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Conference Courses 18 May

Multi-phase Flow and Bubble Management in Anion Exchange Membrane Water Electrolysis for Green Hydrogen Production

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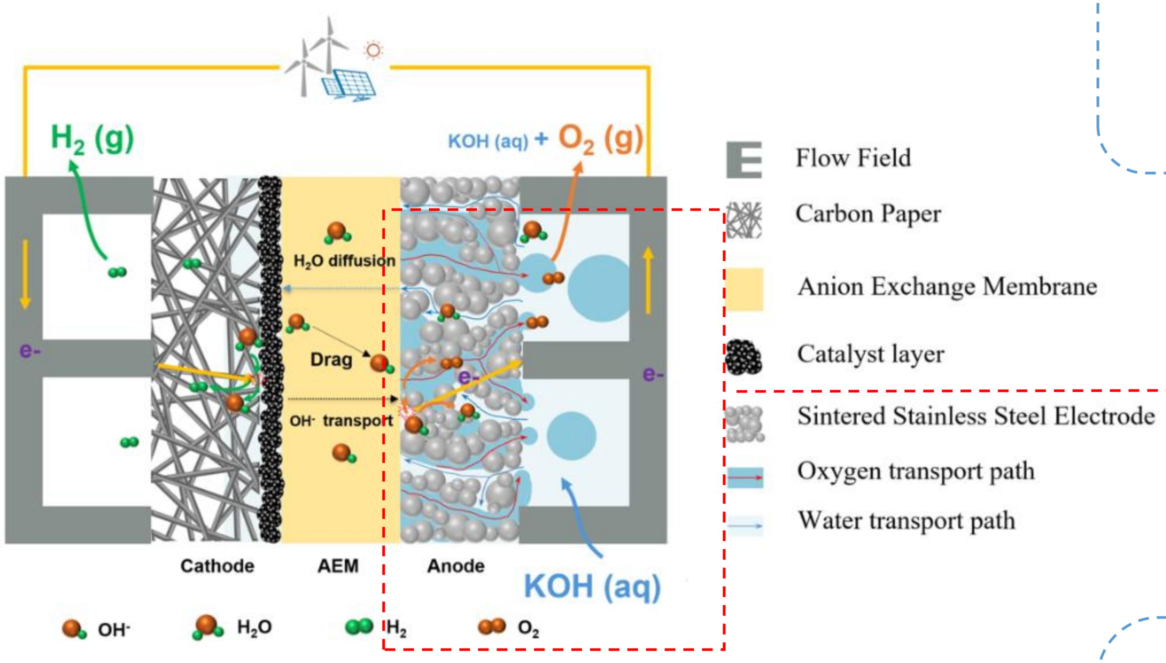
Outline

- Background and bubble issues
- Methodology
- Pore size and thickness optimization
- Hierarchical bubble-management design
- Summary

Background

➢ Water electrolysis for green hydrogen production

Taking the AEMWE as an example:

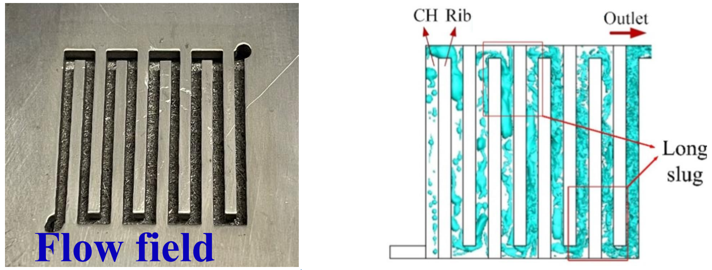


Anode: $2OH^- \rightarrow 1/2O_2\uparrow + H_2O + 2e^-$ $E^0 = 0.40$ V vs SHE

Cathode: $2H_2O + 2e^- \rightarrow 2OH^- + H_2\uparrow$ $E^0 = -0.83$ V vs SHE

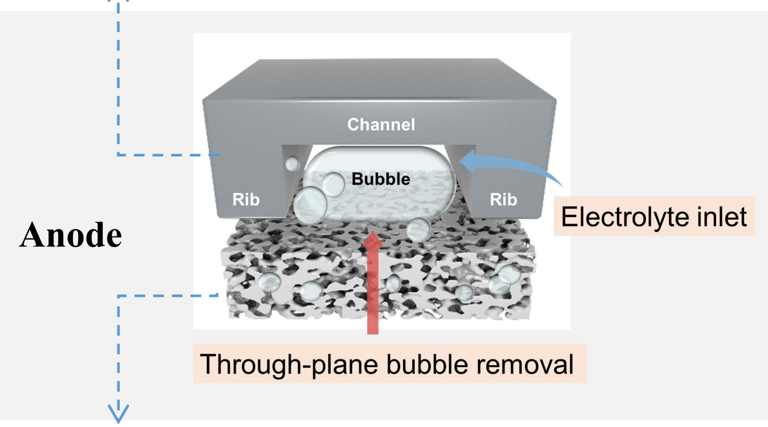
Overall: $H_2O \rightarrow 1/2O_2\uparrow + H_2\uparrow$ $E^0 = 1.23$V vs SHE

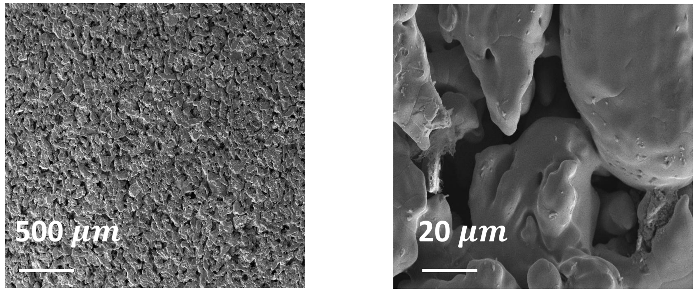
Anion Exchange Membrane Water Electrolysis



- Bubble removal
- Electrolyte supply

Anode





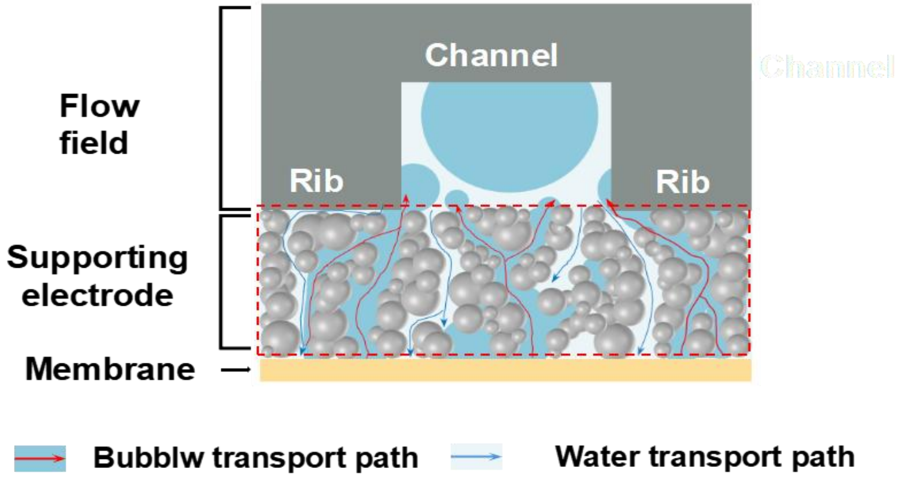
Porous Electrode

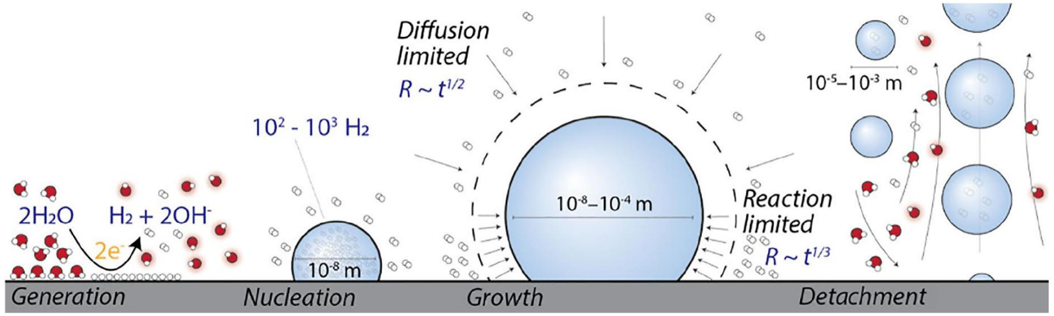
- Providing active sites
- Bubble generation
- Bubble transport
- Electrolyte distribution

Applied Energy 323 (2022) 119651

Bubble issues

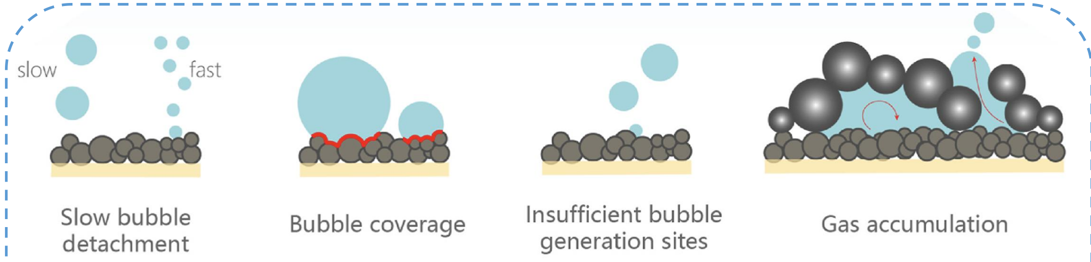
➢ Bubble issues in the porous electrode





Bubble life cycle

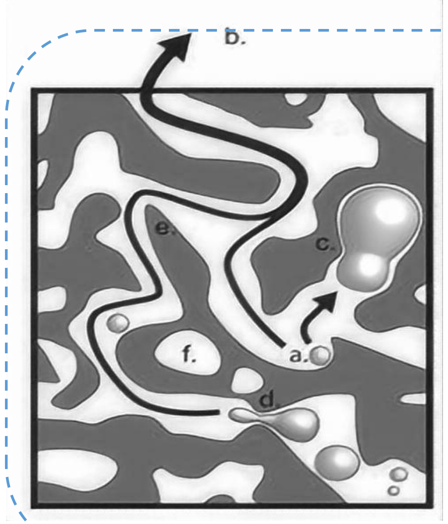
☐ Bubbles cover the active electrode surface

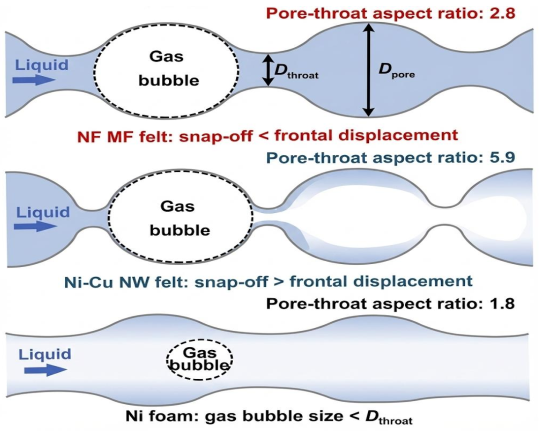


Bubble shielding effect

Electrochemical Active Surface Area (ECSA) ↓

☐ Bubbles block electrolyte transport pathways

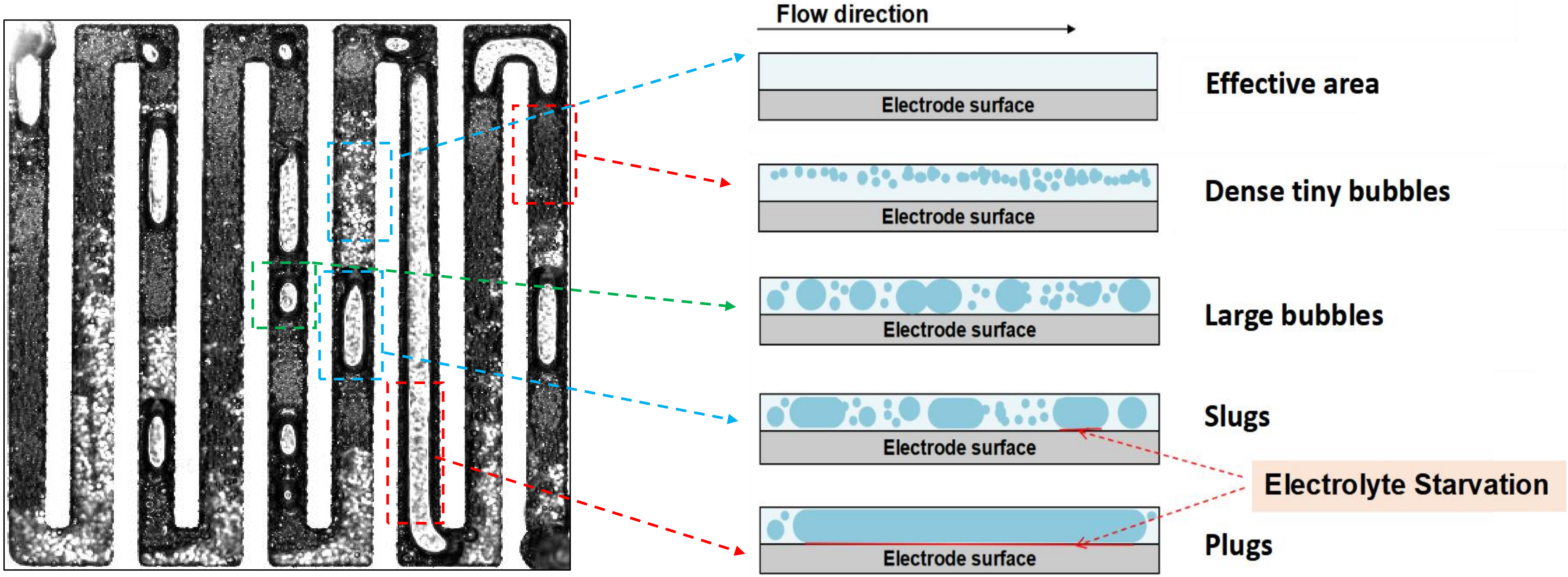




Progress in Energy and Combustion Science 96 (2023) 101075
Chem. Rev. 2024, 124, 10964−11007

Bubble issues

➢ Bubble issues in the flow field



Two-phase flow in the flow field

- Bubble coalescence and blockage restrict liquid transport pathways, leading to electrolyte starvation

Bubble issues

➢ **Why bubble management matters?**

How to maximize H_2 production and minimize cost ?

Hydrogen production at high current densities:

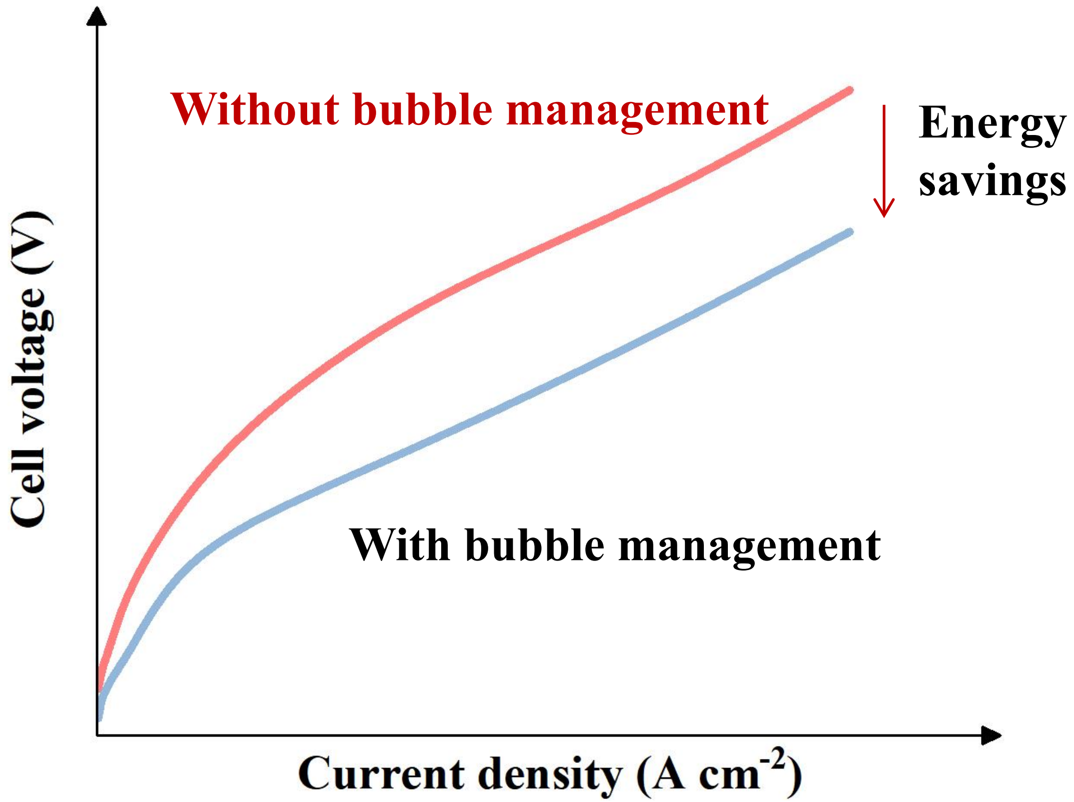
Current density ↑

⇩

H_2 (i) ↑ ⟶ Bubble ↑ ⟶ Voltage ↑ ⟶

Bubble shielding effect
Water starvation

Bubble and water management ⟶ Voltage ↓ ⟶ Cost ↓



- Effective bubble management lowers the cell voltage at high current densities, enabling energy savings during hydrogen production

Bubble issues

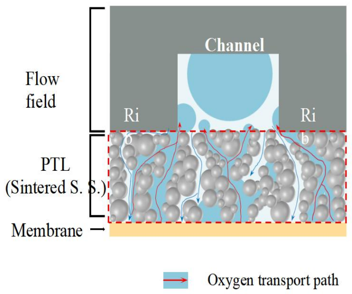
Research objective

- To investigate the impact of electrode structural parameters on electrochemical performance and mass transport via numerical and experimental methods
- To elucidate bubble dynamics and mass-transfer mechanisms at high rates via in-situ visualization
- To design hierarchical grooves for improved bubble evacuation and liquid supply

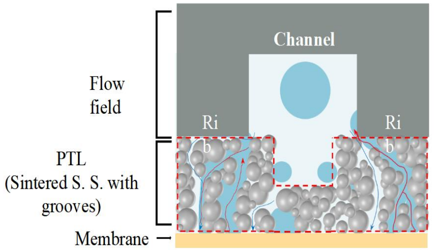
Sintered stainless steel electrodes (low-cost)

Electrode pore size

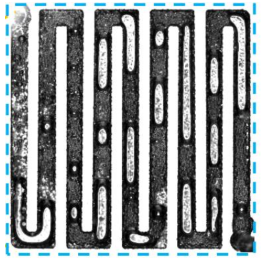
Electrode thickness



Optimization of electrode structure parameters



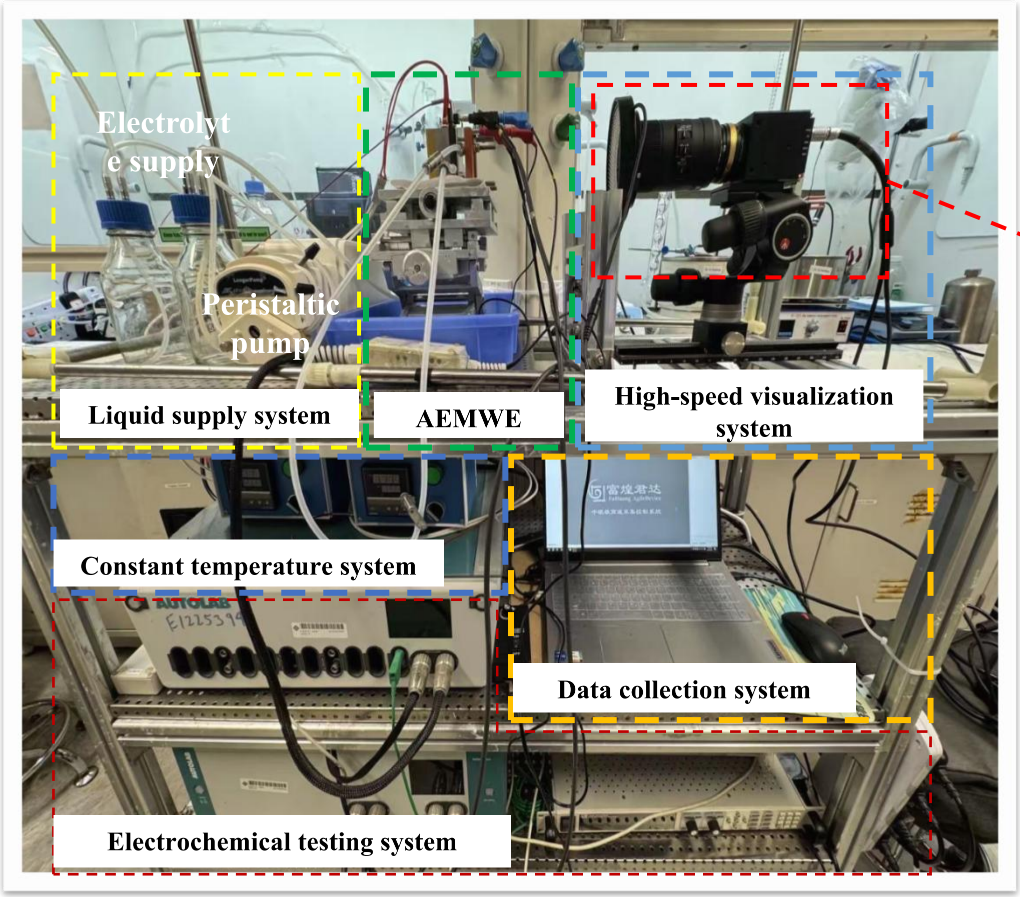
Hierarchical electrode



Bubble dynamics

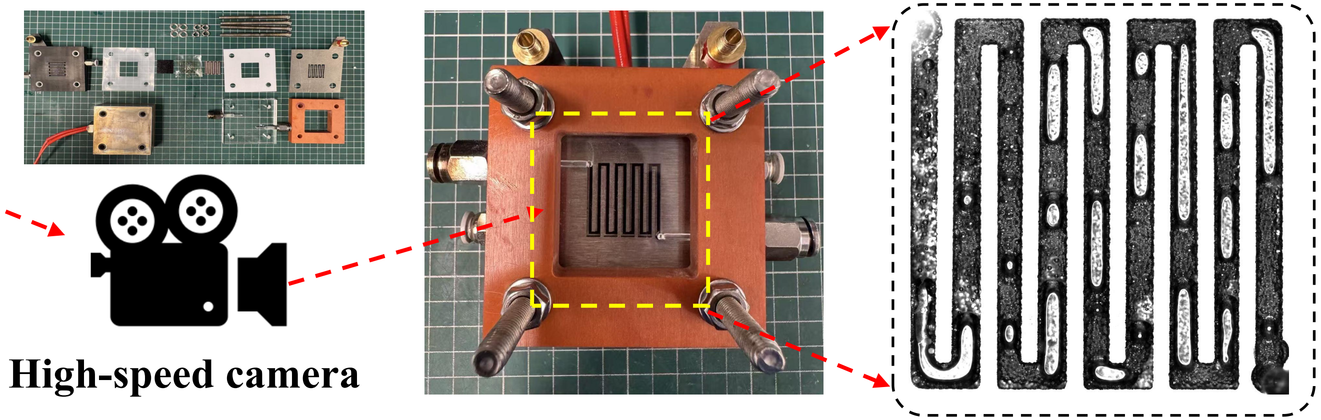
Methodology

➢ Electrochemical testing platform and in-situ visualization system



Electrochemical testing platform

Visualize bubble behavior in flow fields

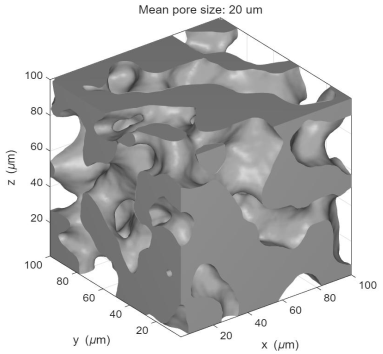


Operating condition and components

- **Operating Temperature:** 80 ˚C; Electrolyte: 1 M KOH
- **Electrolyte flow rate:** 5.0 mL min^{-1};
- **Anode CL and PTL:** Sintered S. S. electrode;
- **Cathode CL and GDL :** Carbon paper coated with 0.5 mg cm^{-2} Pt/C;
- **Membrane:** Nafion 115
- **Flow field plate:** Graphite plate(cathode), Nickel plate(anode)

Methodology

➢ Pore-scale numerical simulation of porous electrode



Size:

$100 \times 100 \times 100\ \mu m^3$

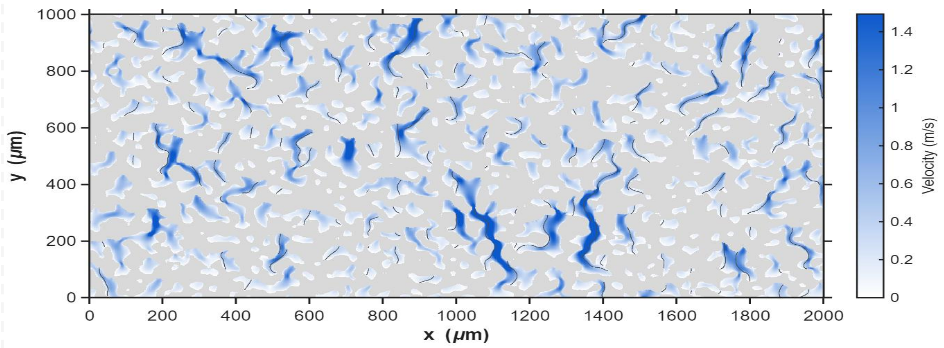
Lattice:

$80 \times 80 \times 80$ nodes

($1.25\ \mu m$/grid)

REV (Gaussian Random Field)

Study on the effect of electrode pore size



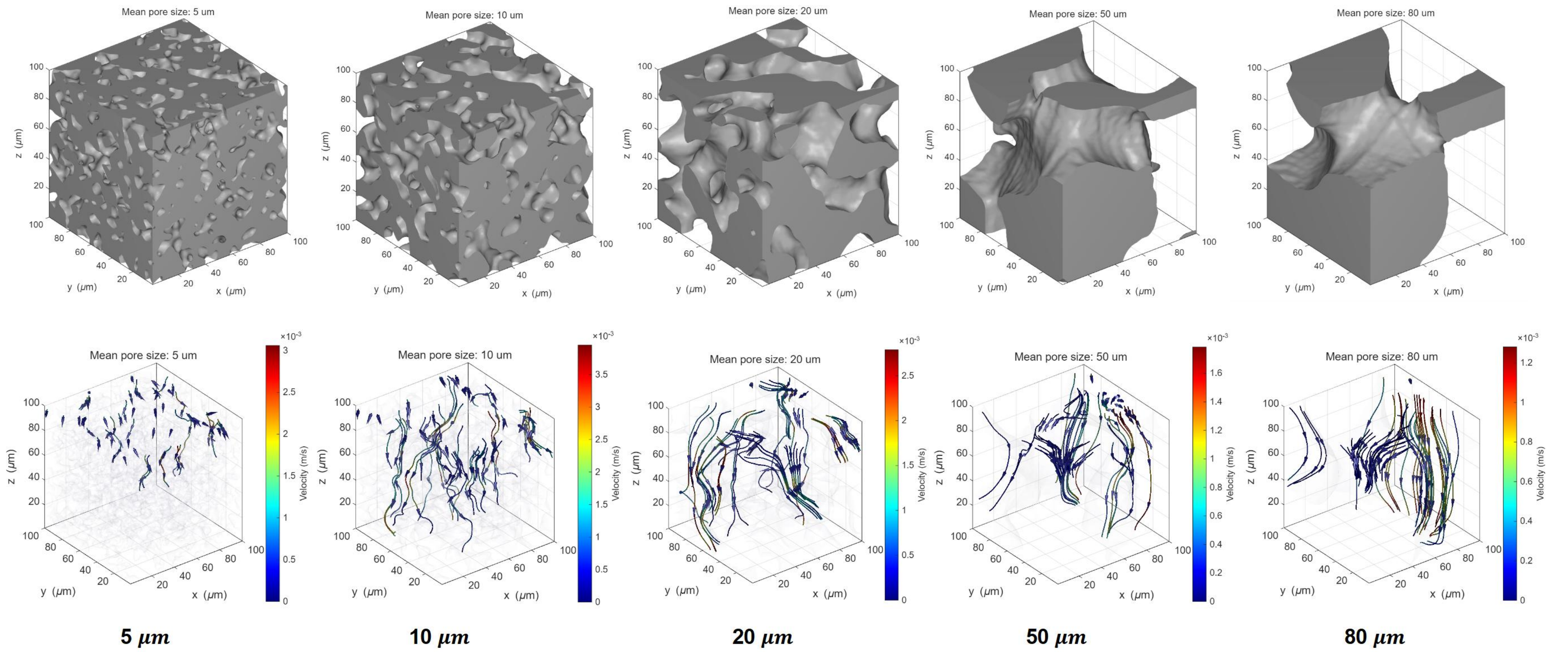
Study on the effect of electrode thickness

Transport properties and electrochemical properties

- ✓ Permeability
- ✓ Pressure drop (ΔP)
- ✓ Tortuosity
- ✓ Specific surface area (SSA)
- ✓ Area specific resistance (ASR)
- ✓ The local effective active area density
- ✓ Effective reaction area utilization (U)

Research results

➢ Pore-size-dependent flow transport in porous electrodes

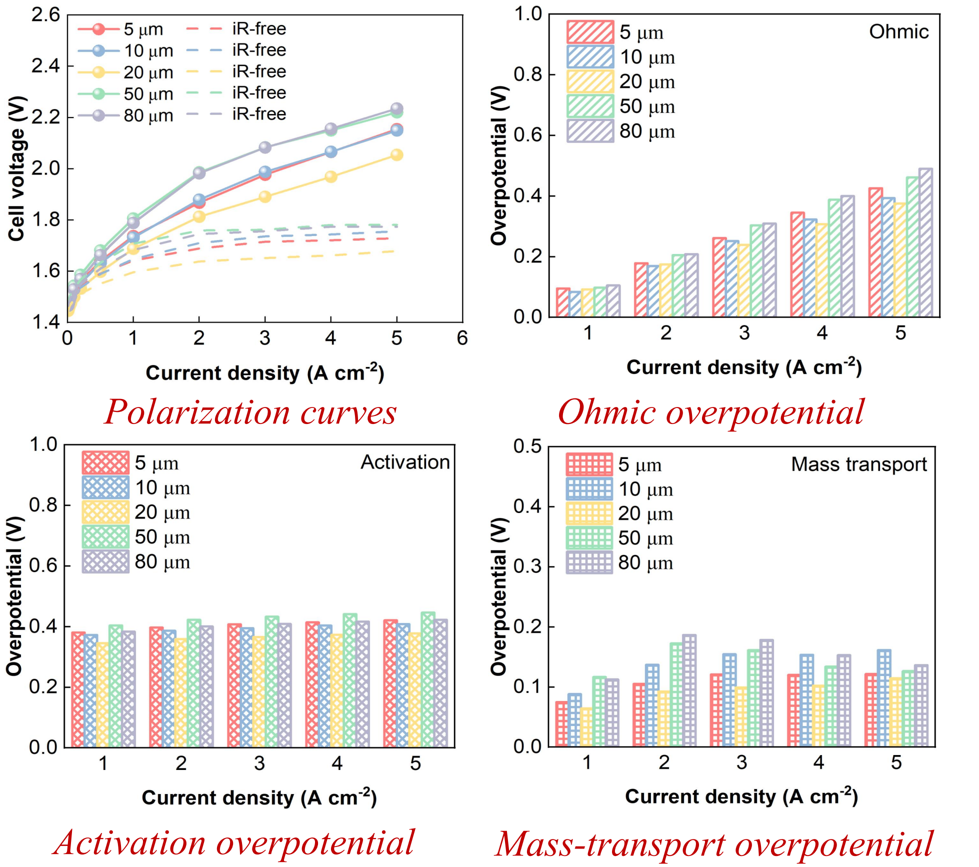


Reconstructed 3D microstructures of stainless steel electrodes and flow velocity streamlines

- Pore-scale simulations identify 20 μm as the optimal pore size, balancing pore connectivity, flow uniformity, and transport resistance.

Research results

➢ **Pore-size-dependent cell performance and loss breakdown**



Key finding:

- 20 μm shows the lowest cell voltage by balancing active surface area and transport resistance

Small pores → poor liquid/bubble transport

Large pores → reduced surface area/contact quality

- An intermediate pore size minimizes cell voltage by balancing active surface area, contact resistance, and mass-transport loss

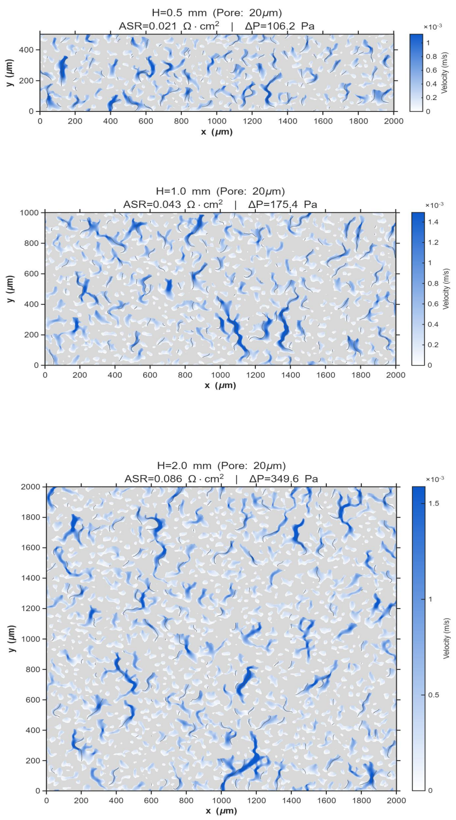
Research results

➢ Thickness-dependent flow transport in porous electrodes

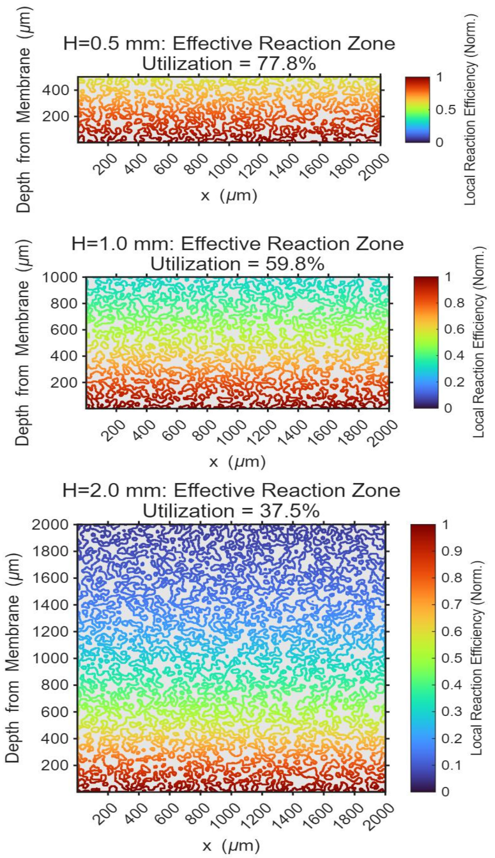
0.5 mm

1.0 mm

2.0 mm



Electrolyte flow velocity distribution



Distribution of the effective reaction zone

77.8%

59.8%

37.5%

Thickness ↑

→ longer pathway

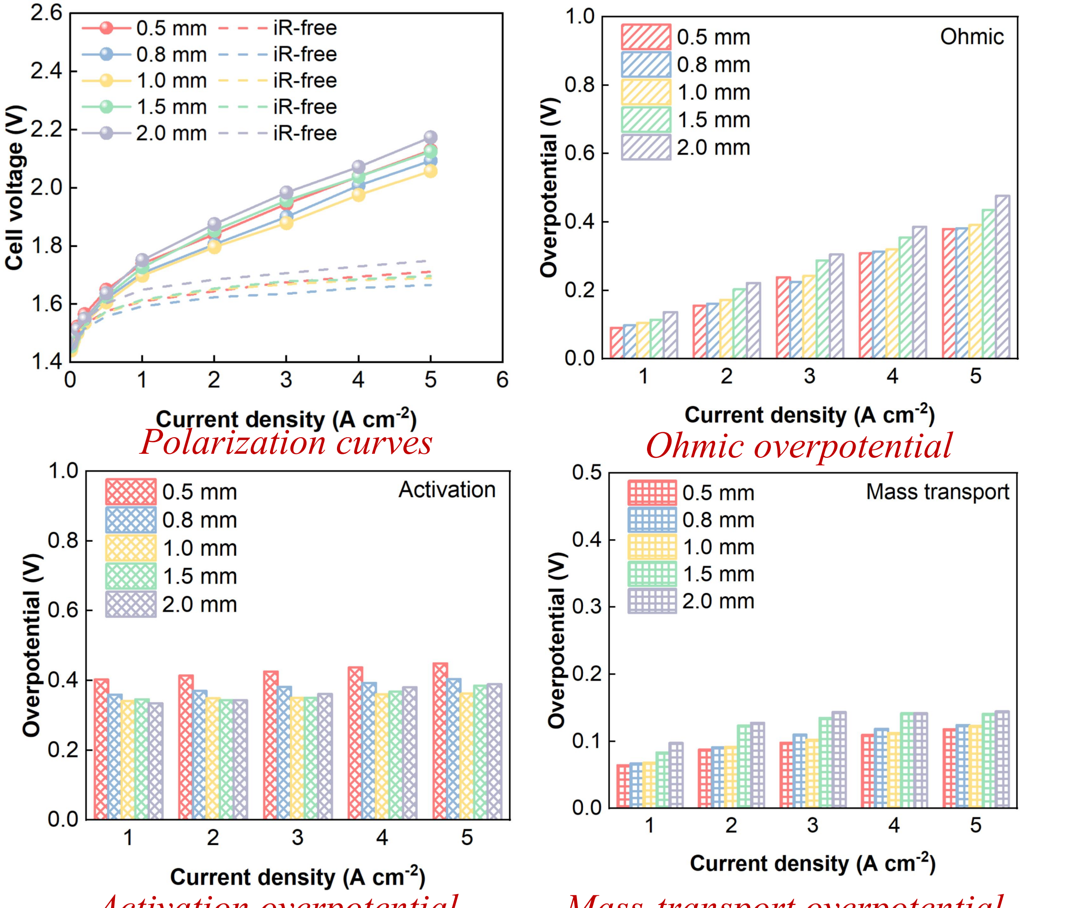
→ higher pressure drop

→ lower ECSA utilization

- Excessive electrode thickness extends transport pathways, promotes gas accumulation, and reduces effective reaction-zone utilization

Research results

➢ Thickness-dependent cell performance and loss breakdown



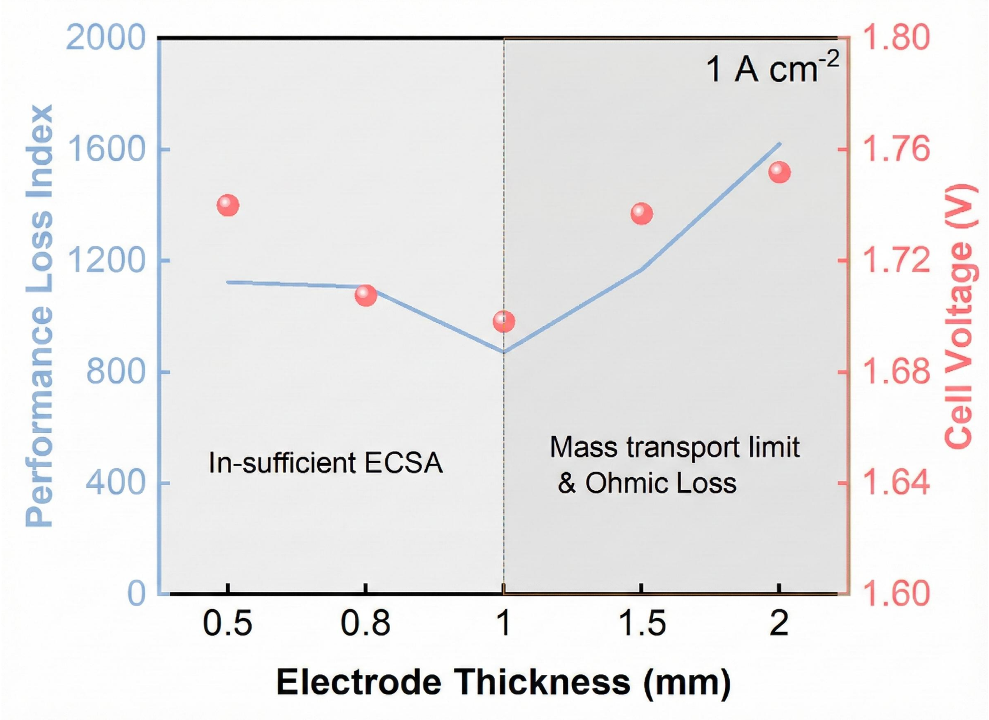
Polarization curves

Ohmic overpotential

Activation overpotential

Mass-transport overpotential

> **Performance Loss Index (PLI):**
>
> $$\mathrm{PLI} = \frac{1}{(ECSA \cdot U)^2} + 40\sqrt{j(i)} \cdot (ASR \cdot \Delta P)$$

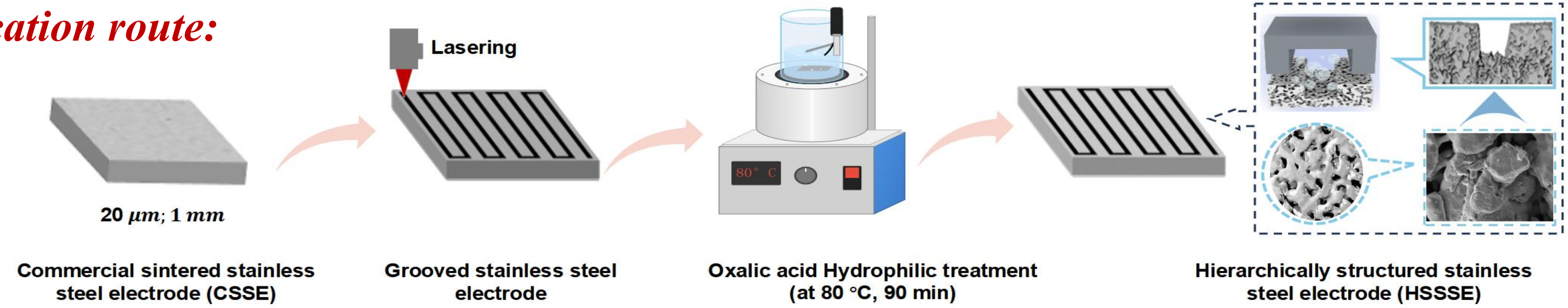


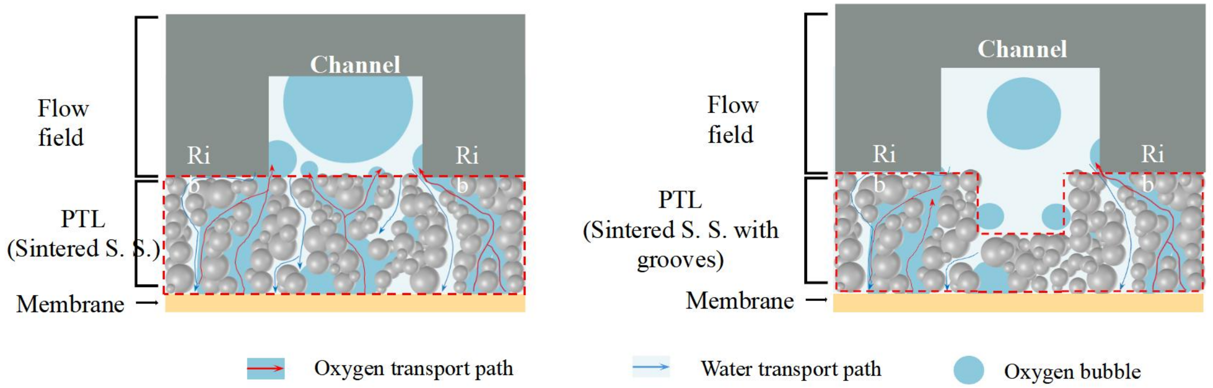
- The 1.0 mm electrode achieves the lowest cell voltage by balancing active surface area, ohmic resistance, and mass-transport loss.

Research results

➢ **Hierarchical grooves for guided bubble removal**

Fabrication route:





Decoupling bubble removal from liquid supply

- Hierarchical grooves are introduced into the optimized 20 μm, 1.0 mm electrode to create preferential bubble-removal pathways while maintaining liquid supply.

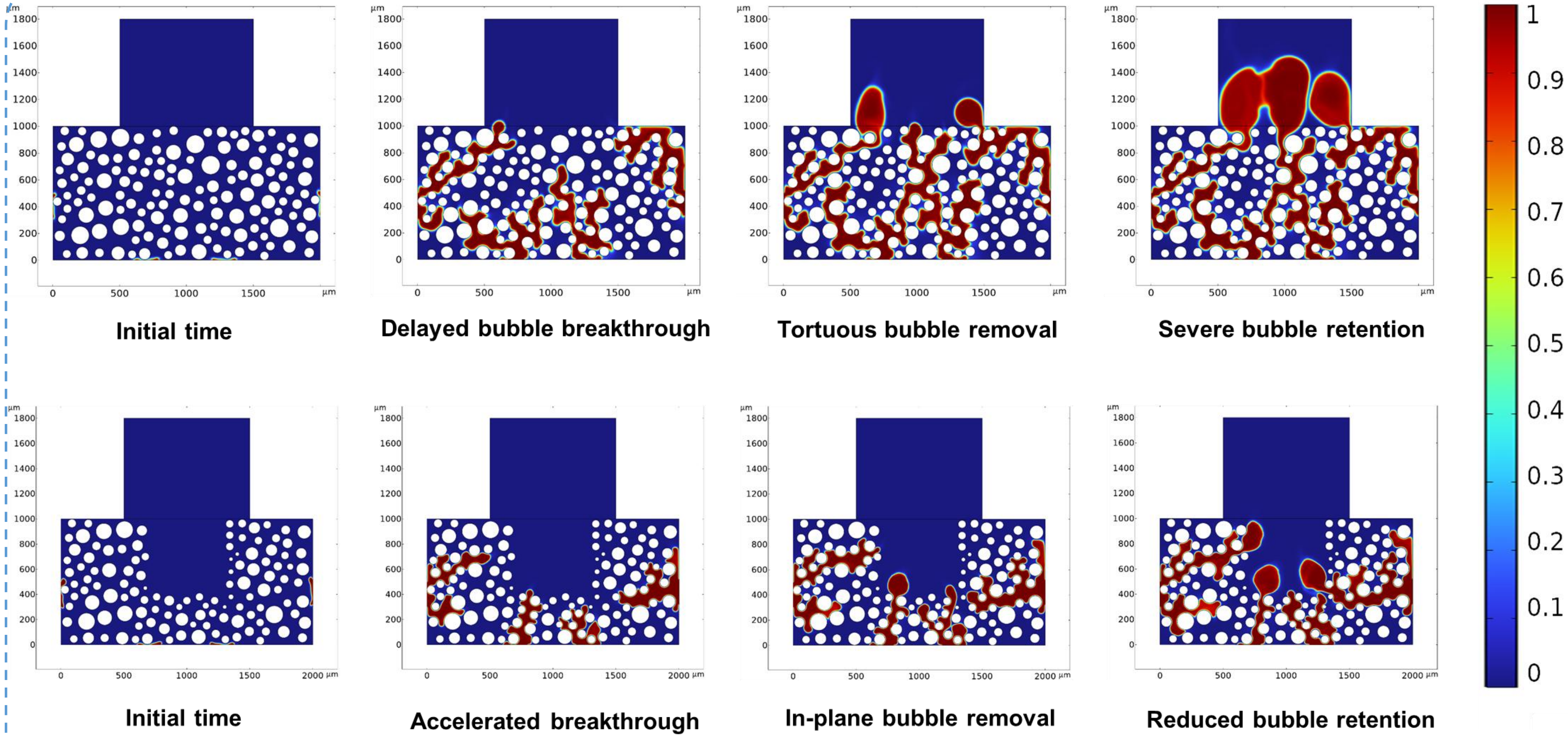
Research results

➢ Hierarchical grooves accelerate bubble evacuation in porous electrodes

Conventional electrode

Hierarchical electrode

Underwater bubble contact angle indicates weaker bubble adhesion

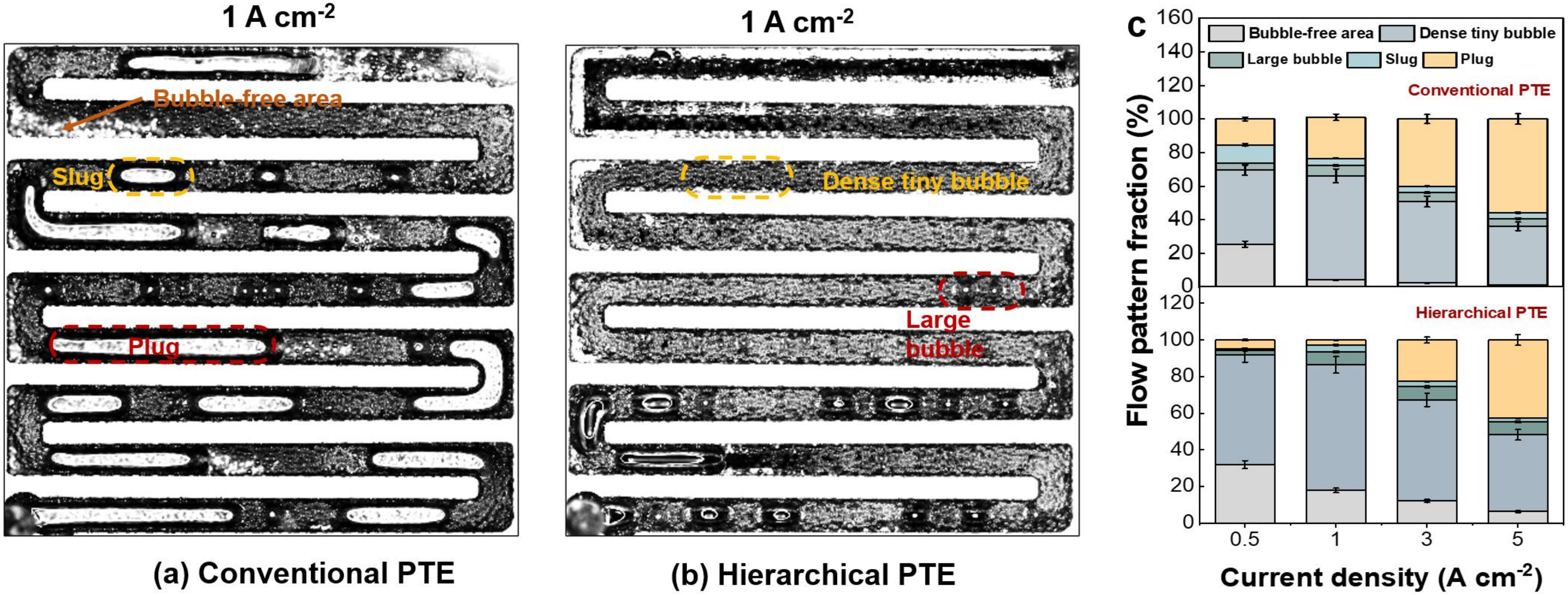


Bubble evacuation in porous media

- Hierarchical grooves weaken bubble adhesion and accelerate bubble evacuation, reducing bubble retention inside the porous electrode.

Research results

➢ **Flow-field visualization confirms enhanced bubble removal**



- The hierarchical electrode suppresses slug and plug flow, thereby maintaining liquid-accessible pathways in the flow field

Summary

- **20 μm pore size：** balances pore connectivity, active surface area, and transport resistance
- **1.0 mm electrode thickness：** achieves the lowest cell voltage by balancing active area and transport losses
- **Hierarchical grooves：** accelerate bubble evacuation and reduce bubble retention inside the porous electrode
- **Flow-field visualization：** confirms suppressed slug/plug flow and improved liquid accessibility

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Thank you!