Modeling and Simulations of Multiphysics Phenomena and Performance in Proton Exchange Membrane Fuel Cells

2019 | MVKF25 Hydrogen, Batteries and Fuel Cells
Outline

(1) Modeling of PEMFCs
(2) Examples
Modeling of PEMFCs

- Numerical methods at three levels?

1. **Macroscale**
   Based on the continuum assumption: FVM, FEM etc.

2. **Mesoscale**
   Lattice-Boltzmann method (LBM)

3. **Microscale**
   Molecular dynamics simulation (MDS)
Modeling of PEMFCs

- Macroscale modeling approaches

- In-house codes
- Commercial softwares
  - ANSYS-FLUENT
  - COMSOL Multiphysics
  - OPEN FOAM (open source code)
  - ...
Modeling of PEMFCs

❖ What is ANSYS Fluent?

ANSYS Fluent is a commercial software for modeling fluid flow and several other related physical phenomena.

❖ ANSYS Fluent applications

Aerodynamics, heat transfer, combustion, reacting flows, mixtures of liquids/solids/gas, particle dispersions, hydrodynamics, and much more.
Modeling of PEMFCs

- Numerical simulation procedure

1. Define goals
2. Identify domain
3. Geometry
4. Mesh
5. Physics
6. Solver Settings
7. Compute solution
8. Examine results
9. Update Model
Modeling of PEMFCs

❖ How to model PEMFCs in Fluent

❖ Add-on modules
❖ Models developed using UDFs
  • General CFD code
  • Additional submodels

General CFD code:
Mass conservation equation
Momentum conservation equation
Species conservation equation
Energy conservation equation

Additional submodels:
Charge conservation equation
Liquid water transport equation
Dissolved water transport equation
Modeling of PEMFCs

- ANSYS Fluent fuel cell add-on module
Introduction

- How do PEM fuel cells work?

**Fuel Cell Stack**

**Overall**: \( H_2 + \frac{1}{2} O_2 \rightarrow H_2O \)

**Anode**: \( H_2 \rightarrow 2H^+ + 2e^- \)

**Cathode**: \( \frac{1}{2} O_2 + 2H^+ + 2e^- \rightarrow H_2O \)

http://www.intelligent-energy.com/technology/technology-faq/ (Animation)
Introduction

❖ Why do we need PEM fuel cells?
  • Fuel efficient energy conversion
  • High power density
  • Environmental friendliness

❖ PEM fuel cell applications
Introduction

- PEM fuel cell components?

Mathematical Model

❖ Governing equations

- **Mass conservation equation**
  \[ \nabla \cdot (\rho \vec{u}) = S_{mass} \]

- **Momentum conservation equation**
  \[ \nabla \cdot (\rho \vec{u} \vec{u}) = \nabla \cdot (\mu \nabla \vec{u}) - \nabla P + S_{mom} \]

- **Species conservation equation**
  \[ \nabla \cdot (\rho \vec{u} Y_i) = \nabla \cdot (\rho D_{eff,i} \nabla Y_i) + S_i \]

- **Energy conservation equation**
  \[ \nabla \cdot (\rho c_p \vec{u} T) = \nabla \cdot (k_{eff} \nabla T) + S_T \]

- **Charge conservation equation**
  \[ \nabla \cdot (\sigma_{eff,s} \nabla \phi_s) + S_s = 0 \]
  \[ \nabla \cdot (\sigma_{eff,m} \nabla \phi_m) + S_m = 0 \]
Mathematical Model

❖ Governing equations

• Liquid water transport equation
  \[ \nabla \cdot \left( \rho_l \frac{K_{rl} \mu_g}{K_{rg} \mu_l} \vec{u} \right) = \nabla \cdot (\rho_l D_s \nabla s) + S_l \]

• Dissolved water transport equation
  \[ -\nabla \cdot \left( \frac{n_d}{F} \sigma_m \nabla \phi_m \right) = \nabla \cdot \left( \rho_m \frac{D_\lambda}{M_m} \nabla \lambda \right) + S_\lambda \]
Results - Case 1

Geometry description
Results – Case 1

- Cell performance

![Graph showing cell performance compared to straight and wavy channels. The graph plots cell voltage (V) and power density (W/m²) against current density (A/m²).]
Results - Case 1

❖ Pressure
Results - Case 1

- Oxygen mass fraction

![Graph showing oxygen mass fraction over length (m)]
Results - Case 1

- Liquid water saturation

![Graph showing liquid water saturation for different channel types and lengths.](image-url)
Results - Case 1

- Local current density

![Graph showing current density vs length for straight and wavy channels]
Results - Case 2

Results - Case 2

- Local thickness and porosity
Results - Case 2

- Cell performance

![Graph showing cell performance with different assembly forces and current densities]
Results - Case 2

- Oxygen concentration
Results - Case 2

- Temperature distribution
Results - Case 2

- Liquid water saturation
Results - Case 2

- Local current density
Results - Case 3

- Schematic of the HT-PEMFCs
Results - Case 3

❖ Cell performance

![Graph showing cell performance for Case A and Case B vs. current density and power density.](image-url)
Results - Case 3

- Temperature distribution

Case A

Case B
Results - Case 3

- Oxygen mass fraction

![Graph showing oxygen mass fraction over X (m) for Case A Line-1, Case A Line-2, Case B Line-1, and Case B Line-2.]
Results - Case 3

- Local current density

![Graph showing current density vs. X (m) for different cases: Case A Line-1, Case A Line-2, Case B Line-1, Case B Line-2.](image)
Results - Case 4

- Geometry description
Results - Case 4

- Cell performance

![Graph showing cell voltage and power density vs. current density for Cases A, B, and C.](image-url)
Results - Case 4

- Oxygen mass fraction
Results - Case 4

- Temperature distribution

![Temperature distribution graphs](image)
Results - Case 4

- Local current density
Summary

- The PEM fuel cell working

**Overall:** \( H_2 + \frac{1}{2} O_2 \rightarrow H_2O \)

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