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

2020 | MVKF25 Hydrogen, Batteries and Fuel Cells
See also Chapter 10 in course book
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

Problem Identification

3. Geometry
4. Mesh
5. Physics
6. Solver Settings

Pre-Processing

7. Compute solution

Solve

8. Examine results

Post Processing

9. Update Model

[Diagram showing a flowchart with steps 1 to 9 and a color gradient graph]
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?

**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

\[ \nabla \cdot \left( \rho_l \frac{K_{rl} \mu_g}{K_{rg} \mu_l} \bar{u} \right) = \nabla \cdot (\rho_l D_s \nabla S) + S_l \]

- Dissolved water transport equation

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

- Geometry description
Results – Case 1

❖ Cell performance

![Graph showing cell performance comparison between straight and wavy channels](image)
Results - Case 1

❖ Pressure

![Graph comparing pressure in straight and wavy channels](image-url)
Results - Case 1

❖ Oxygen mass fraction

![Graph showing oxygen mass fraction against length for different channel types and lines.](image)
Results - Case 1

- Liquid water saturation

![Graph showing liquid water saturation for straight and wavy channels.](image-url)
Results - Case 1

❖ Local current density

![Graph of current density vs. length for straight and wavy channels.](image-url)
Results - Case 2


- Current collector
- Catalyst layer
- Gas diffusion layer
- Membrane

(a)  
- Anode
- Cathode

(b)  
- Channel region
- Rib region
- Channel region
- Line-1
Results - Case 2

❖ Local thickness and porosity

(a)

(b)
Results - Case 2

❖ Cell performance

- Cell voltage (V)
- Power density (W/cm²)
- Current density (A/cm²)

Graph showing performance with different assembly forces and without compression.
Results - Case 2

- Oxygen concentration

![Diagram showing oxygen concentration levels across different cases](image-url)
Results - Case 2

❖ Temperature distribution

(a) Temperature distribution

(b) Temperature distribution

(c) Temperature distribution

(d) 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 against 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 vs X (m) for Case A and Case B with Line-1 and Line-2 comparisons.]
Results - Case 3

❖ Local current density
Results - Case 4

❖ Geometry description
Results - Case 4

❖ Cell performance

![Graph showing cell performance for Case A, Case B, and Case C](image)
Results - Case 4

❖ Oxygen mass fraction
Results - Case 4

❖ Temperature distribution
Results - Case 4

❖ Local current density
The PEM fuel cell working:

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

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

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

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