Meshing Strategy for PEM Fuel Cells CFD Modelling – A Systematic Approach

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Abstract. Typical PEM fuel cell models usually involve more than 10^6 mesh elements making the computation very intense. This necessitates an effective way to mesh the computational domain with a minimum number of mesh points while, at the same time, maintaining good accuracy. The meshing strategy in each flow direction is investigated systematically in the current study and it has been found that mesh resolution in different directions has a different degree of influence on the accuracy of solutions. The proposed meshing strategy is capable of greatly reducing the number of mesh elements, hence computation time, while preserving the characteristics of important flow-field variables.

Introduction

A polymer electrolyte membrane (PEM) fuel cell is the most promising potential candidate that may replace conventional internal combustion engine (ICE) in the near future due to its high efficiency and environmental friendliness. However, significant technical challenges such as durability, performance, and cost-effective manufacturing method [1], [2] have to be addressed to bring it to commercialisation.

Computational Fluid Dynamics (CFD) has been playing a major role in gaining an insight to the flow physics of the cell and increasing cell performance through a better design in the past few decades. However, a typical three-dimensional single-channel fuel cell model requires at least 10^4 cell elements which can increase by many folds if more than one channels are included. Combined with extra equations for a multi-species, two-phase, non-isothermal flow problem, this can be extremely computationally intense. An effective meshing strategy giving good resolution and hence accurate results while keeping the number of elements to a minimum is therefore needed.

Methodology

A representative section of a single-serpentine flow-field consisting of two straight channels connected by a 180-degree bend, shown in Figure *1*, is used as a computational domain consisting of, from top to bottom, anode flow channels, anode gas diffusion layers (GDL), anode catalyst layer (CL), polymer electrolyte membrane (PEM), cathode CL, cathode GDL, and cathode flow channel. The cell dimensions are summarised in Table 1. To aid in the discussion of the results, a PEM fuel cell-specific direction convention based on the Cartesian coordinate system is used where the x-, y-, and z-axes are referred to as an in-plane, along-the-channel, and through-plane direction, respectively.

There is no established rule on how a PEM fuel cell model should be meshed and below is brief summary of basic rules used for mesh generation in the current study.

- It is usually laminar flow in fuel cells due to small Reynolds numbers and hence the near-wall mesh does not need to be very dense.
- Structured, hexahedral mesh elements are used with conforming mesh at all interfaces.
- Low-to-zero cell skewness and close-to-unity cell orthogonality for good convergence rate.
- Cell aspect ratio is kept below 200 (special care is required in the catalyst layers).

- A large jump in size of adjacent cells is avoided (smooth transition between layers).

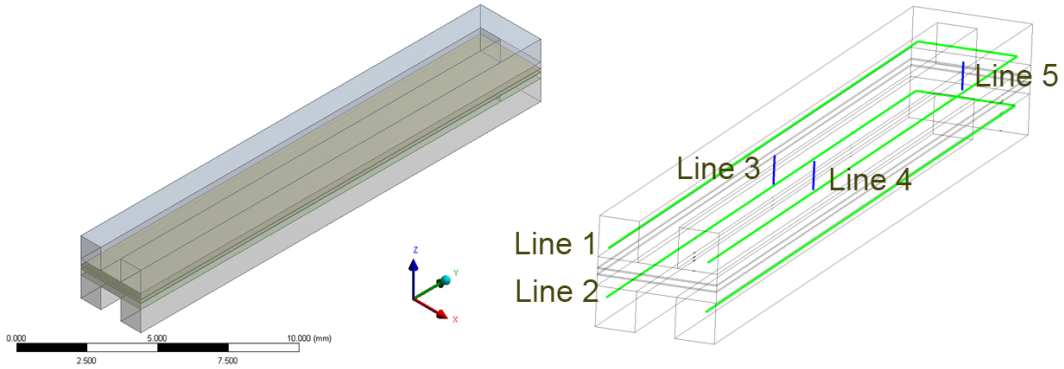

Figure 1. A 180-degree U-bend computational domain and pre-defined lines used in results discussion.

Table 1. Cell dimensions and mechanical properties.

Cell Parameter	Value
Channel width (mm)	1
Channel depth (mm)	1
Rib width (mm)	1
Channel length (from inlet to bend, mm)	20
GDLs thickness (µm)	260
CLs thickness (µm)	28
PEM (Nafion 115) thickness (µm)	127
GDLs porosity	0.5
CLs porosity	0.82
Specific surface area of CLs (m^{-1})	1.25×10^{7}

The governing equations and operating conditions are the same as used in the authors' previous publications [3, 4] and Fluent Fuel Cells module manual [5] which not be repeated here. The problem is solved in a commercial CFD code, ANSYS Fluent with a PEM fuel cells add-on package. The properties of all the meshes are summarised in Table 2 while results are presented and discussed in the next section.

Table 2. Statistics of all meshes used in the study.

Mesh	Element	Orthogonal	Skewness (avg)	Aspect Ratio
M_1	1 904 000	1	0	12/4
M_2	1 520 000	1	0	7/3
M_3	1 328 000	1	0	5/2
M_4	992 000	1	0	2/1
M_5	952 000	1	0	23/9
M_6	761 600	1	0	29/11
M_7	476 000	1	0	46/18
M_8	190 400	1	0	116/44
M_9	952 000	1	0	23/9
M_{10}	761 600	1	0	29/11
M_{11}	476 000	1	0	46/18
M_{12}	190 400	1	0	116/44

Results and Discussion

Study 1: Through-plane (z-axis) Mesh

The variation of flow-field variables in this through-plane direction has a strong effect on the local rate of electrochemical reaction which is why most early one-dimensional models were developed in this direction. A typical cross section of the flow channels measures $\mathbf{1} \times \mathbf{1}$ mm^2 and is equally divided up using 100 ($\mathbf{0.1} \times \mathbf{0.1}$ mm^2 each) uniform square cells. As a reference mesh, a $\mathbf{0.05} \times \mathbf{0.05} \times \mathbf{0.05}$ mm^3 cubical element in the flow channels of Mesh 1 is purposely used giving an ultra-fine mesh in which its solution will be used as a reference. Keeping the mesh in the other two directions the same, the mesh in the porous layers are coarsened. The four meshes and the corresponding polarisation curve are shown in **Error! Reference source not found.**.

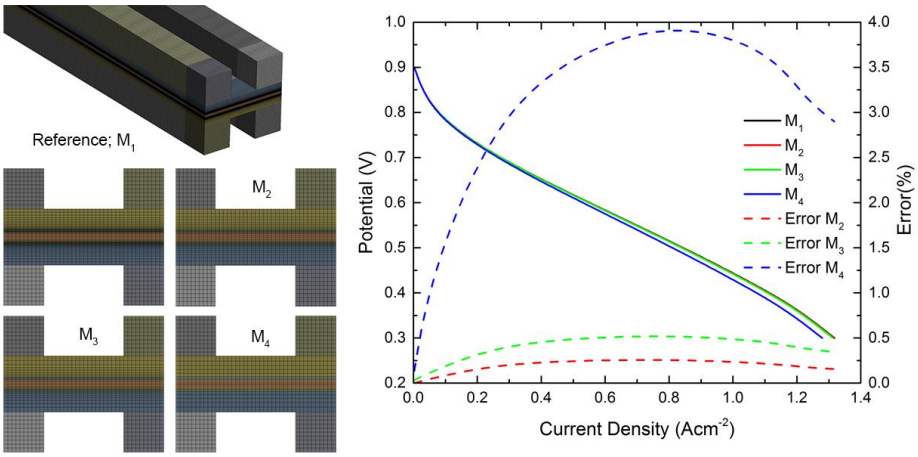

Figure 2. Meshes 1-4 and their corresponding polarisation curve.

Figure 2 shows the percentage errors, defined as the deviation of the average current density of a particular mesh from the reference value. The errors are small at low operating current and increase with the current and peak at the mid-current (ohmic) region. Particularly, both catalyst layers of Mesh 4 have only one element in the through-plane direction hence showing the largest deviation. This is caused by insufficient through-plane mesh elements so that they cannot accurately resolve the transport of electron in the electronically conductive portion in the porous layers. This implies that those early models which treated the catalyst layers as a zero-thickness interface are not a proper representation of a real catalyst layer.

For comparison, the operating voltage corresponding to the highest error, 0.30 V, is chosen and the local distribution of flow-field variables along the flow channels is shown in Figure 3. As can be seen from the figure, the differences of velocity and pressure drop among the meshes are very small suggesting that the effect of through-plane mesh on the flow-field inside the flow channel can be neglected.

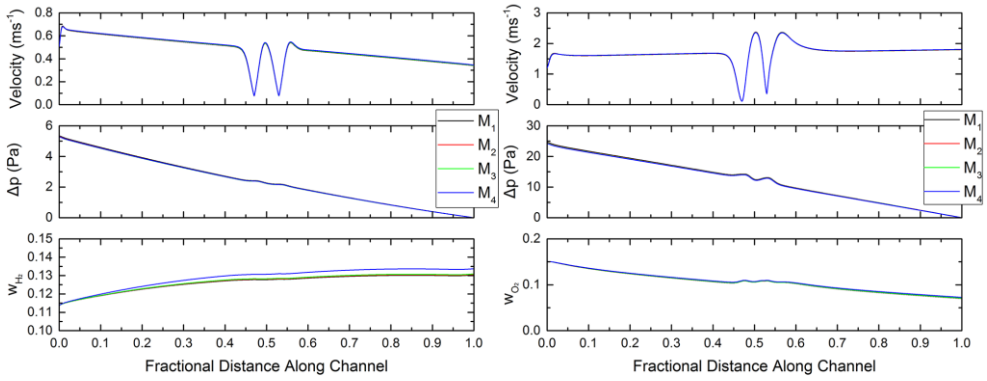

Figure 3. Flow-field variables along the anode (Line1, left) and cathode (Line 2, right) channels.

The current, however, is not a sole function of species concentrations and hence differs notably among the four meshes despite a similar species distribution. This is confirmed by the profile of local overpotential in Figure 4. Clearly, the through-plane mesh has a strong influence on the determination of current density through the accuracy of predicted electron-transport-related variables.

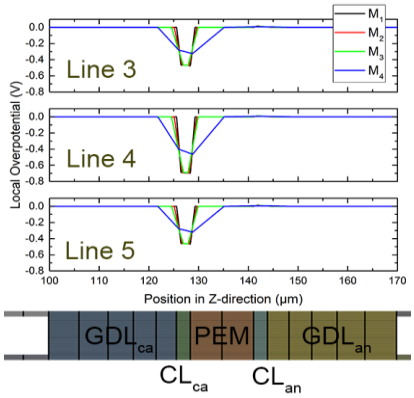

Figure 4. Overpotential profiles across porous layers.

Study 2: In-plane (x-axis) Mesh

The effect of the lateral mesh is now investigated by coarsening the mesh elements in this direction to 0.100, 0.125, 0.200, and 0.500 mm for Meshes 5-8, respectively. The four meshes and their corresponding polarisation curves and the percentage errors are shown in Figure 5.

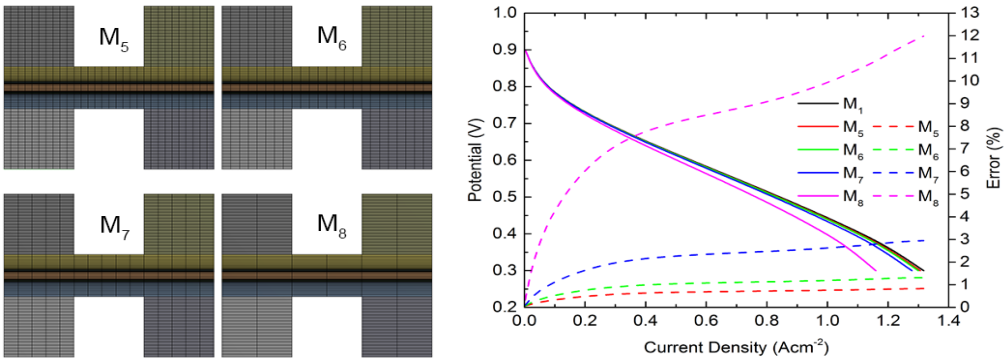

Figure 5. Meshes 5-8 and their corresponding polarisation curves.

The errors increase slightly as expected since fewer cell elements are present in these meshes. However, all error curves are different from those found in Study 1 in which they continually rise with the operating current and the peak values are found in the mass-transport region.

The solution for each mesh at 0.30 V is, again, chosen. Since the lateral mesh is coarsened, a large deviation of flow-field variables in the bend region, where the flow experiences a drastic 180-degree change in direction, is expected. Nevertheless, Figure 6 shows that where there is a negligible difference between the velocities in the bend region in contrast to the ones in the channel region where they differ markedly. This can be explained by the deficiency of near-wall cells which cannot accurately resolve the boundary layer in the channel region. At the bend, on the other hand, the primary flow and subsequently its boundary layer are now aligned with the y-axis where the mesh remains unchanged.

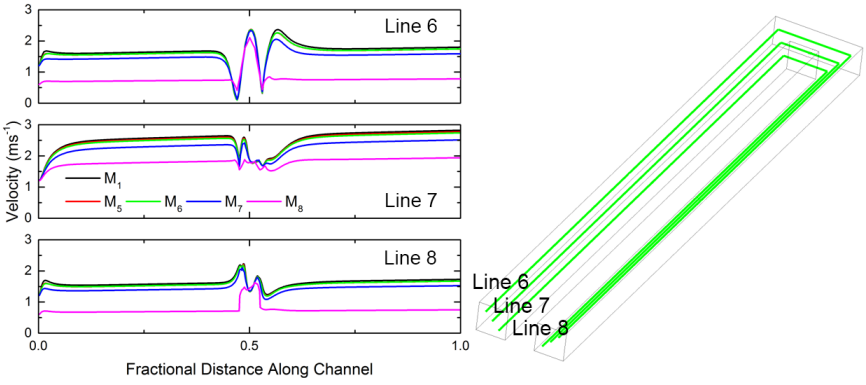

Figure 6: Velocity profiles along the cathode channel. The red arrows indicate the direction vector for the plot.

Study 3: Along-the-channel (y-axis) Mesh

In this study, the mesh in the streamwise direction is stretched to 0.100, 0.125, 0.200, and 0.500 mm in Meshes 9, 10, 11, and 12, respectively. The maximum size is, however, limited to 0.500 mm (Mesh 12) to maintain the cell aspect ratio below 200.

The four meshes give impressive results as can be seen in 7. The errors are much smaller than those produced by Meshes 5, 6, 7, and 8 despite the fact that the same number of elements are used. The largest deviation of 0.45% is found in Mesh 12 at the mass-transport region. As already revealed in Study 2, a large discrepancy of flow-field variables among the four meshes in the bend region is expected because the mesh in the y-direction has been lengthened.

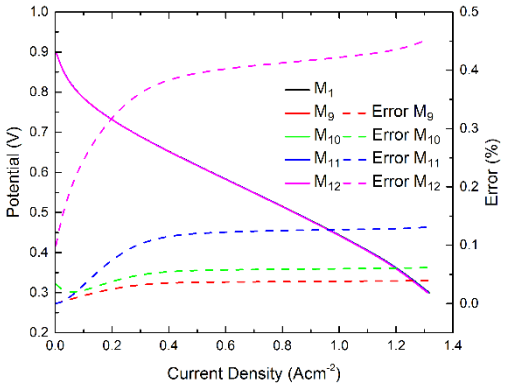

Figure 7: Polarisation curves and percentage errors for Meshes 9-12.

Clearly, the streamwise mesh has little effect on the solutions compared to the other two directions. This can be thought of as highly advantageous since this streamwise mesh can be relaxed to reduce the number of mesh elements. It should be noted that the mesh in this direction cannot be coarsened entirely independently.

Summary

A meshing strategy study for PEM fuel cells CFD modelling has been carried out and it has been found out that:

1. The through-plane mesh has the strongest effect on the predicted current density.
2. The in-plane mesh has a moderate effect on the solution.
3. The streamwise mesh has the least effect on the solution which offers a great benefit from a computational standpoint.

References

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