Numerical Simulation of a Proton Exchange Membrane Fuel Cell

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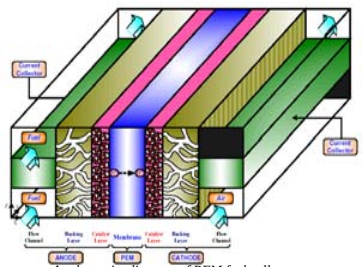
The objective of this study is to design a robust algorithm to solve PDEs arising from proton exchange membrane fuel cell problems. Here we will focus on one major component of fuel cell-Gas Diffusion layer(GDL).

Introduction

A fuel cell is a clean energy device which has potential to substitute the internal combustion engine. A fuel cell has seven components: gas channel, gas diffusion layer(GDL), catalyst layer in both cathode and anode side, and proton exchange membrane.



A schematic diagram of PEM fuel cell

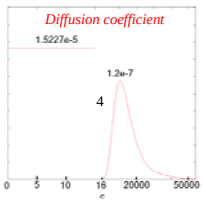
Water management is the key issue in the Proton Exchange Membrane(PEM) fuel cell. Too many liquid water will block the open pores in the porous media of the Gas Diffusion Layer(GDL) and cover the surface of Catalyst Layer, too little water will dry out the membrane. In both cases, the fuel cell cannot operate. Correct understanding of the liquid water transport in the fuel cell is essential to designing the fuel cell device.

Model equations

Generally, fuel cell operation under isothermal conditions is described by mass, momentum, species, and charge conservation principles in all fuel cell components. We mainly focus on the model developed by Chao-Yang Wang and his co-wokers. In this study, we concentrate on GDL. Solve for C (concentration), P (pressure) and u (velocity).

$$\begin{cases} -\nabla\cdot(\Gamma(C)\nabla C)+\nabla\cdot(\gamma_c\vec{u}C) &= 0 \\ \nabla\cdot(\frac{K}{\mu}\nabla p) &= 0 \\ \vec{u} &= -\frac{K}{\mu\rho}\nabla p \end{cases}$$

In the above equation, all coefficients except K depend on the concentration C. Especially, the diffusion coefficient is nonlinear, discontinuous and vanishes at some points. This property is a major source of numerical difficulties. The diffusion coefficient is defined by



$$\Gamma(C)=\begin{cases}\Gamma_{capdiff} & (if\quad C\geq C_{sat})\\ D_g^{eff}=\epsilon^{1.5}D_{gas} & (if\quad C<C_{sat})\end{cases}$$

Numerical methods and results

We use the finite element method to discretize the PDE. Multilevel Newton's method, Full approximation scheme and global Kirchhoff transformation are used.

Multilevel Newton's method

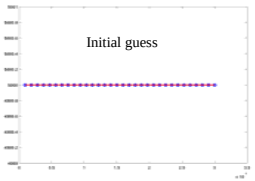
Simplified 1d model.

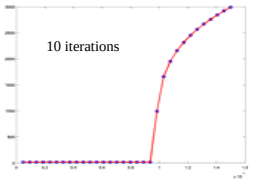
$$\begin{cases} -(\Gamma(C)C')'-dC' &= 0 \\ C(0) &= 15 \\ \Gamma(C)C'+dC|_{x=L} &= \frac{I}{2F} \end{cases}$$

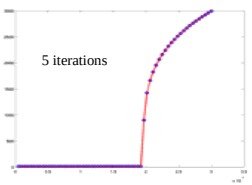
In order to make Newton's iteration robust in the practical problem the following things are crucial.

- Good initial guess
- Make the iteration in the definition domain

We choose the initial guess from the solution on the coarser level. Using this idea recursively, we can get a good initial guess. This method is equivalent to adaptively smoothing the discontinuous diffusion coefficient.



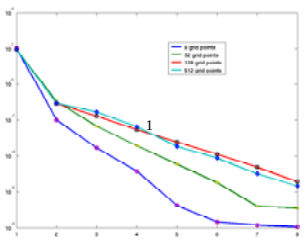




The coarse grid is used to find a initial guess that is "close enough" to the final solution so that we insure convergence. Without a coarse grid, the method doesn't always converge.

Full Approximation Scheme

We use operator induced prolongation and a nonlinear pointwise Gauss-Seidel method as a smoother. We get the following uniform convergence numerical result for the simplified 1d model.



Convergence behaviour for different mesh sizes

Global Kirchhoff transformation

From an approximation point of view, smooth functions can be well represented on a coarse grid. The concentration profile has a sharp interface because of the big discontinuity of the diffusion coefficient. Using a Kirchhoff transformation, we introduce a new variable w.

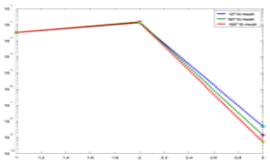
$$w(C)=\int_{C_0}^{C}\Gamma(s)ds \longrightarrow \nabla w=\Gamma(C)\nabla C$$

We get new PDEs

$$\begin{cases} -\Delta W-\nabla\cdot(\gamma_c\nabla pC) &= 0 \\ \nabla\cdot(\frac{1}{\mu}\nabla p) &= 0 \end{cases}$$

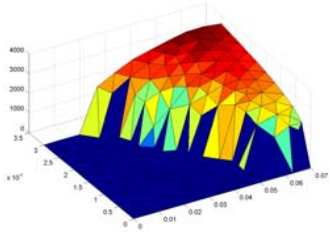
The new variable is much smoother than the original one. Also the diffusion term changes to a linear one.

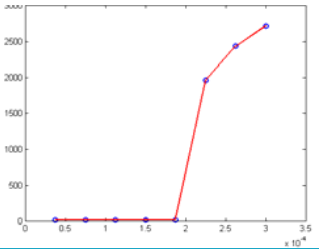
In the case that the convection term is small, the nonlinear iteration converges very fast.



Convergence behaviour for different mesh sizes

Typical solution profile for concentration of 1d and 2d





Conclusions and future work

Conclusions

- The multilevel Newton's method provides a good initial guess that makes Newton's method robust.
- The full approximation scheme with operator dependent prolongation exhibits good convergence behaviour.
- The global Kirchhoff transformation is very effective when the convection term is small.

Future work

- Develop multigrid algorithms that converge uniformly for degenerate problems in higher dimensions (2d and 3d).
- Consider the problem that couples both the GDL and gas channel, and develop a solver for it.
- Consider the full seven-domain fuel cell problem.

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