

# Multiphysics Model of an Electrochemical Hydrogen Compressor

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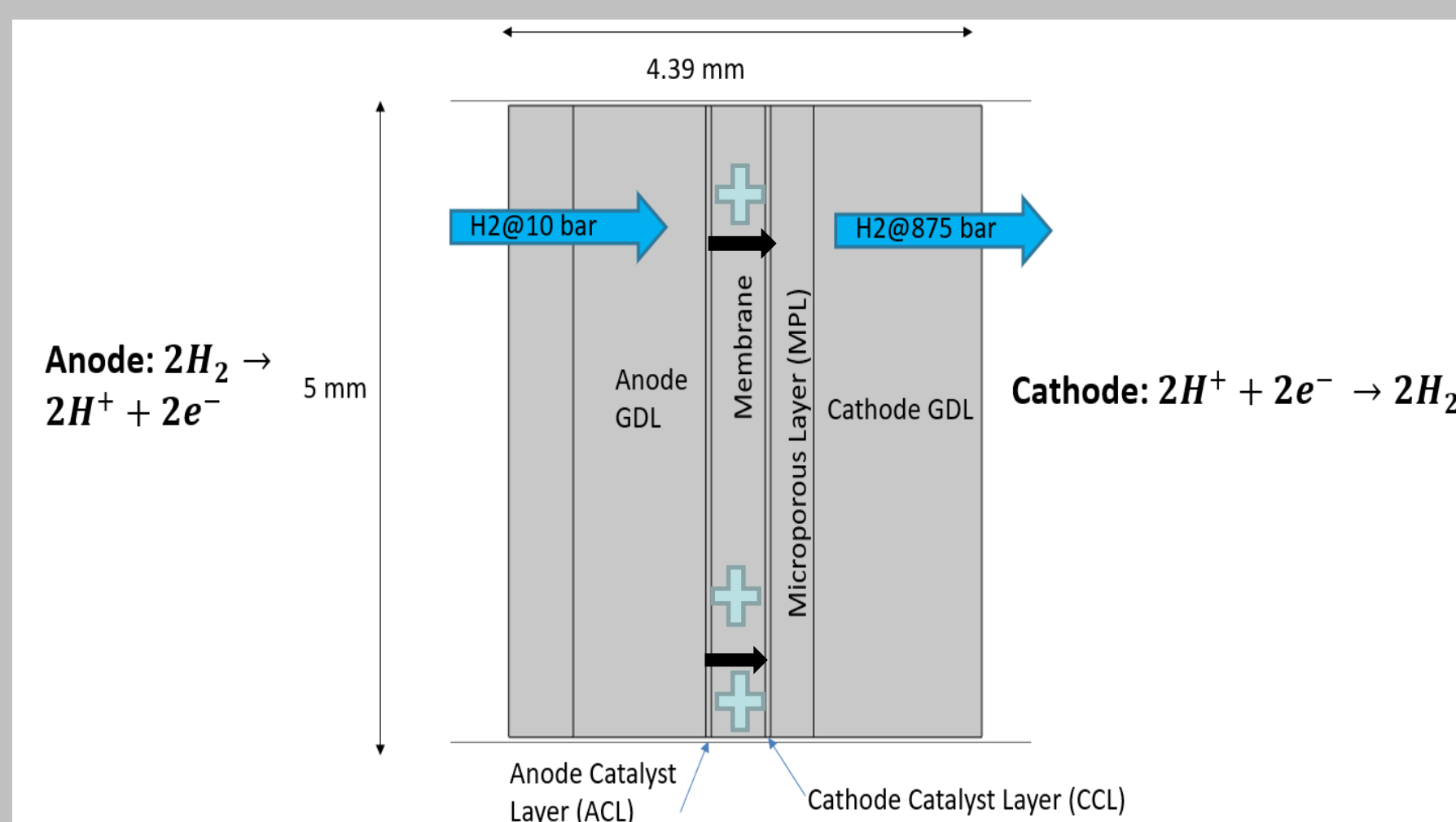
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## Abstract

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.

## Introduction

- The EHC has the potential to beat traditional mechanical compressors in terms of efficiency, purity, and maximum compression pressure
- How does the EHC work?**



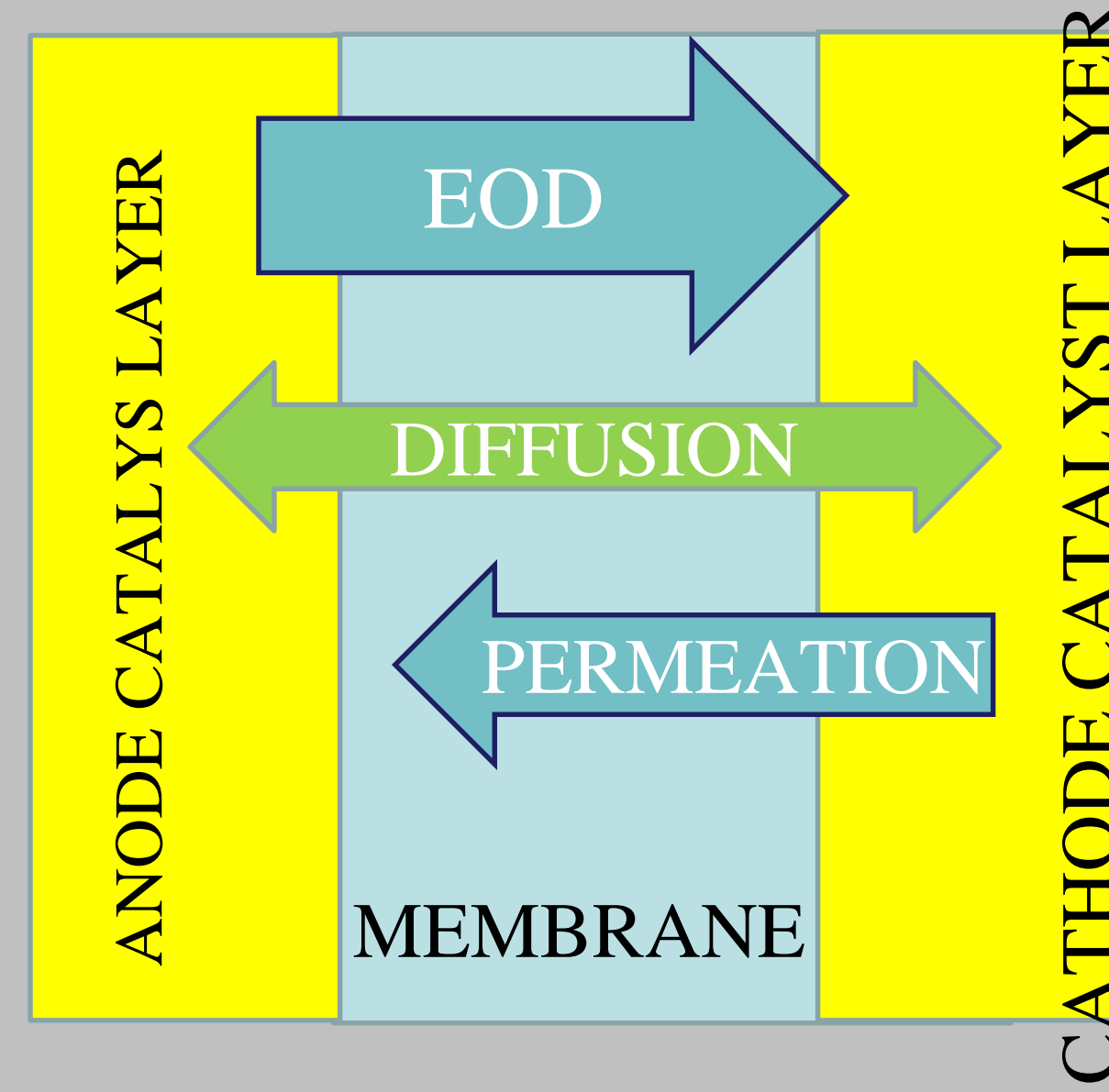
### EHC Operating Principles

- Humidified hydrogen gas is split into electrons and protons on anode side
- Protons cross membrane to cathode side due to applied potential, converting electrical power into compression work
- Protons recombine with electrons in cathode catalyst layer (CCL) to reform H2
- Pressurized H2 exits cathode side

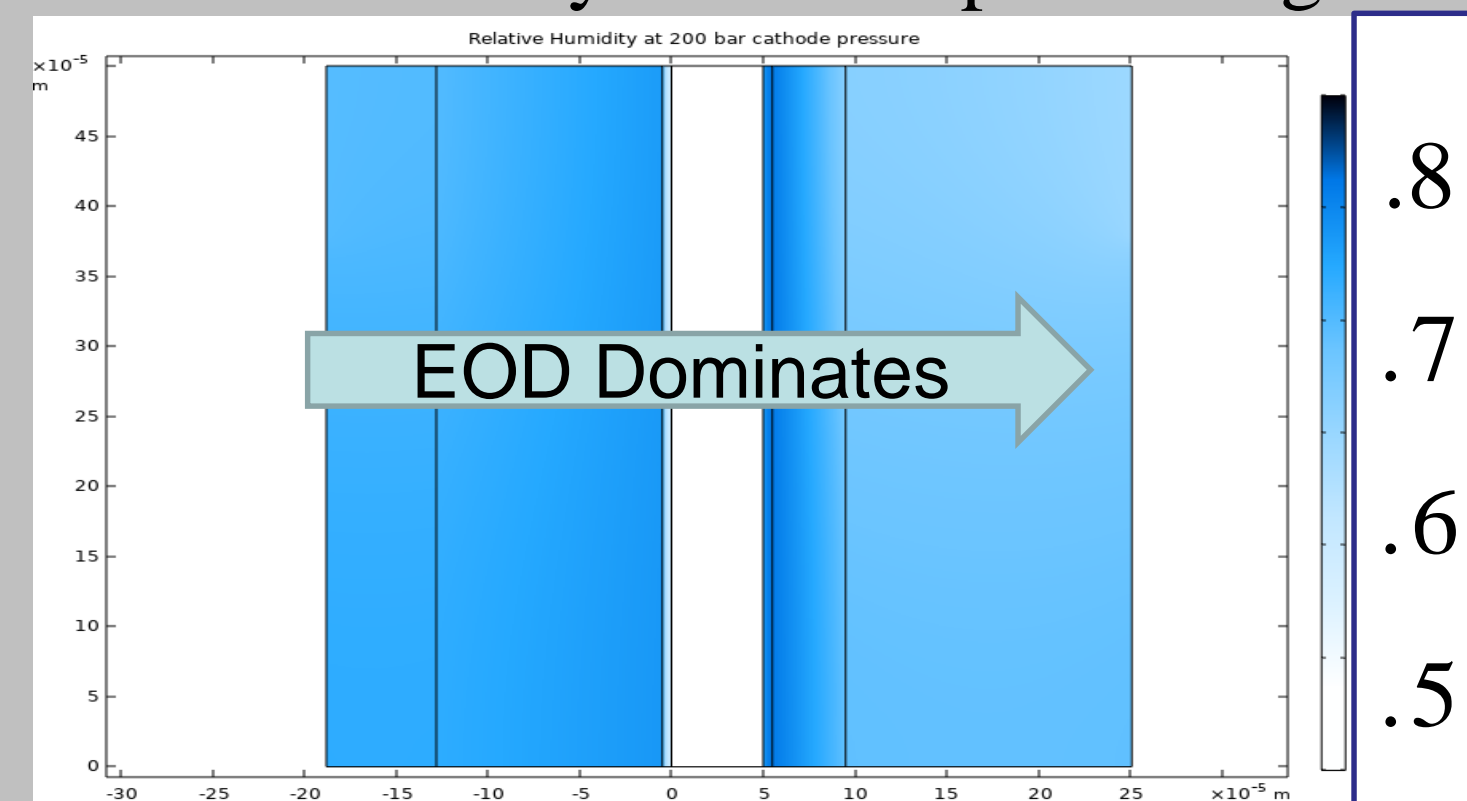
How can EHC performance and design be improved based on insights from the computational model?

## Water Management

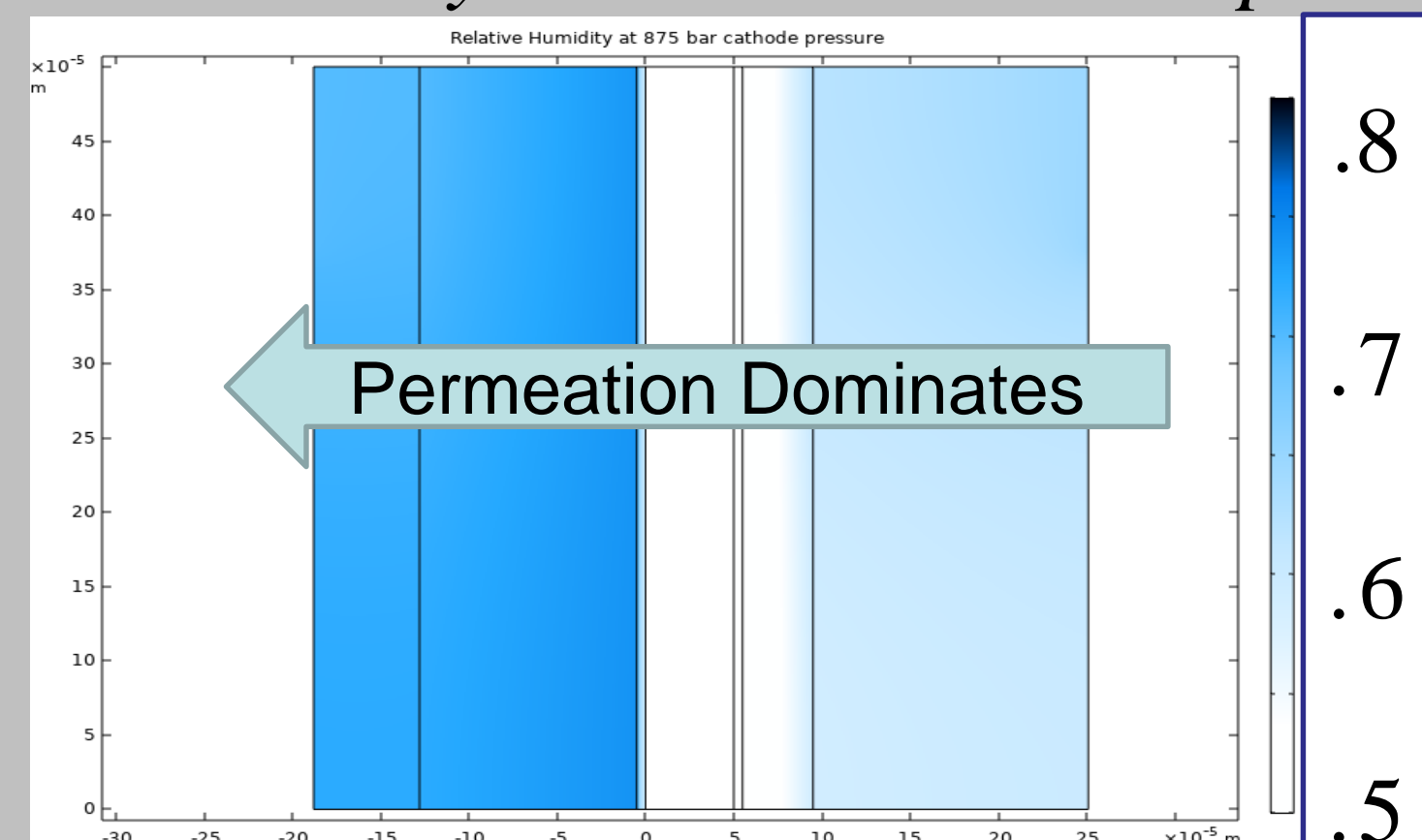
- Water management in membrane-electrode-assembly (MEA) is a balance between forces:



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



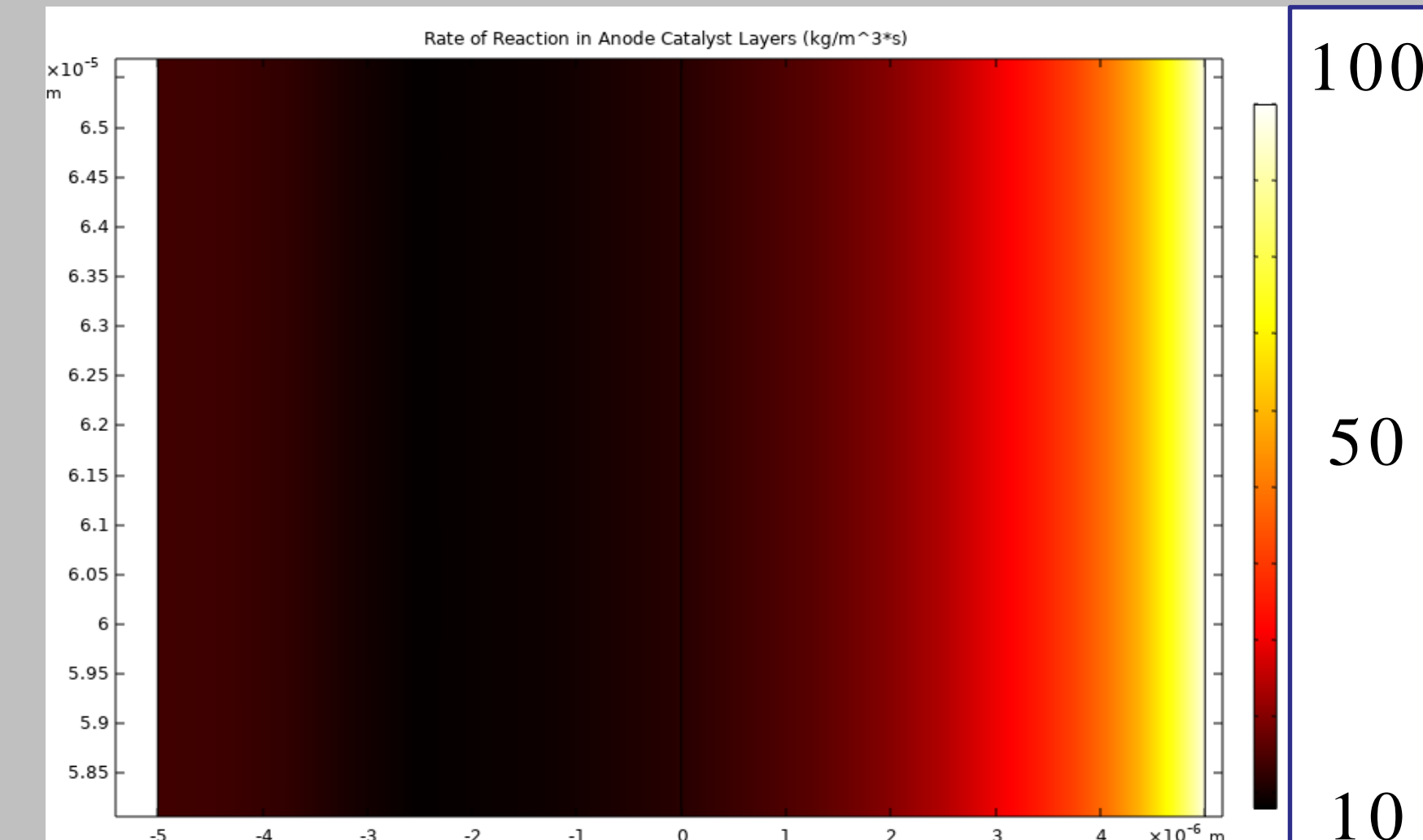
Relative humidity at 200 bar cathode pressure



Relative humidity at 875 bar cathode pressure

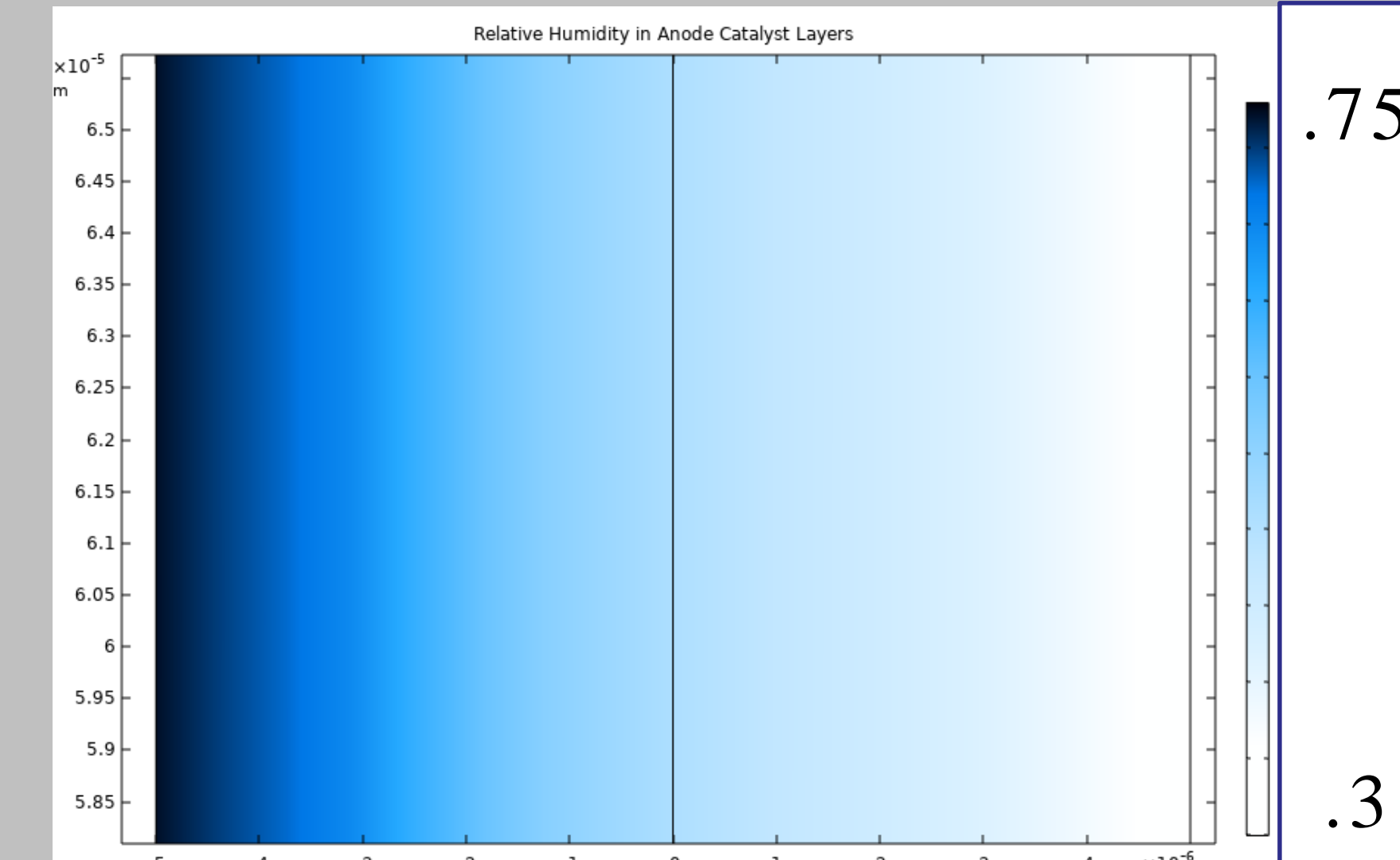
## Effect of Multiple Anode Catalyst Layers

### 1 Catalyst Layer, 10 micron thickness



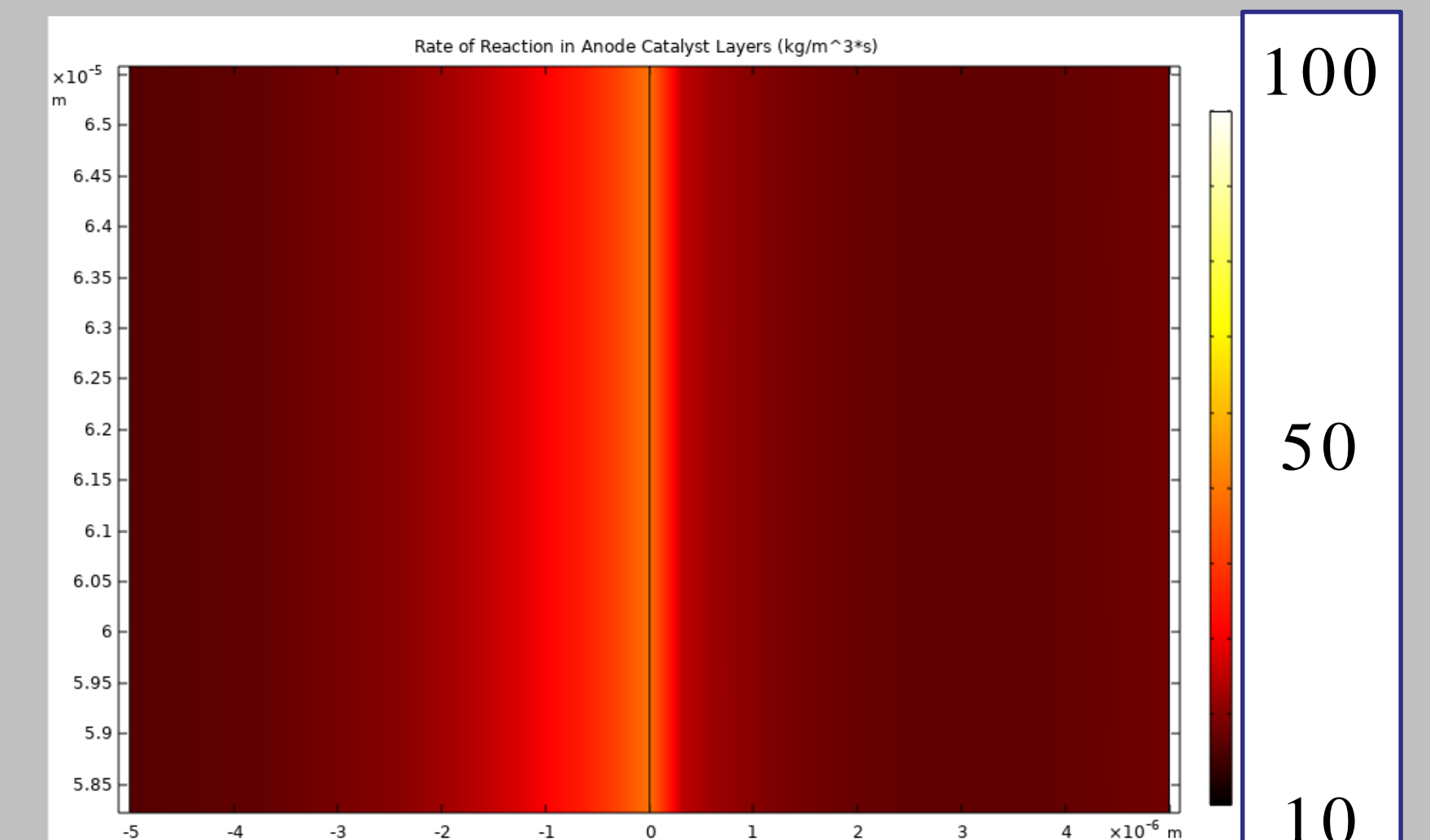
Reaction rate ( $\text{kg/m}^3\text{s}$ ) in anode catalyst layer with 40% porosity, 18% ionomer

Reaction rate **concentrated at membrane interface** and **water unevenly distributed**



Relative humidity in MEA with single CL

### 2 Catalyst Layers, 5 micron thickness each



Reaction rate ( $\text{kg/m}^3\text{s}$ ). Left-hand CL: high porosity, low ionic conductivity. Right hand CL: low porosity, high ionic conductivity

Reaction rate and water **distributed more evenly** in both catalyst layers



Relative humidity in MEA with two CLs

How does having two anode CLs improve performance?

- First CL has high reactant saturation → 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

## Mathematical Model

- Computer modeling gives us detailed information about cell conditions on a microscopic scale, and allows us to simulate experiments by varying cell properties and conditions

Transport in Porous Media	Membrane Transport
Darcy's Law: $u_i = \frac{k_{r,i} k_0}{\eta_i} \nabla p_i$	Two-phase transport: ( <i>Weber and Newman, 2004</i> ) $j_{rxn,m} = \nabla \cdot [(1 - S_m)(-k_{m,v}^{eff} \nabla \phi_m) - \frac{k_{m,v}^{eff} \epsilon_{m,v}^{eff}}{F} \nabla \mu_w] + S_m(-k_{m,l}^{eff} \nabla \phi_m - \frac{-k_{m,l}^{eff} \epsilon_{m,l}^{eff}}{F} \nabla \mu_w)$
Diffusion: $J_i = -\rho_g \omega_i \sum_k \tilde{D}_{ik} (\nabla x_k - \omega_k) \nabla p_g$	Reaction Kinetics Butler-Volmer equation: $i_{rxn} = A S_G i_0 \left[ \frac{c_o}{c_{ref}^o} \exp\left(\frac{\alpha_a F}{RT} \eta\right) - \frac{c_r}{c_{ref}^r} \exp\left(-\frac{\alpha_c F}{RT} \eta\right) \right]$

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**HyET Hydrogen**

