A Numerical Investigation on the Flow, Thermal and Electrical Coupling in a PEMFC Stack

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Abstract

This paper reports on numerical investigations for a proton exchange membrane fuel cell stack using a CFD-based simulation tool. The stack simulation tool is constructed based on unit cells in parallel that have all components resolved and major transport equations solved in a two-dimensional configuration. The transport equations considered in the model are modified from a complete set of conservation equations (mass, momentum, energy, species and electrical potential). The stack tool also incorporates a flow network solution procedure for all gas and coolant channels to account for flow sharing of fluids at the stack level. The unit cell model in the 2D stack tool is validated with a 3D, comprehensive CFD model. The parameters used in the flow network model are calibrated from experimental data. The stack tool is used to determine the sensitivities of the baseline design of a stack with respect to design parameters, e.g. the dimensions of headers and unit cell components, and operating conditions such the oxidant stoichiometric ratio and coolant flow rate, and so on. Simulation results for the baseline stack with an anomalous unit cell (ill-behaving in flow, thermal or electrical transport) are presented to show how a stack's performance would deviate from the design point due to unfavorable conditions.

Introduction

Flow sharing and thermal management play an important role in the overall efficiency and system stability of a PEMFC fuel cell stack. In a typical plate-and-frame design of PEMFCs for automotive applications, there exist gradients of temperature, electrical potentials and gas concentration in different directions of the stack. The coupling of flow, thermal and electrical transfer in a stack is very involved, hence the design of unit cell and stack hardware is a rather complicated process. In the literature there have been several reports for stack modelling based on reduced dimensional and physical models, e.g. [1] and [2]. These models were implemented using proprietary computer codes, which were thus limited in their capabilities in application to common design practice. In order to better integrate into existing design environment, the CFD methodology is adopted for the development of a stack simulation tool. The CFD-based stack tool thus developed takes the standard procedure of preprocessing (mesh generation), solution of the governing conservation equations, and post-processing. The objective of the present study is to report on the development of the CFD-based simulation tool for the optimal design of PEMFC stacks.

Mathematical Formulation

Figure 1 shows a typical plate-and-frame type of PEMFC. A unit cell is primarily a membrane electrode assembly (MEA) sandwiched by two bipolar plates. The MEA is made of a membrane (proton conductor), coated by catalyst layers, and hot-pressed to gas diffusion layers on both sides.

There are three primary directions of transport, i.e., the direction perpendicular to the MEA, along the flow direction in the unit cell, and along the headers in the stack. These directions correspond to coordinate of z, x, and z in Fig. 1, respectively. Since the thickness of the MEA is the smallest length scale in the stack, the gradients of species and potentials are likely the largest. Along the gas/coolant channels of the unit cell, significant variation of concentration and temperature exist because of stoichiometric ratio and thermal management requirements. The flow sharing in the headers of the stack is expected to be smaller than the former two directions, however, the impact of stack level variations is tremendous because the flow and thermal distribution of the unit cells are closely coupled. To simplify the analysis, the present model makes the following assumptions: (1) The stack operation reaches a steady state; (2) The flow in the porous media and gas channels is in vapor phase; (3) Negligible contact resistance for heat and electron conduction. Because of a 2-D configuration adopted for the computational domain, further simplifications are needed: (1) The flow resistance in the fluid channels is adjusted to reflect the hydraulic diameter of the channel geometry to obtain similar pressure drop; (2) The inlet velocity of gas channels is adjusted to achieve the same stoichiometric ratio as the actual 3-D channel; (3) The thermal and electrical conductivities of the fluid channels are adjusted to allow heat flux and current density to be comparable to the actual geometry.

Governing Equations

Conservation equations of mass, momentum, energy, gas species and charged species (electron) are solved in the present study. For a steady state, the conservation equations can be expressed in the following form:

$$\rho\vec{u}\nabla\cdot\phi = \nabla\cdot\vec{J}_{\phi} + S\,, \tag{1}$$

with $\phi = 1, \vec{u}, h, Y_i, \Phi$ for conservation of mass, momentum, energy, gas species and charged species, respectively. The source terms for gas species and energy conservation as function of local current density are:

$$S_{Y_{O_2}} = \frac{-\nabla\cdot\vec{i}}{4F} \tag{2}$$

$$S_{Y_{H_2}} = \frac{-\nabla\cdot\vec{i}}{2F} \tag{3}$$

$$S_{Y_{H_2O}} = \frac{\nabla\cdot\vec{i}}{2F} \tag{4}$$

$$S_h = i^2 R\,, \text{ where} \tag{5}$$

R is the sum of electrical resistance for ohmic loss and equivalent resistance for the activation overpotential.

Numerical Method and Computational Domain

The stack tool in the present study is built by assembling a group of unit cells. Figure 2(a) shows the computational domain of a unit cell. In a unit cell the governing equations (1)-(5) are solved. The catalyst layers and the membrane are treated as solid, within which electrical and thermal

conduction is considered. The GDLs as well as the fluid channels are treated as porous media. The stack tool is constructed by combining unit cells. A flow network model is implemented on the stack domain and the results appear as the inlet flow rate for the fluid channels, cf. Fig. 2(b). The stack simulation passes the flow resistance of the fluid channels back to the flow network model and this forms an iterative solution procedure. During the iteration, a current density profile is determined from potential solution for each unit cell. The current density profile is then used in evaluation of the source terms, i.e., equations (2)-(5). There are several sub-models for selected regions in the unit cell model, which are explained as follows.

Sub-models: Membrane

simplified model for the membrane is used in the present study. The model considers water transport due to electro-osmotic drag and diffusion. For simplicity the diffusivity of water in the membrane is assumed to be constant, which then makes an analytical solution of the water transport across the membrane possible:

$$\lambda = \lambda_a + \frac{e^{c_3 x}}{e^{c_3 l_m} - 1}(\lambda_c - \lambda_a) \tag{6}$$

where

$$c_1 = \frac{e^{c_3 l_m}\lambda_a - \lambda_c}{e^{c_3 l_m} - 1}, \tag{7}$$

$$c_2 = \frac{\lambda_c - \lambda_a}{e^{c_3 l_m} - 1}, \tag{8}$$

$$c_3 = \frac{2.5i}{22FD}. \tag{9}$$

Sub-model: Catalyst layer

The overpotential in the catalyst layer is expressed as a voltage drop across a resistor. The equivalent resistance at a given current density based on the Butler –Volmer equation can be computed as:

$$R_\eta = \frac{\eta}{i^N} = \frac{RT}{\alpha_c F \cdot i^N} \log\left(\frac{i^N}{a i_0 (C_{O_2})^\gamma}\right). \tag{10}$$

$i^N \equiv i$ at previous iteration

Results and Discussion

Figure 3 shows a comparison of predicted polarization for the baseline case. The computational result for a 3D model are used as the “true solution” with which all other results obtained using reduced dimensional models and simplified model are compared against. Figure 4 shows a typical result of predicted relative humidity (RH) for a 10-cell stack operated at stoichiometric factor of 5 for the cathode flow. The cathode flow and the coolant flow are from left to right in the figure, whereas the anode flow goes in the opposite direction against the cathode and coolant flows.

Conclusions

In this paper we report the numerical implementation of a stack simulation tool based on CFD framework and present some computational results obtained using the stack simulation tool. The simulation tool takes into account flow sharing, thermal and electrical coupling in a stack. The unit cell model in the simulation tool has advantages in detailed account for the flows in gas and coolant channels. The flow network model incorporated in the tool adds capabilities to predict the flow sharing in the stack headers.

Acknowledgement

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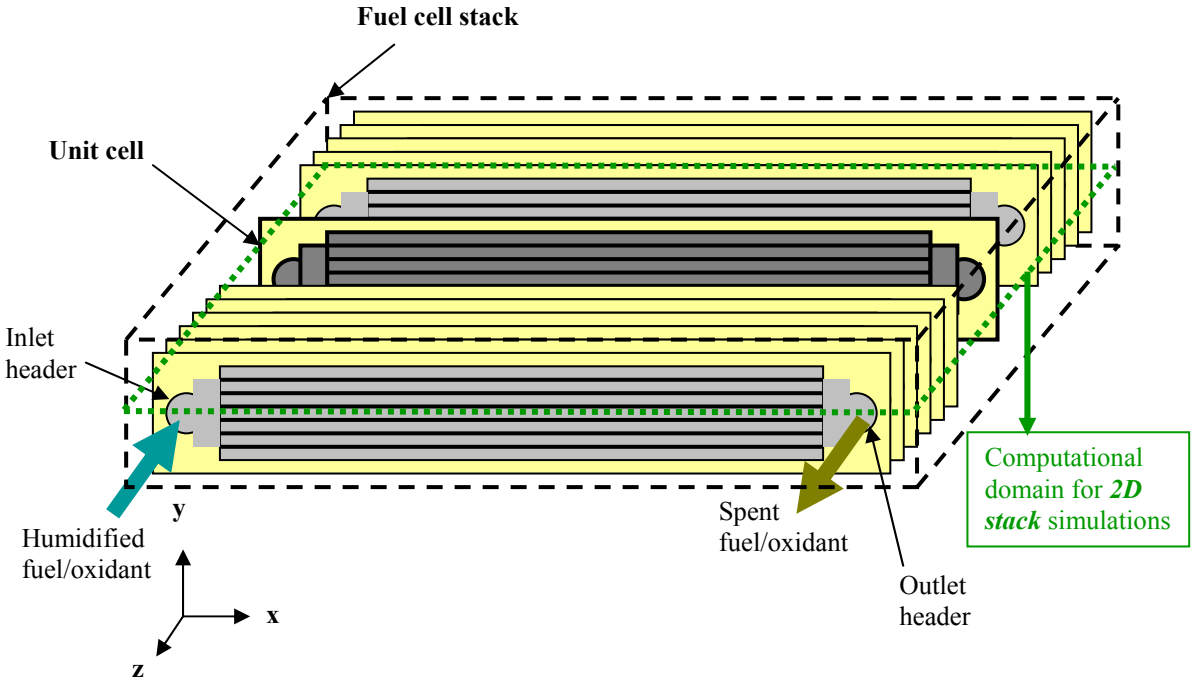
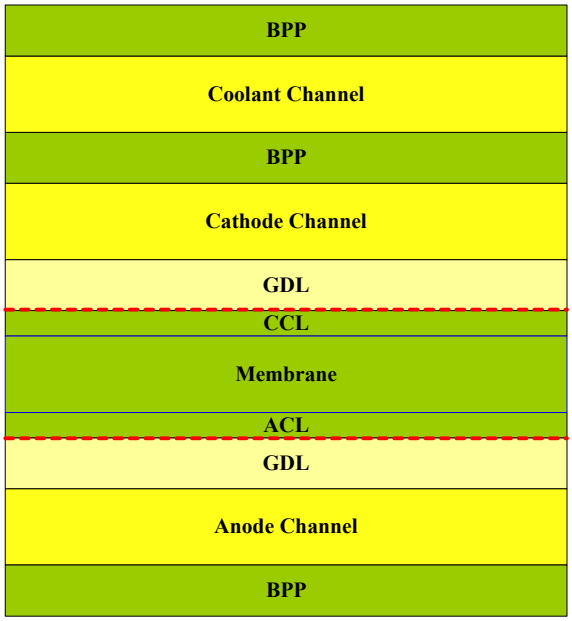
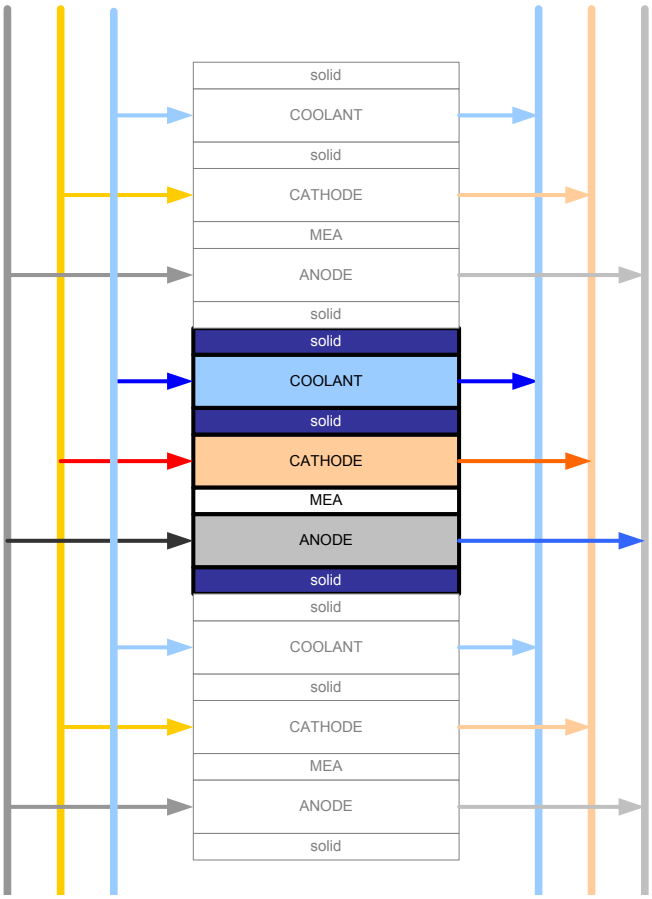


Figure 1.Schematic of a PEMFC stack

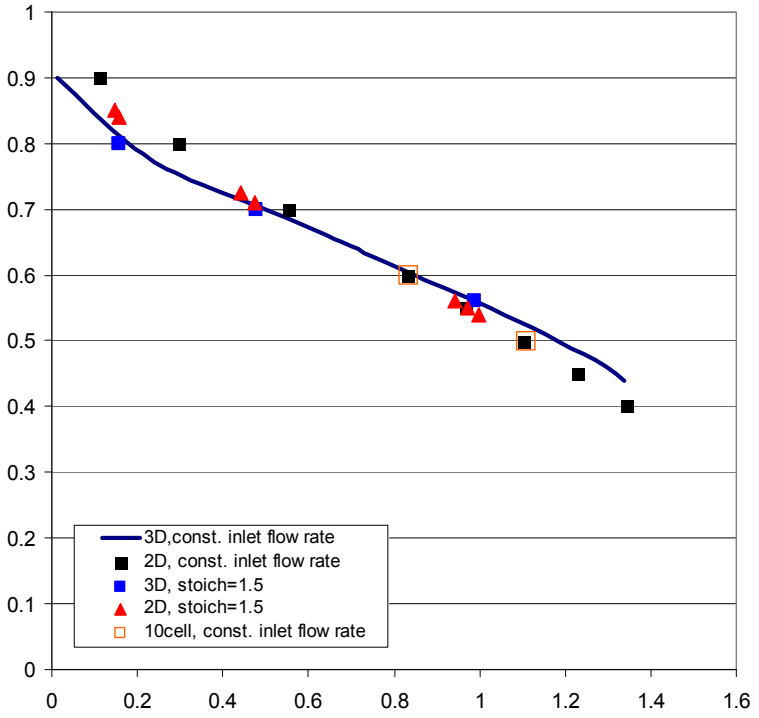


(a)



(b)

Figure 2. Schematic of the stack model (a) components of a unit cell unit (b) cell in a stack model and relation to flow network model.



(b)

Figure 3. Comparison of predicted results, (a) species flow rate along the gas channel, (b) current density and membrane resistance

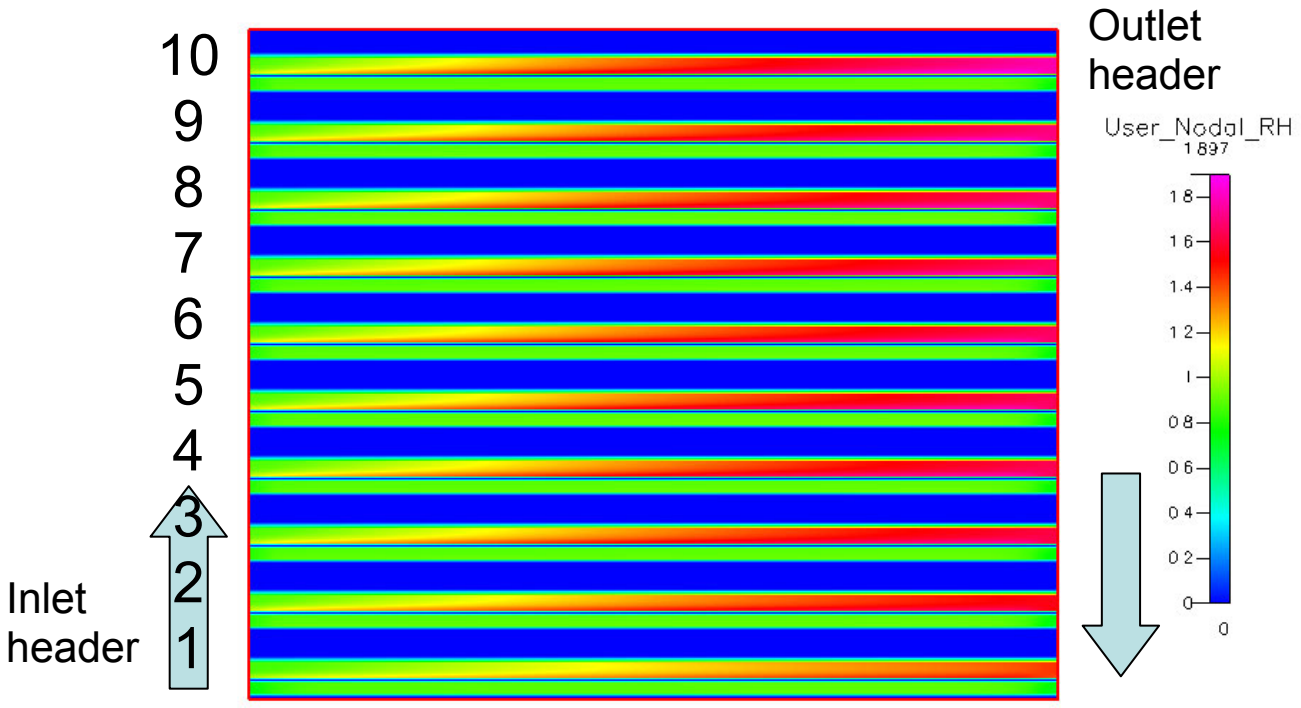


Figure 4. Relative humidity of a 10-cell stack operated at stoichiometric factor 5.

References

[1] Karimi, G., .Baschuk, J.J., Li, X. Performance analysis and optimization of PEM fuel cell stacks using flow network approach. Journal of Power Sources, 147(1-2):162–177, 2005.

[2] Kim, G.S., St-Pierre, J., Promislow, K., Wetton, B. Electrical coupling in proton exchange membrane fuel cell stacks. Journal of Power Sources, 152(1):210–217, 2005.

[3] Mackie, R., Sui, P.C. Djilali, N. Modelling and simulation of flow distribution in a PEMFC stack. ASME Fourth International Conference on Fuel Cell Science, Engineering and Technology, Irvine, CA, 2006.

[4] Springer T.E., Zawodzinski T.A., Gottesfeld S. Polymer electrolyte fuel cell model. J. Electrochem. Soc. 1991; 138(8), 2334–2342

[5] CFD-ACE+ User's Manual, v. 2006, ESI-CFD, Huntsville, AL, U.S.A.

[6] Sui P.C., Kumar S., Djilali N. Advanced computational tools for PEM fuel cell design – Part 1: Development and Base Case Simulations. J. Power Sources, in press.

[7] Sui P.C., Kumar S., Djilali N. Advanced computational tools for PEM fuel cell design Part 2. Detailed experimental validation and parametric study. J. Power Source, in press.