Development of Unified PEM Fuel Cell Models

DOE CARAT Program

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DOE Fuel Cells for Transportation Program
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Objective

- Demonstrate the feasibility of unified model approach to eliminate errors due to approximate boundary conditions at various interfaces
- Develop a comprehensive 3-D fuel cell model
- Develop reliable tools for design and optimization of fuel cells, stacks, and systems (long-term)

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Approach

- Develop general mathematical models valid in different parts of a fuel cell
- Eliminate boundary conditions at the various interfaces
- Adaptability: different levels of model complexity, easy to update, custom model incorporation
- Independent package (not based on any CFD package) - economical
- Robust and high-speed

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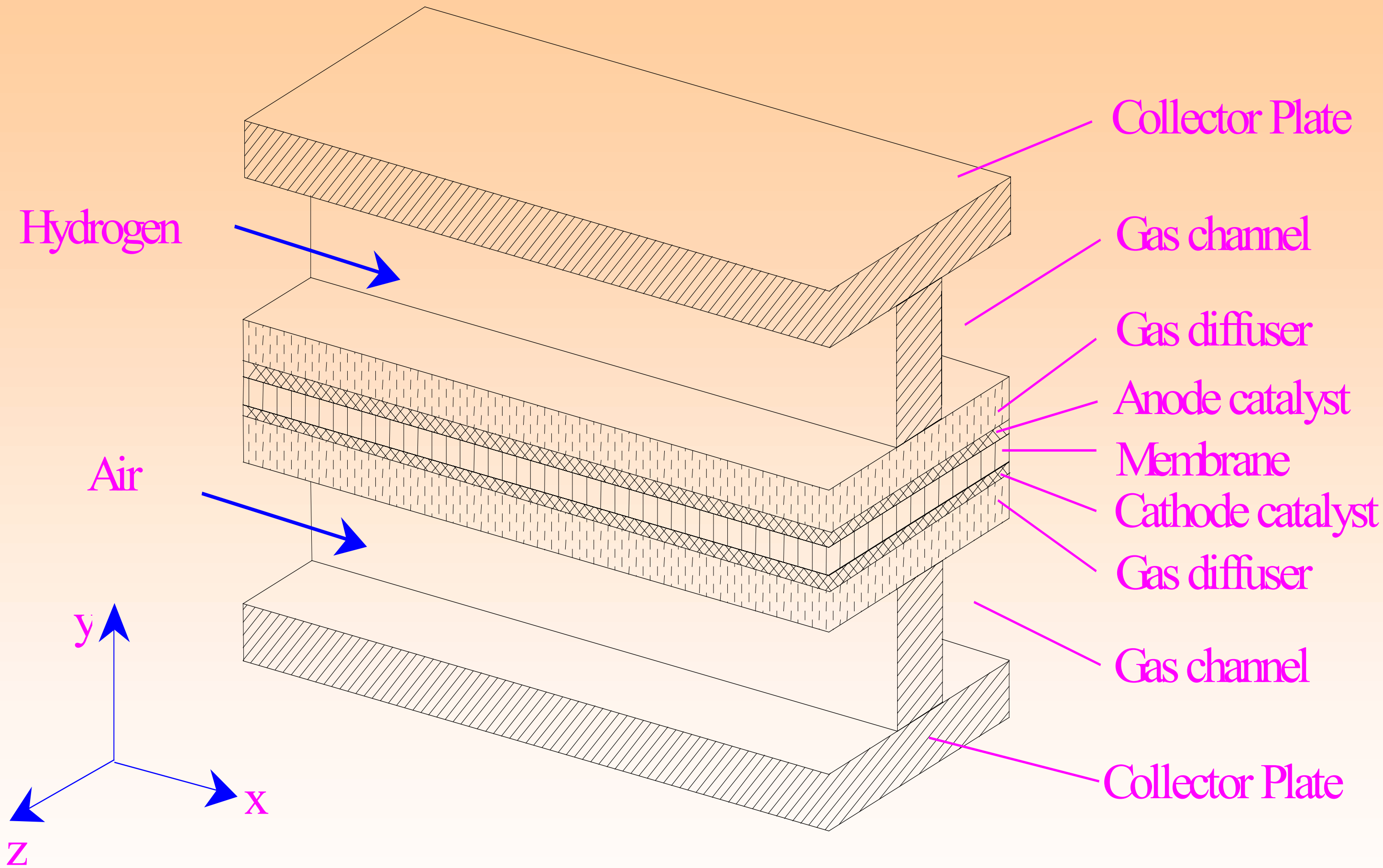
3D fuel cell model



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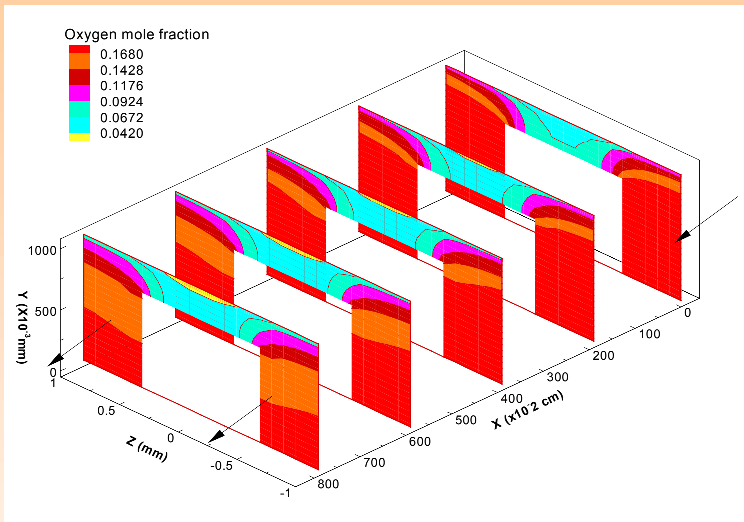
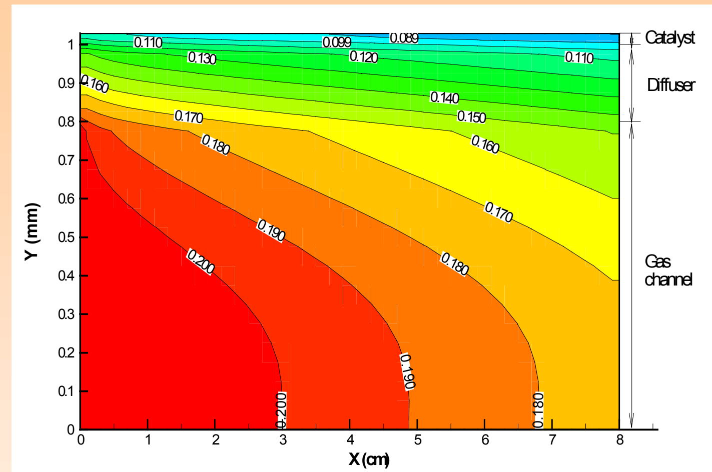
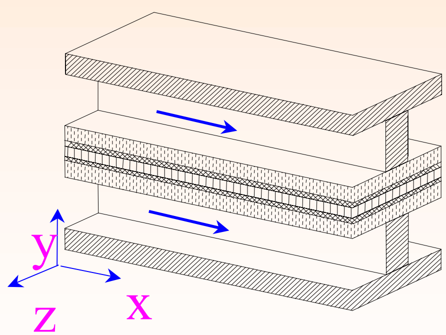
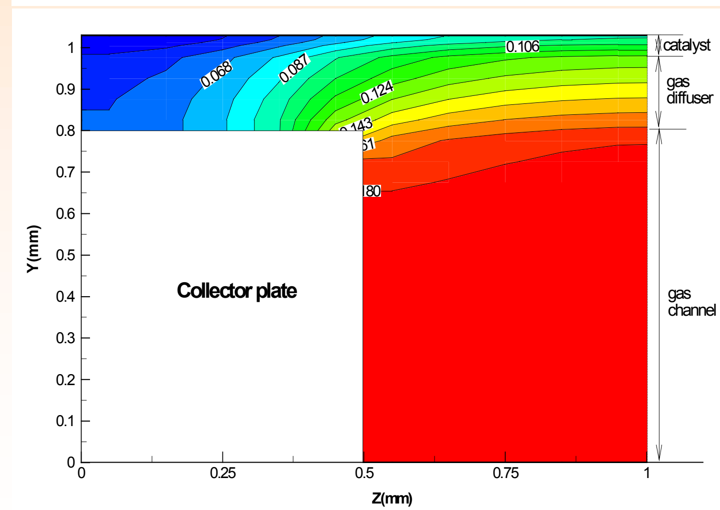
Sample results-3D model: oxygen molar fraction

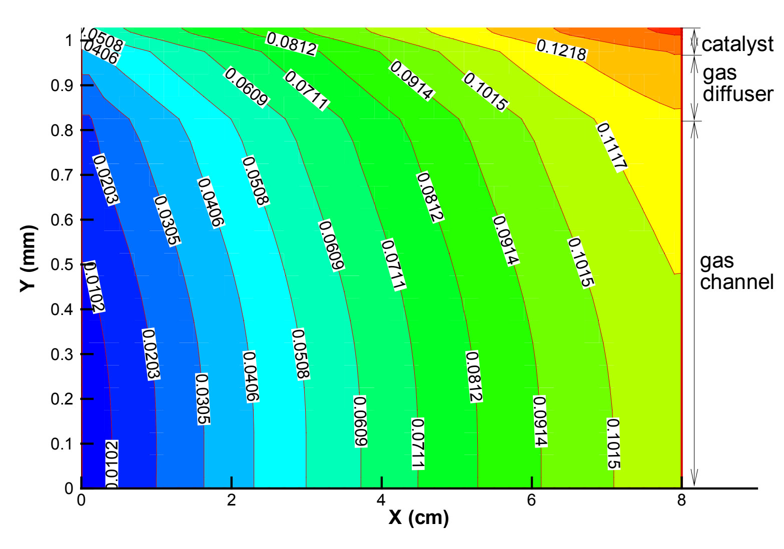


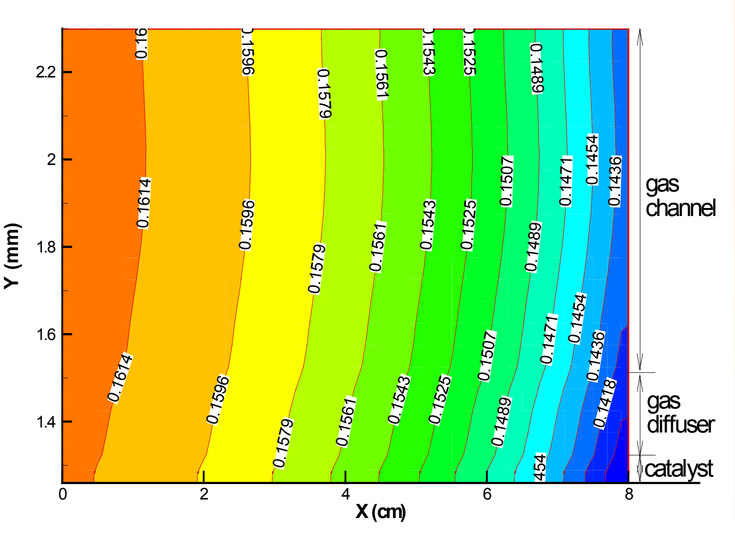






Sample results - 3D model: water contours





Cathode side

Anode side

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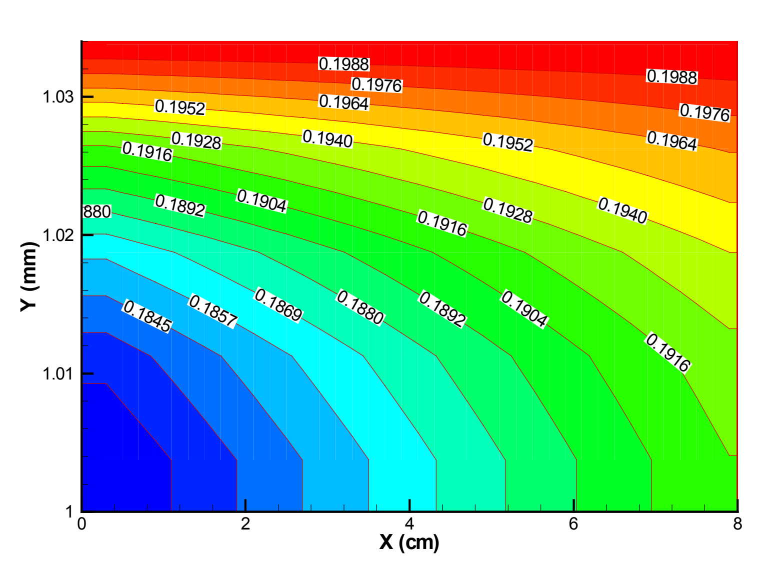
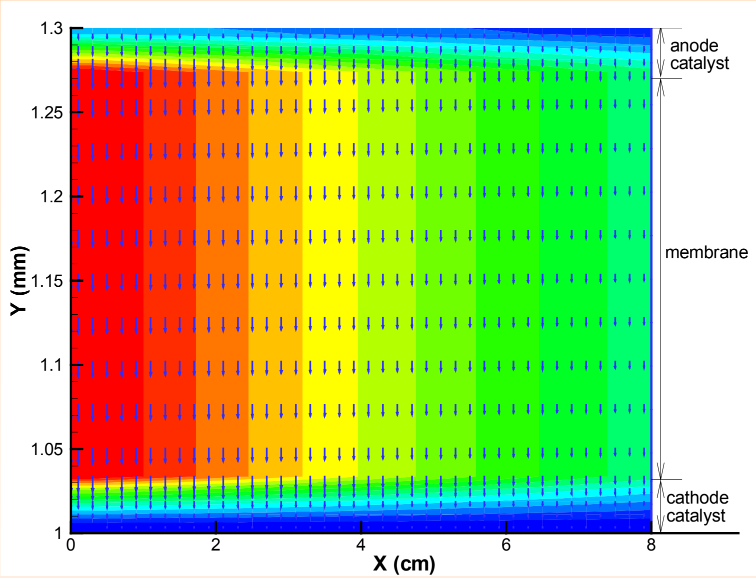
Sample results - 3D model



Overpotential distribution within the cathode catalyst layer



Current density distribution within the PEM

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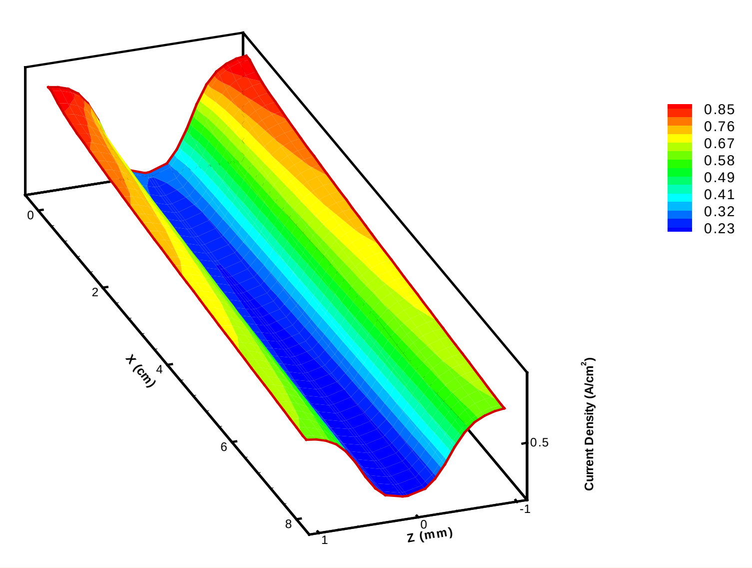
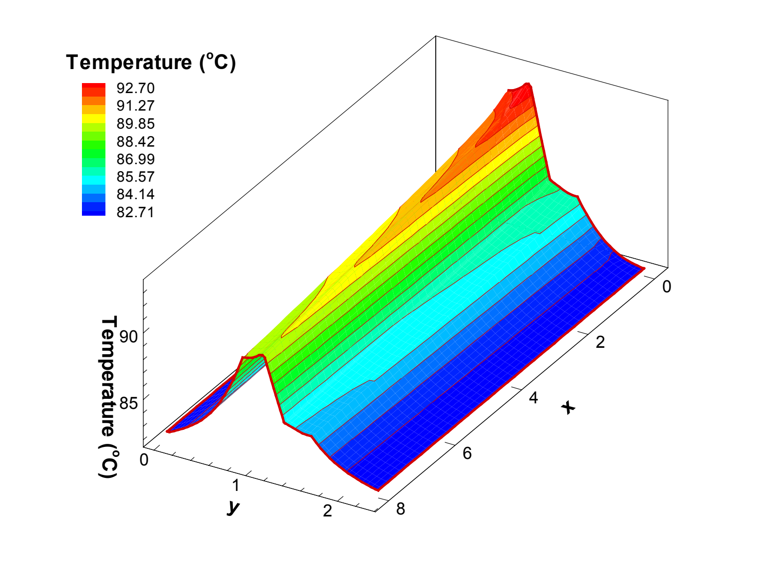
Sample results – 3D model





Current density distribution **Temperature distribution**

UM fuel cell test station

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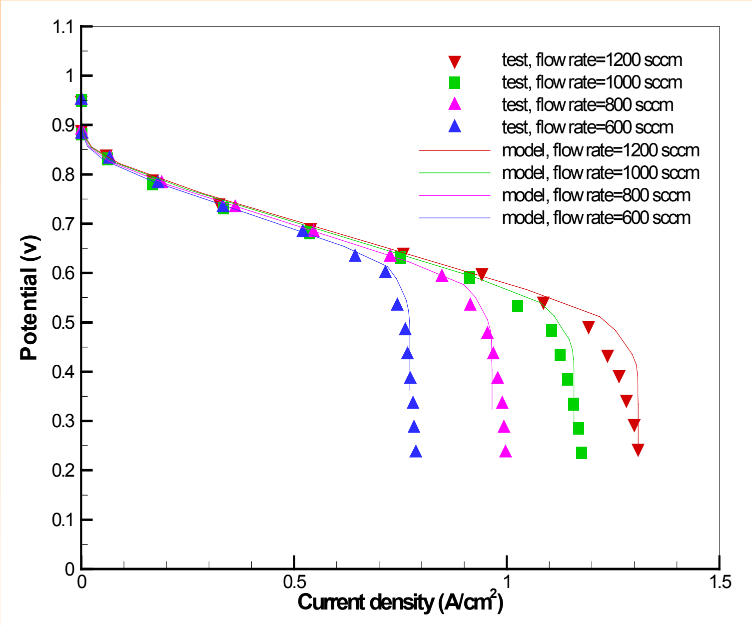
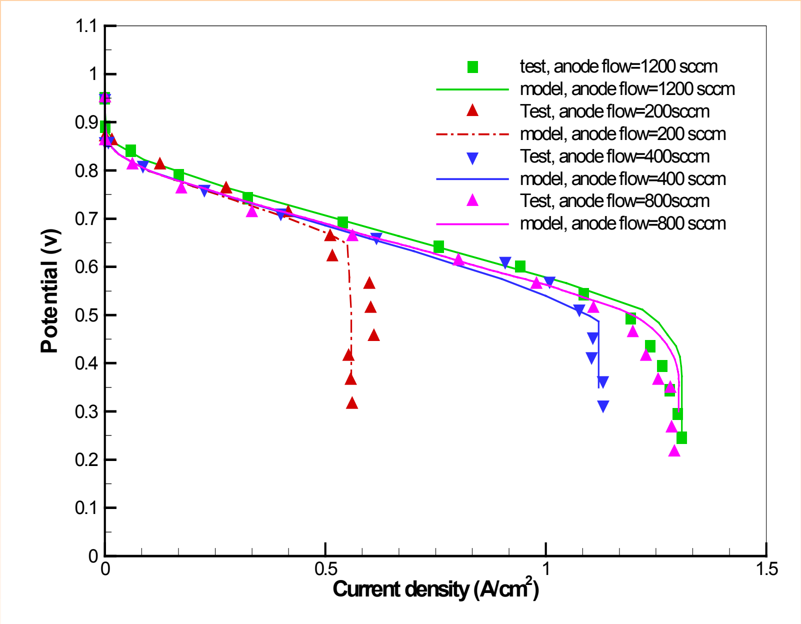
Comparison of 3D model with experiments





Different air flow rates

Different hydrogen flow rates

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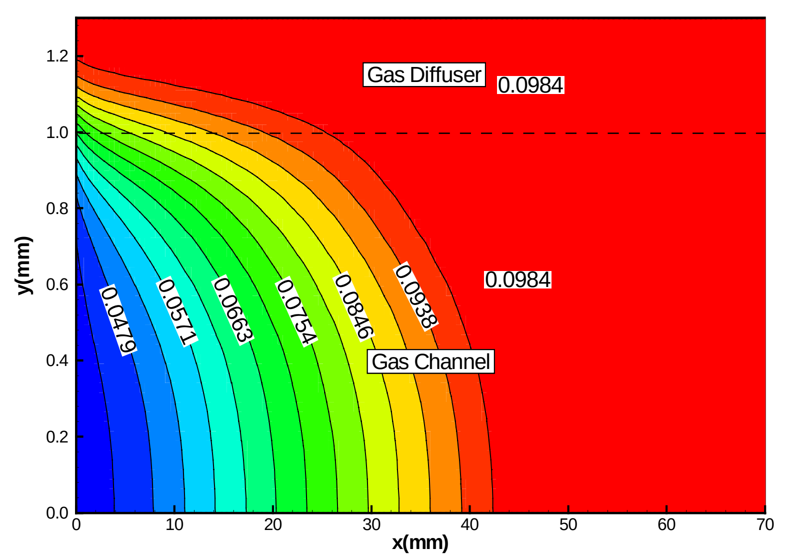
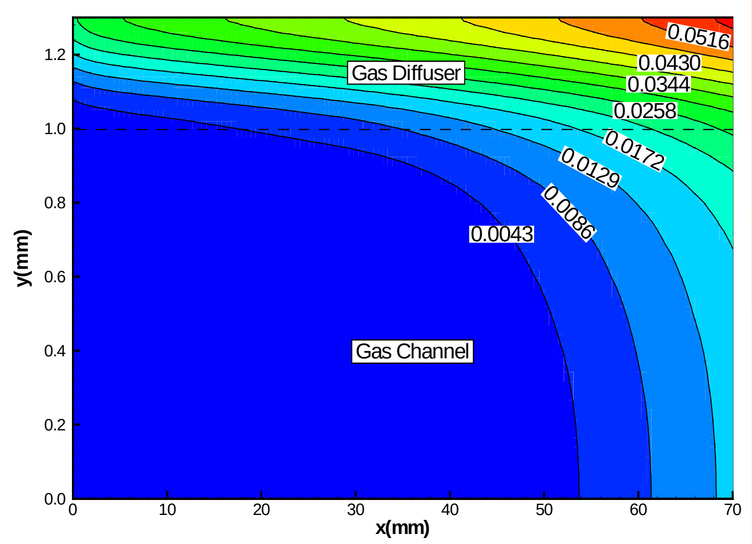
Sample results - 2-phase model

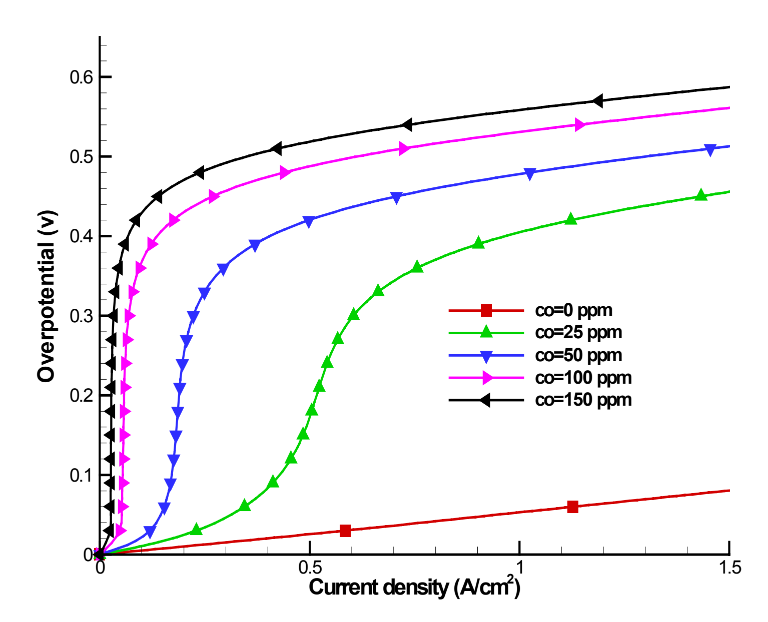


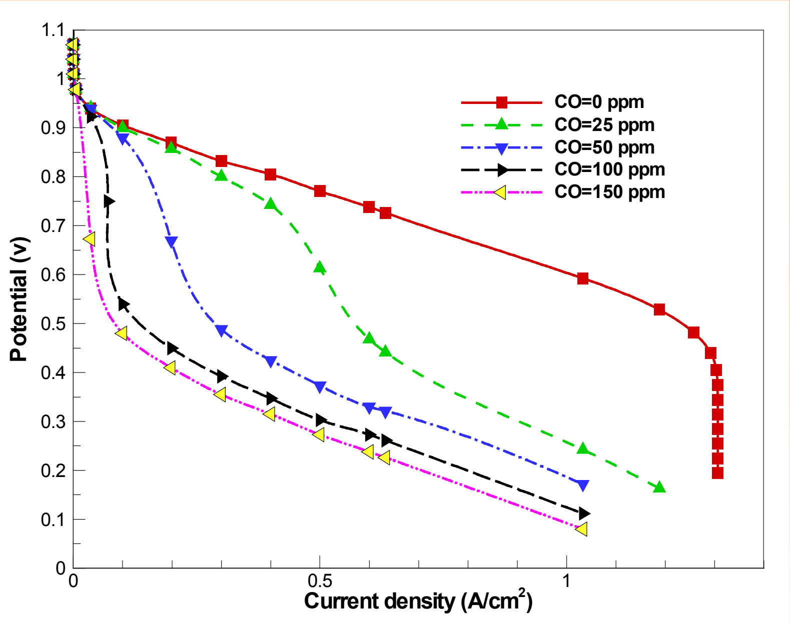


Vapor water fraction

Liquid water fraction

Sample results 3D – reformate feed





Current densities vs. overpotentials

Polarization curves

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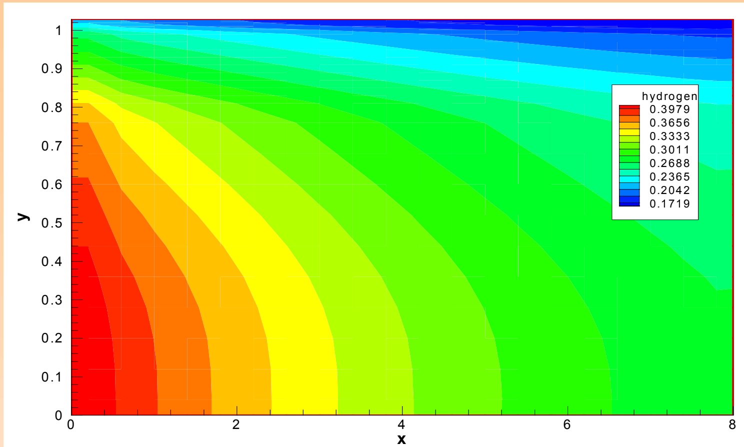
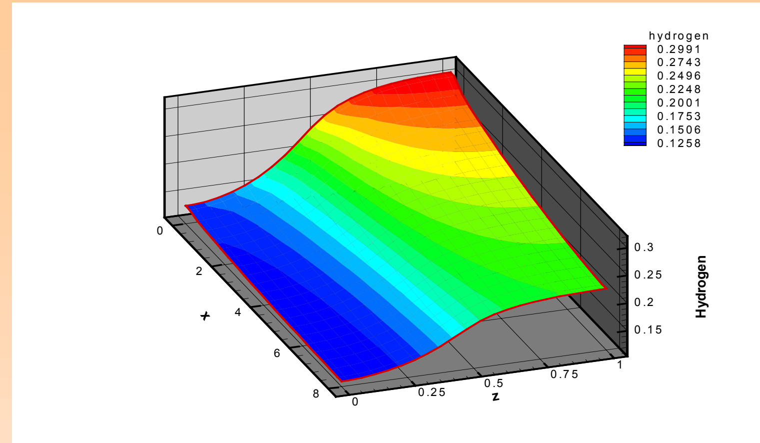
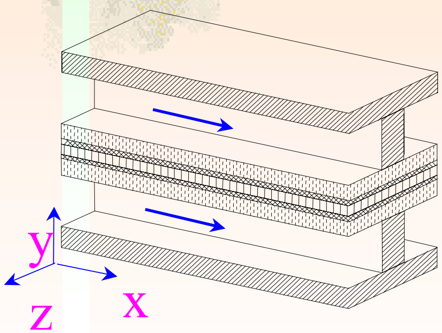
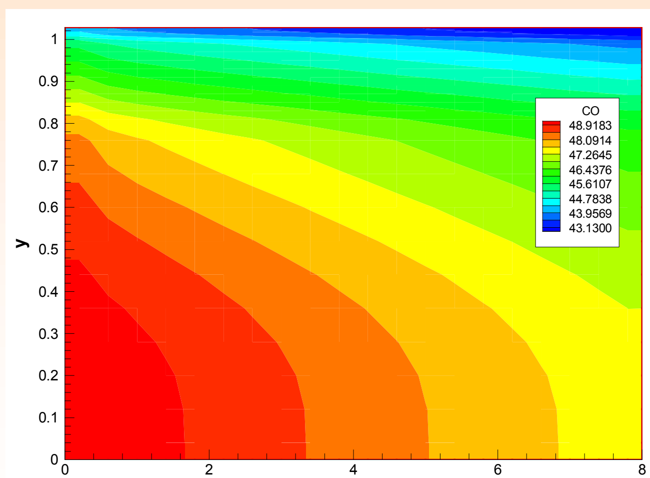
3D results – reformate feed

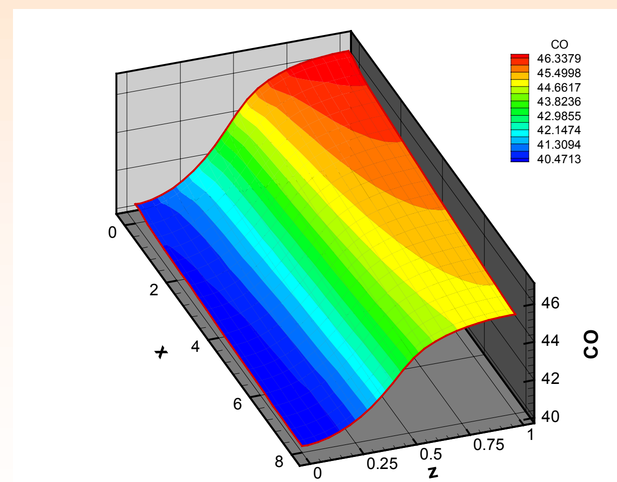




Hydrogen molar fraction at i=0.7 A/cm^2

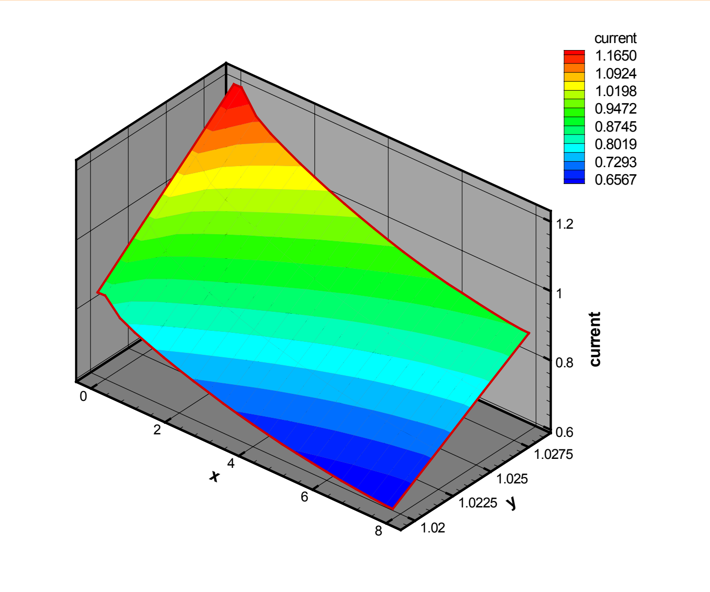


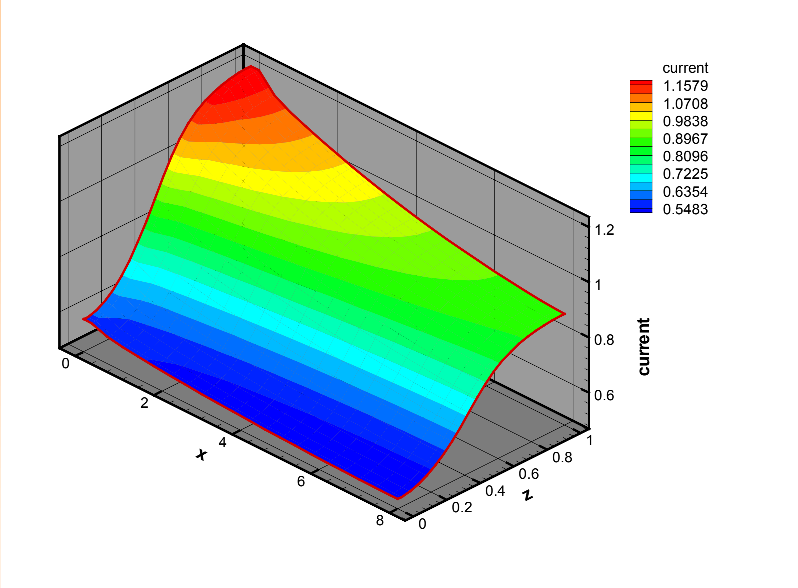




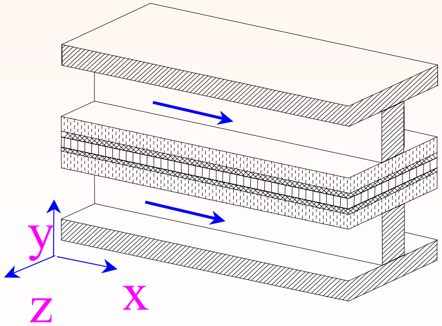
CO variation (ppm) at i=0.7 A/cm^2

3D results – reformate feed

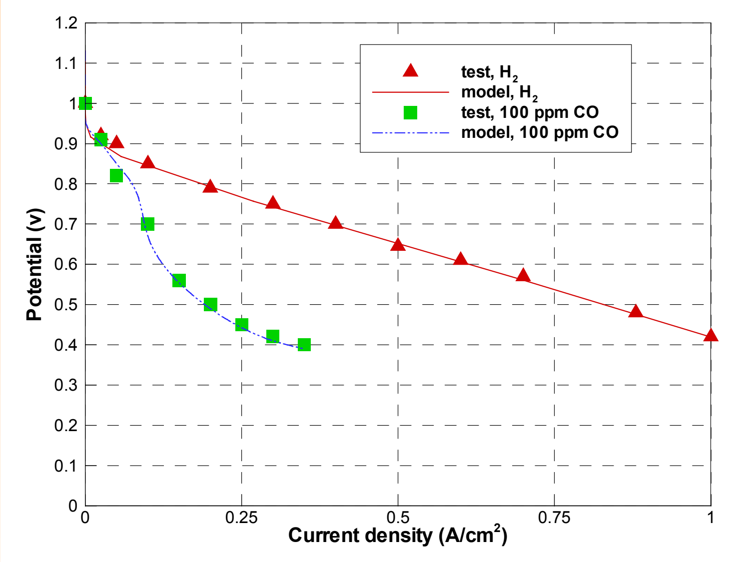


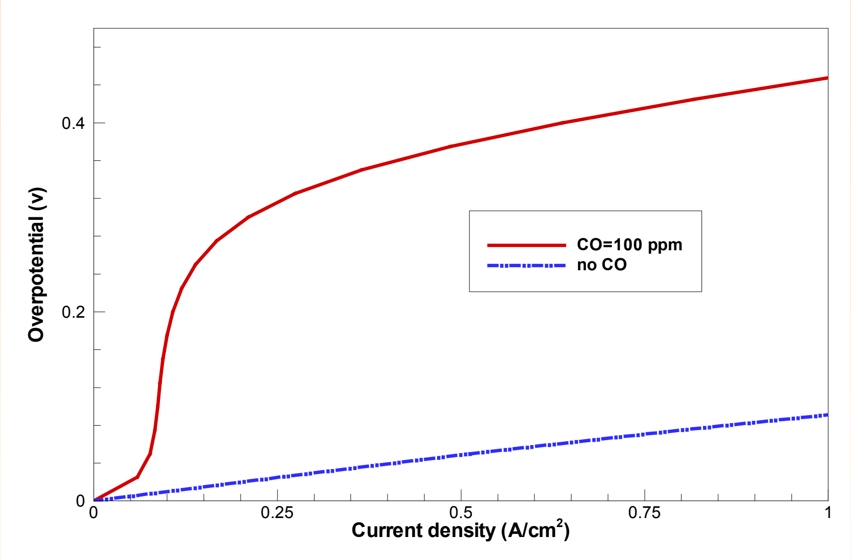


Local current density distributions



3D results – reformate feed





Comparison with experimental data

Current density vs. surface overpotential at the anode

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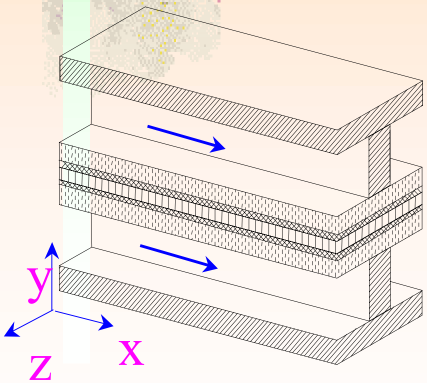
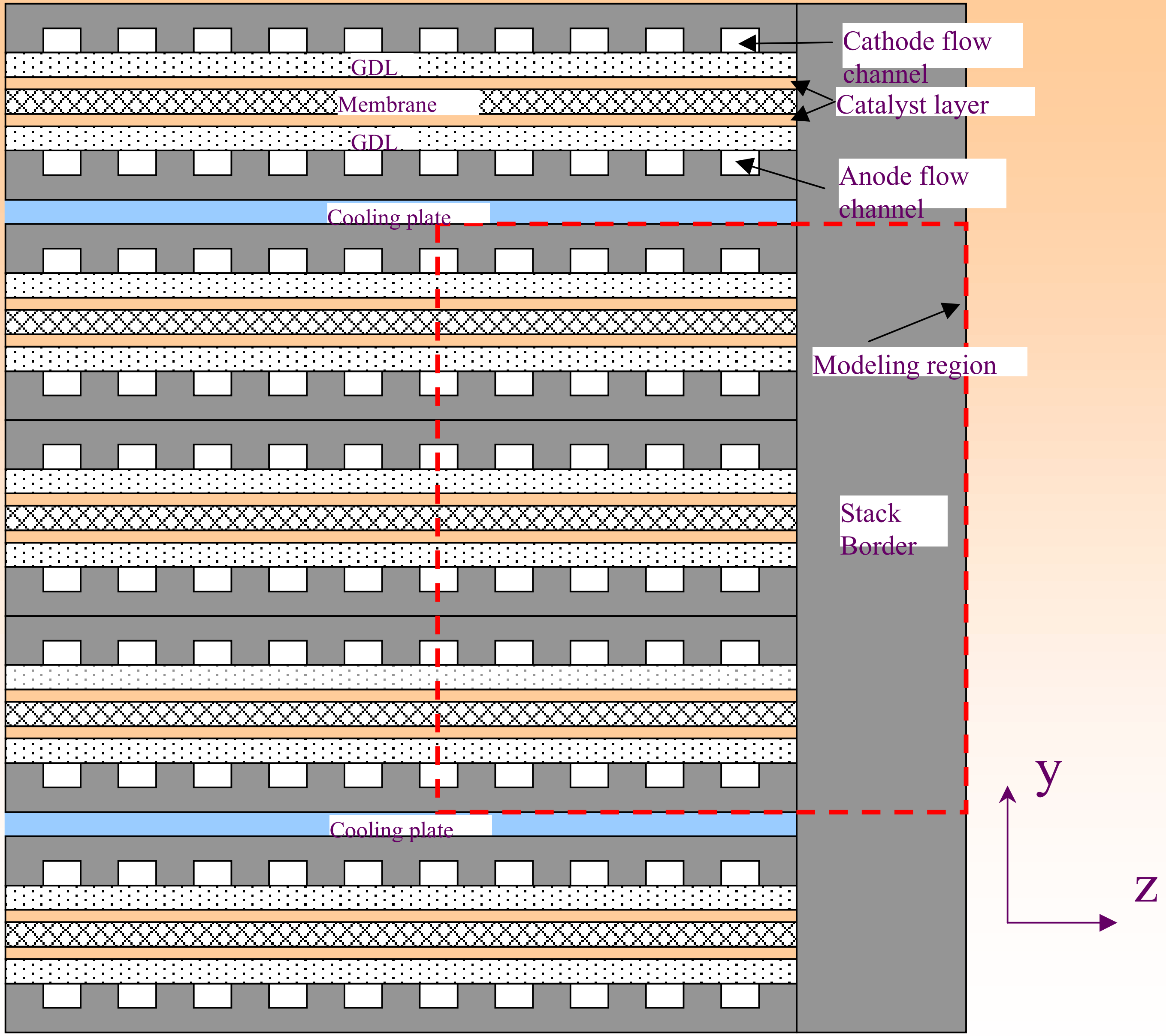
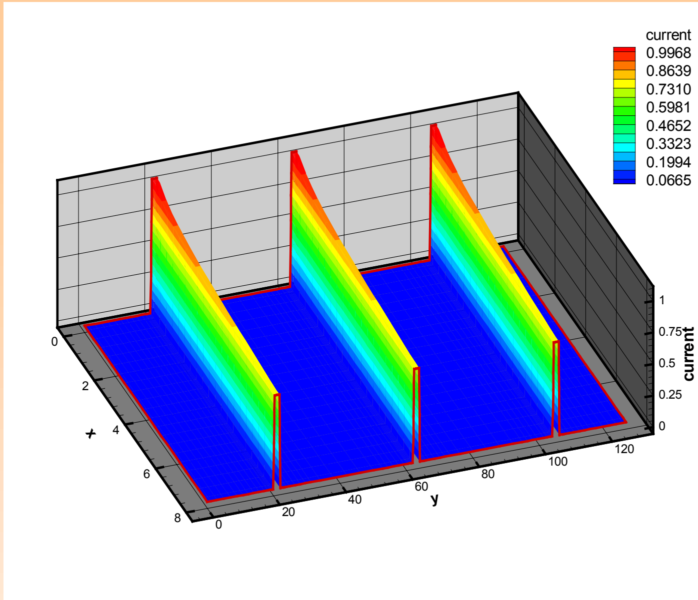
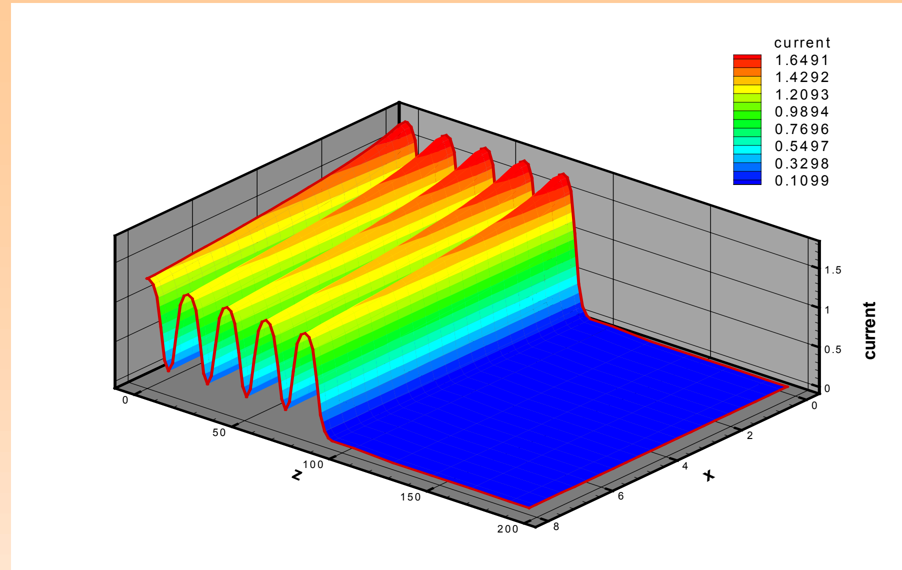
Preliminary stack model

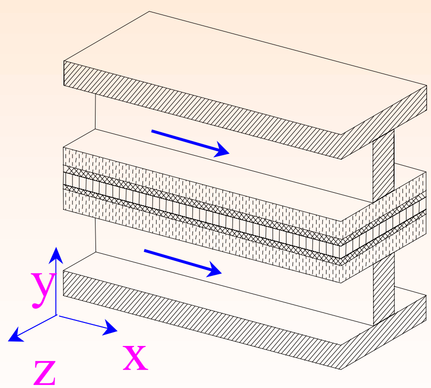


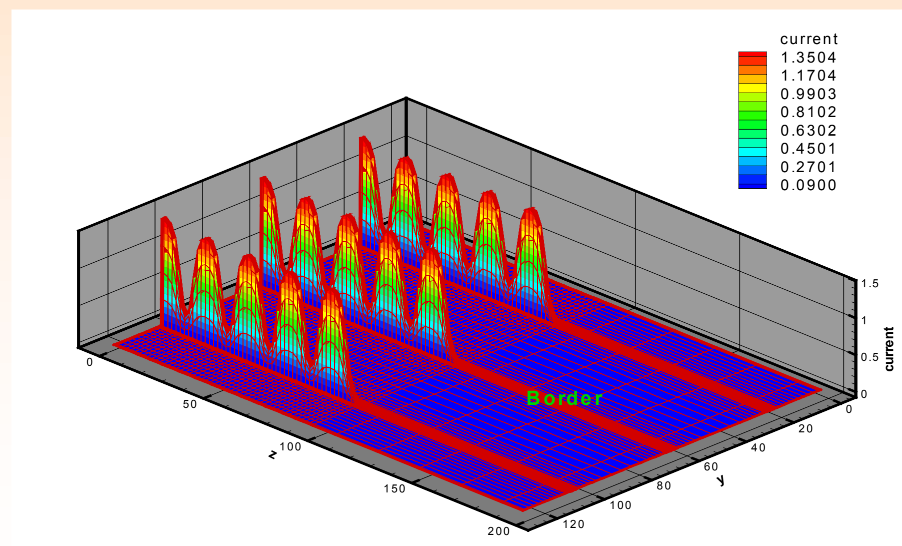


Current density distributions









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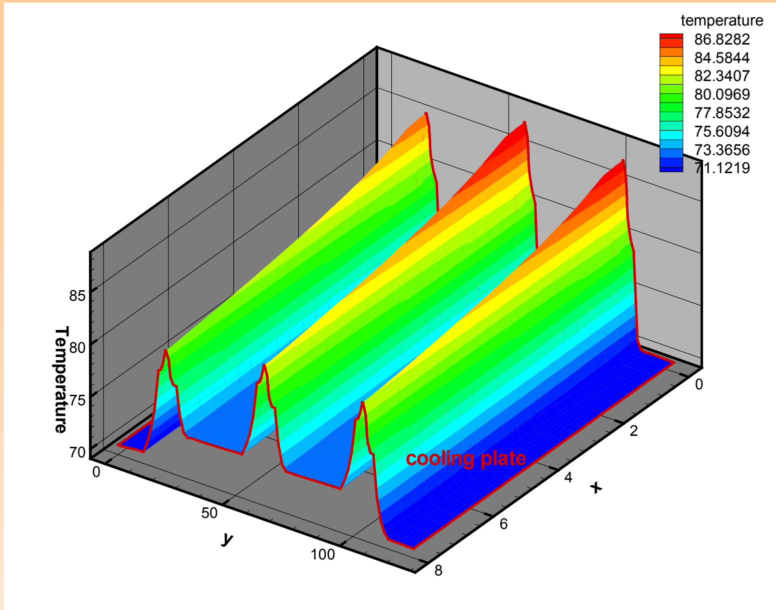
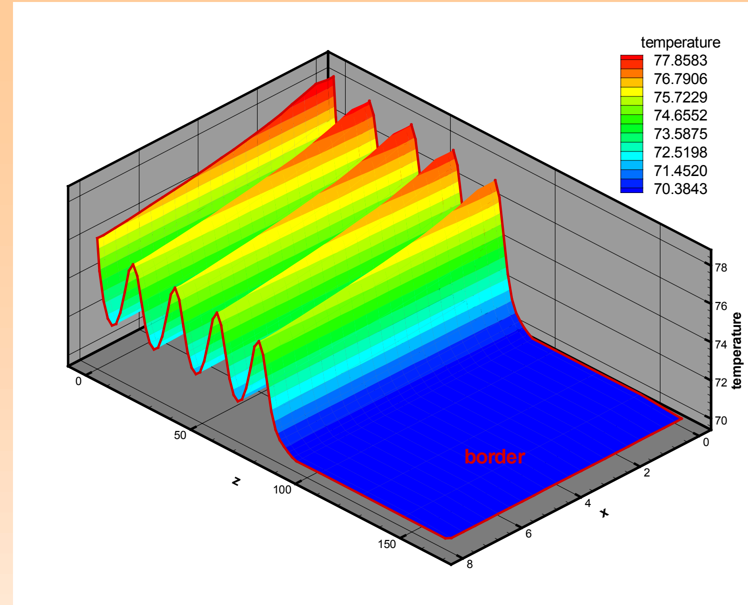
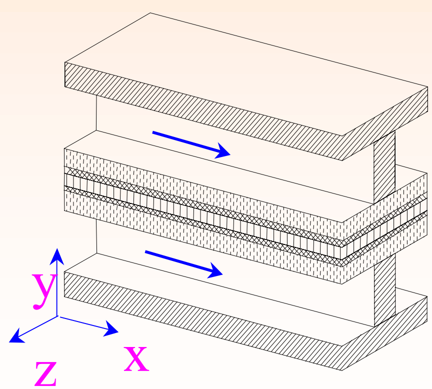
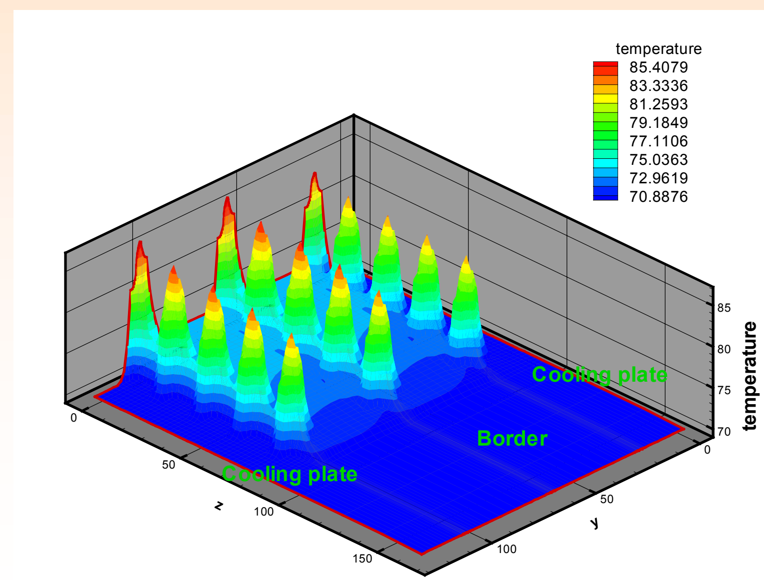
Temperature distributions









Summary and Highlights

- The unified approach is successfully used in the 3-D model and partially in the two-phase model.
- Developed a fully functional “prototype”
- The models has been tested against experimental results (ours, in literature, and FC industry)
- The models are independent, no need of any CFD package
- 7 journal papers published since 11/1998 (3 in FY02)
- 14 conference papers published/presented
- 2 journal and 3 conference papers accepted/submitted

Major Publications

- ***AIChE Journal***, pp. 2410 – 2422, Vol. 44, Nov. 1998.
- ***Journal of Applied Electrochemistry***, pp. 1409 – 1416, Vol. **29**, Dec. 1999.
- ***Journal of The Electrochemical Society***, Vol. 147 (7), pp. 2468 – 2477, 2000.
- ***Int. J. Hydrogen Energy***, Vol. 26, pp. 991-999, 2001.
- ***Int. J. Transportation Phenomena***, Vol. 3, pp. 177 – 198, 2001.
- ***Int. J. Heat Mass Transfer***, Vol. 45, pp. 2277 –2287, 2002.

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Future Plans

- Further development of the 3-D single-phase model: improve on reformate, different flow fields.
- Develop a 3-D two-phase model.
- Improve the a stack model.
- Couple the stack model with a system model.
- Extend the models to other type of fuel cells.
- Further interactions with industry and national labs.