, we can not only maintain appropriate lateral current distribution but also obtain correct cell performance.

Because the contact resistance between MEA and GDL varies under the gas channel and the current-collecting land, it is appropriate to include the reduced through-plane resistance into the contact resistance between GDL and the current-collecting land. Furthermore, since current density increases when passing through the GDL/land interface, assuming a uniform current distribution in the lateral direction, an extra contact resistance accounting for the reduced through-plane resistance should be corrected as

$$R_c = \frac{(W - w)}{W} R_r. \tag{8}$$

where the parameter W is the half-width of the current-collecting plate.

In practical fuel cell simulations, the extra contact resistance should be slightly adjusted, like a number of other model parameters, based on a set of experimental data, including the overall cell performance and the along-channel current variations, as discussed in [10]. Afterwards, it should be fixed for all other simulations.

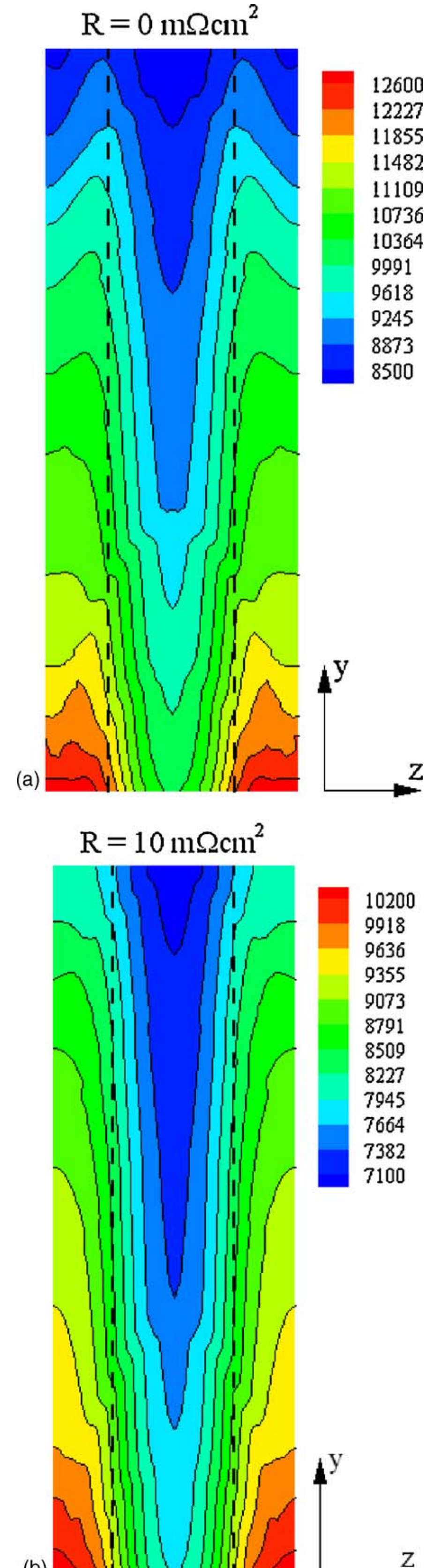

Fig. 3. Current distribution in the middle of the membrane, (a) without contact resistance, and (b) with contact resistance.

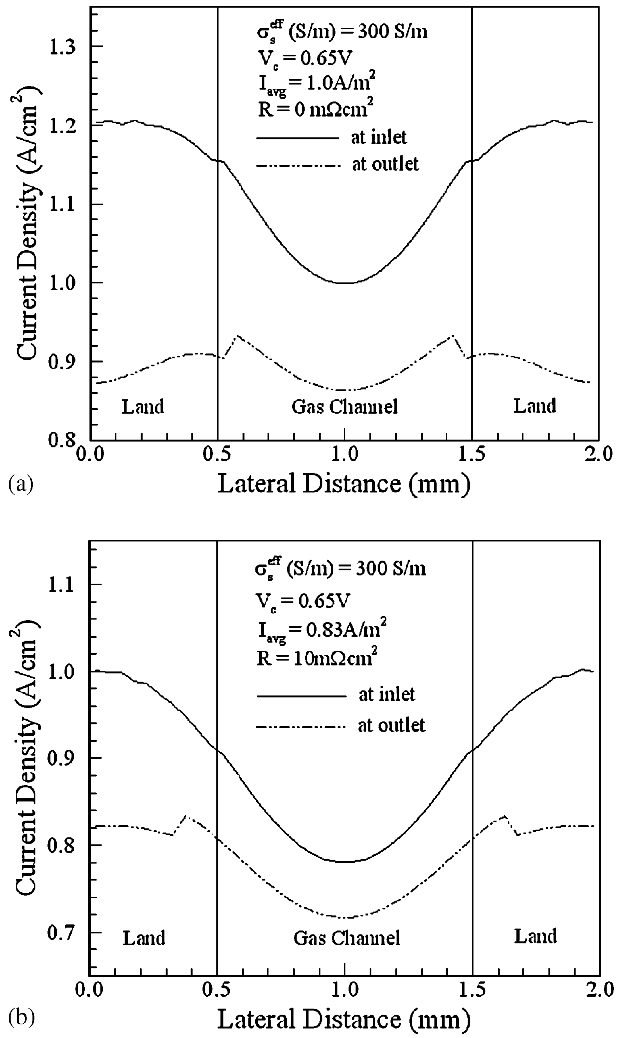

Fig. 4. Variation of current density in the lateral direction at the inlet and outlet regions, (a) without contact resistance, and (b) with contact resistance.

In order to examine the effects of the extra contact resistance on the current distribution and cell performance, two cases are calculated with and without the contact resistance. The current distributions are illustrated in Fig. 3, and the variations of the lateral current density are compared in Fig. 4. With a contact resistance of $10\,m\Omega\,cm^2$ added between GDL and the current-collecting land, the cell performance decreases to $0.83\,A\,cm^{-2}$, from an average current density of $1.0\,A\,cm^{-2}$ without the contact resistance. The variations of the current density in the lateral direction are very similar, especially near the inlet region; near the outlet region, the current density under the land, calculated with the contact resistance, becomes higher because of the low cell performance, which leaves higher oxygen concentration in this region.

Since we have encountered numerical convergence problems in our attempts to directly solve anisotropic electron transport in a three-dimensional PEM fuel cell model, which fully couples various transport phenomena and the electrochemical kinetics [5,8,9], it seems that the present simplified isotropic method is more appropriate for solving this anisotropic phenomenon. This method improves numerical stability and convergence in large-scale simulations.

Because heat is transferred out of a PEM fuel cell mainly in the form of thermal conduction through the current-collecting land [11], this simplified isotropic treatment could be applied to solve the anisotropic heat transport phenomenon in a PEM fuel cell, as well.

3. Conclusion

In this technical note, a simplified numerical method for solving the anisotropic electron transport phenomenon in a PEM fuel cell is addressed. In order to obtain appropriate lateral current distribution, an isotropic treatment using the in-plane electronic conductivity has been proposed. An extra contact resistance is added between GDL and the current-collecting land to compensate the reduced through-plane electronic resistance. This simplified isotropic method can also be applied to solve the anisotropic heat transfer phenomenon in a PEM fuel cell, since heat is transported out of the cell almost exclusively in the form of thermal conduction through the current-collecting land. This simplified isotropic method for solving anisotropic transport phenomena in a PEM fuel cell improves numerical convergence and stability in three-dimensional large-scale simulations.

References

[1] S. Dutta, S. Shimpalee, J.W. Van Zee, Three-dimensional numerical simulation of straight channel PEM fuel cells, J. Appl. Electrochem. 30 (2000) 135.
[2] T. Zhou, H. Liu, A general three-dimensional model for proton exchange membrane fuel cells, Int J. Transp. Phenom. 3 (2001) 177.
[3] T. Berning, D.M. Lu, N. Djilali, Three-dimensional computational analysis of transport phenomena in a PEM fuel cell, J. Power Sources 106 (2002) 284.
[4] S. Um, C.Y. Wang, Three-dimensional analysis of transport and electrochemical reactions in polymer electrolyte fuel cells, J. Power Sources 125 (2004) 40.
[5] C.Y. Wang, Fundamental models for fuel cell engineering, Chem. Rev. 104 (2004) 4727.
[6] R. Sousa Jr., E.R. Gonzalez, Mathematical modeling of polymer electrolyte fuel cells, J. Power Sources 147 (2005) 32.
[7] D. Cheddie, N. Munroe, Review and comparison of approaches to proton exchange membrane fuel cell modeling, J. Power Sources 147 (2005) 72.
[8] H. Meng, C.Y. Wang, Electron transport in PEFCs, J. Electrochem. Soc. 151 (2004) A358.
[9] H. Meng, C.Y. Wang, Multidimensional modeling of polymer electrolyte fuel cells under a current density boundary condition, Fuel Cells 5 (2005) 455.
[10] H. Ju, C.Y. Wang, Experimental validation of a PEM fuel cell model by current distribution data, J. Electrochem. Soc. 151 (2004) A1954.
[11] H. Ju, H. Meng, C.Y. Wang, A single-phase non-isothermal model for PEM fuel cells, Int J. Heat Mass Transfer 48 (2005) 1303.