DOE Hydrogen Program

Development of Novel PEM Membrane and Multiphase CFD Modeling of PEM Fuel Cell

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Project ID # **FC_15_Das**

Overview

Overview

Timeline

- Start – July 2006
- Finish - June 2008
- 98% Complete

Budget

- Total project funding
  - DOE - $600K
- Funding received in FY06
  - $150K
- Funding received in FY07
  - $300K
- Funding for FY08
  - $150K

Barriers

- Barriers
  - A. Materials and manufacturing costs
  - B. Membrane performance
  - C. Water and thermal management
- Targets –Improved conductivity & membrane stability
  - Efficient water & thermal management

Partners

- Bei-Tech – Polymer membranes
- MEA development

Objectives

Overall	• Development of novel proton exchange membrane (PEM) for fuel cells • Development of multiphase CFD model of PEM fuel cell for improved water and thermal management
2006-2007	• Low-cost, high-performance membrane - Design and manufacturing processes - Experimental testing and performance validation
2008-2009	• Low-cost, high-performance membrane - Real-time membrane testing for single cell and stack - Real-time testing for stability and materials properties • Integrated multiphase CFD model for PEM fuel cell - Performance evaluation for different parametric conditions

Approach

Plan & Approach

100% Completed

- **Task 1:** New fuel cell membrane
  - Literature survey
  - Theoretical analysis and model development
  - Inexpensive materials search

95% Completed

- **Task 3:** Thermal stability and water management
  - Test of water uptake and thermal stability
  - Improved durability and efficiency
  - Test of stable proton conductivity

100% Completed

- **Task 2:** Chemical modification
  - Modification of polymer backbone
  - Increased proton conductivity
  - Reduced resistance than peer

98% Completed

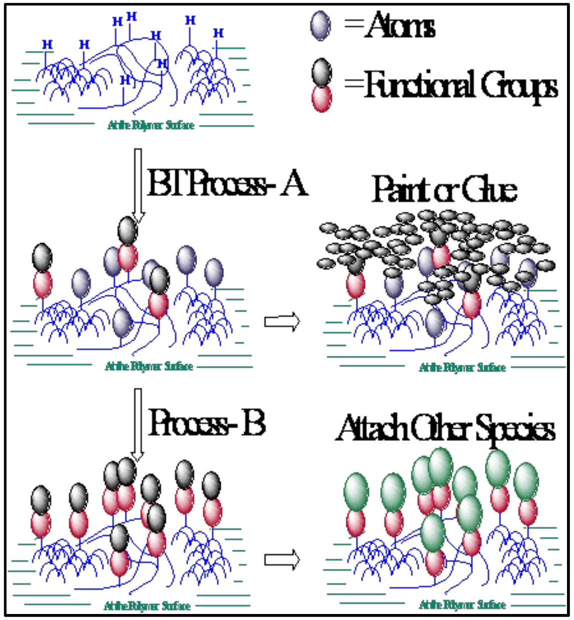
- **Task 4:** CFD multiphase model for PEM fuel cell
  - Literature survey
  - Developed CFD multiphase mathematical model
  - Developed graphical user interface

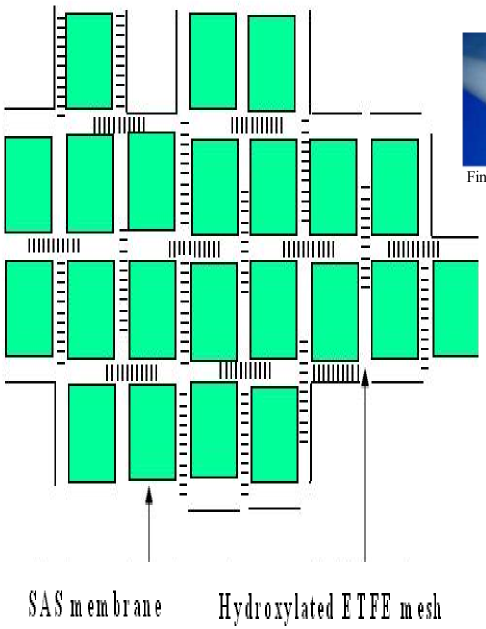
Approach

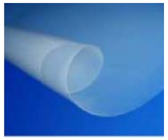
Approach Overview

- We used novel patented polymer chain modification technology through chemical treatment onto an inexpensive robust polymer backbone

- Patented Polymer Backbone Modification Technology
- New SAS Polymer Membrane
- Performance Validation






Finished SAS Membrane

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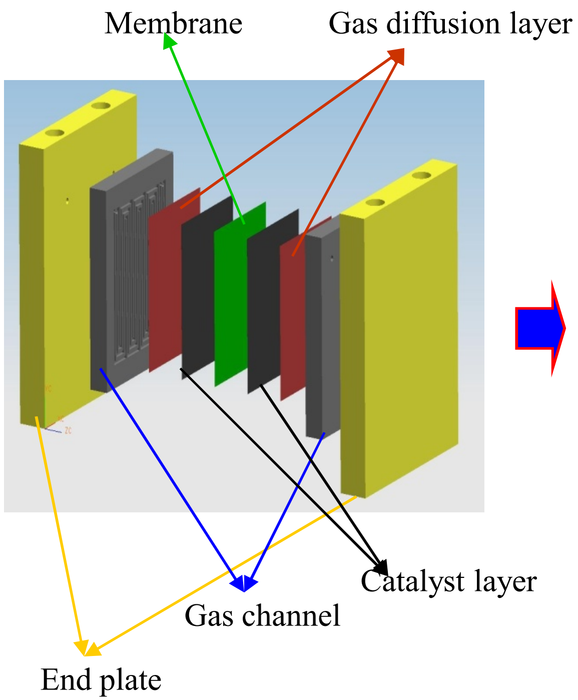
Approach

Approach Overview for CFD Modeling

- Multiphase CFD analysis of PEM fuel cell for water & thermal management

- Geometry



Membrane

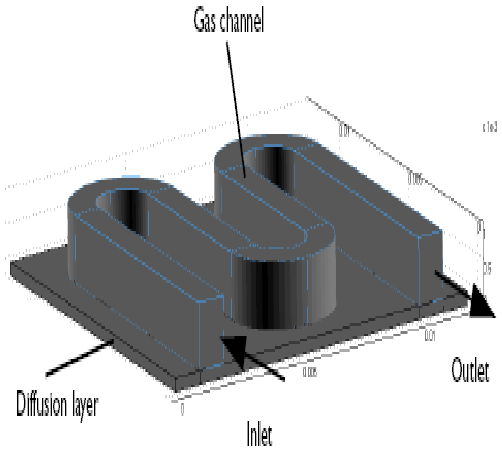
Gas diffusion layer

Catalyst layer

Gas channel

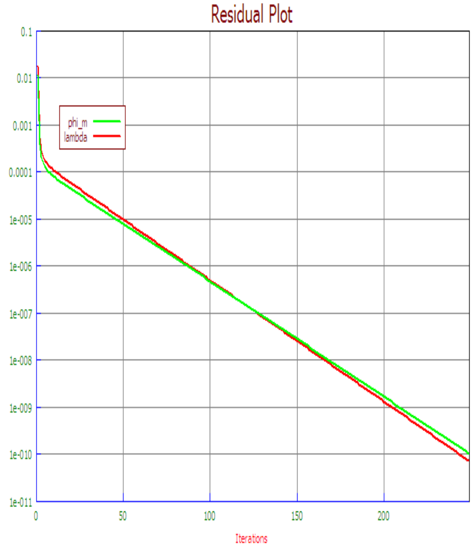
End plate

- Simulation



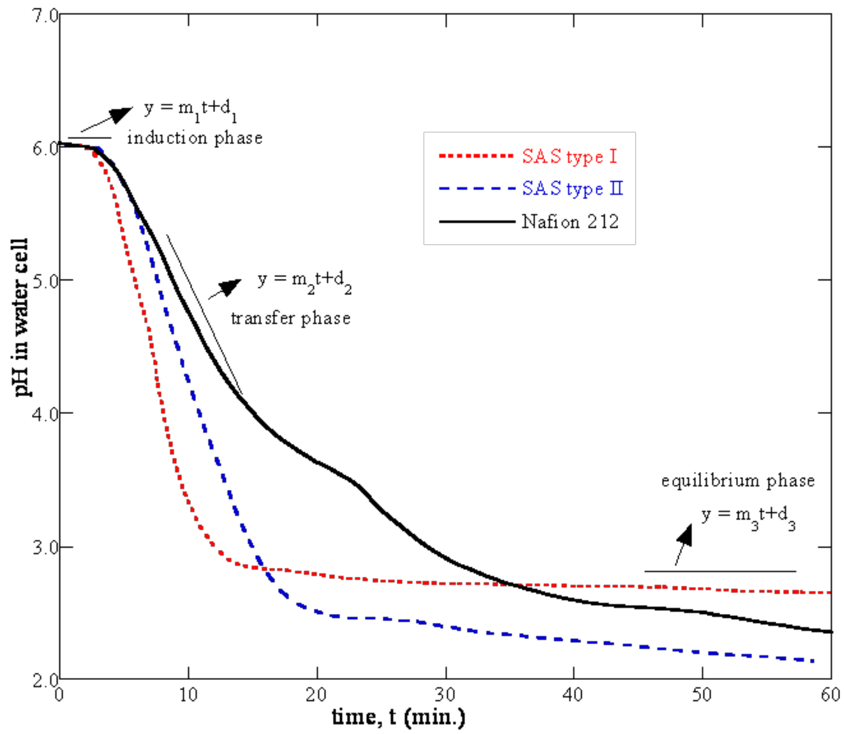
- Post Processing

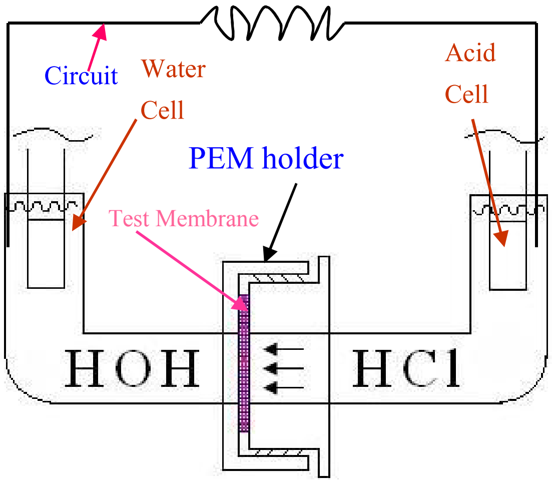
Result Validation



Proton Conductivity

- Membrane’s proton exchange capacity



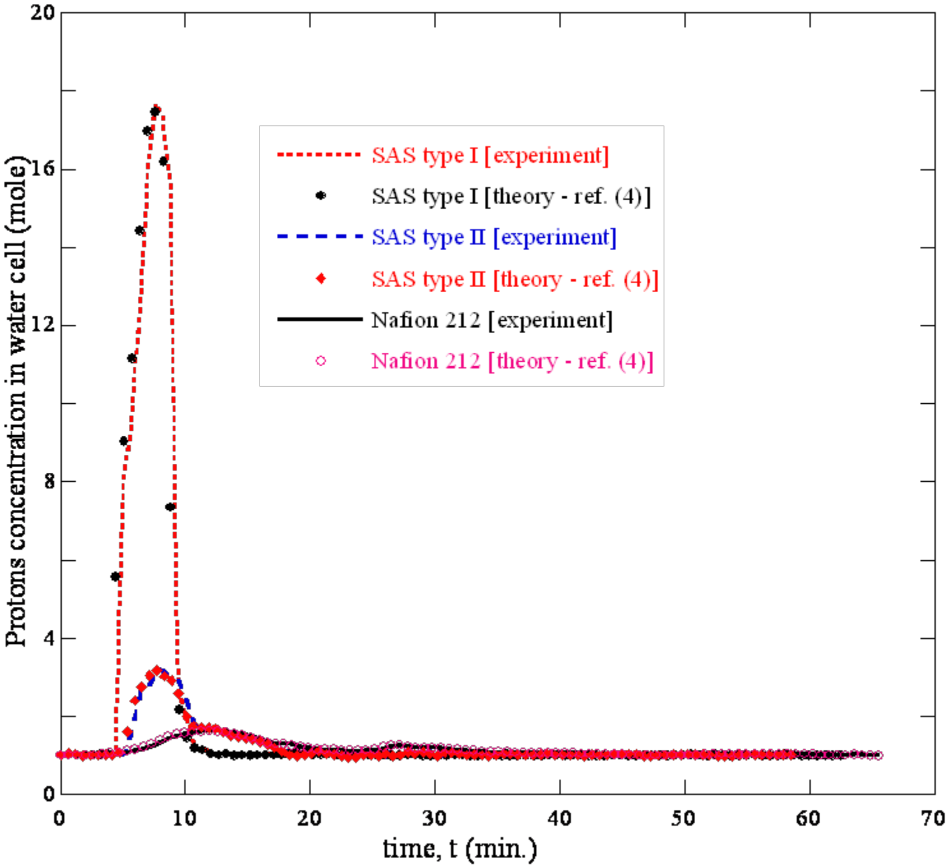


Schematic of proton exchange capacity test method

- Induction time (time required to start proton transfer) is lower than Nafion$^{®}$ 212
- Higher proton transfer rate than peer membrane (Nafion$^{®}$ 212) materials
- Steady proton transfer capacity at higher rate than Nafion$^{®}$ 212 for extended period of time
- Very inexpensive membrane materials and easy to manufacture than Nafion$^{®}$ 212

Comparison of Membrane Conductivity

- **Proton conductivity through the membrane**



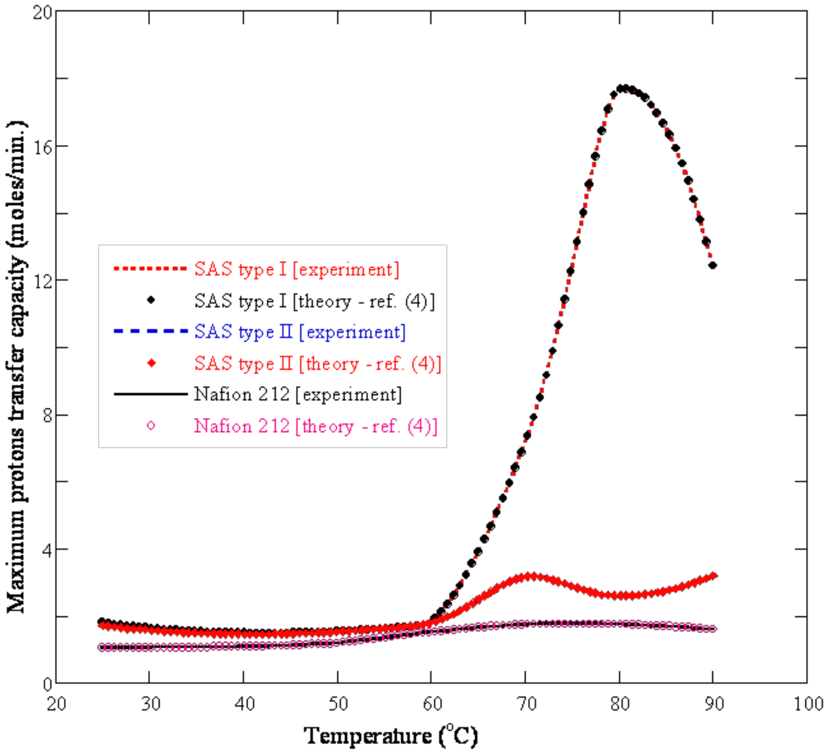
Proton Concentration: 10^{-pH}

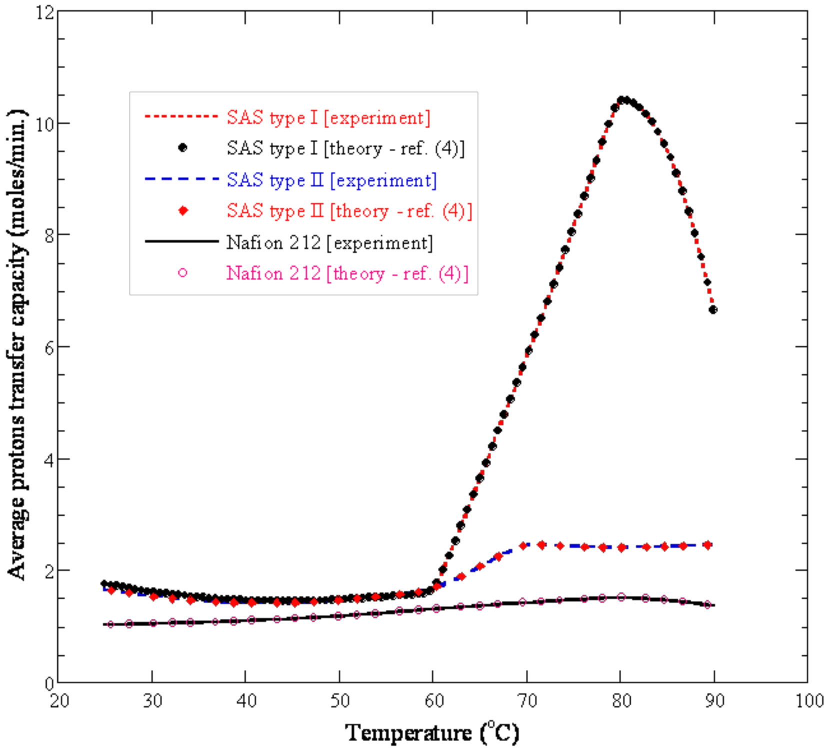
- SAS type I has higher proton conductivity than peer materials
- Excellent agreement between experimental and theoretical results
- Ability to reach equilibrium state quickly

** ref. (4) is our published paper number 4 (publication list is given at the end of this presentation) where theoretical model is presented.

Proton Transfer Capacity

- Comparison of proton transfer capacity

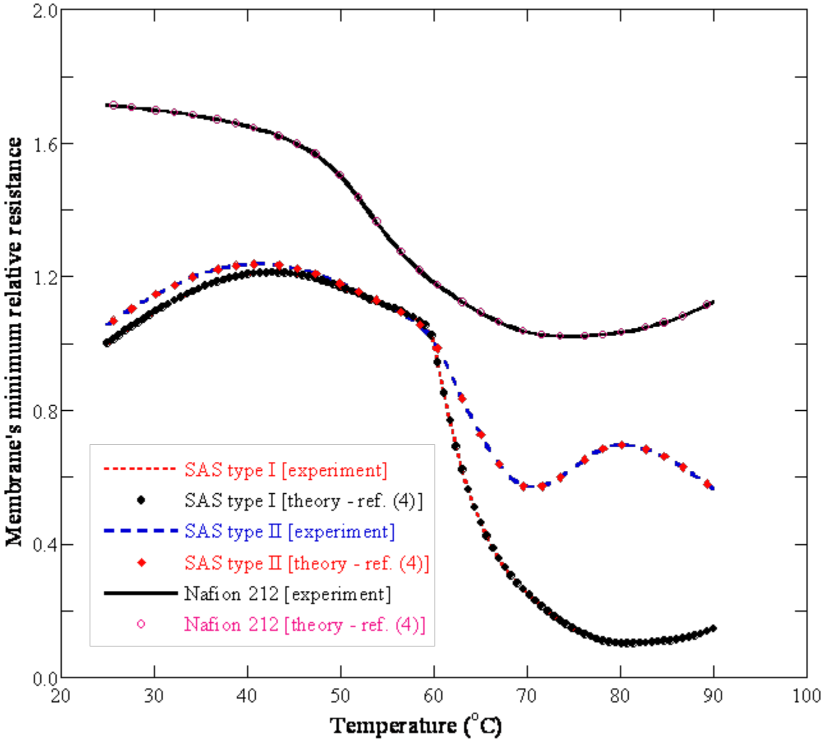


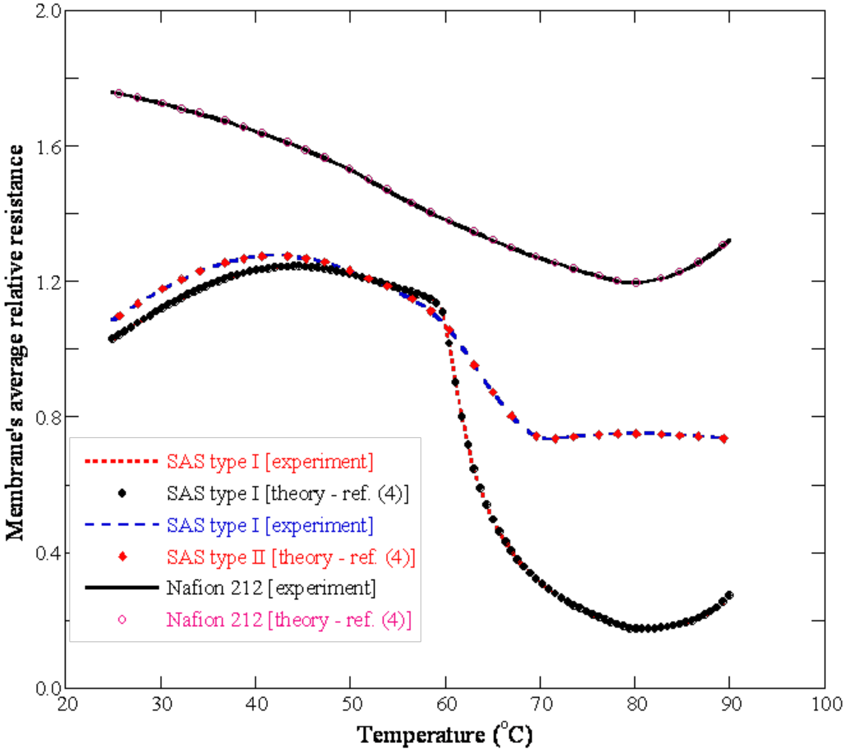


- Maximum 16 times higher proton transfer rate than Nafion® 212 at 80°C
- Average 10 times faster proton transfer rate than Nafion® 212 at 80°C
- Since the protons present in water cell are in the form of H_3O^+ and not simply H^+, it is not known what the significance of the shifted trend after 80°C when considering a hydrogen fuel source, it requires further experimental investigations to understand the trend.

Membrane Resistance

- Comparison of relative membrane resistance

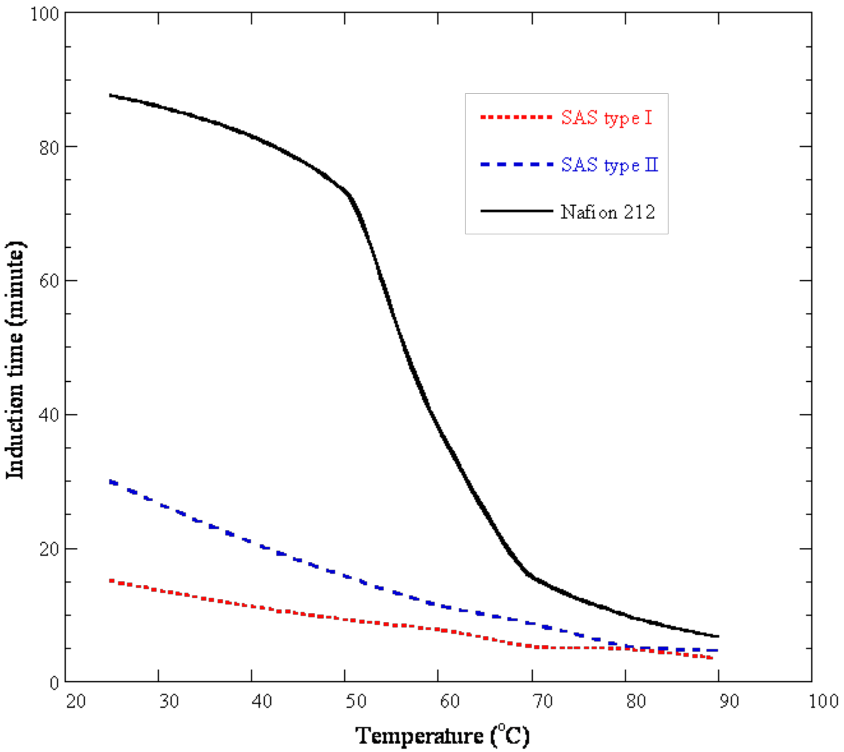


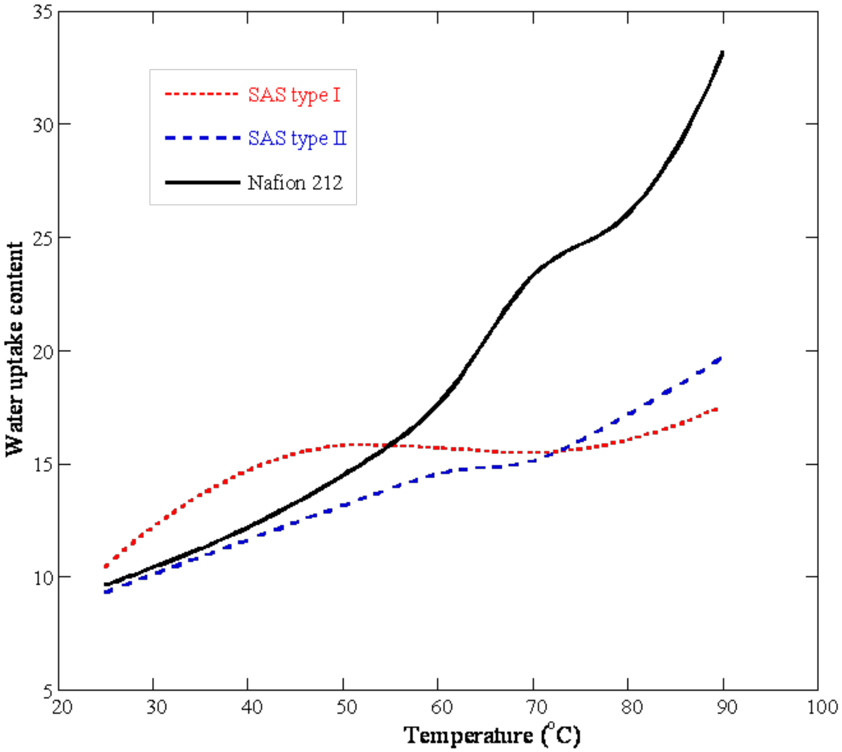


- Membrane's minimum resistance is reduced 87% than Nafion® 212 at 80°C
- Average resistance is reduced 80% than Nafion® 212 at 80°C

Water Uptake

- Comparison of induction time & water uptake content





- Induction time of SAS membrane is reduced significantly than the peer Nafion® 212
- SAS type membranes are capable of transferring protons efficiently at low water content i.e. at low humidity level than Nafion® 212

Industry Standard Testing

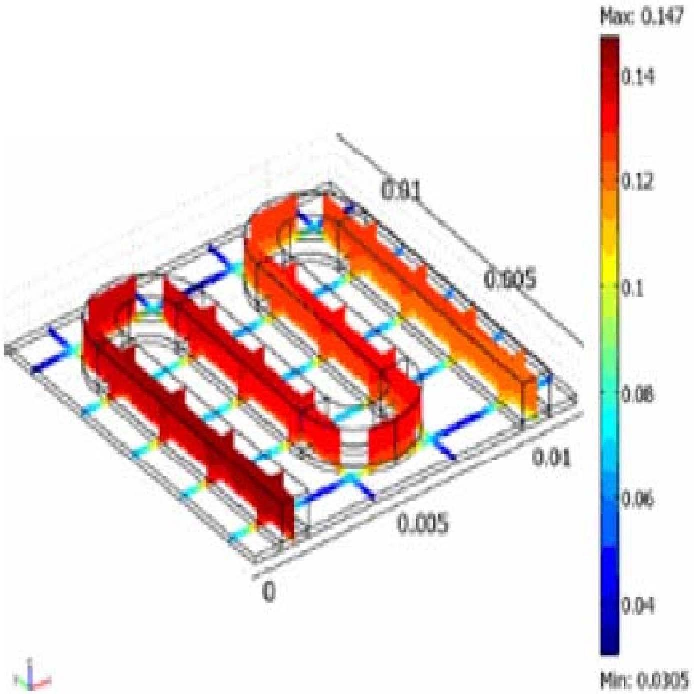
- Conductivity, Resistance, RH Cycle measurement of SAS PEM using industry standard technique

- The samples of our finished SAS PEM membrane has to be sent shortly to the BekkTech. LLC, Colorado (a service provider for conductivity, resistance and RH cycle measurement of fuel cell membrane) for membrane performance measurement using industry standard techniques.

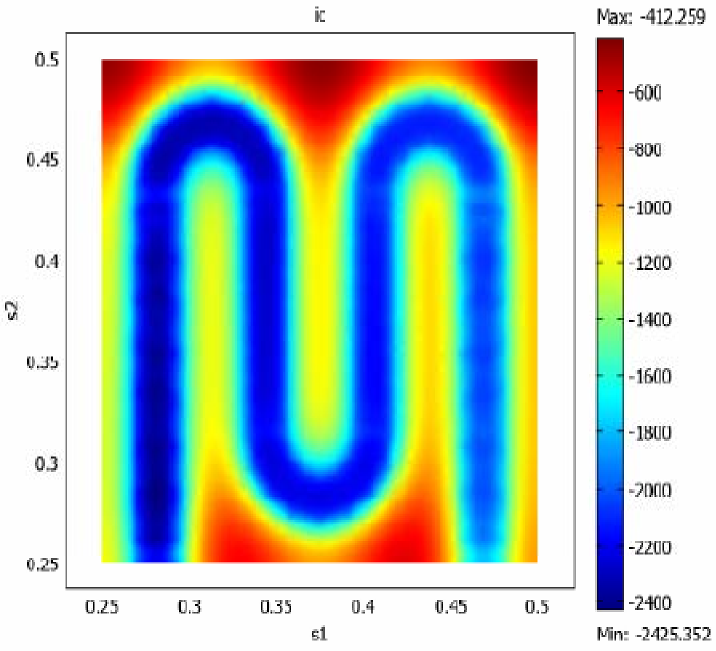
- The results will be presented during DOE review meeting presentation.

Base Case: CFD Results

- Multiphase CFD analysis of PEM fuel cell



- Mass fraction of oxygen in the channel and the porous cathode



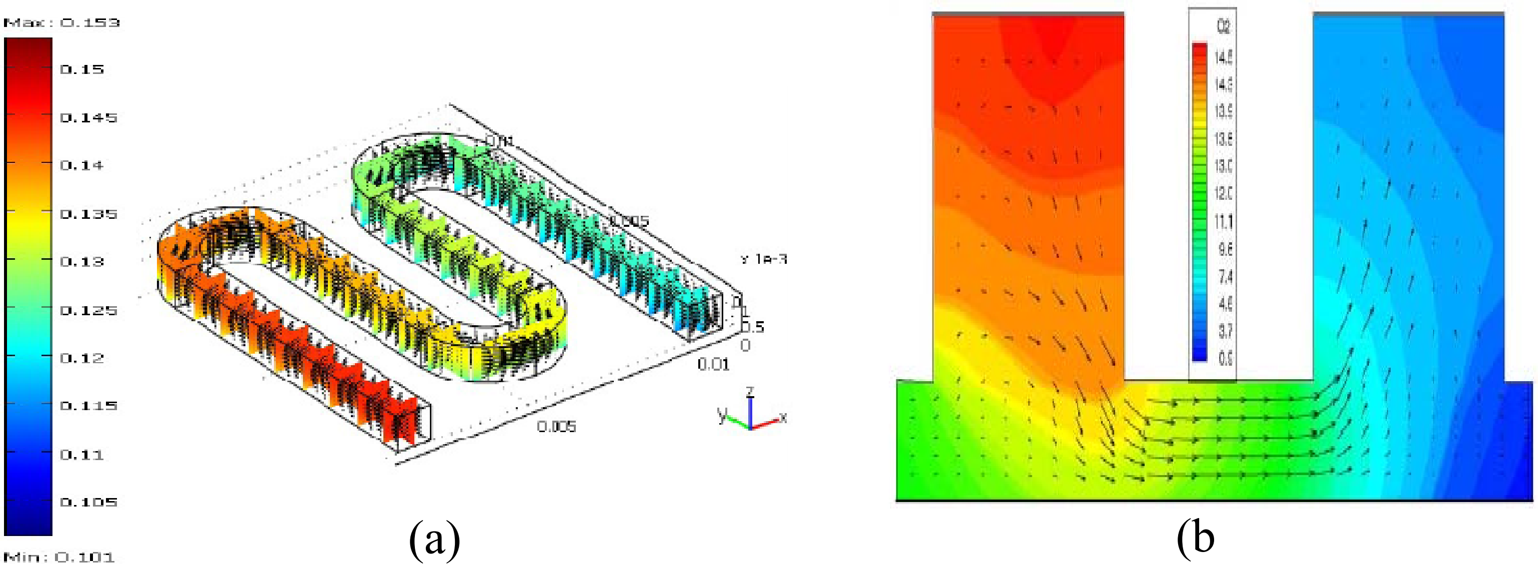
- Top view of the current-density distribution on the surface of the catalytic active layer.

- High current density results in substantial oxygen depletion in the regions far away from the gas channel. Substantial decrease in oxygen weight fraction along the gas channel from inlet to outlet, from 0.145 to approximately 0.1.

- The current density is significantly higher below the gas channels.

Comparison of CFD Results

- Comparison of multiphase CFD analysis of PEM fuel cell



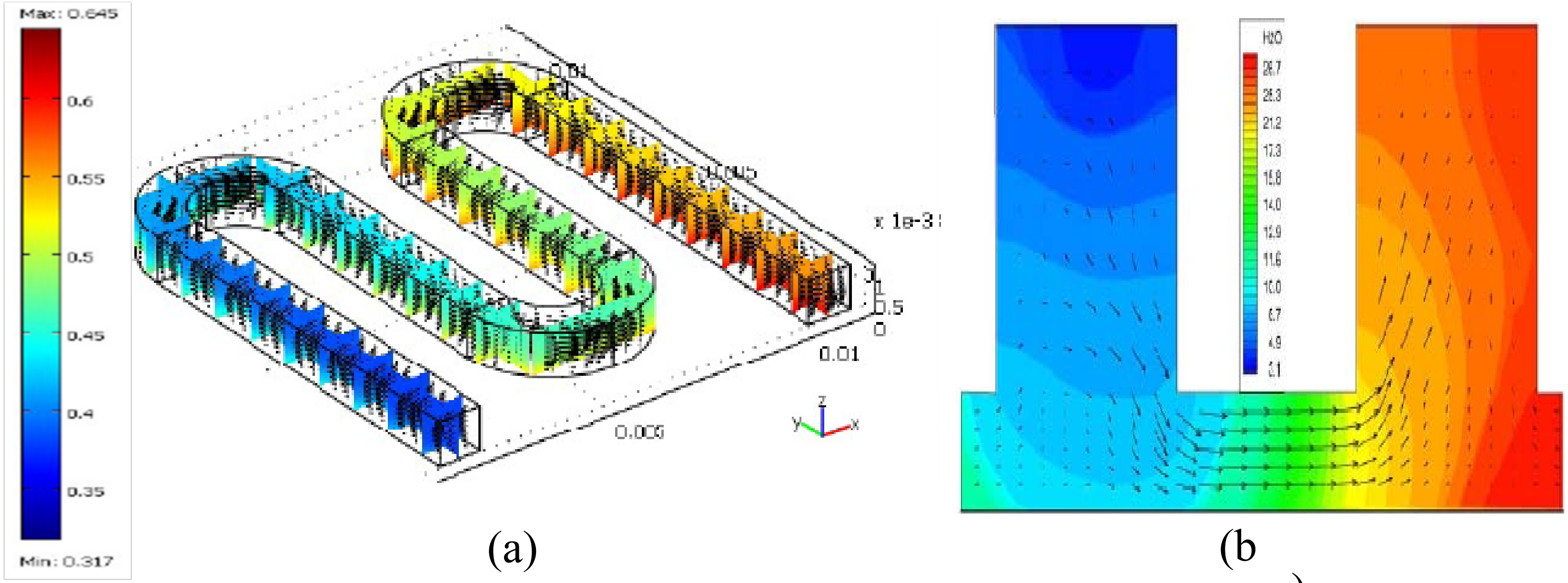
(a) (b)

Figure: Concentration distribution of gas phase (O2) in the cathode channel. (a) 3D simulation of cathode with present multiphase model, (b) 2D model simulation of Wang and Wang [1]. Black arrow indicates cathode gas velocity inside the channel.

- A typical laminar gas flow profile is present in the straight sections. In the curved sections, the gas velocity distribution is asymmetric, resulting in an asymmetric concentration of gas distribution there.

Comparison of CFD Results

- Comparison of multiphase CFD analysis of PEM fuel cell



(a) (b)

Figure: Concentration distribution of liquid phase (water - H2O) in the cathode channel. (a) 3D simulation of cathode with present multiphase model, (b) 2D model simulation of Wang and Wang [1]. Black arrow indicates cathode gas velocity inside the channel.

- Water fraction increases significantly in the electrode. It is probably the fact that water droplets would start forming at the cathode. To avoid this problem, in the design we should decrease the inlet water fraction and increase the thickness of the diffusion layer.

Parametric Values for CFD Model

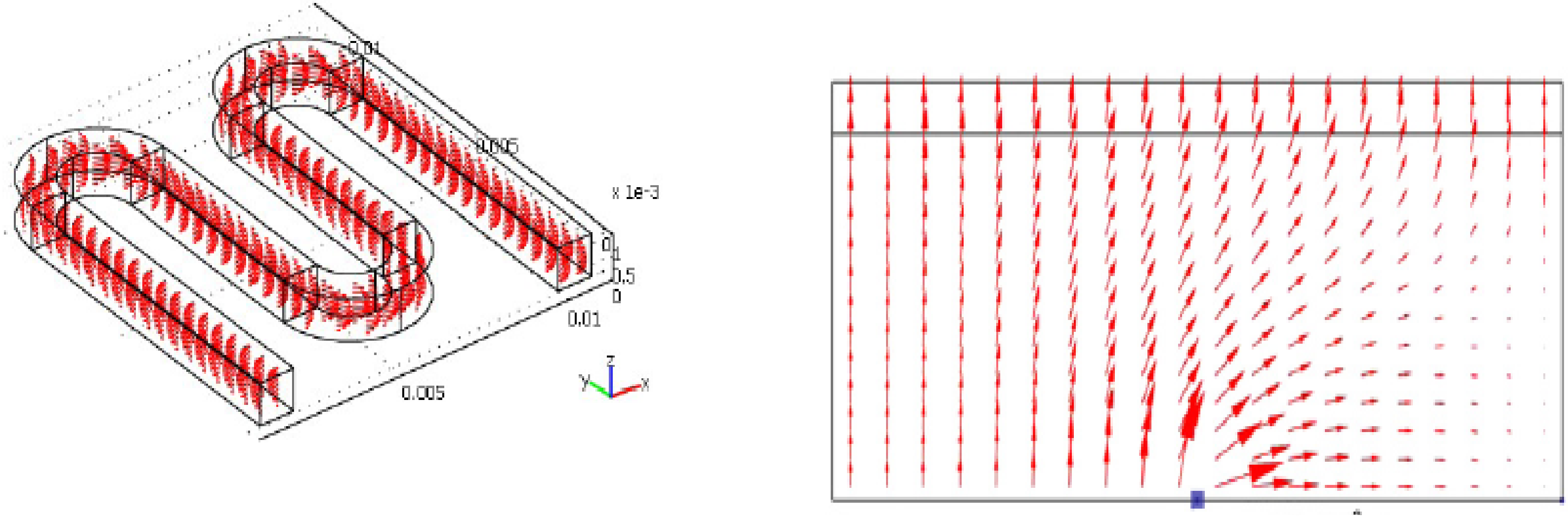
- Multiphase CFD analysis of PEM fuel cell

Quantity/Parameter	Value
Gas channel depth	1 mm
Gas channel height	1 mm
Gas channel width	1 mm
Diffusion layer thickness	0.3 mm
Catalyst layer thickness	0.01 mm
Pressure difference between cathode inlet and outlet	0.2 atm
Reference current density	1.0 amp/cm^2
RH (Relative Humidity) of cathode inlet	90%
Temperature of Fuel cell cathode	80^oC
Porosity of the cathode GDL [5]	0.6
Porosity of catalyst layer [5]	0.4
Permeability of the GDL, K (m^2) [5]	10^{-12}
O_2 diffusivity in cathode gas at standard condition [6]	3.2348×10^{-5}
H_2O diffusivity in cathode gas at standard condition [6]	7.35×10^{-5}

- Parametric values used to compute gas and liquid phase presented in the previous Figures.

Comparison of CFD Results

- Comparison of multiphase CFD analysis of PEM fuel cell



(a)

(b)

Figure: Distribution of gas-phase velocity in the cathode gas mixture. (a) 3D multiphase model present and (b) 2D two-phase model [2]. The red arrow indicates gas-phase velocity.

- **The gas-phase velocity vectors shown in Fig. 3 induce the gaseous mixture from the flow channel into the porous cathode. This is in contrast with the results obtained by the single-phase model [6] in which the gaseous-mixture velocity is directed from the porous cathode to the flow channel.**

Parametric Values for CFD Model

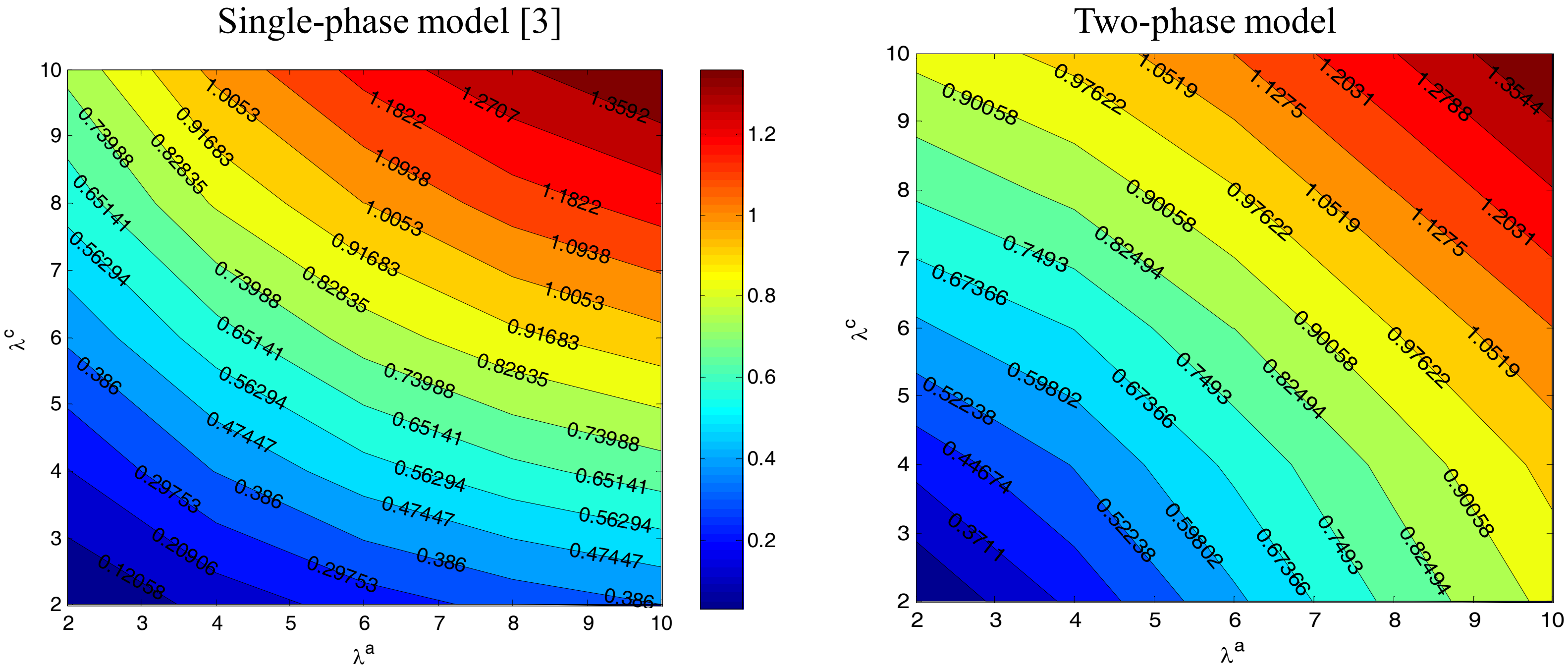
- Multiphase CFD analysis of PEM fuel cell

Parameter	Value
Gas channel depth	1 mm
Gas channel height	1 mm
Gas channel width	1 mm
Diffusion layer thickness	0.3 mm
Catalyst layer thickness	0.01 mm
Pressure difference between cathode inlet and outlet	0.2 atm
Reference current density	0.5amp/cm^2
RH (Relative Humidity) of cathode inlet	90%
Temperature of Fuel cell cathode	80^{o}C
Porosity of the cathode GDL [2]	0.48
Porosity of catalyst layer [2]	0.42
Permeability of the GDL, K (m^2) [2]	2.55x10^{-13}
Reference mole fraction of O_2 [2]	3.6641 molm^{-3}
Reference mole fraction of H_2O [2]	0.0703 molm^{-3}
Inlet water-vapor mass fraction	0.0198
Inlet O_2 mass fraction	0.2284
Inlet N_2 mass fraction	0.7518

- Parametric values used for porous-electrochemical variables in the model simulation presented in previous Figure.

Comparison of CFD Models

- Comparison of single phase and multiphase model



Single-phase model [3]

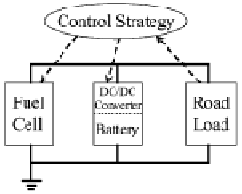
Two-phase model

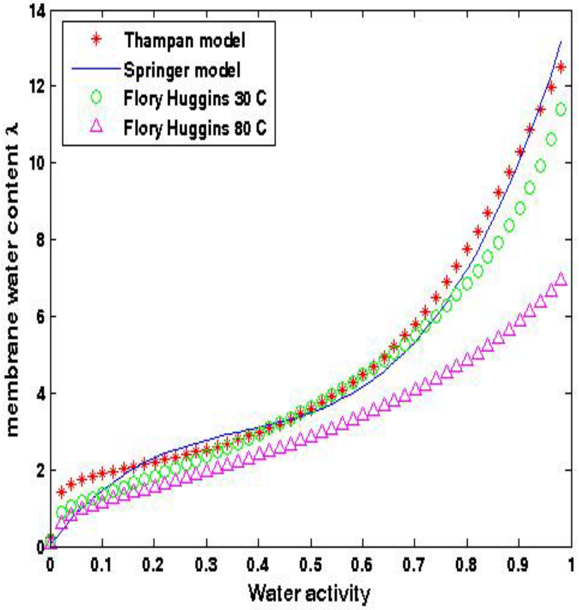
- Current density across the membrane at 80°C

- Significant improvement in current density in two-phase model compared to single-phase model, in particular, at low membrane water contents.
- The predictions of two-phase flow model will be beneficial to improve PEM fuel cell designs.

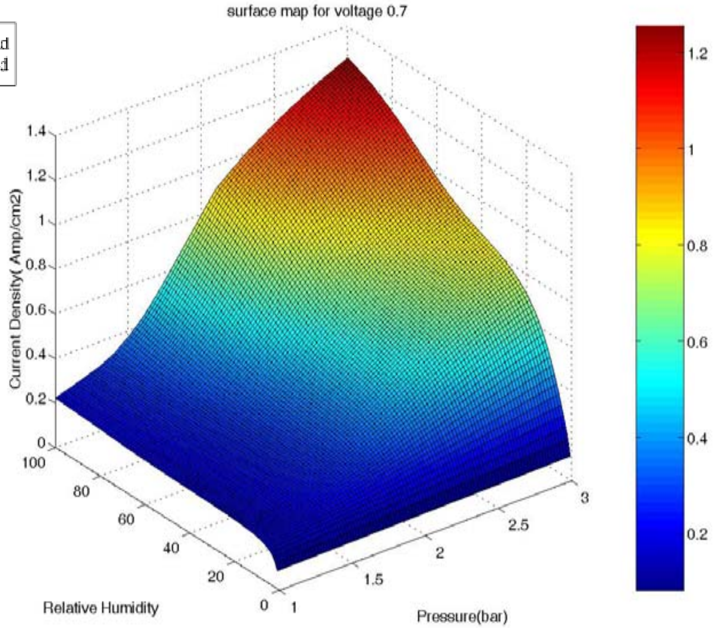
Control-Oriented CFD Model

- Control strategy for PEM fuel cell stack





- Water activity in the membrane

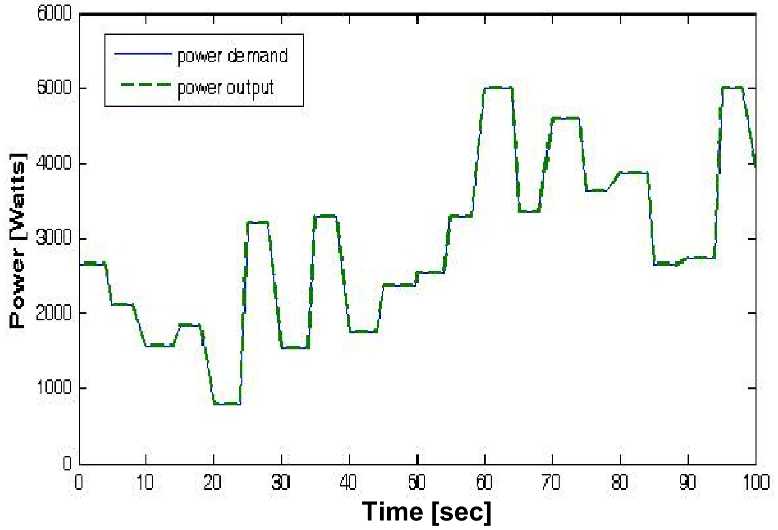


- 3D surface map for a voltage of 0.7V

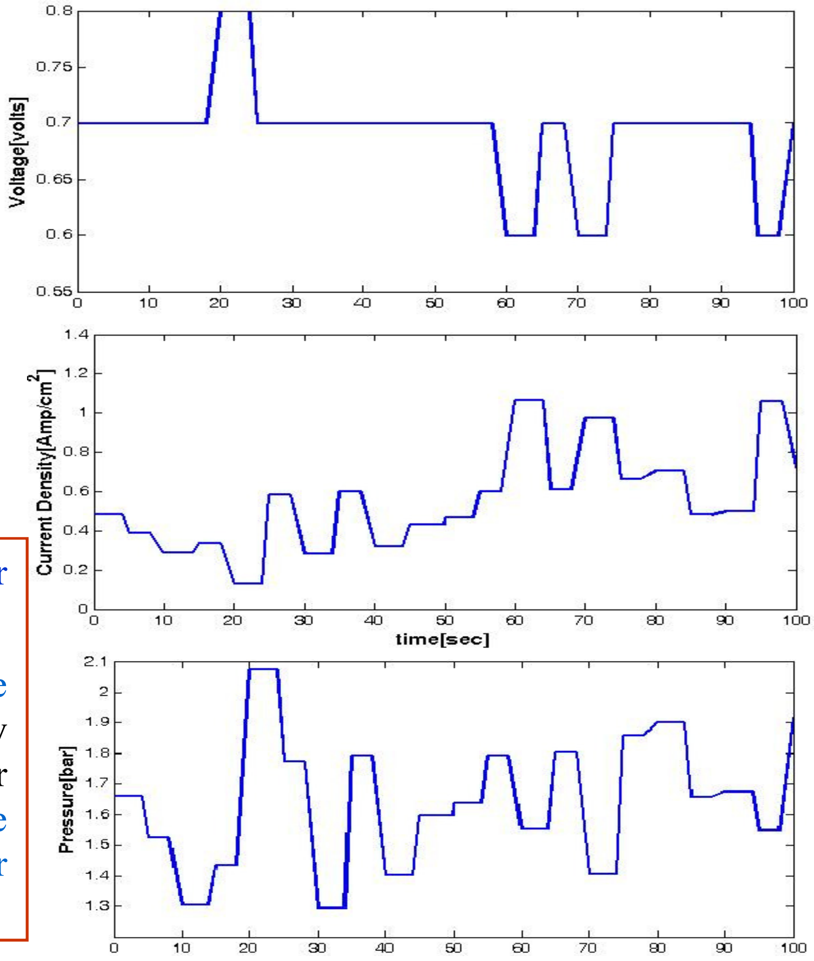
- **Developed membrane hydration model for efficient water management.**
- **Developed 3D surface map of cathode pressure, current density and membrane humidity at different voltages ranging 0.5~0.9V. Use these maps in a feed-forward control system to adapt the output voltage of the fuel cell by calculating the optimum operating conditions for input pressure at various power requirements.**

Dynamic Model Simulation

- Control strategy for PEM fuel cell stack



- The control strategy ensures that the requested power demand is met for both small and large changes.
- For small changes in power demand the voltage remains constant but the current density is changed by changing the pressure. For larger changes in power demand - a new voltage is chosen, both the voltage and current density are constant at constant power demand.



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Validation of Control Model

- Experimental validation of control strategy

Greenlight PEMFC test stand at Kettering

Ballard 4.8kW PEM fuel cell stack

- **We developed a 3D water management control surface for PEM fuel cell stacks.**
- **This control strategy will be tested using a Ballard 4.8kW fuel cell stack on a Greenlight Fuel Cell Test Stand as shown to the right.**
- **The primary theory is that for a gas of known or desired humidity we can calculate the pressure to operate the fuel cell from the 3D surface map of current density, humidity, and pressure.**
- **The pressure can be used in a feed forward control strategy to meet the power requirement. As such we will evaluate a humidity driven power management strategy.**

Protocol for Experimental Validation

- Test protocol for experimental validation of control strategy

  - **STEP 1 : Set the pressure to *P***
  - **STEP 2 : Set the Relative humidity to *RH=70%***
  - **STEP 3 : Apply the load.**
  - **STEP 4 : Allow to stabilize and record stack voltage (*Vstack*) and voltage of the individual cells (*Vcell*)**
  - **STEP 5 : Increase the load by *loadstep*, until *Vcell >Vmin*** (to meet stack safety requirements).
  - **STEP 6 : Increase Relative humidity be *RHstep*, reset the load and repeat steps 3 -5 until *RH=100%***
  - **STEP 7 : increase the pressure by *Pstep*, reset *RH* and go to STEP 2 until *P =3 bar*.**

This stack test protocol is being implemented using a scripting software (HYAL). The test results will be presented during the DOE review meeting presentation.

Future Work

- Future Work (FY09)

- Performance improvement of SAS membrane
  - Apply cross-linking agent to make membrane chemically inert towards reactant gases
  - Test thermal effect and life-cycle sensitivity
  - Map membrane water history

- Development of integrated CFD porous media multiphase model
  - FEA graphical user interface for unit PEM fuel cell
  - Effect of flow, heat transfer and electrochemistry on fuel cell performance
  - Improve design of single cell
  - Experimental testing of 3D surface map obtained by CFD analysis for effective control of fuel cell systems

Future Work

- Future Work (FY09)

- Explore other avenues for membrane performance enhancement
  - Real-time test of membrane performance with single cell and stack
  - Test of SAS PEM membrane performance using industry standard devices if fund is available

- Improve design of unit cell and stack based on CFD modeling results
  - Perform parametric study for design sensitivity analysis
  - Calculation of optimal combination of operating conditions based on CFD surface map
  - Identify water production and management precursors
  - Identify self-humidifying mechanism for effective fuel cells water management

Summary

Project Summary

Relevance: **Help to develop advanced membrane materials for fuel cell applications. CFD model helps to understand water-thermal couple-system in PEMFC.**

Approach: **Using patented polymer structure modification technology, develop and experimentally characterize new membrane properties and validated with peers. Use multiphase CFD model to understand water & thermal management in PEMFC.**

Technical Accomplishments and Progress: **Advanced fuel cell membrane manufacturing procedure has been developed. CFD multiphase porous media flow model is developed and investigated to improve PEMFC design.**

Technology Transfer/Collaborations: **Active partnership with Bei-Tech, presentations, publications and patents.**

Proposed Future Research: **Seek answers by identifying factors limiting PEM fuel cell performance and industrial applications.**

References

[1] Y. Wang and C. Y. Wang, J. Power Sources, **147**, 148-161 (2005).

[2] J. J. Hwang, J. Power Sources, **164**, 174-181 (2007).

[3] T. E. Springer, T. A. Zawodzinski, and S. Gottesfeld, *J. Electrochem. Soc.,* **138**, 2334 (1991).

[4] Susanta K. Das, and K. J. Berry, *Journal of Power Sources*, 173, p. 909-916 (2007).

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[6] R.B. Bird, W.E. Stewart, E.N. Lightfood, Transport Phenomena, John Wiley & Sons, New York (1960).

[7] J.J. Hwang, C.H. Chao, W.Y. Ho, C.L. Chang, D.Y. Wang, J. Power Sources, **157**, 85 (2006).