An Overview of Fuel Cells

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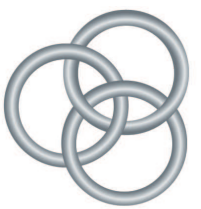

Outline

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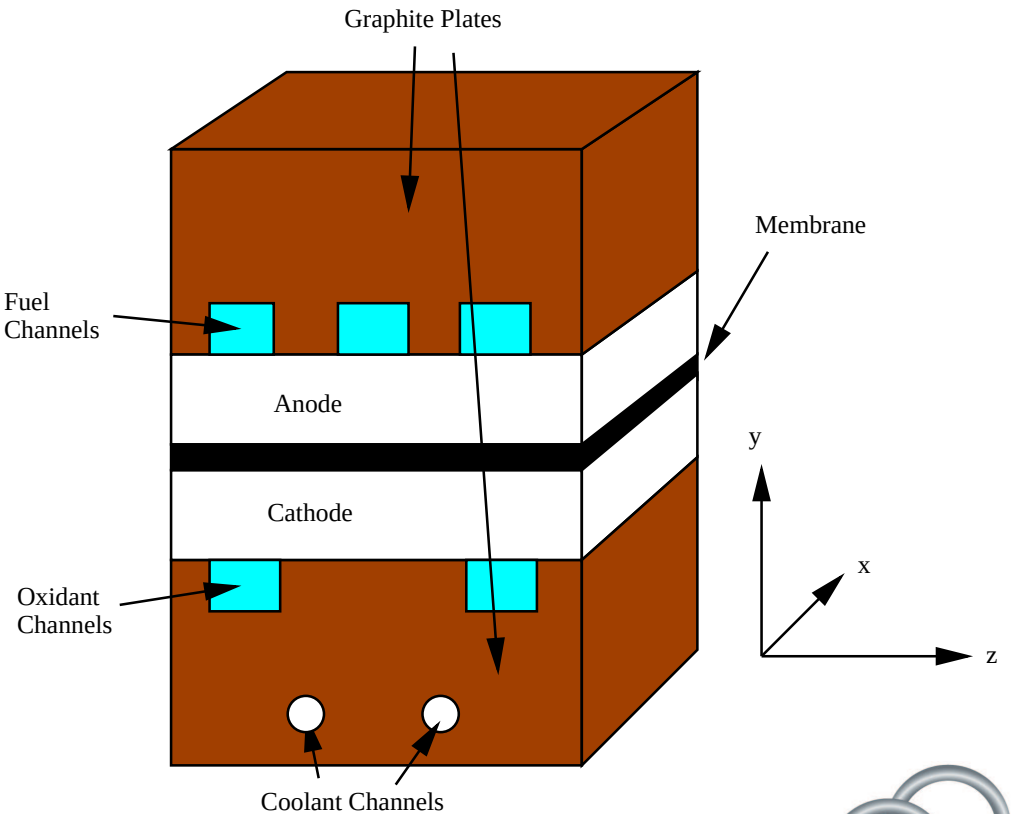
Introduction to PEM Fuel Cells

Unit Cells

- Membrane Electrode Assembly (MEA):
  1. Electrodes
  2. Catalyst Layers
  3. Membrane
- Plates, Gas Channels, Coolant
- Large Aspect Ratio



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Introduction to PEM Fuel Cells

Electrochemical Reactions

Main reactions under normal conditions:

- Hydrogen oxidation at the anode (Platinum catalyst):

$$H_2 \rightarrow 2p^+ + 2e^-$$

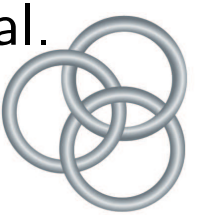
  occurs at low electrochemical potential.
- Oxygen reduction at the cathode (Platinum):

$$O_2 + 4e^- + 4p^+ \rightarrow 2H_2O$$

  occurs at high electrochemical potential.

Some additional reactions that can occur that lead to degradation:

- Carbon oxidation of catalyst support, occurs at high potential.
- Intermediate product of hydrogen peroxide that destroys the membrane material, occurs at intermediate potential.
- Platinum agglomeration.



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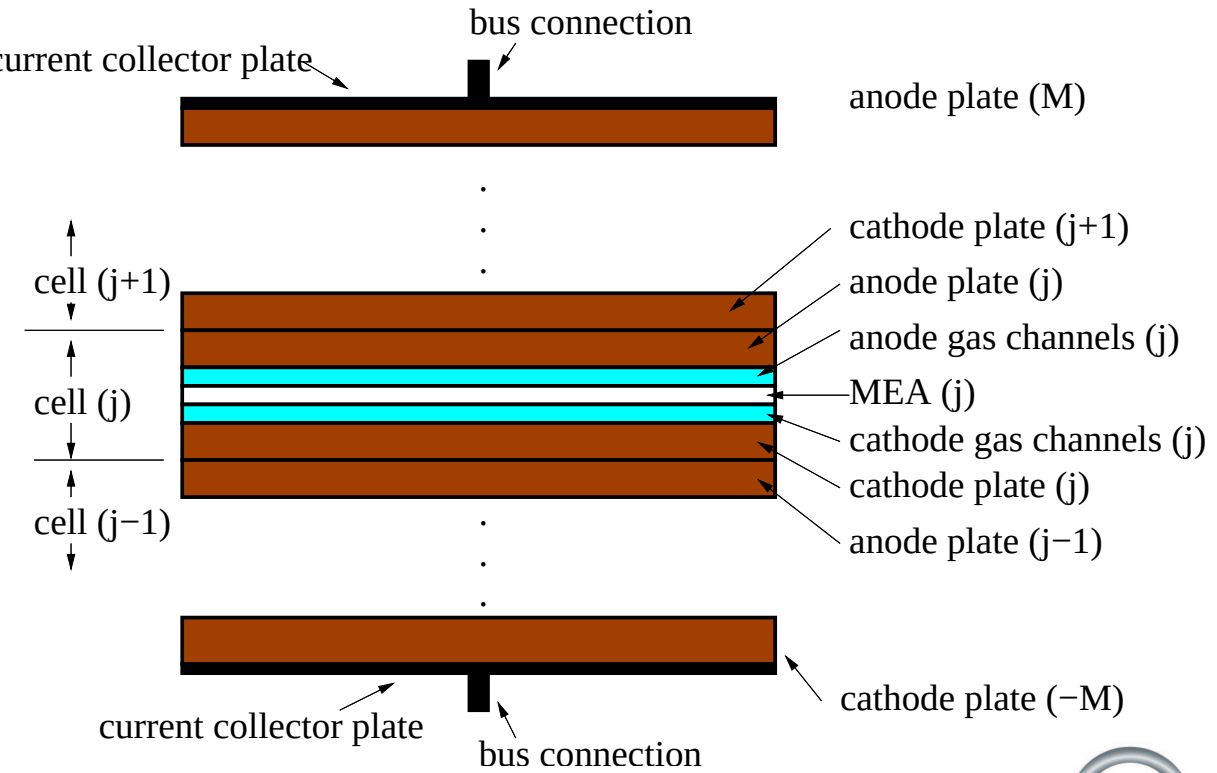
Introduction to PEM Fuel Cells

Fuel Cell Stacks

- Bipolar Plates
- Same Total Current Through Each Cell
- Electrical Coupling
- Thermal Coupling
- End Cell Effects



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Introduction to PEM Fuel Cells

The Bigger Picture

There are other kinds of fuel cells:

- Direct Methanol
- Solid Oxide
- Molton Carbonate

There are external systems:

- Fuel Production
- Fuel Storage
- Reformers
- Humidifiers
- Oxygen Enrichment
- Compressors
- Power Conditioning
- System Control

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Fuel Cell Community Goals

- Increase performance
- Decrease cost
- Make components more durable
- Make the devices safer

- Improve components
- Improve systems

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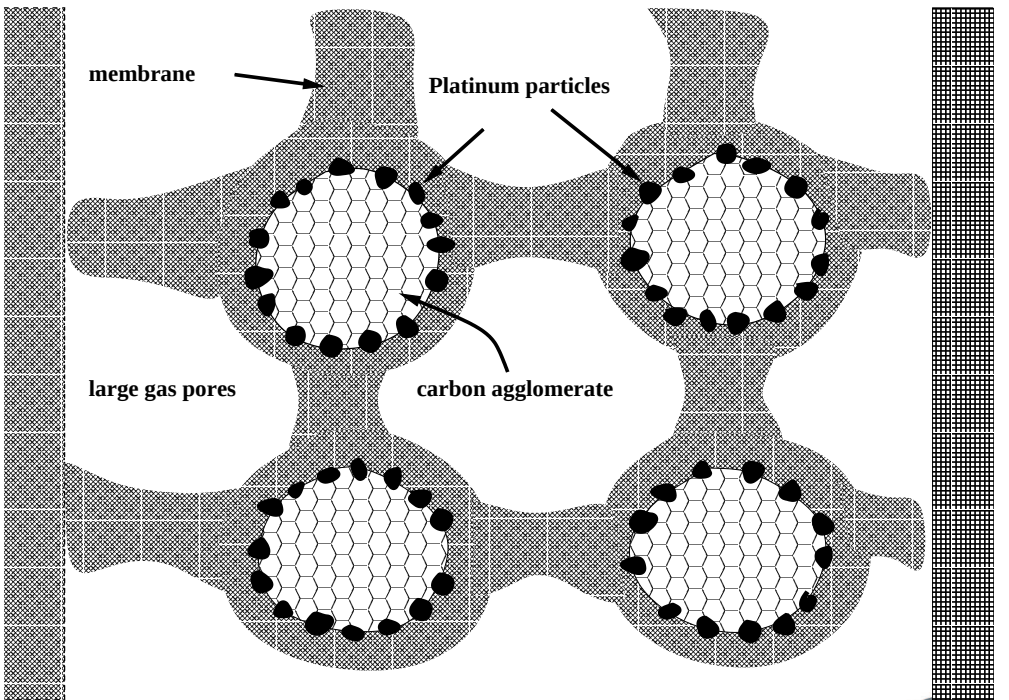
Component Modelling

Example: Catalyst layer

- Composite Material: Pores, carbon particles, Pt particles, and ionomer.
- On either side: electrode (microlayer) and membrane
- Issues: multi-phase transport, water removal, "sluggish" oxygen reduction reaction, Pt cost.



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Component Modelling

Example: Catalyst layer, cont.

Modelling goals:

- Optimization of structure (performance, Pt usage)
- Identification of limiting behaviour
- Effect of contaminants
- Degradation mechanisms

Major Difficulty in Modelling: materials used in fuel cells are changing rapidly.

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System Modelling

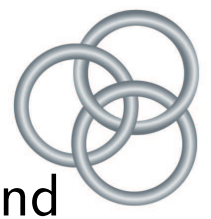
Example: Stack Modelling

Multiscale problem, but there is scale separation

Unit Cell Models:

- Couple channel transport, MEA transport, electrochemistry, temperature.
- Understanding "water management" is a key goal.
- Liquid water transport in the electrodes and channels is the least well understood.
- 3D models - often based on commercial CFD codes.
- Reduced dimensional models:
  1. Cross plane transport decouples from channel transport (3D $\rightarrow$ 2+1D).
  2. Averaging over cross-channel transport (2+1D $\rightarrow$ 1+1D).

Stack Models combine multiple unit cell models with electrical and thermal interactions.



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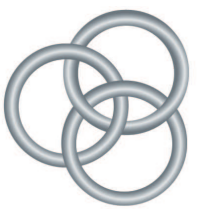
System Modelling

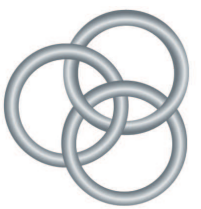
Uses of Modelling

- System optimization
- Identification of system limiting components
- Virtual testing of new components in system environment
- Identification of component tolerances
- Insight into the closed system
- Tool for experimental design



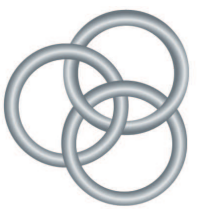
Scientific Questions

- Two phase flow:
  1. Mechanisms of liquid water flow in channels (droplets).
  2. Mechanisms of liquid water flow in electrodes.
- Catalyst layer microstructure and its relation to performance.
- Structure and property changes of membrane due to hydration.
- Degradation mechanisms.
- Development of new materials.



Mathematical Fields

1. Homogenization (microstructure to macroscopic behaviour)
2. Free boundary problems (liquid water fronts)
3. PDE modelling
4. Numerical Analysis



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