



# **Development of Novel PEM Membrane and Multiphase CFD Modeling of PEM Fuel Cell (Kettering University's Fuel Cell Program)**

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**June 9-13, 2008**

**Project ID # FCP14**

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# Overview

## Overview

### Timeline

- Start – July 2006
- Finish - June 2008
- 80% 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
- Umicore Fuel Cells
  - MEA development

# Objectives

Overall	<ul style="list-style-type: none"><li>• Development of novel proton exchange membrane (PEM) for fuel cells</li><li>• Development of multiphase CFD model of PEM fuel cell for improved water and thermal management</li></ul>
2006	<ul style="list-style-type: none"><li>• Low-cost, high-performance membrane<ul style="list-style-type: none"><li>- Design and manufacturing processes</li><li>- Experimental testing and performance validation</li></ul></li></ul>
2007-2008	<ul style="list-style-type: none"><li>• Low-cost, high-performance membrane<ul style="list-style-type: none"><li>- Real-time membrane testing for single cell and stack</li><li>- Real-time testing for stability and materials properties</li></ul></li><li>• Integrated multiphase CFD model for PEM fuel cell<ul style="list-style-type: none"><li>- Complete unit fuel cell performance evaluation</li><li>- Performance evaluation for fuel cell stack</li></ul></li></ul>

# Approach

## Plan & Approach

### ➤ Task 1: New fuel cell membrane

Completed  
95%

- Literature survey
- Theoretical analysis and model development
- Inexpensive materials search

### ➤ Task 2: Chemical modification

Completed  
80%

- Modification of polymer backbone
- Increased proton conductivity
- Reduced resistance than peer

### ➤ Task 3: Thermal stability and water management

Completed  
75%

- Test of water uptake and thermal stability
- Improved durability and efficiency
- Test of stable proton conductivity

### ➤ Task 4: CFD multiphase model for PEM fuel cell

Completed  
80%

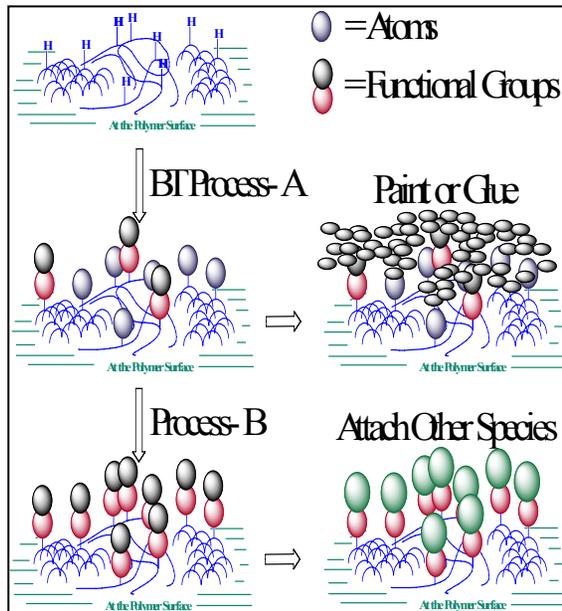
- Literature survey
- Developed CFD multiphase mathematical model
- Developed graphical user interface

# Approach

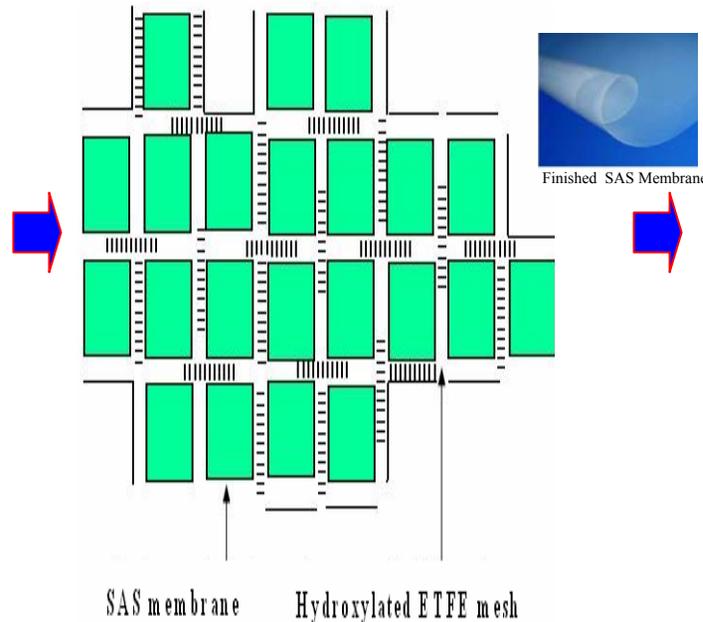
## Approach Overview

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

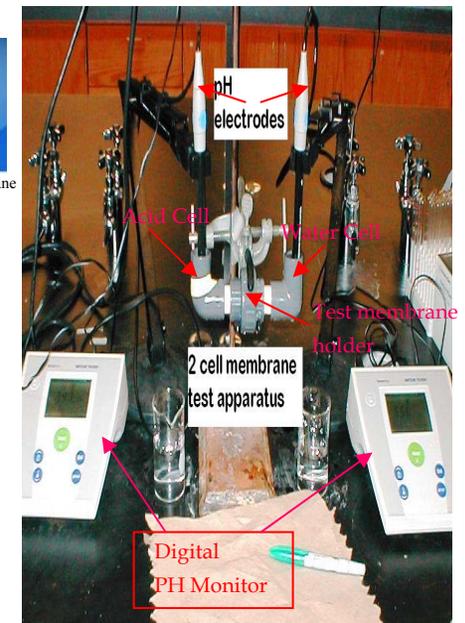
- Patented Polymer Backbone Modification Technology



- New SAS Polymer Membrane



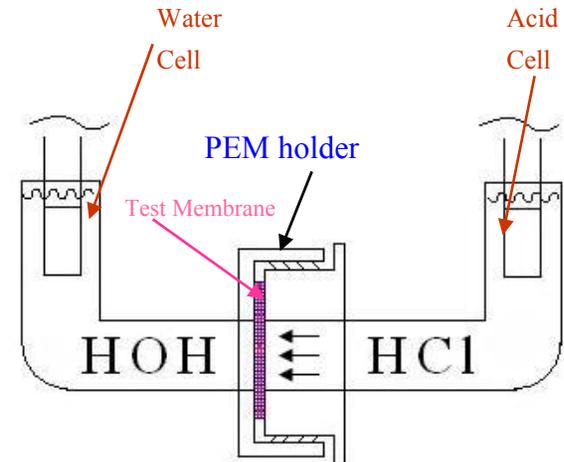
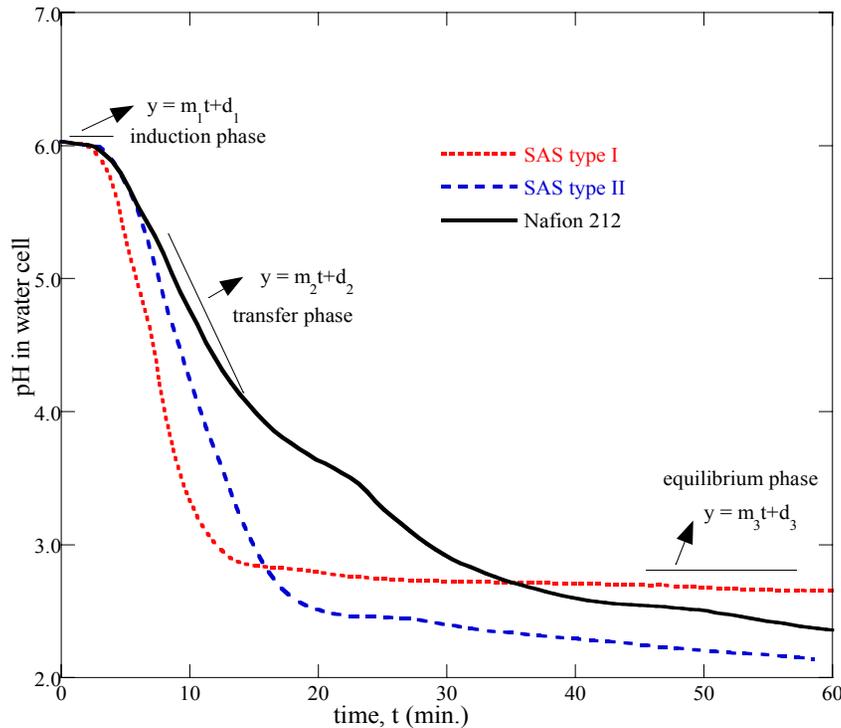
- Performance Validation





# Accomplishments/Progress/Results

- Membrane's proton exchange capacity

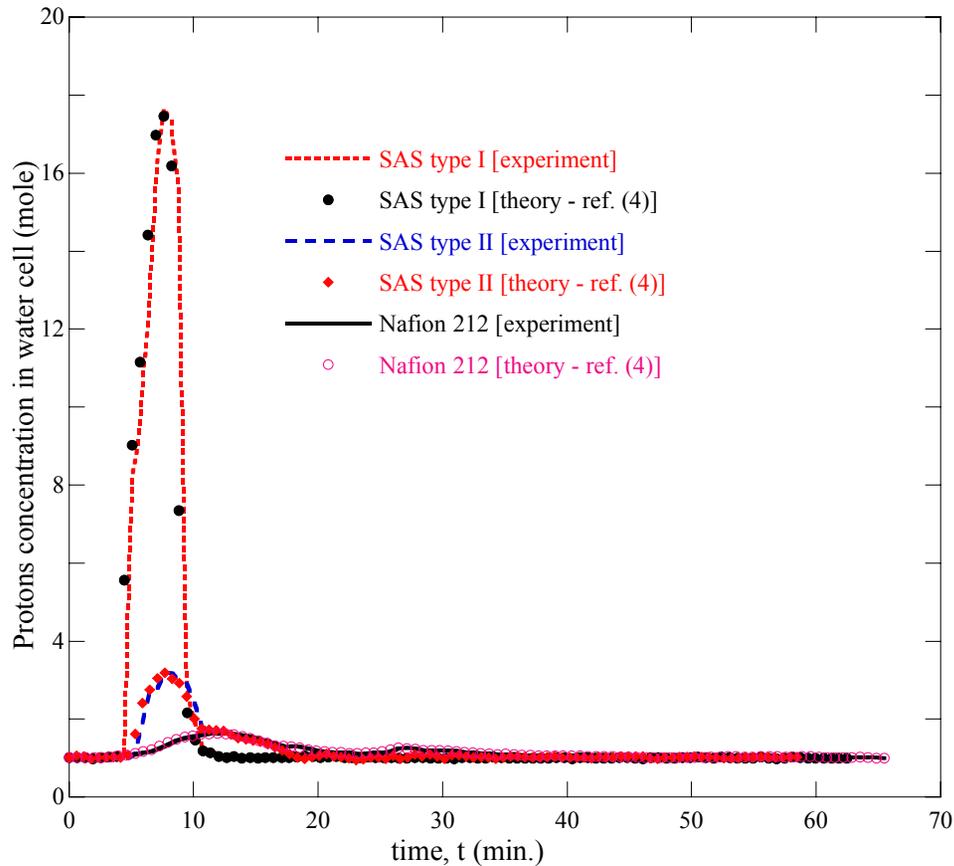


Schematic of proton exchange capacity test method

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

# Accomplishments/Progress/Results

- Proton conductivity through the membrane

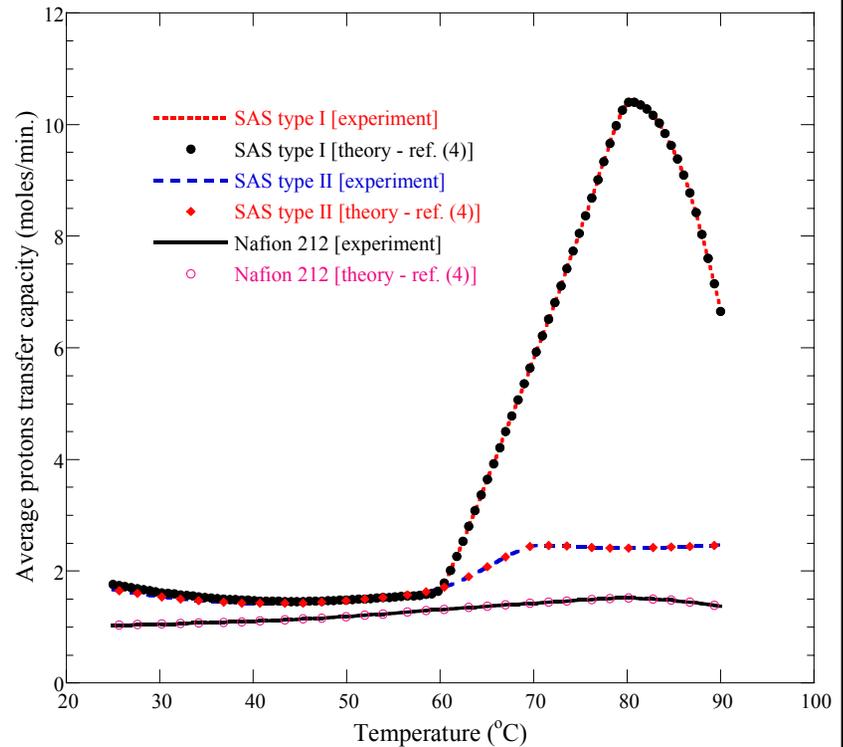
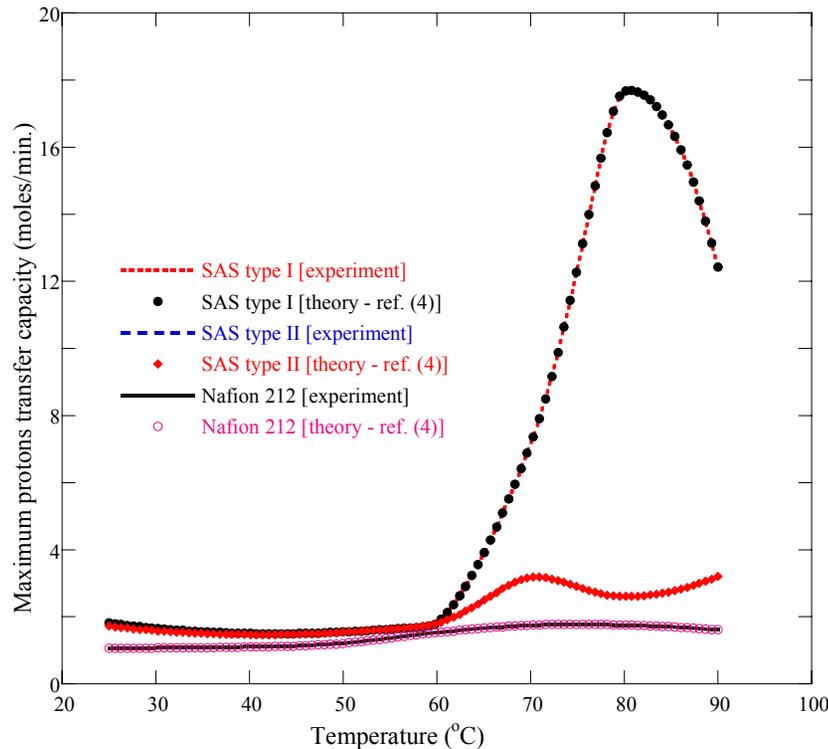


- SAS type I has higher proton conductivity than peer materials
- Excellent agreement between experimental and theoretical results
- Ability to reach equilibrium state quickly

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

# Accomplishments/Progress/Results

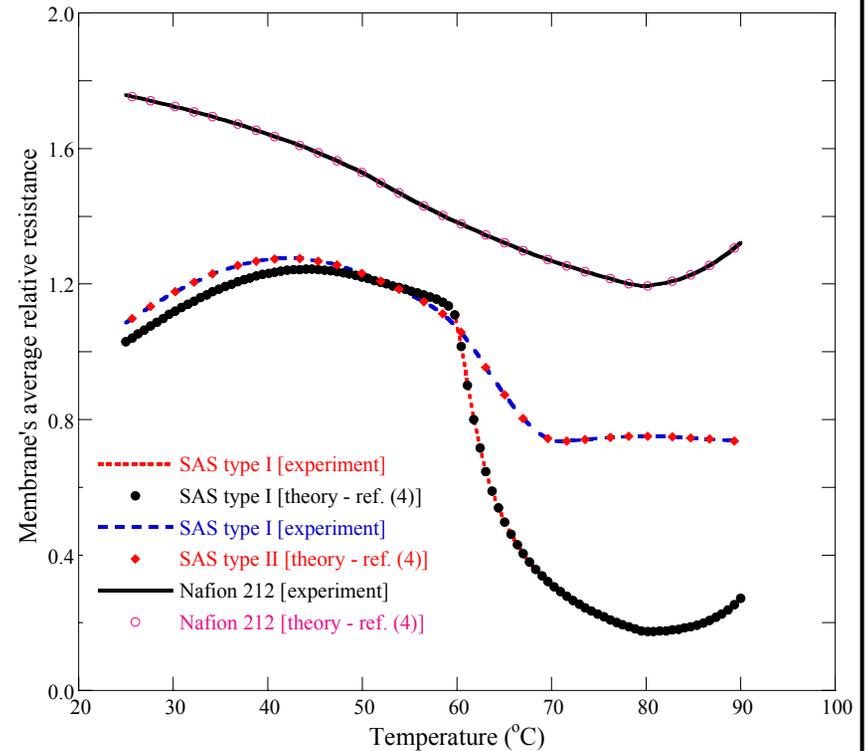
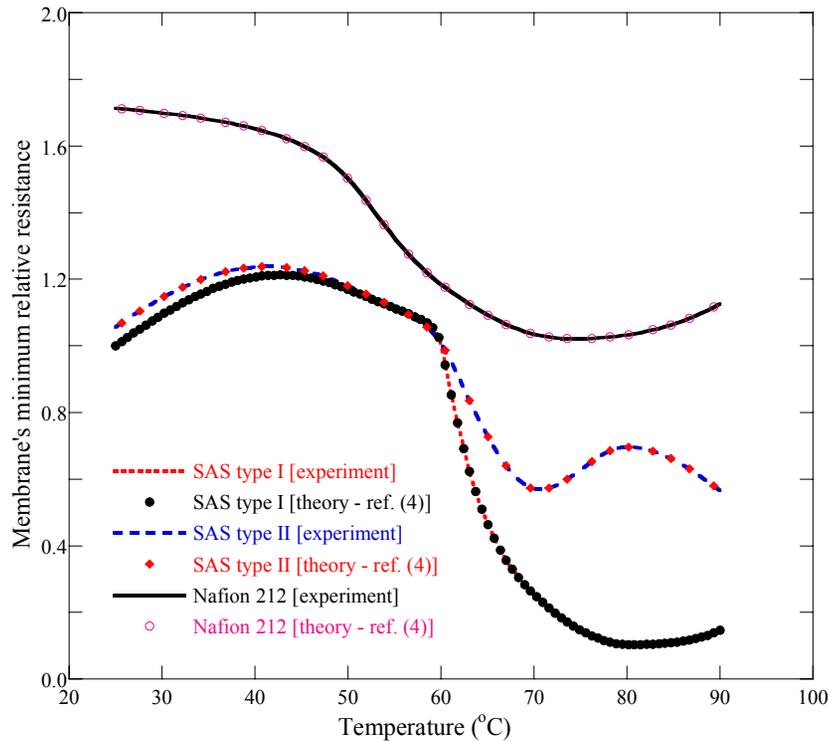
- Comparison of proton transfer capacity



- Maximum 16 times higher proton transfer rate than Nafion<sup>®</sup> 212 at 80°C
- Average 10 times faster proton transfer rate than Nafion<sup>®</sup> 212 at 80°C
- Since the protons present in water cell are in the form of  $\text{H}_3\text{O}^+$  and not simply  $\text{H}^+$ , 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.

# Accomplishments/Progress/Results

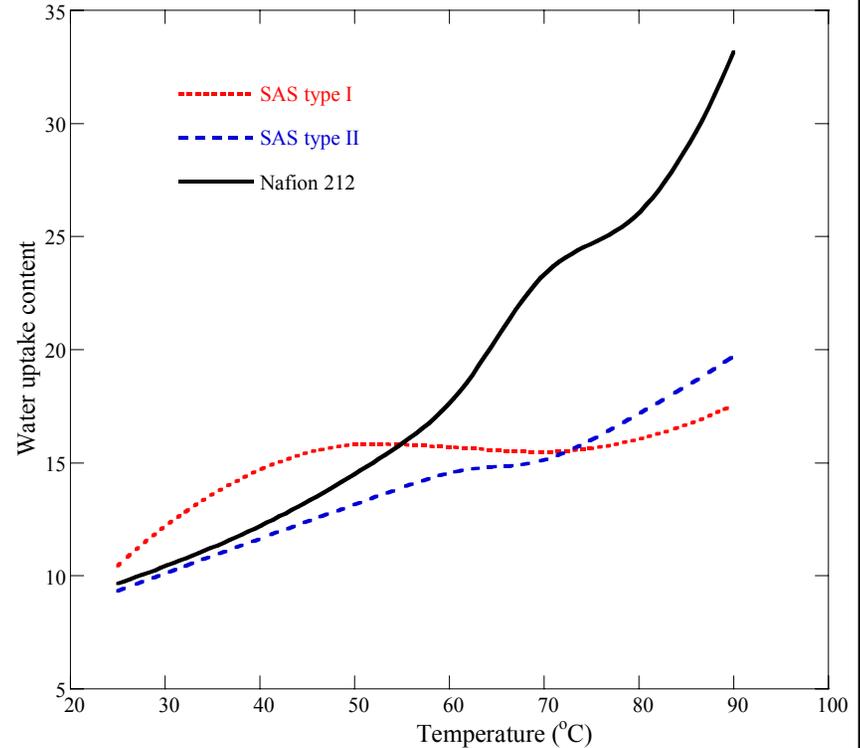
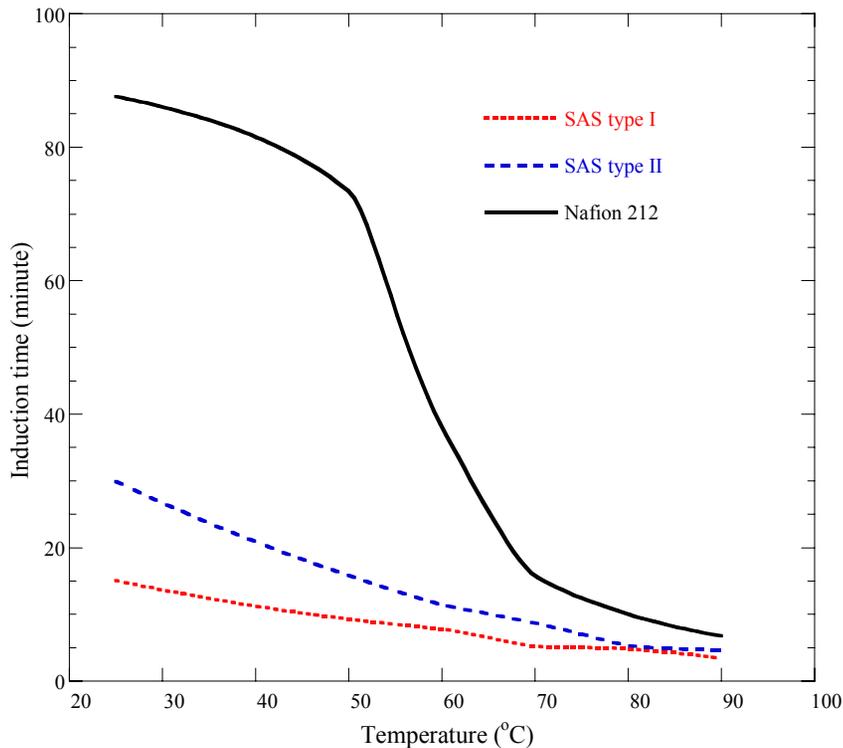
- Comparison of relative membrane resistance



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

# Accomplishments/Progress/Results

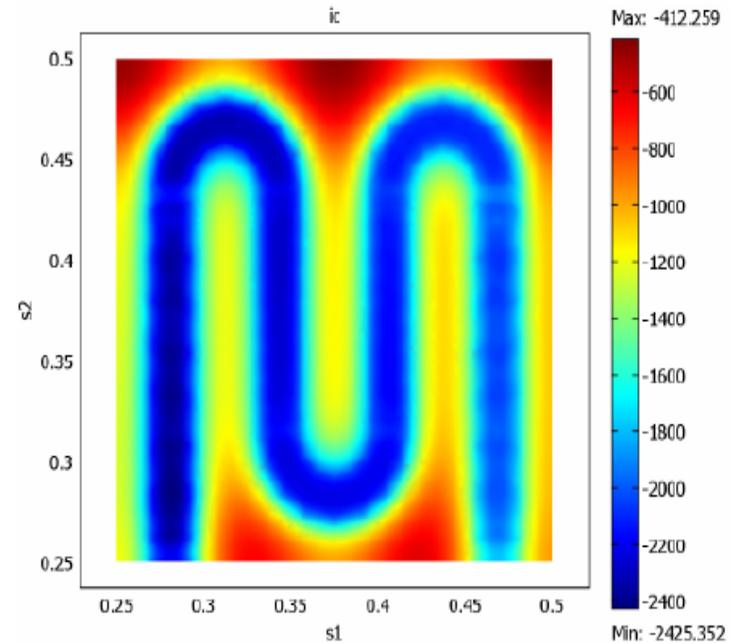
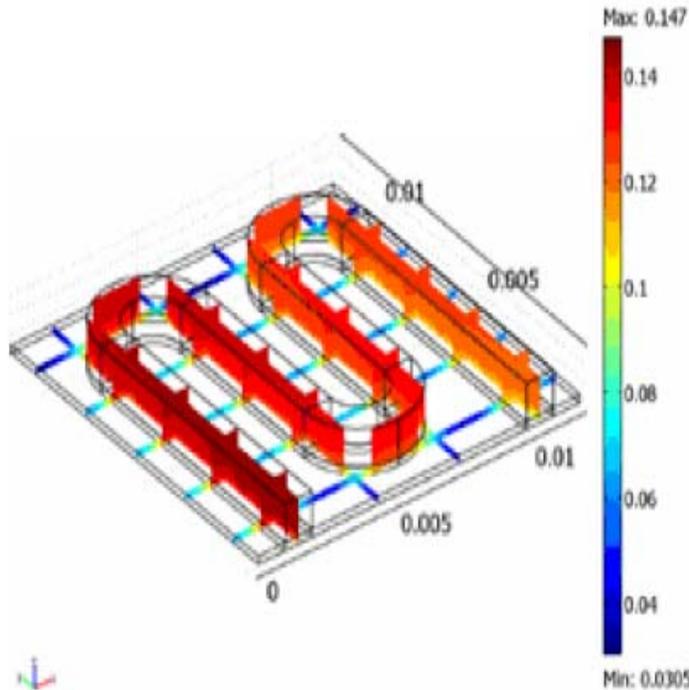
- Comparison of induction time & water uptake content



- 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

# Accomplishments/Progress/Results

- Multiphase CFD analysis of PEM fuel cell



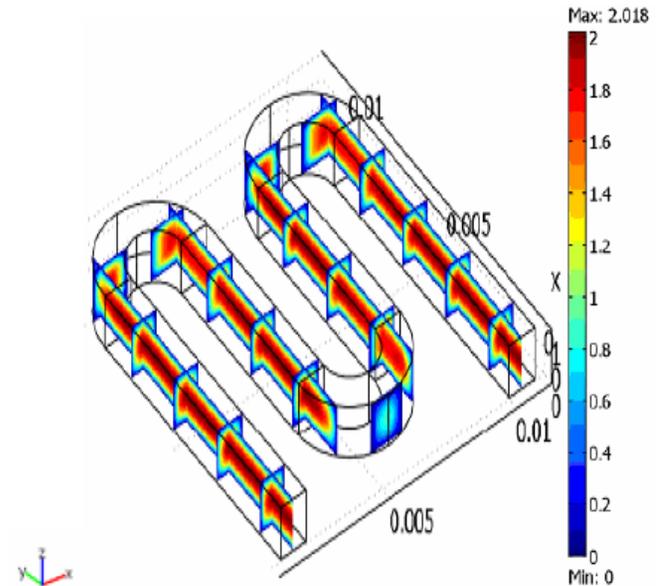
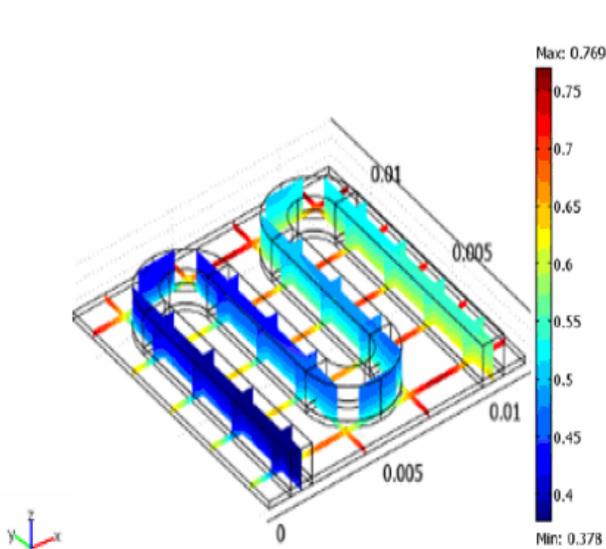
- Mass fraction of oxygen in the channel and the porous cathode

- 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.

# Accomplishments/Progress/Results

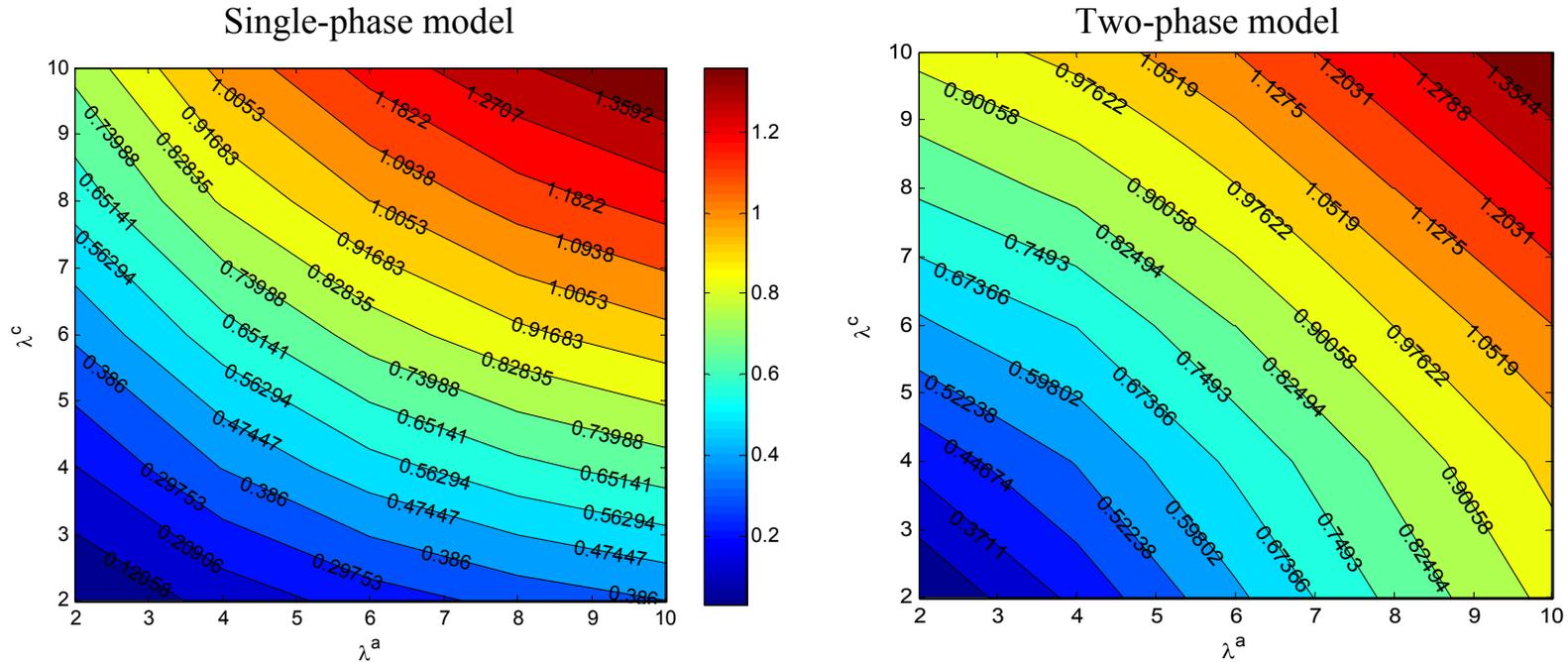
- Multiphase CFD analysis of PEM fuel cell



- Weight fraction of liquid phase (water) in the cathode gas.
  - Gas-velocity (gas phase) distribution in the gas channel for a 25 Pa pressure drop between the inlet and outlet.
- 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.
  - 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.

# Accomplishments/Progress/Results

- Multiphase CFD analysis of PEM fuel cell

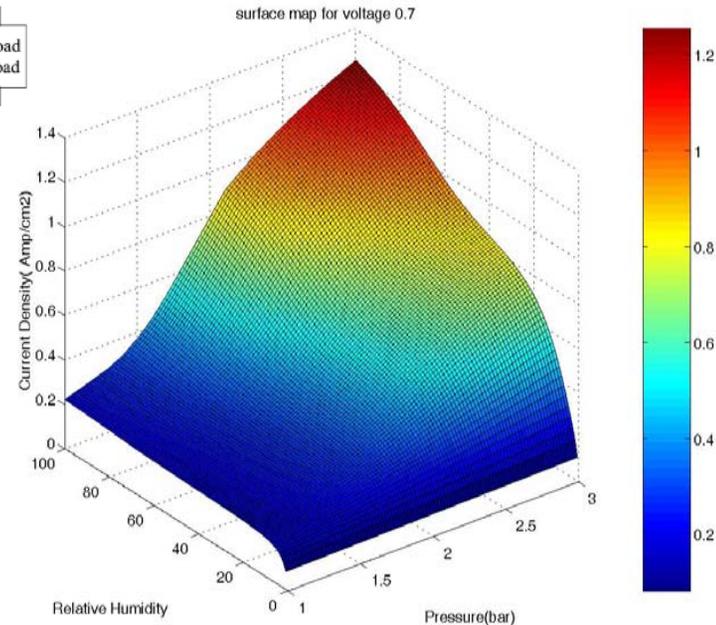
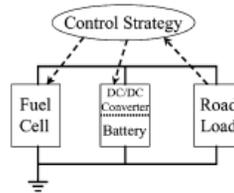
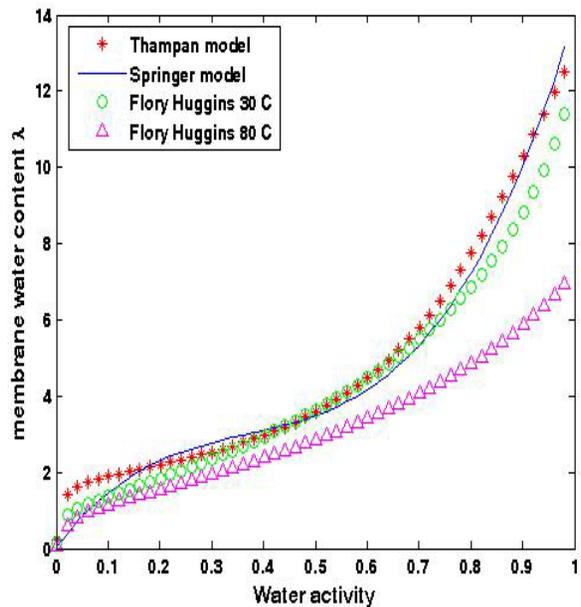


- Current density across the membrane at 80°C

- 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 air breathing fuel cell designs.

# Accomplishments/Progress/Results

- Control strategy for PEM fuel cell applications



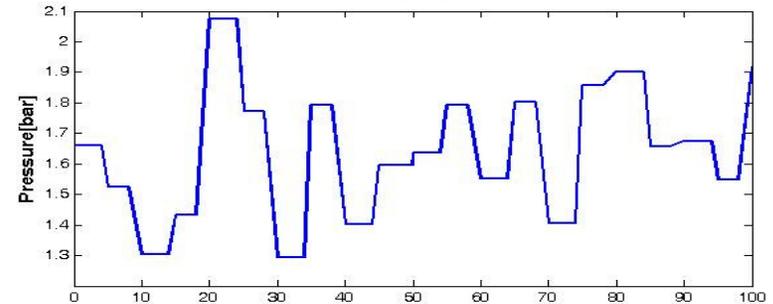
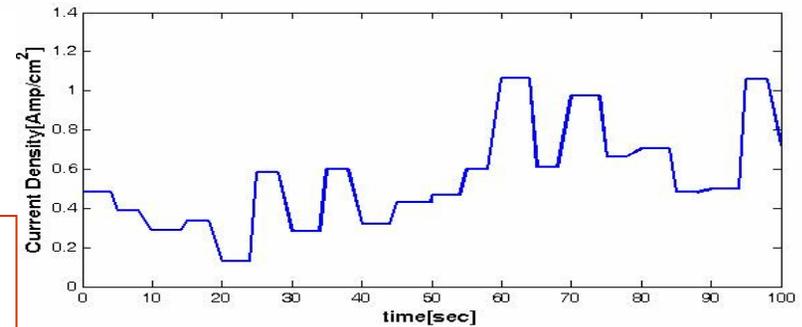
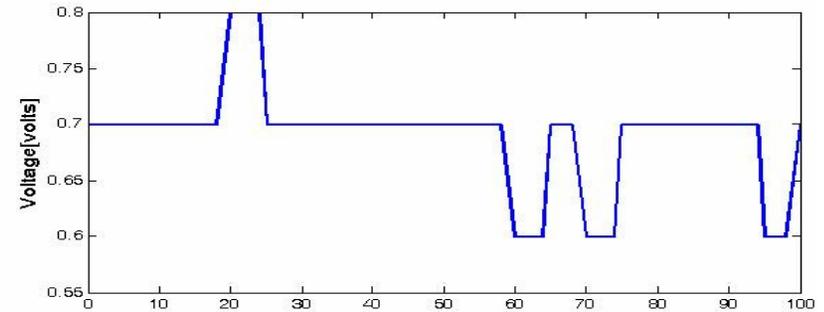
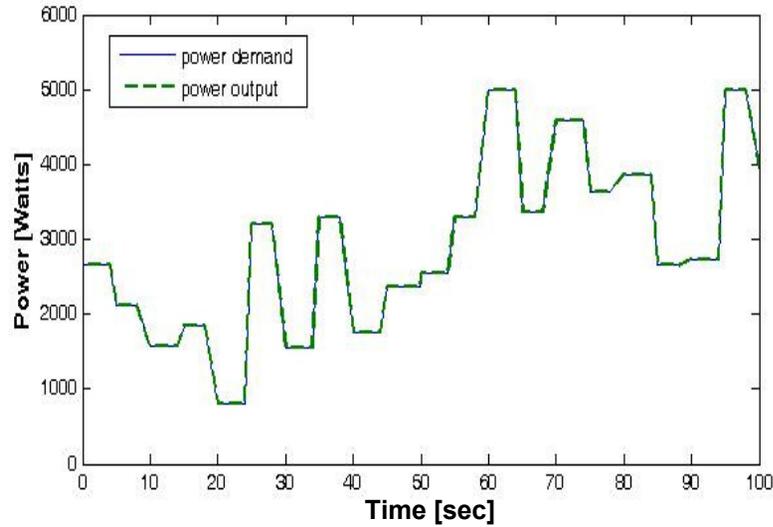
- Water activity in the membrane

- 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.

# Accomplishments/Progress/Results

- Control strategy for PEM fuel cell applications



- 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.

# Future Work

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- Future Work (FY08)

- 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 and stack
- Effect of flow, heat transfer and electrochemistry on fuel cell performance
- Improve design of single cell and stack
- Experimental testing of 3D surface map obtained by CFD analysis for effective control of fuel cell systems

# Future Work

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- Future Work (FY08)

- Explore other avenues for membrane performance enhancement

- Replace sulfate group with phosphate group for better water management
- Real-time test of membrane performance with single cell and stack
- Characterization of membrane properties 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, Unicore fuel cell**, presentations, publications and patents.

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