Multiphysics Model of an Electrochemical Hydrogen Compressor

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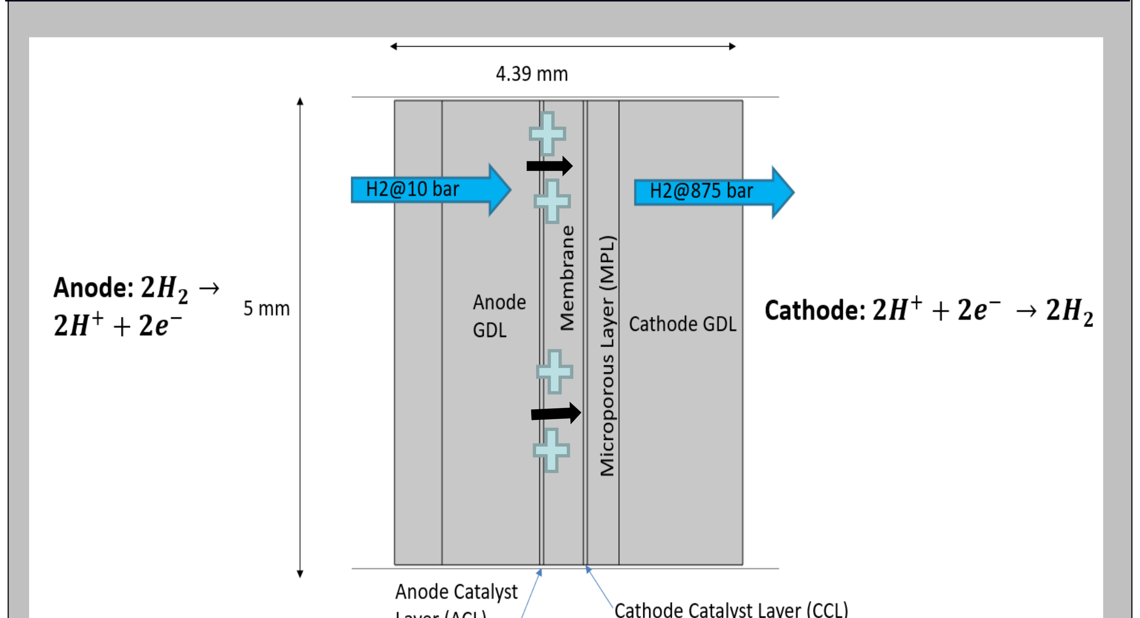
ABSTRACT

The electrochemical hydrogen compressor (EHC) is a technology that has the potential to play an important role in the hydrogen economy. The EHC utilizes a proton exchange membrane (PEM) and electrical power to pressurize hydrogen, which can then be used for applications such as fuel cells. It has several advantages over traditional mechanical compressors: lower costs, higher efficiency, and purer produced hydrogen. Performance of the EHC is dictated by complex interactions between water management, multiphase transport, and material properties of cell layers. The EHC has been studied experimentally, but there is a need for a sophisticated mathematical model that can be used to examine cell performance in higher detail in order to make suggestions for optimal design. The model is two-dimensional and steady-state. We use the model to analyze the role of water management in the membrane-electrode assembly (MEA) and the role of the catalyst layer and membrane in cell performance. Water is the critical factor for determining protonic conductivity in the MEA, and plays a role in kinetics of the catalyst layer. The use of multiple catalyst layers with varying compositions is explored, along with various membrane properties.

RESEARCH QUESTION

How can EHC performance and design be improved based on insights from the computational model?

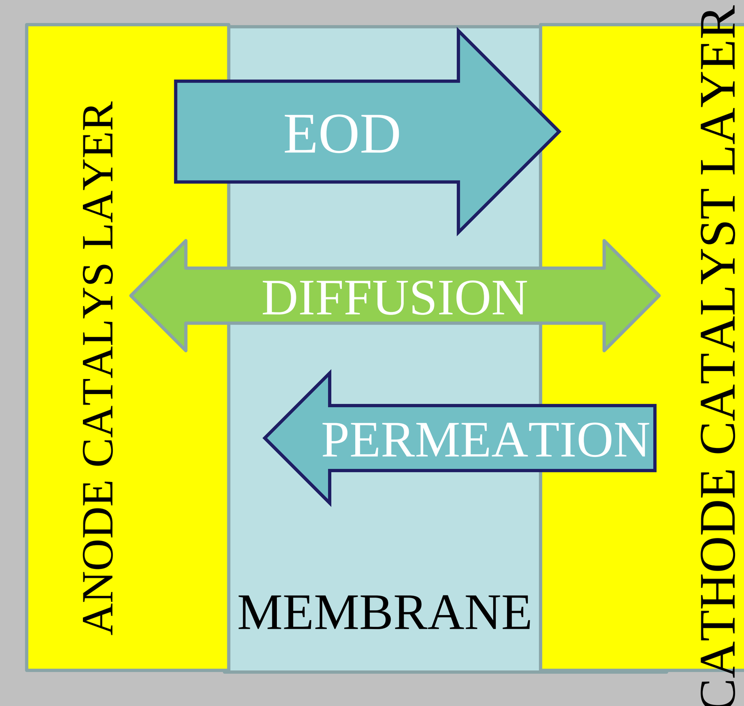
Operating Principles



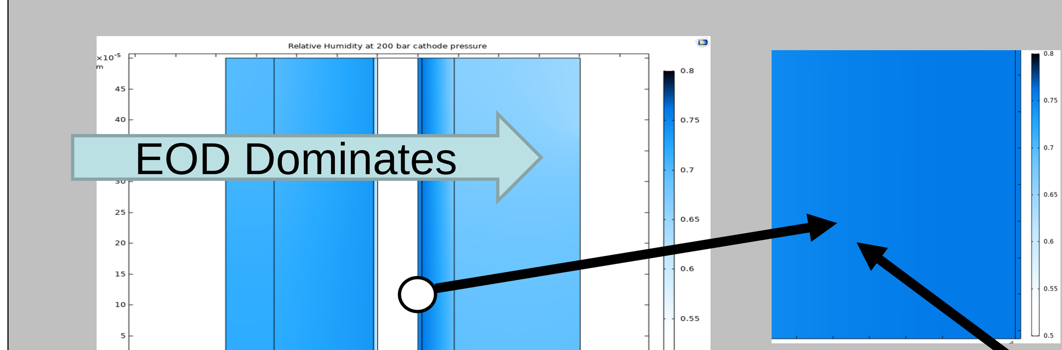
- Humidified hydrogen gas enters anode and moves through gas diffusion layer (GDL) toward anode catalyst layer (ACL)
- Reaction in ACL splits H2 into 2 electrons and 2 protons
- Protons cross membrane to cathode side due to potential difference applied to cell, converting electrical power into compression work
- Protons recombine with electrons in cathode catalyst layer (CCL) to reform H2
- Pressurized H2 exits cathode side

Water Management

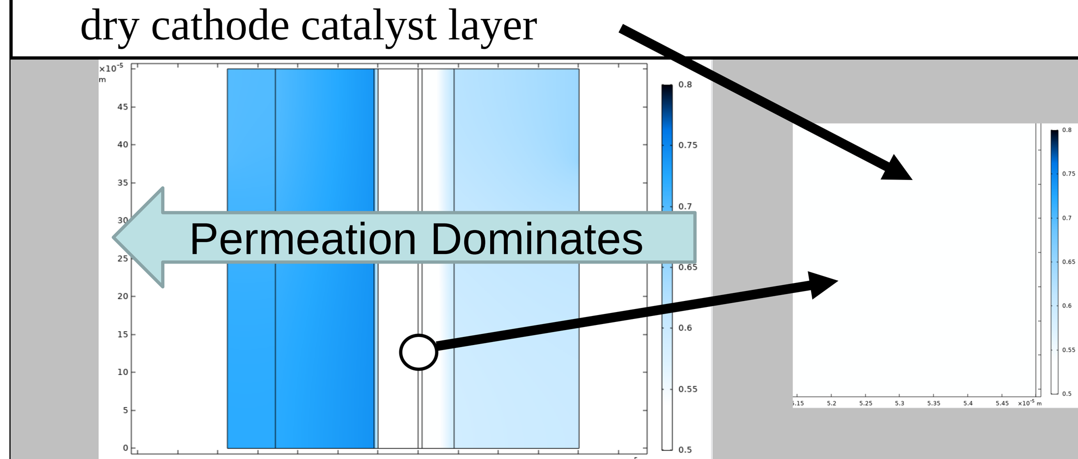
- Water management in membrane-electrode-assembly (MEA) is a balance between forces:



- Electroosmotic drag (EOD) is a phenomena in which protons drag water molecules across membrane
- Water is driven from cathode to anode by pressure differential
- Water diffuses from catalyst layer into and out of membrane driven by chemical potential gradients



- Top: Relative humidity at 200 bar cathode pressure – wet cathode catalyst layer
- Bottom: Relative humidity at 875 bar cathode pressure – dry cathode catalyst layer

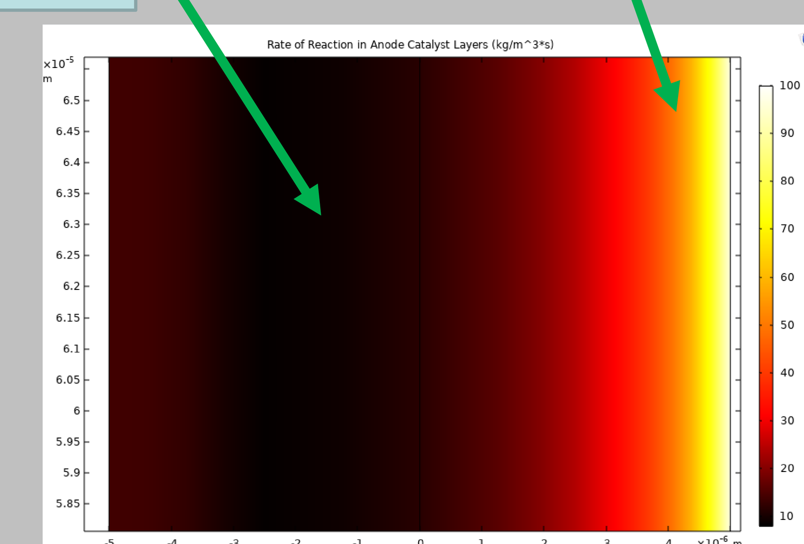


Effect of Multiple Anode Catalyst Layers

1 Catalyst Layer, 10 micron thickness

- Baseline values:
- 40% porosity
- 18% ionomer

Reaction concentrated at membrane interface

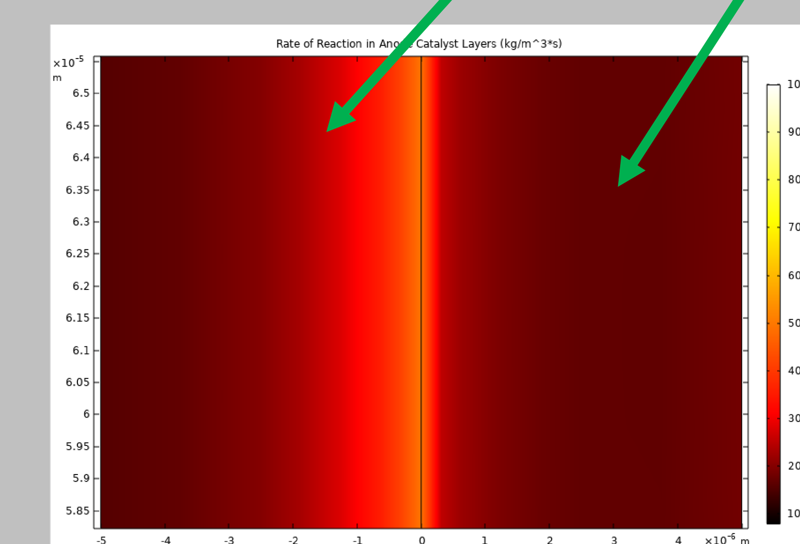


2 Catalyst Layers, 5 micron thickness each

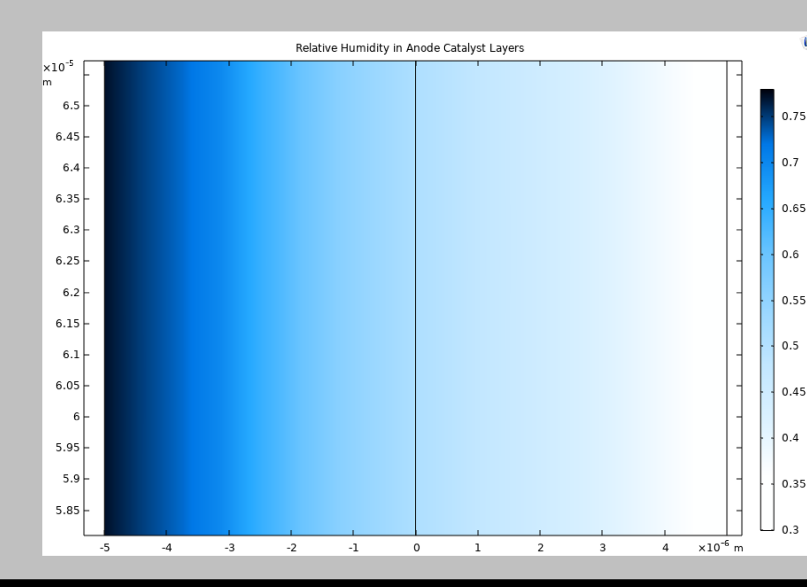
Reaction distributed more evenly in both catalyst layers

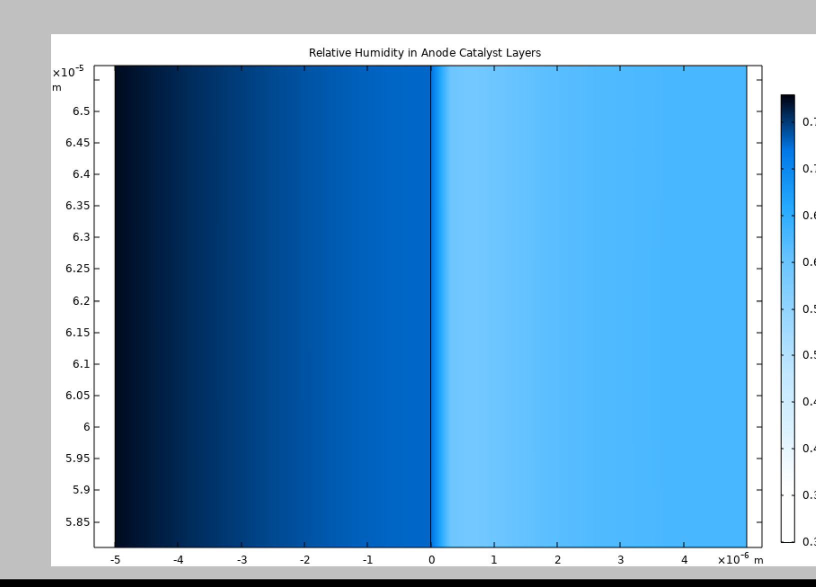
1
- High porosity
- Low conductivity

2
- Low porosity
- High conductivity



- Top: Reaction Rate [kg/m^3*s]
- Bottom: Relative Humidity

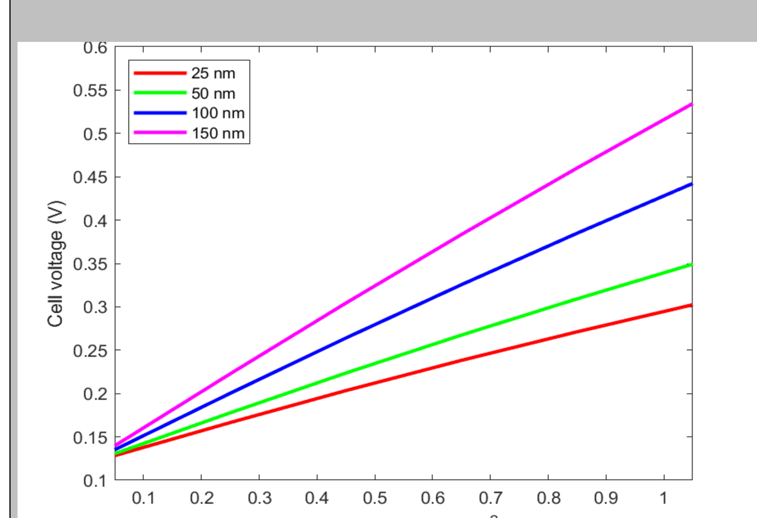




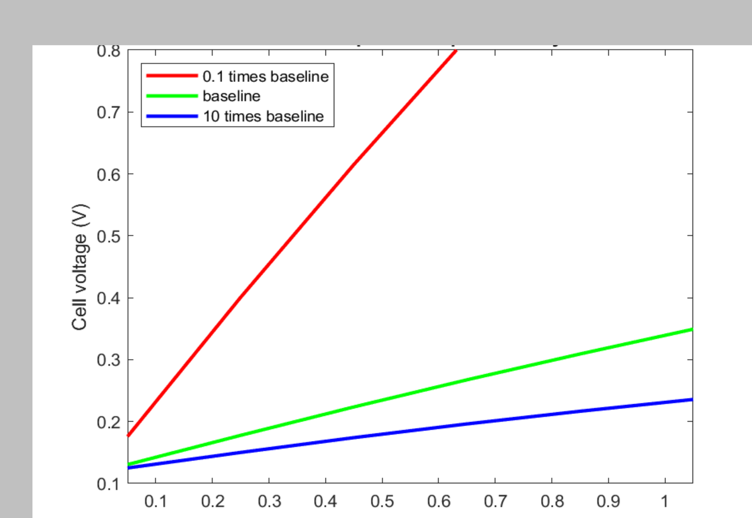
How does having two anode CLs improve performance?

- First CL has high reactant saturation → easier reaction, second has high conductivity → easier reaction → even reaction rate
- Even reaction rate → **lower ohmic losses and even water distribution**
- With one CL, reaction occurs as close as possible to membrane to reduce ohmic losses → much of catalyst layer is underutilized

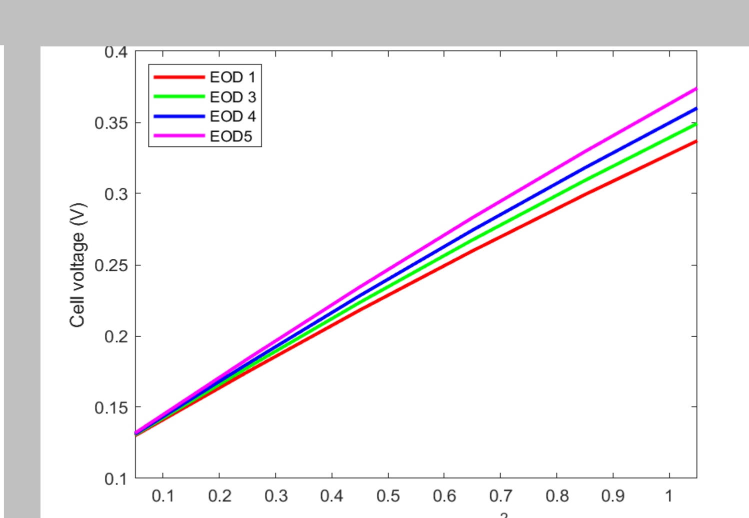
Effect of Membrane Properties



Effect of varying membrane thickness → **thinner is better**



Effect of varying membrane conductivity → **higher conductivity is better**



Effect of varying membrane EOD coefficient → **lower EOD coefficient is better**

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