Encontro Nacional do Programa de Formação de Recursos Humanos da ANP – 2026

Otimização orientada por simulação numérica de eletrolisadores PEM para produção de H2 verde a altas densidades de corrente e elevadas pressões

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Tipo de bolsa: Doutorado

Universidade Federal de Santa Catarina (UFSC)

Gestão:

Introdução

Contexto

- Transição energética -> renováveis em crescimento.
- Fósseis ainda por anos, mas eólica/solar e carros elétricos são tendência.

Desafio

- Intermitência -> dificulta equilíbrio oferta x demanda na rede.

Hidrogênio Verde Como Solução

- Produzido por eletrólise da água (fontes renováveis).
- Armazena energia e gera eletricidade limpa em células combustíveis.

Outras aplicações

- Setor de transportes, indústria (fertilizantes, metalurgia) estações off-grid.

Desafio Atual

- Hidrogênio é leve, armazenamento exige alta pressão (700 bar em FCEVs).

Eletrolisadores PEM

- Vantagens: Compacto, resposta rápida, temperatura moderada, alta eficiência, alta pureza, alta densidade de corrente, alta pressão.
- Desvantagens: Durabilidade (corrosão) + alto custo.

OBJETIVOS

Objetivo Geral

- Desenvolver modelo CFD preditivo para escoamento em eletrolisadores PEM.
- Construir bancada experimental para operar a alta pressão (100 bar).
- Usar dados experimentais para validar o modelo.

O que já foi feito (2022–2025)

- Modelo iniciado em 2022 no software OpenFOAM.
- Artigo publicado em 2025 no *International Journal Of Hydrogen Energy*.
- Modelo contendo:
  - Reação de evolução do oxigênio (OER) no ânodo;
  - Escoamento multifásico na camada porosa;
  - Formação de grandes bolhas de oxigênio nos canais do ânodo.

O que está sendo feito (atualmente)

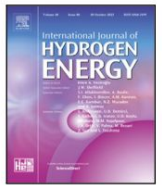
- Expansão do modelo CFD para:
  - Lado do cátodo.
  - Crossover de gás.
  - Equação da energia.
  - Modelos de compressibilidade.
- Bancada experimental: fase de projeto e orçamento.

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journal homepage: www.elsevier.com/locate/he

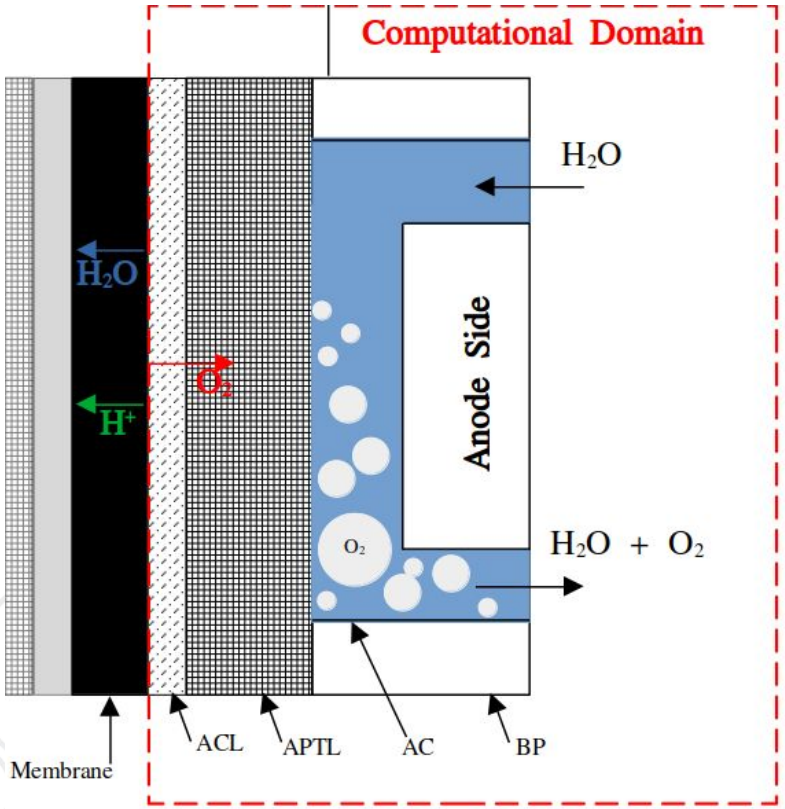


Hybrid multi-scale multiphase flow modeling of proton exchange membrane electrolyzers for green hydrogen production

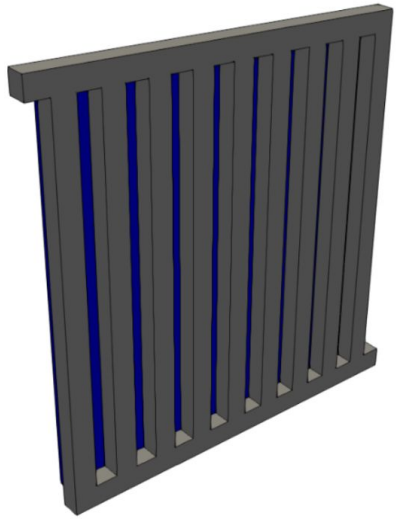
Vittorio Nardin *, Emilio E. Paladino

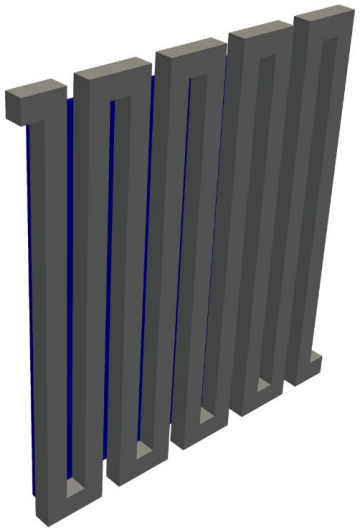
SINMEC Lab, Department of Mechanical Engineering, Federal University of Santa Catarina, Campus Reitor Joao David Ferreira Lima, Florianopolis, 88040-900, Santa Catarina, Brazil

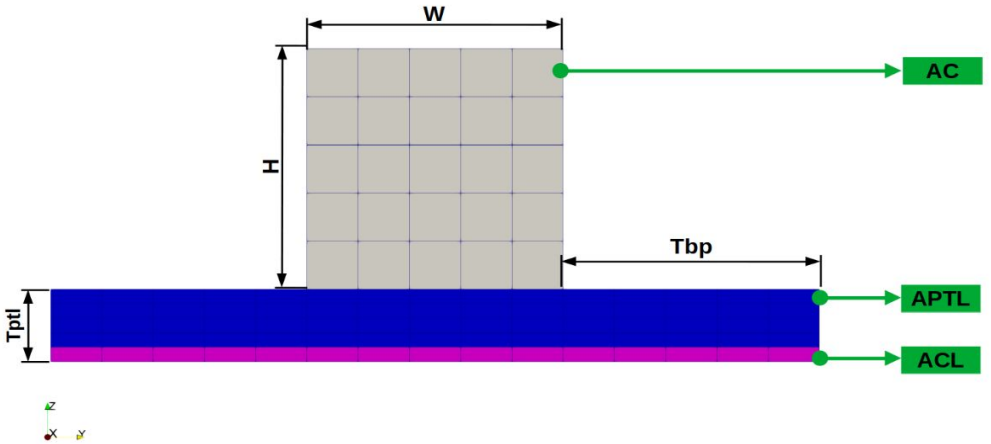
METODOLOGIA









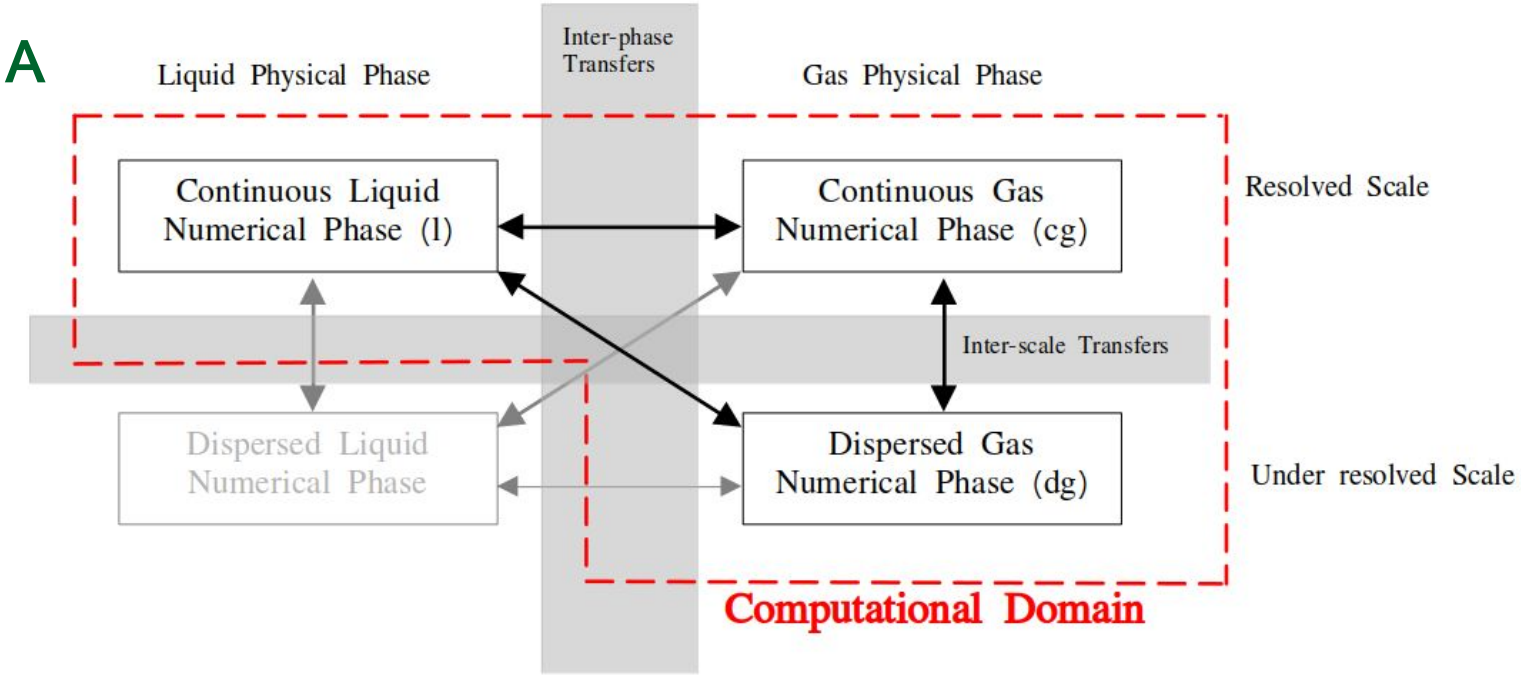


$$H_2O \rightarrow H_2 + \frac{1}{2}O_2$$

$$H_2O_{(l)} \rightarrow \frac{1}{2}O_{2(g)} + 2H^+ + 2e^-$$

$$2H^+ + 2e^- \rightarrow H_{2(g)}$$

METODOLOGIA



Continuity equations

The liquid phase continuity equation is given by [6]

$$\frac{\partial(\varepsilon S_l \rho_l)}{\partial t} + \nabla \cdot \left(\varepsilon S_l \rho_l \mathbf{U}_l\right) = \Gamma_{\mathrm{H_2O},l}$$

The discrete gas phase continuity equation is given by [6]

$$\frac{\partial(\varepsilon S_{dg} \rho_{dg})}{\partial t} + \nabla \cdot \left(\varepsilon S_{dg} \rho_{dg} \mathbf{U}_{dg}\right) = \Gamma_{\mathrm{O_2},dg} + \Gamma''_{\mathrm{O_2},dg}$$

The continuous gas phase continuity equation is given by [23]

$$\frac{\partial(\varepsilon S_{cg} \rho_{cg})}{\partial t} + \nabla \cdot \left(\varepsilon S_{cg} \rho_{cg} \mathbf{U}_{cg}\right) + \nabla \cdot \left(\varepsilon S_{cg} \left(1 - \varepsilon S_{cg}\right) \mathbf{U}_c\right) = \Gamma''_{\mathrm{O_2},cg}$$

METODOLOGIA

Momentum conservation

The liquid phase momentum conservation equation is given by [6]

$$\frac{\partial(\varepsilon S_l \rho_l \mathbf{U}_l)}{\partial t} + \nabla \cdot \left(\varepsilon S_l \rho_l \mathbf{U}_l \mathbf{U}_l\right) = \nabla \cdot \left(\varepsilon S_l \tau_l\right) - \varepsilon S_l \nabla P + \varepsilon S_l \rho_l \mathbf{g} + \mathbf{S_l} + \mathbf{M}_l$$

The discrete gas phase momentum conservation equation is given by [6]

$$\frac{\partial(\varepsilon S_{dg} \rho_{dg} \mathbf{U}_{dg})}{\partial t} + \nabla \cdot \left(\varepsilon S_{dg} \rho_{dg} \mathbf{U}_{dg} \mathbf{U}_{dg}\right) = \nabla \cdot \left(\varepsilon S_{dg} \tau_{dg}\right) - \varepsilon S_{dg} \nabla P + \varepsilon S_{dg} \nabla P_c + \varepsilon S_{dg} \rho_{dg} \mathbf{g} + \mathbf{S_{dg}} + \mathbf{M}_{dg}$$

The continuous gas phase momentum conservation equation is given by [20]

$$\frac{\partial(\varepsilon S_{cg} \rho_{cg} \mathbf{U}_{cg})}{\partial t} + \nabla \cdot \left(\varepsilon S_{cg} \rho_{cg} \mathbf{U}_{cg} \mathbf{U}_{cg}\right) = \nabla \cdot \left(\varepsilon S_{cg} \tau_{cg}\right) - \varepsilon S_{cg} \nabla P + \varepsilon S_{cg} \nabla P_c + \varepsilon S_{cg} \rho_{cg} \mathbf{g} + \mathbf{S_{cg}} + \mathbf{M}_{cg}$$

$$\Gamma_{\mathrm{H_2O},l} = -\frac{i \cdot M_{\mathrm{H_2O}}}{2F}$$

$$\Gamma_{\mathrm{O_2},dg} = \frac{i \cdot M_{\mathrm{O_2}}}{4F}$$

Butler–Volmer Equation [24]

$$i_a = S_l i_{0,a} \left\{ \exp\left[+\frac{\alpha_{\mathrm{Red},a} z F \eta_{act,a}}{RT}\right] - \exp\left[-\frac{\alpha_{\mathrm{Ox},a} z F \eta_{act,a}}{RT}\right] \right\}$$

METODOLOGIA

$$V_{th}{}^{0} = \frac{\Delta H^{0}}{zF} = 1.481 \text{ [V]}$$

$$V_{PEM} = V_{th} + \eta_{act,a} + \eta_{act,c} + \eta_{ohm} + \eta_{diff} + \eta_{bub}$$

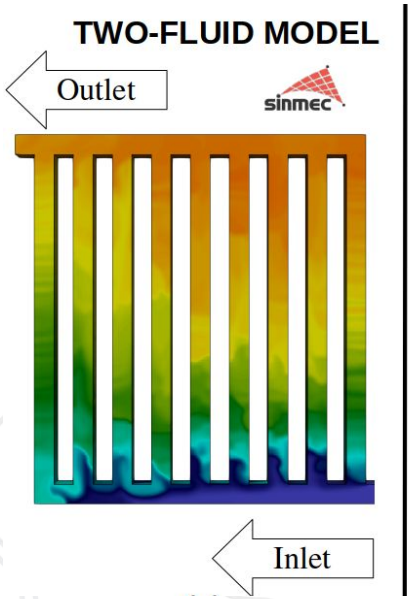
$$\eta_{act} = \frac{RT}{z\alpha F} \ln\left(\frac{i}{i_0}\right) = a \ln\left(\frac{i}{i_0}\right)$$

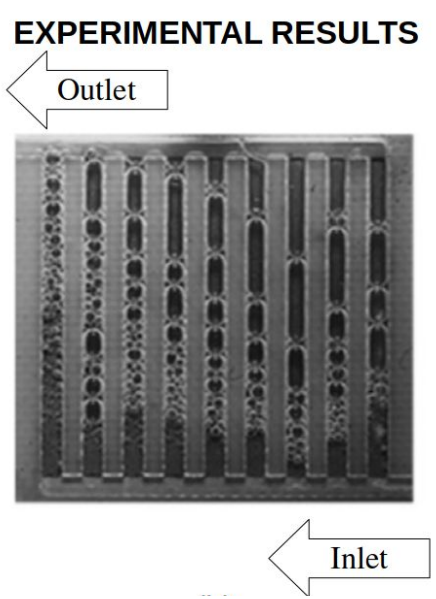
$$\eta_{ohm,mem} = \frac{i\delta_{mem}}{\sigma_{mem}} \qquad \sigma_{mem} = (0.005139\lambda - 0.00326) \exp\left[1268\left(\frac{1}{303} - \frac{1}{T}\right)\right]$$

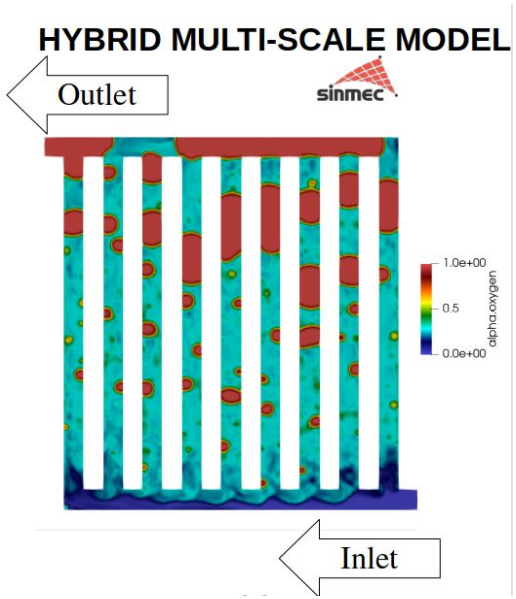
$$\eta_{diff,a} = \frac{RT}{4F} \ln\left(\frac{S_{O_2,mem}}{S_{O_2,mem,0}}\right) \qquad \eta_{diff,c} = \frac{RT}{2F} \ln\left(\frac{S_{H_2,mem}}{S_{H_2,mem,0}}\right)$$

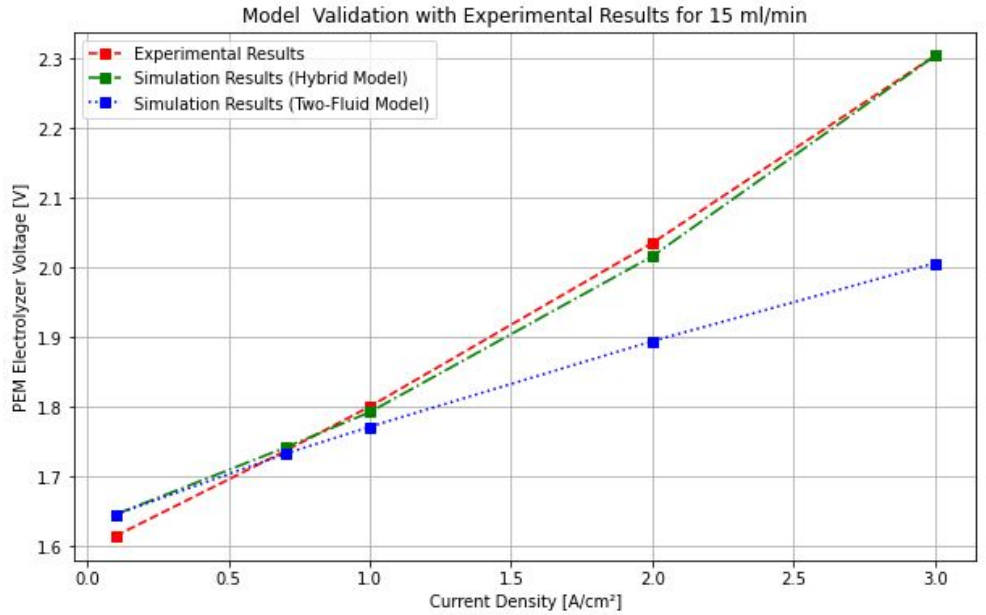
$$\eta_{bub} = \frac{RT}{4F}\left(\frac{\forall_r}{\forall_{crit}}\right)^2$$

RESULTADOS

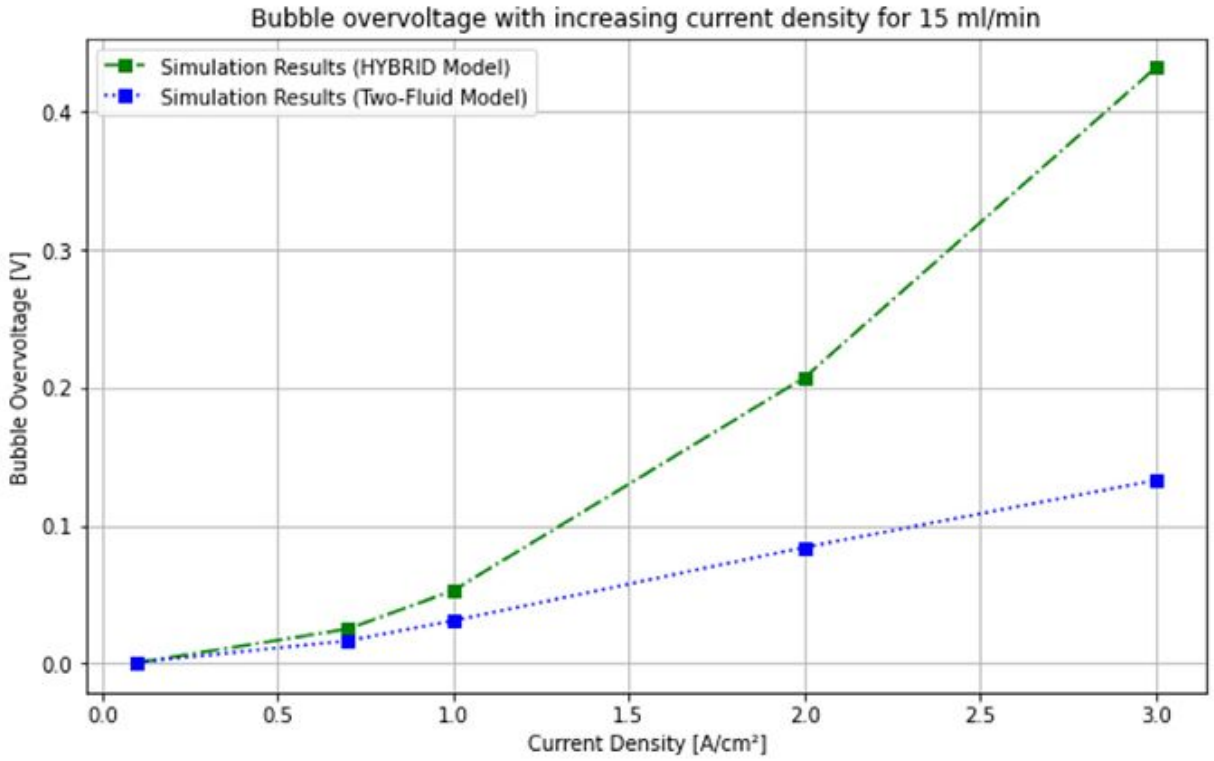

TWO-FLUID MODEL
Outlet
sinmec
Inlet


EXPERIMENTAL RESULTS
Outlet
Inlet

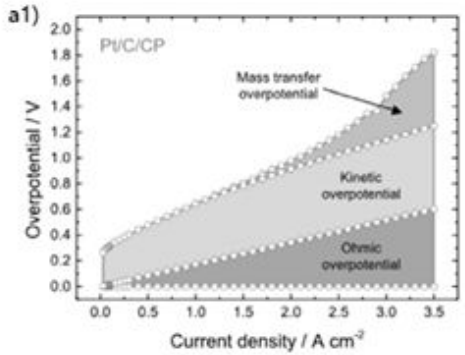

HYBRID MULTI-SCALE MODEL
Outlet
sinmec
1.0e+00
0.5
0.0e+00
alpha.oxygen
Inlet


Model Validation with Experimental Results for 15 ml/min
Experimental Results
Simulation Results (Hybrid Model)
Simulation Results (Two-Fluid Model)
PEM Electrolyzer Voltage [V]
Current Density [A/cm²]
1.6
1.7
1.8
1.9
2.0
2.1
2.2
2.3
0.0
0.5
1.0
1.5
2.0
2.5
3.0

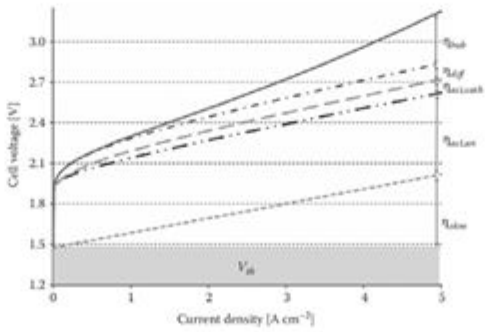
RESULTADOS



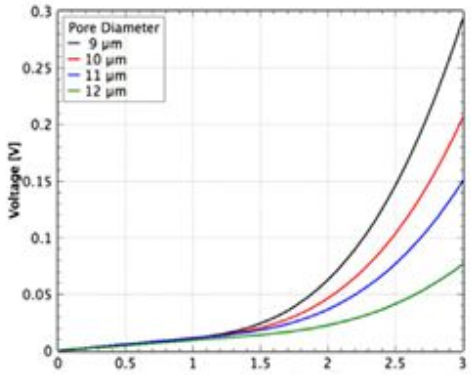
(a)



(b)



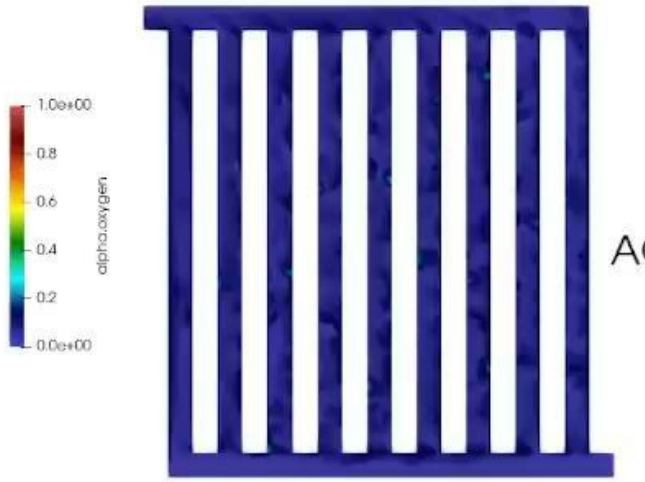
(c)



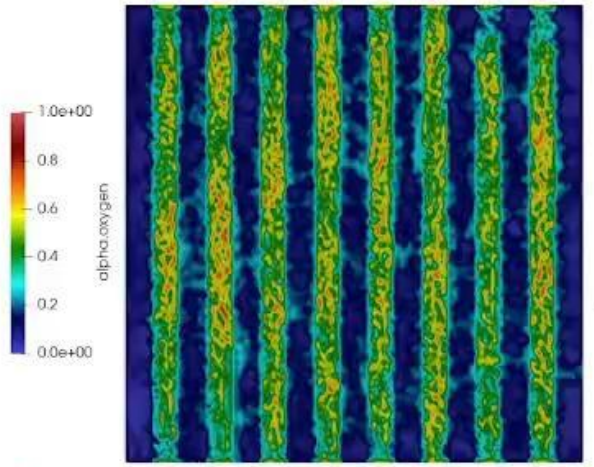
(d)

RESULTADOS

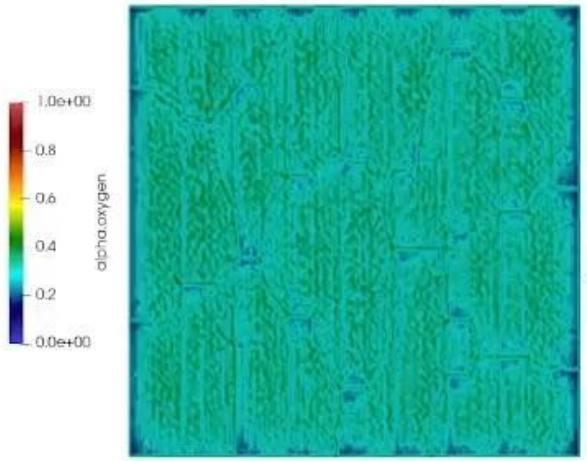




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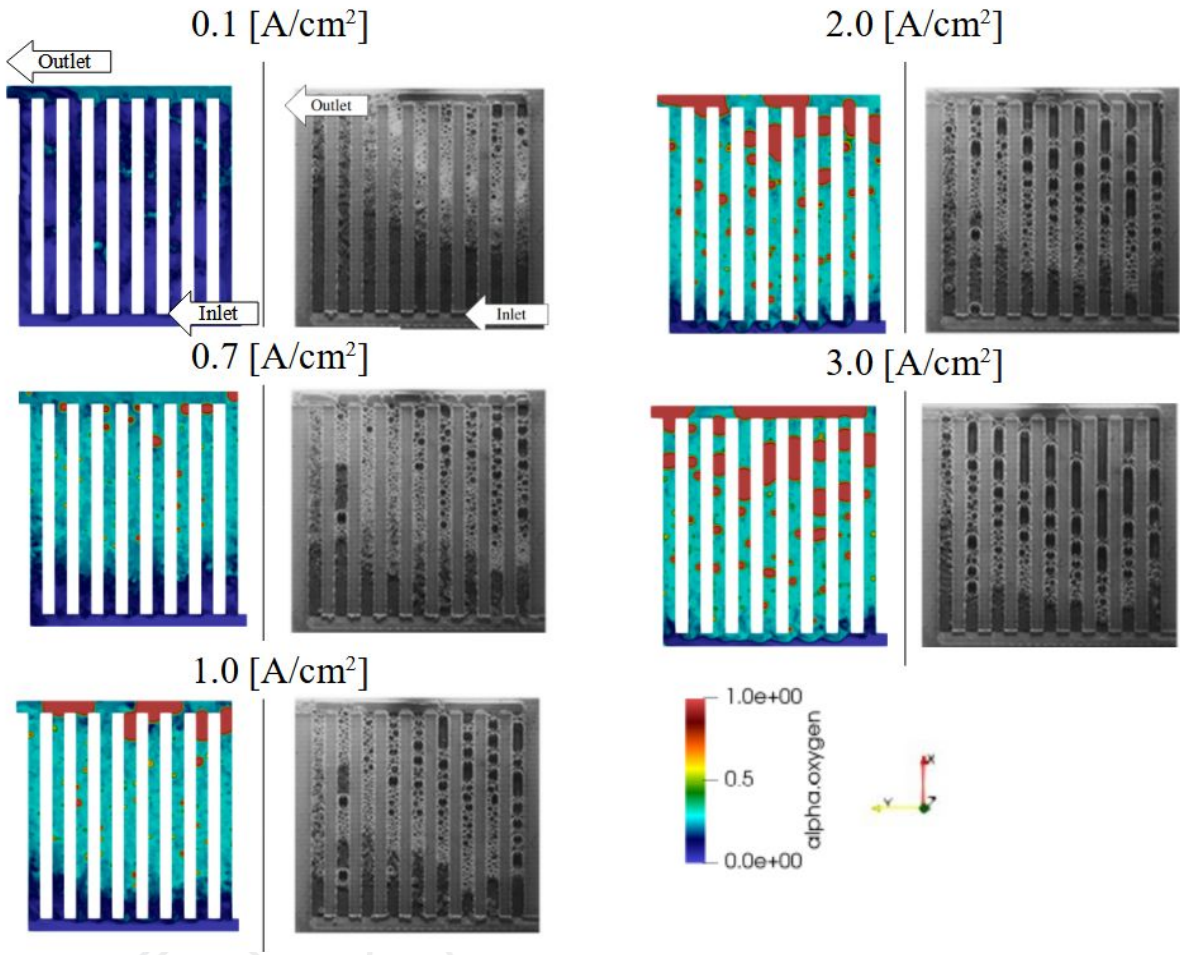


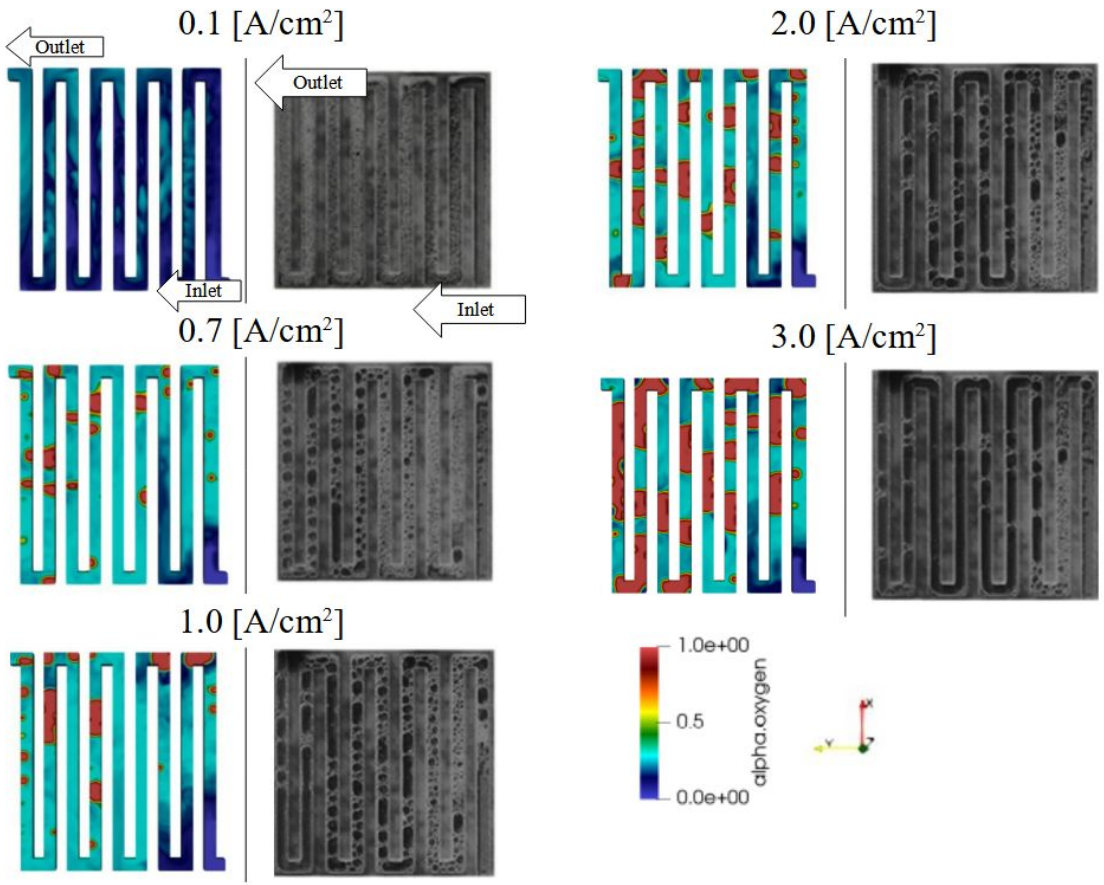
ACL



ACL

RESULTADOS


0.1 [A/cm²]
Outlet
Outlet
Inlet
Inlet
2.0 [A/cm²]
0.7 [A/cm²]
3.0 [A/cm²]
1.0 [A/cm²]
1.0e+00
0.5
0.0e+00
alpha.oxygen

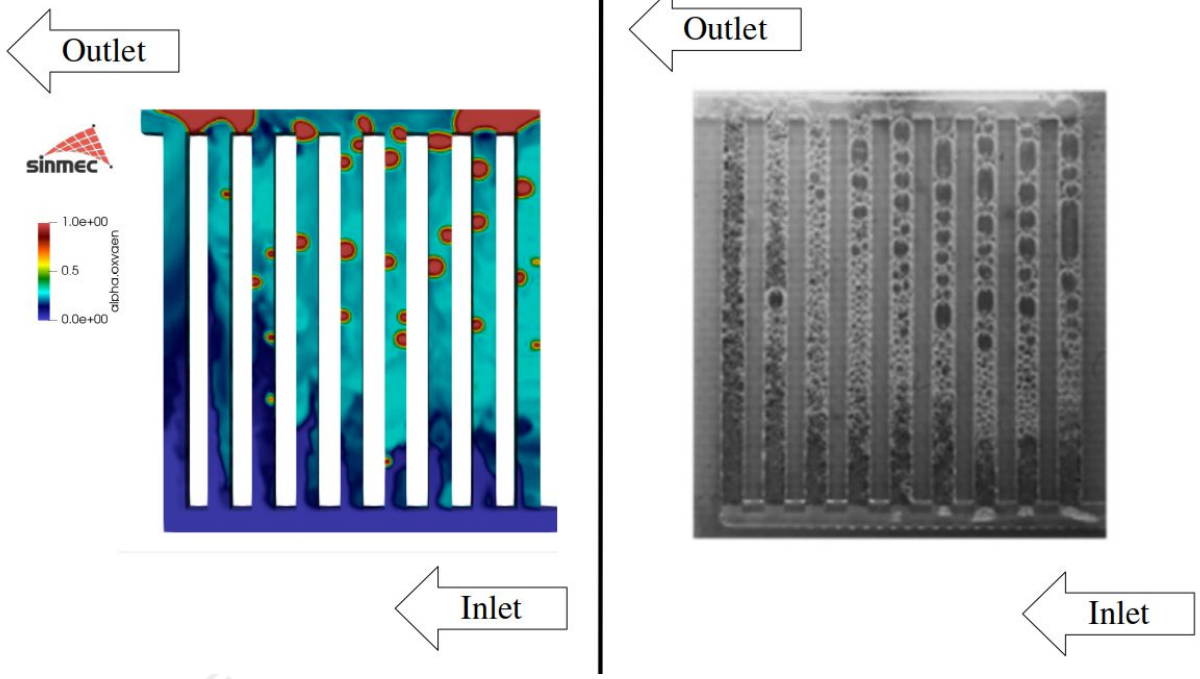

0.1 [A/cm²]
Outlet
Outlet
Inlet
Inlet
2.0 [A/cm²]
0.7 [A/cm²]
3.0 [A/cm²]
1.0 [A/cm²]
1.0e+00
0.5
0.0e+00
alpha.oxygen

RESULTADOS

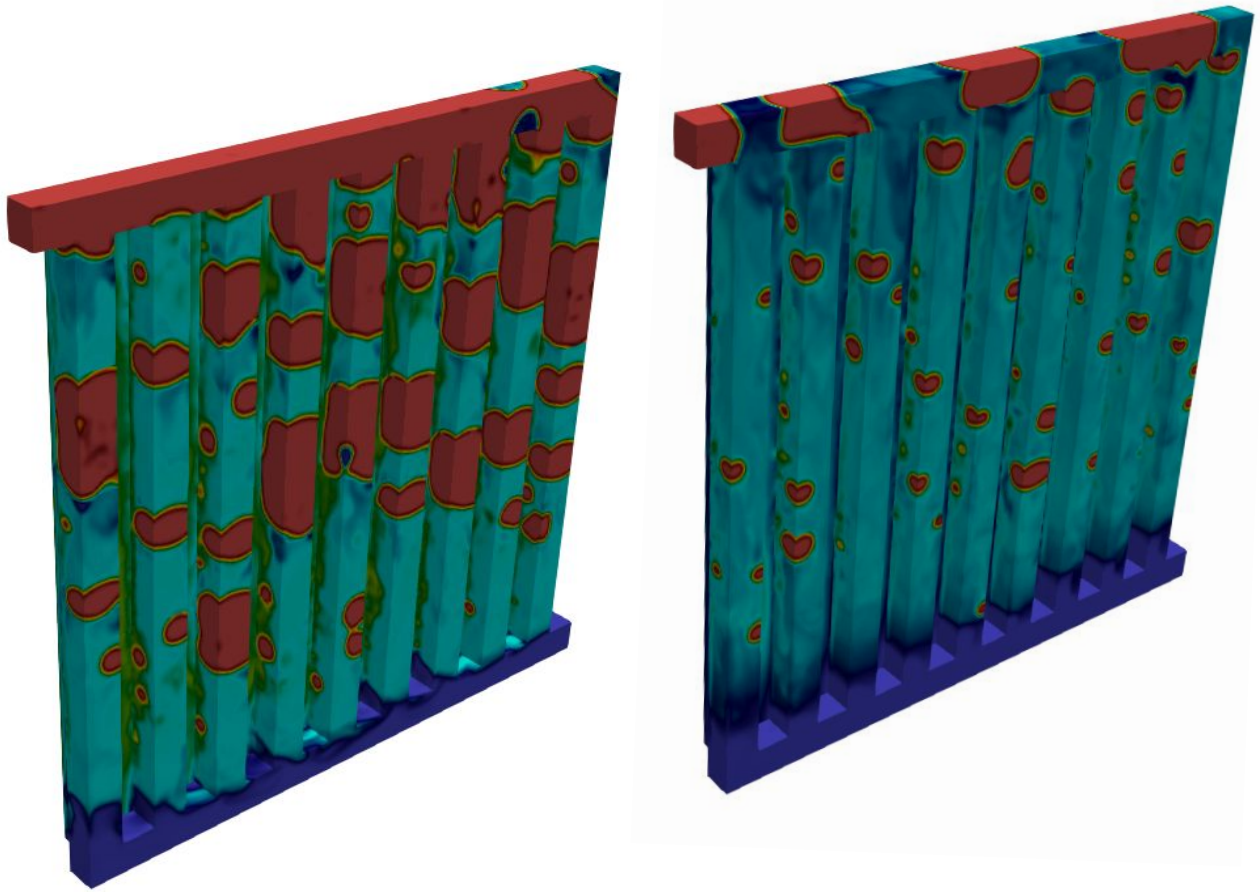
$i = 2.0\ [A \cdot cm^{-2}]$

HYBRID MULTI-SCALE MODEL

EXPERIMENTAL RESULTS



1.5 bar x 10 bar



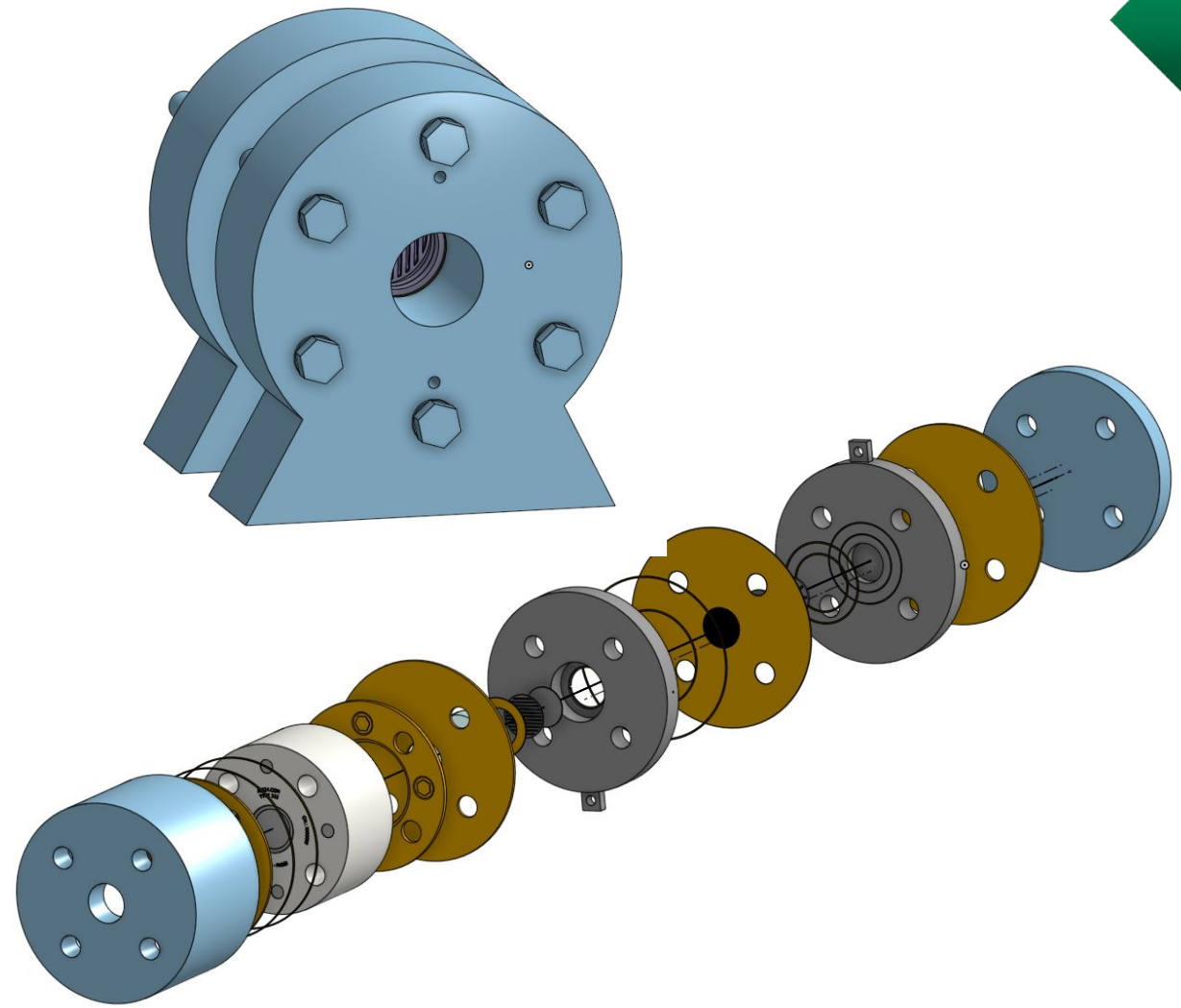
CONSIDERAÇÕES FINAIS

Conclusão

- Transição de morfologia:
- Efeito “shielding” da camada catalítica;
- Comparação de geometrias;
- Impacto da taxa de alimentação de água.

Trabalhos Futuros

- Expansão do modelo;
- Montagem da bancada experimental.



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REFERÊNCIAS

Li and Liao. "PEM Water Electrolysis - Fundamentals And Practice." Elsevier. 2025. DOI: https://doi.org/10.1016/C2023-0-01237-7.

Majasan, Cho, and Dedigama. " Two-Phase Flow Behavior And Performance Of Polymer Electrolyte Membrane Electrolysers: Electrochemical And Optical Characterisation." International Journal of Hydrogen Energy. 2018. DOI: https://doi.org/10.1016/j.ijhydene.2018.07.003.

Meller, Schlegel, and Lucas. "Basic Verification Of A Numerical Framework Applied To A Morphology Adaptive Multifield Two-Fluid Model Considering Bubble Motions." International Journal for Numerical Methods in Fluids. 2020. DOI: https://doi.org/10.1002/fld.4907.

Nardin and Paladino. "Hybrid Multi-Scale Multiphase Flow Modeling of Proton Exchange Membrane Electrolyzers For Green Hydrogen Production." International Journal of Hydrogen Energy. 2025. DOI: https://doi.org/10.1016/j.ijhydene.2025.151764.

UNEP. "Emission Gap Report: Off Target - Continued Collective Inaction Puts Global Temperature Goal At Risk." United Nations Environment Programme. 2025. DOI: https://doi.org/10.59117/20.500.11822/48854.



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Gestão:

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