

Processes

Supporting Information

Numerical Simulation of Gradient Pore Structures in Anodes for Anion Exchange Membrane Water Electrolysis

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Table S1. Nomenclature of Physical Quantities

Symbol	Definition	Symbol	Definition
a_v	Active specific surface area (m^{-1})	μ_g	Gas phase dynamic viscosity ($\text{Pa}\cdot\text{s}$)
α_f	Forward charge transfer coefficient	μ_l	Liquid phase dynamic viscosity ($\text{Pa}\cdot\text{s}$)
α_θ	Beavers-Joseph empirical constant	μ_m	Mixture dynamic viscosity ($\text{Pa}\cdot\text{s}$)
C_O	Oxidized species concentration correction factor	n	Boundary normal vector
C_R	Reduced species concentration correction factor	P_{H_2}	Hydrogen partial pressure (atm)
C_{in}	Inlet KOH concentration (mol/L)	P_{O_2}	Oxygen partial pressure (atm)
C_K	Potassium ion concentration (mol/L)	P_{out}	Outlet pressure (Pa, gauge pressure)
C_{OH}	Hydroxide ion concentration (mol/L)	P_{ref}	Reference pressure (atm)
$C_{OH,ref}$	Reference hydroxide ion concentration (mol/L)	p_c	Capillary pressure (Pa)
C_w	Water concentration (mol/L)	p_g	Gas phase pressure (Pa)
$C_{w,ref}$	Reference water concentration (mol/L)	p_l	Liquid phase pressure (Pa)
d	Average pore diameter (mm)	R	Gas constant (8.314 J/mol/K)
D_{OH}	Bulk diffusion coefficient of KOH (m^2/s)	R_{lg}	Mass transfer rate (liquid to gas) ($\text{kg}/(\text{m}^3\cdot\text{s})$)
$D_{e,OH}$	Effective diffusion coefficient of OH^- (m^2/s)	R_{OH}	Hydroxide ion reaction rate ($\text{mol}/(\text{m}^3\cdot\text{s})$)
E_{act}	Electrode reaction activation energy (kJ/mol)	ρ_g	Gas phase density (kg/m^3)
E_{eq}	Actual equilibrium potential (V)	ρ_l	Liquid phase density (kg/m^3)

$E_{eq,T}$	Temperature-corrected equilibrium potential (V)	ρ_m	Mixture density (kg/m ³)
$E_{eq,ref}$	Reference equilibrium potential (V)	s_g	Gas phase volume fraction
dT/dE_{eq}	Temperature coefficient of equilibrium potential (mV/K)	$s_{g,in}$	Inlet gas volume fraction
F	Faraday's constant (C/mol)	s_l	Liquid phase volume fraction
γ	Average activity coefficient of KOH	σ	Surface tension coefficient (N/m)
ε	Electrode porosity	$\sigma_{e,l}$	Effective ionic conductivity (S/m)
ε_m	Membrane porosity	$\sigma_{e,s}$	Effective electronic conductivity (S/m)
i	Current density (A/m ²)	σ_l	Intrinsic ionic conductivity (KOH) (S/m)
i_{cell}	Cell operating current density (A/cm ²)	σ_s	Intrinsic electronic conductivity (S/m)
i_l	Ionic current density (A/m ²)	T	Operating temperature (°C)
i_{loc}	Local reaction current density (A/m ²)	T_{ref}	Reference temperature (K)
i_0	Actual exchange current density (A/m ²)	t_K	Potassium ion transference number
$i_{0,T}$	Temperature-corrected exchange current density (A/m ²)	t_{OH}	Hydroxide ion transference number
$i_{0,ref}$	Reference exchange current density (mA/cm ²)	t_K^0	K ⁺ transference number (infinitely dilute)
i_s	Electronic current density (A/m ²)	t_{OH}^0	OH ⁻ transference number (infinitely dilute)
I	Identity matrix	ϑ	Contact angle (°)
j_{OH}	Hydroxide ion molar flux (mol/(m ² ·s))	u_g	Gas phase velocity (m/s)
j_v	Volumetric current density (A/m ³)	u_{in}	Inlet velocity (m/s)

J	Leverett J-function	u_l	Liquid phase velocity (m/s)
K_{ab}	Absolute permeability (m ²)	u_m	Mixture average velocity (m/s)
$K_{r,g}$	Gas phase relative permeability	u_t^f	Free flow tangential velocity (m/s)
$K_{r,l}$	Liquid phase relative permeability	u_t^p	Porous medium tangential velocity (m/s)
λ^0	Limiting molar conductivity (S/m)	φ_l	Ionic phase potential (V)
M	Molar mass (kg/mol)	φ_s	Electronic phase potential (V)
μ	Dynamic viscosity (Pa·s)	z	Charge number

S1. Model Assumptions and Selection Reasons

To simplify the multi-physics coupling solution process and reduce the computational complexity and convergence difficulties of the model, the two-phase flow numerical model for the anion-exchange membrane water electrolysis cell (AEMWE) in this study was developed based on the following assumptions[1].

(1) The fluid flow within the electrolytic cell is in a laminar state with $Re < 2300$. The simulation system is in a steady state, where the distributions of all physical fields do not change with time, and the partial derivatives of physical quantities with respect to time are zero. Rationale: Under typical AEMWE channel dimensions and feed flow rates, the flow naturally falls within the laminar range. The steady-state assumption aligns with the stable operating conditions of the electrolyzer, which involves constant current and constant flow rate, thereby significantly reducing the number of control equations and lowering computational costs.

(2) Gaseous products such as H_2 and O_2 within the cell follow the ideal gas equation of state, neglecting intermolecular forces and the volume of the molecules themselves, while also neglecting water vapor evaporation from the electrolyte. Reason for selection: Under the standard low-temperature, low-pressure operating conditions of AEMWE, deviations in gaseous properties from those of an ideal gas are negligible, and water vapor evaporation is extremely low; this assumption simplifies the calculation of gaseous properties.

(3) Within the flow channel, the gas and liquid phases are in uniform flow; the flow velocities of the gaseous reaction products and the liquid electrolyte are equal, with no interphase slippage. Rationale: This assumption forms the core foundation of two-phase flow models for mixtures. It allows complex two-fluid models to be simplified into single-fluid mixture models, significantly reducing the difficulty of solving two-phase flow problems. Under normal operating conditions, bubble sizes are much smaller than the flow channel dimensions, ensuring good inter-phase tracking; errors caused by slip velocity remain within an engineering-acceptable range.

(4) The AEM membrane has an ample supply of liquid water; its internal pores are filled with water, maintaining a 100% saturated state at all times, ensuring stable ionic

conductivity. Reason for selection: This assumption avoids the need to introduce multi-mechanism water transport equations within the membrane, simplifying the membrane ionic conductivity to a constant value and greatly simplifying the coupled solution of the ionic conduction field; simultaneously, it aligns with the AEMWE's operating mode of excess electrolyte feed, eliminating the risk of membrane drying under normal operating conditions and preventing interference from moisture content fluctuations on electrochemical performance.

(5) AEM membranes exhibit excellent gas impermeability and electrical insulation; gas molecules cannot permeate the membrane, and electrons form a circuit solely through the external circuit. Rationale: The gas permeability coefficient and electronic conductivity of high-performance AEM membranes are extremely low; the effects of gas permeation and electronic leakage on electrolytic performance can be neglected.

(6) The entire electrolytic cell system is isothermal, with constant and uniform temperatures across all components. Reaction heat, frictional heat, and heat transfer processes are neglected, and temperature is treated as a constant boundary condition. Rationale: AEMWE is routinely equipped with a constant-temperature circulation control system; at low to medium current densities, heat generation is minimal, and the temperature distribution within the cell is uniform. This assumption eliminates the need to solve the energy conservation equation, avoids strong coupling between thermal, flow, electrical, and chemical fields, and significantly reduces model complexity.

(7) Ignore interfacial contact resistance between functional layers; layers are in close contact, and charge transport is influenced only by electrode polarization resistance and electrolyte ohmic resistance. Rationale: Under standardized hot-pressing and constant-torque assembly processes, interfacial contact resistance is far smaller than the bulk ohmic resistance and polarization resistance, and its impact on overall performance is negligible; this assumption simplifies the solution of the charge conservation equation and eliminates the interference of assembly process variations on simulation results.

(8) The effect of gravity on the flow of the gas-liquid mixture is not considered; fluid flow is driven solely by pressure gradients, viscous forces, and interphase forces between the gas and liquid phases. Rationale: Within the millimeter-scale channels of the AEMWE, the influence of gravity on the distribution of the two-phase flow is negligible; this

assumption simplifies the source terms of the momentum conservation equation and reduces the convergence difficulty and computational complexity of the flow field solution.

(9) The electrolyte is treated as an incompressible fluid, with constant physical properties such as density and viscosity, to simplify the solution of the momentum conservation equation. Rationale: Under ambient pressure conditions, the compressibility of the electrolyte is extremely low; the incompressibility assumption fully aligns with the physical characteristics of the liquid. Constant physical properties avoid nonlinear coupling between these parameters and multiphysics fields, significantly simplifying the solution of the continuity and momentum equations.

(10) Only the core electrolysis reaction of water decomposition is considered. In contrast, side reactions between bubbles and the electrolyte are neglected, and the focus is on the flow and mass-transfer characteristics of the gas-liquid two-phase system. Rationale: Under conditions of high-purity electrolyte and high-performance membranes, the current efficiency of the electrolytic cell can reach over 99%, making the impact of side reactions negligible; this assumption establishes a direct linear relationship between current density and reaction rate, simplifying the solution of electrochemical reaction kinetics.

(11) The channel walls are treated as smooth surfaces, disregarding wall roughness, and a no-slip boundary condition is adopted to simplify the calculation of flow resistance. Rationale: Under laminar flow conditions, the effect of wall roughness on flow is far smaller than that of viscous forces; the no-slip boundary condition is a classic and universal condition for laminar flow walls; this assumption reduces the need for mesh refinement in the near-wall region and simplifies the configuration of wall boundary conditions.

S2. Control Equations and Boundary Conditions

This section describes the coupled processes of “fluid flow—mass transfer—charge transport—electrochemical reaction” in AEM water electrolysis. The conservation equations are as follows[2]:

S2.1 Equations of Fluid Flow (for Solving the Velocity Field, Pressure Field, and Phase Fractions)

(1) Flow domain: Navier-Stokes equations (N-S equations)

The Navier-Stokes (N-S) equations govern the flow of fluid within the channel. Based on the assumption of a common velocity for the gas and liquid phases, a mixture model is employed to couple the mass conservation equations for the two phases into a single-phase, continuous-flow model with macroscopic properties. This is used to solve for the velocity, pressure, and volume fraction of each phase within the channel.

Continuity equation (mass conservation constraint)[1]:

$$\nabla \cdot (\rho_m u_m) = 0 \quad (S1)$$

Equations of motion (steady state, neglecting gravity):

$$\rho_m (u_m \cdot \nabla) u_m = \nabla \cdot [-pI + \mu_m (\nabla u_m + (\nabla u_m)^T) - \frac{2}{3} \mu_m (\nabla \cdot u_m) I] \quad (S2)$$

p is the pressure of the electrolyte, measured in Pa, describing the pressure distribution within the fluid. I represents the total pressure and the identity matrix. u_m is the average velocity, measured in m/s, describing the speed and direction of fluid flow. ρ_m and μ_m represent the density and dynamic viscosity of the mixture, respectively, determined using the average method and calculated using the following two equations. s_l is the liquid-phase volume fraction, and s_g is the gas-phase volume fraction. ρ_l is the liquid-phase density, and ρ_g is the gas-phase density. μ_l is the liquid-phase viscosity, and μ_g is the gas-phase viscosity.

$$\rho_m = s_l \rho_l + s_g \rho_g \quad (S3)$$

$$\mu_m = s_l \mu_l + s_g \mu_g \quad (S4)$$

(2) Electrode Region: Darcy's Law (Equation of Flow in Porous Media)

Continuity Equation (Conservation of Mass in Porous Media):

$$\nabla \cdot (\rho_m u_m) = R_{lg} \quad (S5)$$

Velocity-based Darcy correction (phase-by-phase correction, followed by coupling the Darcy flow rates of the two phases back into the mixed-phase flow velocity):

$$u_l = -\frac{\kappa_{r,l}}{\mu_l} \kappa_{ab} \nabla p_l \quad (S6)$$

$$u_g = -\frac{\kappa_{r,g}}{\mu_g} \kappa_{ab} \nabla p_g \quad (S7)$$

$$u_m = \frac{s_l \rho_l u_l + s_g \rho_g u_g}{\rho_m} \quad (S8)$$

R_{lg} represents the mass transfer rate from the liquid phase to the gas phase; its specific expression is shown in Table S2. $\kappa_{r,g}$ and $\kappa_{r,l}$ represent the relative permeability of the gas and liquid phases, respectively. κ_{ab} represents the absolute permeability, which describes the electrode's ability to allow electrolyte passage, and is calculated using the method described in Reference[3]. d represents the pore diameter, describing the size of a single pore in the electrode. p_g represents the gas pressure, and p_l represents the liquid pressure.

$$\kappa_{r,l} = s_l^3 \quad (S9)$$

$$\kappa_{r,g} = s_g^3 \quad (S10)$$

$$\frac{\kappa_{ab}}{d^2} = \frac{\varepsilon [1 - (1 - \varepsilon)^{\frac{1}{3}}]^2}{36 [(1 - \varepsilon)^{\frac{1}{3}} - (1 - \varepsilon)]} \quad (S11)$$

In porous media, the pressure difference between the liquid and gas phases is calculated using the Leverett J-function, and the calculation of capillary pressure is as follows[4]:

$$p_c = p_g - p_l \quad (S12)$$

$$p_c = \sigma \cos(\theta) \left(\frac{\varepsilon}{\kappa_{ab}} \right) J(s_l) \quad (S13)$$

$$J(s_l) = \begin{cases} 1.417(1 - s_l) - 2.120(1 - s_l)^2 + 1.263(1 - s_l)^3 & \theta < 90^\circ \\ 1.417s_l - 2.120s_l^2 + 1.263s_l^3 & \theta > 90^\circ \end{cases} \quad (S14)$$

In this context, σ and θ represent the surface tension coefficient and the contact angle, respectively.

Table S2. Source terms

Source terms	Expression	Unit
Reaction rate of potassium hydroxide	$R_{OH} = \begin{cases} -j_v/F & AGDE \\ -j_v/F & CGDE \end{cases}$	mol/m ³ /s
rate of gas formation	$R_{lg} = \begin{cases} j_v M_{O_2}/4F & AGDE \\ -j_v M_{H_2}/2F & CGDE \end{cases}$	kg/m ³ /s

S2.2 Mass Transfer Control Equation (for Solving the Concentration Field of Components)

(1) Flow channel region: Convection-flux equation

For K⁺, OH⁻, and H₂O in the electrolyte, the convection-flux equations are used to derive the concentrations of all other liquid-phase components based on the OH⁻ concentration, ultimately determining the concentration distributions of each key component within the computational domain. The equation for calculating the OH⁻ concentration in the electrolyte (steady-state, strong solution model[5]) is:

$$\nabla \cdot j_{OH} + u_l \cdot \nabla c_{OH} = 0 \quad (S15)$$

$$j_{OH} = -D_{e,OH} \nabla c_{OH} - \frac{i_l t_{OH}}{F} \quad (S16)$$

Equation for calculating the K⁺ concentration in an electrolyte (electrochemical neutrality equation):

$$z_{OH} c_{OH} + z_{K^+} c_{K^+} = 0 \quad (S17)$$

Equation for calculating the concentration of water molecules in an electrolyte:

$$c_w = [\rho_l - c_l(M_{K^+} + M_{OH^-})]/M_w \quad (S18)$$

The effective overall diffusion coefficient $D_{e,OH}$ is calculated using the Bruggeman correction:

$$D_{e,OH} = D_{OH} s_l^{1.5} \quad (S19)$$

c_{OH} is the concentration of OH⁻. i_l is the liquid-phase current density. F is Faraday's constant. t_{OH} is the mobility of OH⁻ relative to the mass-averaged velocity, calculated as shown in Equation (S20). t_{OH}^0 represents the migration number of OH⁻ in an infinitely dilute

solution; the calculation is given in Equation (S50). z_{OH^-} and z_{K^+} are the charge numbers of OH^- and K^+ , respectively, with values of -1 and +1; c_{OH^-} and c_{K^+} are the molar concentrations of OH^- and K^+ , respectively. c_w is the concentration of water; ρ_l is the density of the KOH solution; D_{OH} is the bulk diffusion coefficient of KOH.

$$t_{OH} = w_K + w_w t_{OH}^0 \quad (S20)$$

(2) Electrode region: Convection-flux equation (modified equation for porous media and reaction source term)

Since the electrodes are porous media, a porosity correction is required. The distribution of OH^- is the primary consideration; the calculation of other components is as described above. The convection-diffusion equation for OH^- concentration in porous media is:

$$\nabla \cdot j_{OH} + u \cdot \nabla c_{OH} = R_{OH} \quad (S21)$$

$$j_{OH} = -D_{e,OH} \nabla c_{OH} - \frac{i_l t_{OH}}{F} \quad (S22)$$

The effective overall diffusion coefficient $D_{e,OH}$ is calculated using the Bruggeman correction:

$$D_{e,OH} = D_{OH} \varepsilon^{1.5} s_l^{1.5} \quad (S23)$$

ε is the porosity of the porous medium; s_l is the volume fraction of the liquid phase; D_{OH} is the overall diffusion coefficient of KOH; R_{OH} is the reaction rate of OH^- (Table S2)

(3) Membrane region: Flux equation (no flow, only ion transport)

There is no convection within the membrane; ion transport is the primary mechanism. The distribution of OH^- is accounted for; the remaining components are as described above.

Convection-diffusion equation for the concentration of OH^- in the membrane:

$$\nabla \cdot j_{OH} = 0 \quad (S24)$$

$$j_{OH} = -D_{e,OH} \nabla c_{OH} - \frac{i_l t_{OH}}{F} \quad (S25)$$

The effective overall diffusion coefficient $D_{e,OH}$ is calculated using the Bruggeman correction:

$$D_{e,OH} = D_{OH}\varepsilon_m^{1.5} \quad (S26)$$

ε_m is the porosity of the membrane.

S2.3 Equations Governing Charge Transport (for Solving the Electric Potential Field and Current Density Field)

Charge transport is divided into electron transport within the electrode and ion transport within the electrolyte and membrane.

(1) Plate region: Electron transport equation

In a conductive nickel plate, electron transport within the electrode follows Ohm's law, and there is no accumulation of electrons during steady-state conditions (charge conservation). The Laplace equation (without a charge source term) is used to solve for the electron potential φ_s and electron current density i_s in the BP plate.

Ohm's Law (Steady State):

$$\nabla \cdot i_s = \nabla \cdot (-\sigma_s \nabla \varphi_s) = 0 \quad (S27)$$

s denotes the electronic phase. σ_s denotes the intrinsic conductivity of nickel. φ_s is the potential within the nickel material.

(2) Flow channel region: Ion transport equation

The transport of ions within the flow channel follows Ohm's law; the solution current consists of both the current resulting from the potential difference and the current resulting from ion migration. Furthermore, during steady-state conditions, there is no accumulation and no charge source term. This section determines the ionic potential φ_l and the ionic current density i_l of the electrolyte within the flow channel.

Ohm's Law (considering potential difference and ionic migration, steady state)[6]:

$$\nabla \cdot i_l = \nabla \cdot \left(-\sigma_l \nabla \varphi_l - \frac{2\sigma_l RT}{F} \left(1 + \frac{\partial \ln \gamma}{\partial \ln c_K} \right) \left(t_K + \frac{c_K}{c_w} \right) \nabla \ln c_K \right) = 0 \quad (S28)$$

l represents the ionic phase. σ_l represents the intrinsic conductivity of the KOH solution. φ_l is the potential of the KOH solution. γ is the average activity coefficient of KOH;

c_w is the concentration of water.

(3) Electrode region: Modified electron transport and ion transport equations for the porous medium in which the reaction takes place

Both electron transport and ion transport occur within the electrode. Since the electrode is itself a porous medium, a porous-medium correction is required. Additionally, electrochemical reactions alter the current, so a source term is added to the right-hand side of the equation. This section is used to solve for the electron potential φ_s and electron current density i_s within the electrode, as well as the corresponding ion potential φ_l and ion current density i_l .

$$\nabla \cdot i_l = \nabla \cdot \left(-\sigma_{e,l} \nabla \varphi_l - \frac{2\sigma_{e,l}RT}{F} \left(1 + \frac{\partial \ln \gamma}{\partial \ln c_K} \right) \left(t_K + \frac{c_K}{c_w} \right) \nabla \ln c_K \right) = j_v \quad (S29)$$

$$\nabla \cdot i_s = \nabla \cdot (-\sigma_{e,s} \nabla \varphi_s) = -j_v \quad (S30)$$

The effective electronic conductivity $\sigma_{e,s}$ and ionic conductivity $\sigma_{e,l}$ are calculated using the Bruggeman correction:

$$\sigma_{e,l} = \sigma_l \varepsilon^{1.5} s_l^{1.5} \quad (S31)$$

$$\sigma_{e,s} = \sigma_s (1 - \varepsilon)^{1.5} \quad (S32)$$

ε is the porosity of the porous electrode. j_v is the current source term, calculated as described in Section 2.4 below.

(4) Membrane region: Modified electron transport and ion transport equations for porous media

The transport of ions within the flow channel follows Ohm's law; the solution current consists of both the current resulting from the potential difference and the current resulting from ion migration. Additionally, since there is no gas in the membrane region, the calculation is corrected for the membrane porosity. This section determines the membrane ionic potential φ_l and the ionic current density i_l .

Ohm's Law:

$$\nabla \cdot i_l = \nabla \cdot \left(-\sigma_{e,l} \nabla \varphi_l - \frac{2\sigma_{e,l}RT}{F} \left(1 + \frac{\partial \ln \gamma}{\partial \ln c_K} \right) \left(t_K + \frac{c_K}{c_w} \right) \nabla \ln c_K \right) = 0 \quad (S33)$$

The effective ionic conductivity $\sigma_{e,l}$ is calculated using the Bruggeman correction:

$$\sigma_{e,l} = \sigma_l \varepsilon_m^{1.5} \quad (S34)$$

ε_m is the porosity of the membrane.

S2.4 Equations for Controlling Electrochemical Reactions (Solving for Reaction Rate and Current Density)

Using the BV equation corrected for concentration and gas fraction, determine the electrochemical reaction rates and reaction current densities at the anode and cathode interfaces.

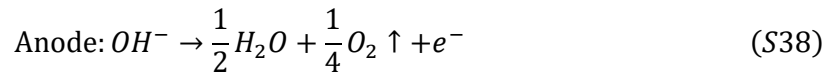
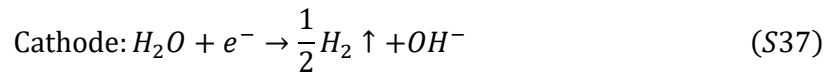
The Butler–Volmer equation[6,7] (corrected for concentration and gas fraction):

$$\begin{aligned} i_{loc} &= s_l i_{0,T} \left[C_R \exp\left(\frac{\alpha_f F \eta_{ref}}{RT}\right) - C_O \exp\left(\frac{-(1 - \alpha_f) F \eta_{ref}}{RT}\right) \right] \\ &= s_l i_0 \left[\exp\left(\frac{\alpha_f F \eta}{RT}\right) - \exp\left(\frac{-(1 - \alpha_f) F \eta}{RT}\right) \right] \end{aligned} \quad (S35)$$

$$i_0 = i_{0,T} C_R^{\alpha_f} C_O^{(1-\alpha_f)} \quad (S36)$$

Here, α_f is the forward transfer coefficient of the electrode reaction. i_0 is the exchange current density under actual conditions. $i_{0,T}$ is the temperature-corrected exchange current density. The other parameters are broken down into the following components.

(1) Concentration correction term (concentration ratio)



The ratio of the concentrations of the reduced and oxidized species in the cathode and anode reactions, C_R and C_O (refer to the chemical equation for the subscripts):

$$C_{R,c} = \left(\frac{c_{OH,c}}{c_{OH,ref}} \right) \left(\frac{P_{H_2}}{P_{H_2,ref}} \right)^{0.5}, C_{R,a} = \left(\frac{c_{OH,a}}{c_{OH,ref}} \right) \quad (S39)$$

$$C_{O,c} = \left(\frac{c_{w,c}}{c_{w,ref}} \right), C_{O,a} = \left(\frac{c_{w,a}}{c_{w,ref}} \right)^{0.5} \left(\frac{P_{O_2}}{P_{O_2,ref}} \right)^{0.25} \quad (S40)$$

Where: $C_{R,c}$: concentration correction factor for the cathode reduction reaction (used to correct for concentration effects related to the cathode reaction). $C_{OH,c}$: actual molar concentration of hydroxide ions (OH⁻) at the cathode. $C_{OH,ref}$: reference molar concentration of hydroxide ions (OH⁻) (comparison concentration). P_{H_2} : The actual partial pressure of hydrogen (H₂). $P_{H_2,ref}$: The reference partial pressure of hydrogen (H₂) (comparison baseline). $C_{R,a}$: The concentration correction factor for the anode reduction reaction (used to correct for concentration effects related to the anode reaction). $C_{O,c}$: The concentration correction factor for the cathode oxidation reaction (used to correct for concentration effects related to the cathodic oxidation reaction). $c_{w,c}$: Actual molar concentration of water molecules (H₂O) at the cathode. $c_{w,ref}$: Reference molar concentration of water molecules (H₂O) (comparison concentration). $C_{O,a}$: Concentration correction factor for the anodic oxidation reaction (used to correct for concentration effects related to the anodic oxidation reaction). $c_{w,a}$: Actual molar concentration of water molecules (H₂O) at the anode. P_{O_2} : Actual partial pressure of oxygen (O₂). $P_{O_2,ref}$: Reference partial pressure of oxygen (O₂) (comparison baseline).

(2) Equilibrium electrode potential (temperature + concentration difference)

The temperature-corrected equilibrium electrode potential $E_{eq,T}$ and the actual equilibrium electrode potential E_{eq} serve as the basis for calculating overpotentials. In conjunction with the Nernst equation:

$$E_{eq,T} = E_{eq,ref} + \frac{dE_{eq}}{dT} (T - T_{ref}) \quad (S41)$$

$$E_{eq} = E_{eq,T} - \frac{RT}{F} \ln \frac{C_R}{C_O} \quad (S42)$$

Here, $E_{eq,ref}$ is the equilibrium electrode potential under reference conditions (reference concentration c_{ref} and reference temperature T_{ref}). dE_{eq}/dT is the temperature coefficient of the equilibrium electrode potential, and T is the actual temperature.

(3) Activation overpotential (temperature + concentration gradient)

Corresponding to the equilibrium potential, the temperature-corrected activation overpotential η_{ref} and the actual activation overpotential η :

$$\eta_{ref} = \varphi_s - \varphi_l - E_{eq,T} \quad (S43)$$

$$\eta = \varphi_s - \varphi_l - E_{eq} \quad (S44)$$

(4) Gas fraction and intrinsic current:

Bubbles occupy the electrode's effective surface area, and this area is influenced by the liquid volume fraction. The effective exchange current density $i_{e,0,T}$ is given by[8,9]:

$$i_{e,0,T} = i_{0,T} S_l \quad (S45)$$

$$i_{0,T} = i_{0,ref} \left[-\frac{E_{act}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right] \quad (S46)$$

Here, $i_{0,ref}$ is the intrinsic exchange current density at the reference temperature, and E_{act} is the activation energy of the electrode reaction.

(5) From surface density to bulk density:

j_v is the current density, i.e., the local current source. The specific surface area of the electrode, a_v (1/m), is calculated using the method described in Reference[10]. For the distribution of the activated specific surface area of the electrodes, refer to Sections 6 and 7.

$$j_v = i_{loc} a_v \quad (S47)$$

$$a_v = \frac{0.7531}{d} \left[(1 - \varepsilon)^{\frac{1}{2}} - (1 - \varepsilon) \right] (1 - \varepsilon)^{-0.2267} \quad (S48)$$

S2.5 Boundary Conditions

The boundary conditions for this simulation model are set as follows:

(1) Boundary conditions for fluid flow

Anode/Cathode Channel Inlet Boundary: Velocity Inlet, inlet velocity $u_{in} = 0.01$ m/s, with the velocity direction aligned with the channel length (x-direction). Rationale: Based on the electrolyte circulation velocity in the experiment, this ensures stable fluid flow within the channel and prevents turbulence caused by excessively high or low velocities.

Anode/Cathode Channel Outlet Boundary: Pressure Outlet, outlet pressure $P_{out} = 0$ (gauge pressure). Rationale: In the experiment, the outlet of the electrolytic cell is open to

the outside environment, resulting in a gauge pressure of 0, which aligns with actual experimental conditions.

Electrolytic cell walls and membrane interface: No-slip boundary condition, with flow velocity $u = 0$; rationale: The walls and membrane are fixed solids, and there is no relative sliding between the electrolyte and the walls.

Electrode-channel interface: The Beavers-Joseph-Saffman (B-J-S) boundary condition is applied; the governing equations are as follows:

$$\frac{\partial \mathbf{u}_t^f}{\partial n} = \frac{\alpha_\beta}{\sqrt{\kappa_{ab}}} (\mathbf{u}_t^f - \mathbf{u}_t^p) \quad (S49)$$

Here, $\mathbf{u}_t^f$ denotes the tangential velocity in the flow channel, $\mathbf{u}_t^p$ denotes the tangential velocity at the electrode, $\partial \mathbf{u}_t^f / \partial n$ denotes the gradient of the flow channel tangential velocity with respect to the normal at the interface, κ_{ab} denotes the absolute permeability of the electrode, and α_β denotes the Beavers-Joseph empirical constant, for which the value of 4.0 from the literature[11] is adopted.

(2) Mass transfer boundary conditions

Anode/cathode flow channel inlet boundary: Inlet concentration of components; OH^- concentration $c_{in} = 1 \text{ mol/L}$. Basis for setting: The electrolyte used in the experiment is a 1 mol/L KOH solution.

Anode/Cathode Channel Outlet Boundary: Convective Outlet, $\nabla c_{out} \cdot n = 0$ (where n is the normal vector of the outlet boundary). Rationale: The concentration of the component at the outlet is unconstrained and is freely discharged with the fluid flow, consistent with actual flow conditions.

Electrode-membrane interface: OH^- is permeable, H_2O is permeable, H_2 and O_2 are impermeable. Rationale: The core function of an AEM is to allow OH^- to pass through while permitting H_2O permeation, and to prevent the cross-permeation of electrolysis products (H_2 and O_2), thereby avoiding side reactions.

Electrode-to-channel interface: Free mass transfer of components; no abrupt changes in concentration gradients. Rationale: There is no mass transfer resistance at the

interface, allowing components to move freely between the channels and the electrodes, consistent with actual mass transfer principles.

Electrolyzer wall: Zero-flux boundary; components cannot pass through. Rationale: The wall is a dense solid that does not allow any components to pass through, ensuring that mass transfer occurs only within the computational domain.

(3) Charge transport boundary conditions

Anode plate interface (connected to the external circuit): Constant current density boundary, $i_s = I_{cell}$. Rationale: In the experiment, a constant current is applied via an external power source; this boundary condition aligns with experimental reality and ensures the driving force for the electrochemical reaction.

Cathode plate interface (connected to the external circuit): Grounded boundary, $\sigma_s = 0$ V. Rationale: To simplify the solution, the cathode electron potential is set to the reference potential (0 V), ensuring the uniqueness of the potential field solution.

Electrode-membrane interface: Charge continuity boundary, $i_s \cdot n = i_l \cdot n$. Rationale: The electron current density and ion current density are continuous at the interface, satisfying the law of charge conservation and ensuring the coupling of electrochemical reactions and charge transport.

Electrolyzer wall: Insulating boundary, $i_s \cdot n = 0$, $i_l \cdot n = 0$. Rationale: The wall is made of insulating material that does not conduct electrons or ions, preventing charge leakage and reflecting actual conditions.

(4) Phase-transfer boundary

Anode/cathode channel inlet boundary: Gas fraction inlet, gas fraction $n_{s,g,in} = 0.01$. Rationale: Only a small amount of gas is present in the circulation, and setting a small value facilitates convergence.

Anode/Cathode Outlet Boundary: Free outlet for gas fraction, $\nabla s_{out} \cdot n = 0$ (where n is the normal vector of the outlet boundary). Rationale: The gas fraction at the outlet is unconstrained and is freely discharged with the fluid flow, consistent with actual flow conditions.

Interface between the electrode and the flow channel: Gases and liquids pass through freely. Basis for the setting: Porous media are unobstructed, allowing free passage.

The relevant parameters used in this physical model are summarized in Supplementary Table 3.

S3. Model Parameters and Solution Methods

The model was solved using COMSOL Multiphysics 6.3. The relative error of the solver was set to 10^{-4} . The solution process was divided into three parts: first, the initial current distributions for the first and second stages were calculated; then, the solution of the momentum transfer equation was obtained; and finally, using these results as initial conditions, a fully coupled solution was performed for all transfer processes.

The material properties relevant to the model are as follows: For the gas phase and liquid phase, the density ρ_k and viscosity μ_k are obtained from the COMSOL Material Library. The intrinsic conductivity σ_l of the KOH solution is calculated using the correlation equation by Gilliam et al.[12]. The average activity coefficient γ of KOH is calculated using the correlation equation by Akerlof et al.[13]. The ionic mobility numbers t_K^0 and t_{OH}^0 for infinitely dilute solutions of K^+ and OH^- are both calculated from the limiting molar conductivities of the ions:

$$t_K^0 = \frac{\lambda_K^0}{\lambda_K^0 + \lambda_{OH}^0}, t_{OH}^0 = \frac{\lambda_{OH}^0}{\lambda_K^0 + \lambda_{OH}^0} \quad (S50)$$

The limiting molar conductivities λ_K^0 and λ_{OH}^0 were calculated using the relationship proposed by Robinson et al.[14]. The bulk diffusion coefficient D_{OH} of KOH was calculated using the relationship proposed by De Vidts et al.[15].

The electrical conductivity, Faraday constant, and gas constant of solid nickel were obtained from the COMSOL material library. The electrode reaction kinetic parameters are listed in Table S3.

Table S3. Electrochemical reaction kinetic parameters

Parameters	value	
	cathode	anode
Reference concentration of potassium hydroxide, $c_{OH,ref}/(\text{mol/L})$	1	1
Reference concentration in water, $c_{w,ref}/(\text{mol/L})$	54.933	54.933
Reference pressure, $P_{ref}/(\text{atm})$	1	1
Reference temperature, $T_{ref}/(\text{K})$	298. 15	298. 15
Reference equilibrium electrode potential[16], $E_{eq,ref}/(\text{V})$	-0.828	0.4011
Temperature coefficient of the equilibrium electrode potential[16], $(dE_{eq}/dT)/(\text{mV/K})$	-0.836	-1.682
Reference exchange current density[17], $i_{0,ref}/(\text{mA/cm}^2)$	7000	0.015
Activation energy[17], $E_{act}/(\text{kJ/mol})$	29.5	12.0
Forward transmission coefficient[17], α_f	0.5	0.96

The boundary conditions for the model solution are listed in Table S4.

Table S4. Reference Conditions

Parameters	Symbol	unit	value
Inlet flow velocity	u_{in}	m/s	0.01
Concentration of the potassium hydroxide solution at the inlet	c_{in}	mol/L	1
Volume fraction of inlet gas	$S_{g,in}$		0.01
Operating temperature	T	°C	80
Average porosity of the electrode	ε		0.75
Membrane porosity[18]	ε_m		0.41
Average pore size	d	mm	0.14
Contact angle[19]	θ	°	80
Surface tension coefficient[20]	σ	N/m	0.0732

S4. Model Validation

S4.1 Testing Platform and Model Validation

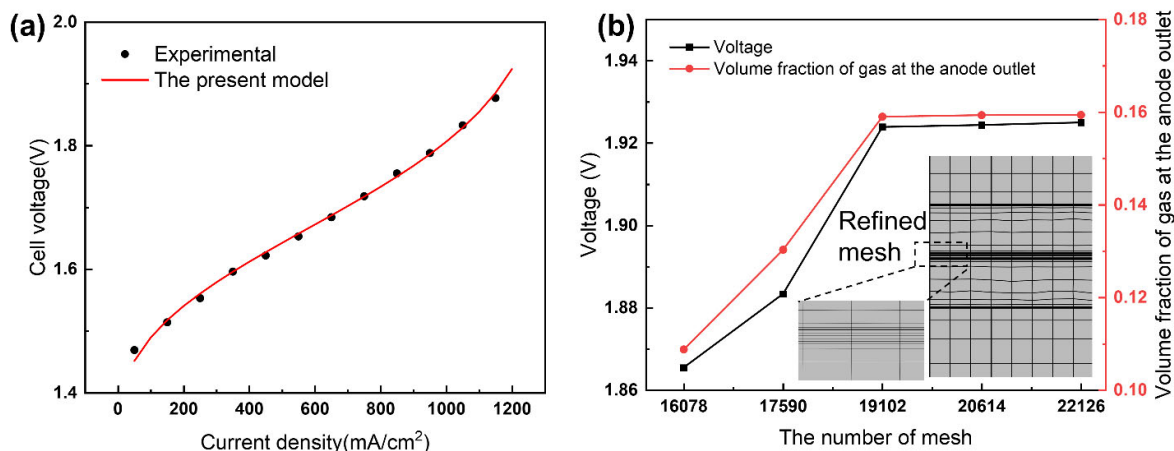


Figure S1 (a) Comparison of simulated and measured polarization curves (in-house experiment) (b) Grid distribution and independence verification results

In this study, a custom-built single-cell testing platform for anion-exchange membrane water electrolysis (AEMWE) was established to characterize the anode electrode performance. The setup, based on Reference [21], was assembled by hot-pressing in the following order: a custom-made NiFe anode catalyst, a commercial anion-exchange membrane, and a Pt/C cathode catalyst layer. Equipped with a potentiostat, an electrolyte circulation system, and a temperature control module, the setup enables simultaneous testing of electrolysis performance and oxygen evolution efficiency. Testing was conducted at 80°C using 1 mol L⁻¹ KOH as the electrolyte. Polarization curves of the single cell were obtained via linear voltammetric scanning to analyze the electrolysis performance of the anode electrode with varying porosity gradients.

By comparing the experimental results of battery voltage as a function of current density with the model's predicted curves, the validity and reliability of the constructed model were verified, providing a theoretical foundation for future research. Supplementary Figure S1(a) shows a comparison between the experimentally measured battery voltage versus current density and the predicted curve from the model developed in this study. As shown in the figure, the battery voltage increases gradually with increasing current density, consistent with the voltage-current response characteristics of electrochemical systems. It can also be observed that the model's predicted curve exhibits a high degree of consistency

with the experimental data points: across all current density ranges (0–1200 mA/cm²), the average relative error between the model's predicted values and the experimental values is 0.45%, with the maximum error not exceeding 1%. This validates the model's validity, and the predicted voltage trend also aligns well with the experimental measurements. This agreement fully validates the model established in this paper for describing the voltage-current density relationship of this electrochemical system, providing effective theoretical support for subsequent research, such as performance analysis and parameter optimization, based on this model.

S4.2 Mesh Partitioning and Independence Study

The computational domain of the AEMWE includes the flow channels on the plane, the electrodes, and the anion-exchange membrane. The entire domain adopts a rectangular grid system, and each functional layer uses a different baseline grid size. In key areas with significant physical field gradients, including the membrane-electrode interface, the flow channel-electrode interface, the entire AEM domain, and the flow channel inlet and outlet, local grid refinement was performed; the detailed fine grid of the core reaction zone is shown in Figure S1(b). This optimization strategy ensures accurate analysis of electrochemical reaction kinetics, interfacial charges, and mass transfer, as well as the two-phase flow of gas and liquid within the cell.

Through grid-independent validation, the optimal number of grids for subsequent numerical simulations is determined, balancing computational accuracy and resource efficiency. Figure S1(b) presents the results of the grid independence verification, illustrating the variation in cell voltage and the anode outlet gas volume fraction with different numbers of grid cells. When the number of grid cells increases from 16,078 to 19,102, both the voltage and the volume fraction of gas at the anode outlet exhibit significant changes, indicating that insufficient grid resolution at this stage can lead to computational errors; However, when the number of grid cells is further increased ($\geq 19,102$), the change in cell voltage is less than 1 mV, and the change in the volume fraction of gas at the anode outlet is less than 0.01. Both the voltage and the gas volume fraction at the anode outlet tend to stabilize, no longer exhibiting significant fluctuations as the grid cell count increases. The above results demonstrate that when the number of grid cells reaches 19,102, the computational results satisfy the grid-independence requirement (i.e., the results are independent of the grid size). Therefore, adopting a grid system with 19,102

grid cells in subsequent numerical simulation studies can effectively avoid wasting computational resources due to excessive grid refinement while ensuring computational accuracy.

S5. The Effect of Porosity Gradient Distribution and Pore Size Distribution on the Distribution of Active Specific Surface Area

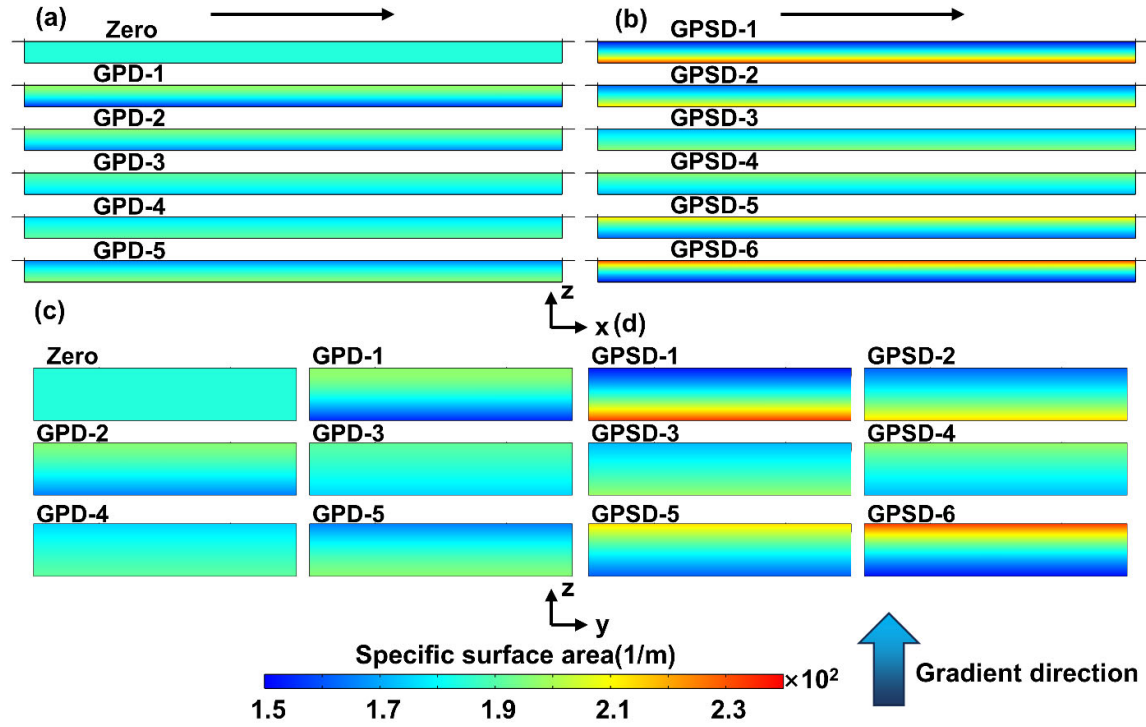


Figure S2 (a) Frontal specific surface area for different porosity gradients; (b) Frontal specific surface area for different pore size gradients; (c) Lateral specific surface area for different porosity gradients; (d) Lateral specific surface area for different pore size gradients ($i_{cell} = 1.2 \text{ A/cm}^2$)

Figure S2 shows the two-dimensional distribution of the active specific surface area within the water-electrolysis anode for structures with different gradient porosity (GPD series) and gradient pore size (GPSD series) at a current density of 1.2 A/cm². The calculation formula is given in Equation (48).

As shown in Figures S2 (a) and (b), the active specific surface area of all structures exhibits no significant fluctuations along the flow direction (x-direction) and remains uniformly distributed. This indicates that the electrolyte flow does not alter the electrode's inherent distribution of active specific surface area; its distribution characteristics are entirely controlled by the gradient design of porosity and pore size. A comparison of the distribution differences among structures with varying gradients reveals that the design of gradient porosity and gradient pore size enables precise control over the distribution of active specific surface area along the electrode thickness direction (z-direction). For the

GPD series, GPD-1 (with porosity increasing from the membrane side to the flow channel side) exhibits a gradient distribution of active specific surface area, decreasing from the membrane side to the flow channel side, with the lowest surface area at the membrane side and the highest at the flow channel side. As the gradient of decreasing porosity intensifies, the direction of the specific surface area gradient reverses; the active specific surface area of GPD-5 exhibits a distribution characterized by a significant increase from the membrane side to the flow channel side. The GPSD series, however, differs from the GPD series. For GPSD-1 (where pore size increases from the membrane side to the flow channel side), the active specific surface area decreases along the electrode thickness from the membrane side to the flow channel side as the pore-size-decrease gradient intensifies (from GPSD-1 to GPSD-6). The high-specific-surface-area region on the flow channel side continues to expand, and GPSD-6 exhibits a strong increasing gradient in active specific surface area, with lower values on the membrane side and higher values on the flow channel side.

Figures S2 (c) and (d) provide a clearer view of the gradient distribution of the active specific surface area along the electrode thickness. The active specific surface area of the gradient-free uniform structure (Zero) is uniformly distributed across the electrode thickness, with no significant gradient. For GPSD-5 and GPSD-1, the high-surface-area regions are concentrated on the membrane side and gradually decrease toward the flow channel side along the z-direction, closely matching the primary electrochemical reaction zone (the membrane-electrode interface). In contrast, for GPSD-1 and GPSD-6, the high-surface-area regions are concentrated on the flow channel side and gradually decrease toward the membrane side along the z-direction, resulting in a spatial misalignment with the core reaction zone.

S6. The Effect of Synergetic Gradient Distribution of Active Specific Surface Area

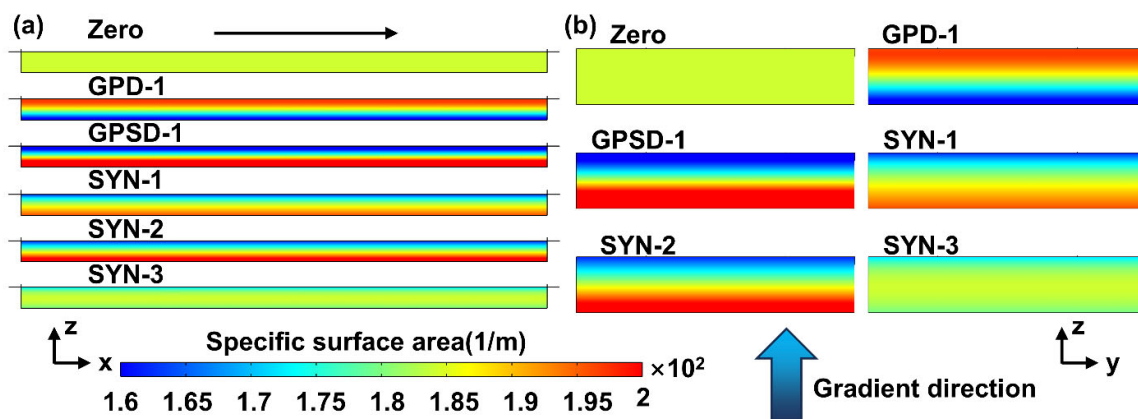


Figure S3 (a) Specific surface area of the synergistic gradient (front side) (b) Specific surface area of the synergistic gradient (side) ($I_{cell} = 1.1 \text{ A/cm}^2$)

Figure S3 presents the two-dimensional specific surface area distributions of uniform, single-gradient and synergistic gradient electrodes at 1.1 A/cm^2 , including the x-z front view (a) and y-z side view (b). The color scale, in units of m^{-1} , quantitatively characterizes the spatial heterogeneity of active-site density across different gradient structures.

As shown in the front-view distribution (Figure S3(a)), the traditional uniform structure (Zero) exhibits a uniform distribution across the electrode thickness. This homogeneous topological structure cannot simultaneously meet the conflicting requirements of “high reactivity near the membrane side” and “high mass transfer permeability on the flow channel side” under high-current-density conditions. Single-parameter gradient designs have limited control dimensions, making it difficult to achieve optimal matching between the active interface and the fluid channel. In contrast, the porosity-pore size synergistic gradient structure (SYN series) achieves precise, coordinated optimization of the SSA distribution. Among these, the SSA distribution of the SYN-1 configuration best meets performance requirements. The membrane side maintains a high density of active sites to ensure kinetic performance, while the SSA on the flow channel side is significantly reduced to maximize fluid transport capacity. Additionally, the distribution along the flow direction is smooth and free of abrupt changes, effectively mitigating the risk of local polarization. SYN-2 and SYN-3 further demonstrate the ability of gradient topologies to control SSA distribution finely; by adjusting the rate of gradient

change, a dynamic balance between active-site distribution and mass-transfer resistance can be achieved.

The cross-sectional distribution (Figure S3(b)) indicates that the SSA of the uniform structure (Zero) is uniformly distributed in the transverse (y-direction) and lacks structural differentiation. In contrast, both the single-gradient and synergistic-gradient structures achieve a good gradient along the thickness (z-direction), with the SYN series maintaining an optimal longitudinal gradient while exhibiting a more uniform transverse distribution. This prevents bubble retention due to excessively high local activity or insufficient reaction due to excessively low local activity.

S7. Specific energy consumption

For the AEMWE system in this work, the lowest cell voltage of SYN-1 necessarily implies higher energy efficiency and lower hydrogen-production energy consumption. The detailed theoretical basis, calculation formulas and quantitative results are supplemented below.

Specific energy consumption (kWh/kg H₂):

$$SEC = \frac{2 \times F \times E_{\text{cell}}}{M_{\text{H}_2} \times 3.6 \times 10^6} \approx 26.58 \times E_{\text{cell}} \quad (S51)$$

where $F = 96487 \text{ C/mol}$ (Faraday's constant), $M_{\text{H}_2} = 0.002016 \text{ kg/mol}$ (molar mass of hydrogen), E_{cell} is the steady-state cell voltage at 1100 mA/cm^2 .

The quantitative calculation results at the core operating condition (1100 mA/cm^2) are as follows:

Table S5. Specific Energy Consumption (kWh/kg H₂)

Sample	Cell Voltage (V)	Specific Energy Consumption (kWh/kg H ₂)
Conventional uniform anode (Base case)	1.854	49.28
SYN-1 (optimal gradient design)	1.812	48.16

Compared with the conventional uniform anode, SYN-1 reduces the specific energy consumption of hydrogen production by 2.27%

References

1. Lee, J.; Alam, A.; Park, C.; Yoon, S.; Ju, H. Modeling of Gas Evolution Processes in Porous Electrodes of Zero-Gap Alkaline Water Electrolysis Cells. *Fuel* **2022**, *315*, 123273, doi:10.1016/j.fuel.2022.123273.
2. Wu, L.; Zhang, G.; Xie, B.; Tongsh, C.; Jiao, K. Integration of the Detailed Channel Two-Phase Flow into Three-Dimensional Multi-Phase Simulation of Proton Exchange Membrane Electrolyzer Cell. *International Journal of Green Energy* **2021**, *18*, 541–555, doi:10.1080/15435075.2020.1854270.
3. Yang, X.; Bai, J.; Lu, T. A Simplistic Analytical Model of Permeability for Open-Cell Metallic Foams. *Chin. J. Theor. Appl. Mech.* **2014**, *46*(6), 982–986. <https://doi.org/10.6052/0459-1879-14-115>
4. Han, B.; Mo, J.; Kang, Z.; Yang, G.; Barnhill, W.; Zhang, F.-Y. Modeling of Two-Phase Transport in Proton Exchange Membrane Electrolyzer Cells for Hydrogen Energy. *International Journal of Hydrogen Energy* **2017**, *42*, 4478–4489, doi:10.1016/j.ijhydene.2016.12.103.
5. Zhou, G.; Chen, L.-D.; Seaba, J.P. Effects of Property Variation and Ideal Solution Assumption on the Calculation of the Limiting Current Density Condition of Alkaline Fuel Cells. *Journal of Power Sources* **2011**, *196*, 4923–4933, doi:10.1016/j.jpowsour.2011.02.026.
6. Tardy, E.; Bultel, Y.; Druart, F.; Bonnefont, A.; Guillou, M.; Latour, B. Three-Dimensional Modeling of Anion Exchange Membrane Electrolysis: A Two-Phase Flow Approach. *Energies* **2024**, *17*, 3238, doi:10.3390/en17133238.
7. Falcão, D.S.; Pinto, A.M.F.R. A Review on PEM Electrolyzer Modelling: Guidelines for Beginners. *Journal of Cleaner Production* **2020**, *261*, 121184, doi:10.1016/j.jclepro.2020.121184.
8. Olesen, A.C.; Frensch, S.H.; Kær, S.K. Towards Uniformly Distributed Heat, Mass and Charge: A Flow Field Design Study for High Pressure and High Current Density Operation of PEM Electrolysis Cells. *Electrochimica Acta* **2019**, *293*, 476–495, doi:10.1016/j.electacta.2018.10.008.
9. Suermann, M.; Schmidt, T.J.; Büchi, F.N. Comparing the Kinetic Activation Energy of the Oxygen Evolution and Reduction Reactions. *Electrochimica Acta* **2018**, *281*, 466–471, doi:10.1016/j.electacta.2018.05.150.
10. Liu, P.; Qing, H. Application of the Octahedral Model Theory to Evaluating the Specific Surface Area of Porous Metal Foams. *Chin. J. Vac. Sci. Technol.* **2025**, *45*(3), 222–228. <https://doi.org/10.13922/j.cnki.cjvst.202411005>
11. Beavers, G.S.; Joseph, D.D. Boundary Conditions at a Naturally Permeable Wall. *J. Fluid Mech.* **1967**, *30*, 197–207, doi:10.1017/S0022112067001375.
12. Le Bideau, D.; Mandin, P.; Benbouzid, M.; Kim, M.; Sellier, M. Review of Necessary Thermophysical Properties and Their Sensivities with Temperature and Electrolyte Mass Fractions for Alkaline Water Electrolysis Multiphysics Modelling. *International Journal of Hydrogen Energy* **2019**, *44*, 4553–4569, doi:10.1016/j.ijhydene.2018.12.222.
13. Akerlof, G.C.; Bender, P. Thermodynamics of Aqueous Solutions of Potassium Hydroxide¹. *J. Am. Chem. Soc.* **1948**, *70*, 2366–2369, doi:10.1021/ja01187a016.
14. Robinson, R.A.; Stokes, R.H. *Electrolyte Solutions*, 2nd rev. ed.; Dover Publications: New York, NY, USA, **2002**.
15. De Vidts, P.; Delgado, J.; Wu, B. A Nonisothermal Nickel-Hydrogen Cell Model. *J. Electrochem. Soc.* **1998**, *145*, 3874–3883. <https://doi.org/10.1149/1.1838870>
16. Bratsch, S.G. Standard Electrode Potentials and Temperature Coefficients in Water at 298.15 K. *Journal of Physical and Chemical Reference Data* **1989**, *18*, 1–21,

doi:10.1063/1.555839.

17. Fei, H.; Ge, S.; Min, L.; et al. A Numerical Simulation of Static Feed Alkaline Water Electrolysis. *Chem. Ind. Eng.* **2022**, *39*, 94–105. <https://doi.org/10.13353/j.issn.1004-9533.20210324>
18. Rakhshani, S.; Araneo, R.; Pucci, A.; Rinaldi, A.; Giuliani, C.; Pozio, A. Synthesis and Characterization of a Composite Anion Exchange Membrane for Water Electrolyzers (AEMWE). *Membranes* **2023**, *13*, 109, doi:10.3390/membranes13010109.
19. Maier, M.; Meyer, Q.; Majasan, J.; Tan, C.; Dedigama, I.; Robinson, J.; Dodwell, J.; Wu, Y.; Castanheira, L.; Hinds, G.; et al. Operando Flow Regime Diagnosis Using Acoustic Emission in a Polymer Electrolyte Membrane Water Electrolyser. *Journal of Power Sources* **2019**, *424*, 138–149, doi:10.1016/j.jpowsour.2019.03.061.
20. Liu, Y.; Diankai, Q.; Xu, Z.; Yi, P.; Peng, L. Comprehensive Analysis of the Gradient Porous Transport Layer for the Proton-Exchange Membrane Electrolyzer. *ACS Appl. Mater. Interfaces* **2024**, *16*, 47357–47367, doi:10.1021/acsami.4c00006.
21. Liu, Y.; Xu, L.; Zhang, J.; Li, G.; Xu, W.; Wang, Y.; Zhang, W. A Rolling Strategy for Layered Double Hydroxide Membrane to Boost Alkaline Water Electrolysis. *Journal of Membrane Science* **2025**, *720*, 123778, doi:10.1016/j.memsci.2025.123778.