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DELYCIOUS

Clean Hydrogen Partnership

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# D5.1 Physical Cell Model Development, Reduction and Database Generation

by University of Twente




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# About DELYCIOUS

As Europe accelerates its transition to clean energy, the Net Zero Industry Act identifies low-carbon hydrogen production as a strategic priority. DELYCIOUS tackles key challenges in water electrolysis technology, focusing on extending electrolyser lifespans and reducing operational costs under variable renewable energy sources. In DELYCIOUS, the development of cost-efficient, innovative, open, universal, and safe diagnostic tools to investigate the chemical and electrochemical properties of electrolysis systems is foreseen. This project combines Raman Spectroscopy (Raman) and Electrochemical Impedance Spectroscopy (EIS), to explore the chemical and electrochemical properties of electrolysis systems. By using both physical and data-driven modeling, it will be possible to identify important degradation parameters. To ensure that the diagnostic tools work effectively in various temperature ranges and across various electrolysis technologies, three technologies namely Alkaline Electrolysis (AEL), Proton Exchange Membrane Electrolysis (PEMEL), and Solid Oxide Electrolysis (SOEL) are addressed in this project, with a demonstration on alkaline electrolysers beyond 100 KW.

## Consortium

Fraunhofer IWES

Coordinator

Air Liquide

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DUMAREY

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# Publishable Summary

A major bottleneck in electrolyzer control is balancing computationally heavy physics simulations with real-time monitoring. We address this with fast, high-fidelity 1D macro-homogeneous digital twins for SOEC, PEM, and Alkaline cells. Deployed as optimized binaries requiring only simple input files, these models execute in approximately 1.5 seconds for PEM and AEL, and mere milliseconds for SOEC. This eliminates the need for further model reduction or standalone offline data generation. By dynamically ingesting experimental EIS and Raman data, the models will couple with an extended Kalman/Particle filter (D 5.2) to fit lumped degradation parameters, ensuring predictive maintenance relies on actual electrochemistry rather than blind data correlations.

The models accurately recreate fundamental operational trends, including expected I-V curve voltage increases and the natural decrease in gas crossover (HTO and OTH) at higher loads due to gas dilution in PEM and AEL cells. To map physical aging of electrodes in all 3 technologies, exchange current density $(i_0)$ derived from EIS is to be updated. Similarly, separator/electrolyte degradation is to be directly incorporated from EIS based Ohmic resistance. To resolve remaining structural and transport decay, the SOEC model tunes Triple Phase Boundary (TPB). Conversely, the PEM and AEL models dynamically fit specific surface area $(a_s)$ to resolve any unaccounted structural degradation and adjust effective gas diffusivities based on Raman evaluated compositions at the outlet to mathematically absorb physical membrane wear and crossover leakage.



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# List of Symbols

| | |
|---|---|
| $a_s$ | Specific surface area (1/m) |
| $c_i$ | Concentration of species i (mol/m³) |
| $c_{th}$ | Threshold concentration for bubble formation (mol/m³) |
| $D_{bulk}$ | Bulk diffusion coefficient (m²/s) |
| $D^{DGM}$ | Effective diffusion matrix (Dusty Gas Model) |
| $D_{eff}$ | Effective diffusion coefficient (m²/s) |
| $F$ | Faraday's constant (C/mol) |
| $i$ | Applied current density (A/cm² or A/m²) |
| $i_0$ | Exchange current density (A/m²) |
| $j_F$ | Faradaic volumetric reaction rate (A/m³) |
| $k_{eff}$ | Effective ionic conductivity (S/m) |
| $M_{sat}$ | Supersaturation multiplier |
| $N_i$ | Flux of species i (mol/(m²·s)) |
| $n$ | Number of electrons transferred in the reaction |
| $R_{ASR}$ | Area Specific Resistance (Ω·m²) |
| $T$ | Temperature (K) |
| $y$ | Mole fraction |
| $\alpha$ | Charge transfer coefficient |
| $\beta$ | Penetration exponent for bubble transport penalty |
| $\varepsilon$ | Porosity |
| $\tau$ | Tortuosity |
| $z_i$ | Charge number of species i |
| $S_i$ | Production/consumption of i (mol/(m³.s)) |



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# 1. Objective

Within the scope of the DELYCIOUS project, a core goal is the development of robust diagnostic tools to extend electrolyzer lifespans and reduce operational costs. A major bottleneck in achieving this kind of real-time monitoring and predictive maintenance is balancing computationally heavy physics simulations with sensor data streams.

Therefore, the primary objective of this task is to provide 1D macro-homogeneous physical cell models for Alkaline Electrolysis (AEL), Proton Exchange Membrane (PEM), and Solid Oxide Electrolysis Cells (SOEC). To serve the project's goal of real-time degradation tracking, these models must maintain high fundamental fidelity while executing rapidly enough to be directly coupled with dynamic filtering algorithms (such as the Extended Kalman Filter). This dynamic coupling ensures predictive maintenance relies on actual physics, and it eliminates the need for further model reduction or standalone, offline data generation. Across all three technologies, the models should be able to predict the overall cell voltage as the primary output. Additionally, for the AEL and PEM models, they should compute gas crossover metrics, Hydrogen-in-Oxygen (HTO) and Oxygen-in-Hydrogen (OTH).

# 2. Strategy

To accurately map physical aging, the models will ingest experimental data directly. Information from Electrochemical Impedance Spectroscopy (EIS) is physically interpreted to update the exchange current density ($i_0$) and the ohmic separator/electrolyte conductivity at every measurement point. Subsequently, hidden degradation phenomena such as structural decay are introduced through scaling factors like the specific surface area ($a_s$). Furthermore, for the AEL and PEM systems, Raman spectroscopy composition data is utilized to adjust scaling factors for gas diffusivities, mathematically absorbing the effects of membrane wear and crossover leakage.

In the following sections, we lay out the core governing physics implemented in each of the three electrolyzer models and present simulation results that demonstrate the model's predicted performance under varying degradation conditions.



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# 3. AEL

## 3.1. Mathematical Model & Governing Physics

We developed a 1D macro-homogeneous porous electrode model designed to simulate the internal physics of an alkaline electrolyzer. The physical laws are expressed as a system of time-dependent partial differential equations (PDEs) that track the conservation of mass (ions and gases) and charge (electrons and liquid potential) across various layers of the cell (Cathode PTL -> Cathode Catalyst Layer-> Separator -> Anode Catalyst Layer -> Anode PTL).

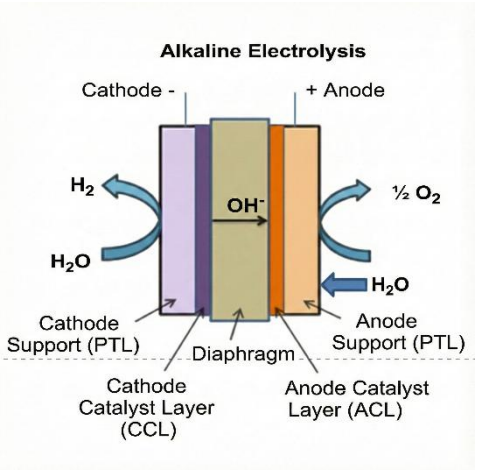



*Figure 1: Schematic of AEL.*

The 1D space across the five layers is sliced into discrete microscopic volumes (Finite Volume Method). The model calculates the flux of species crossing the boundaries of each volume. Because the governing equations are highly coupled and stiff, we use the robust DASKR differential-algebraic solver available in Julia programming language to step the transient system through time until it stabilizes at a steady-state solution.

### 3.1.1. Primary State Variables

The model iteratively solves for 7 primary variables at every spatial node:

- $c_{OH}$: $Hydroxide\ ion\ concentration\ \in\ the\ liquid\ phase\ (mol/m^3)$
- $c_K$: $Potassium\ ion\ concentration\ \in\ the\ liquid\ phase\ (mol/m^3)$
- $c_{H2}$: $Dissolved\ hydrogen\ gas\ concentration\ \in\ the\ liquid\ phase\ (mol/m^3)$
- $c_{O2}$: $Dissolved\ oxygen\ gas\ concentration\ \in\ the\ liquid\ phase\ (mol/m^3)$
- $\Phi_l$: $Liquid\ electrolyte\ potential\ (V)$
- $\Phi_{s,c}$ : $Solid\ phase\ electrical\ potential\ \in\ the\ cathode\ (V)$
- $\Phi_{s,a}$: $Solid\ phase\ electrical\ potential\ \in\ the\ anode\ (V)$



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### 3.1.2. Governing Equations

The solver forces these variables to satisfy the following physical laws simultaneously:

- **Ion Transport (Nernst-Planck Equation)**
  The flux of individual $OH^-$ and $K^+$ ions is driven by both concentration gradients (diffusion) and voltage gradients (migration):

$$N_i = -D_{\text{eff}} \nabla c_i - z_i \left[\frac{(D_{\text{eff}} F)}{RT}\right] c_i \nabla \Phi_l \quad (1)$$

  Mass conservation dictates that the divergence of this flux equals the production rate from the reaction:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot N_i = S_i \quad (2)$$

- **Charge Conservation (Ionic & Electronic Current)**
  The total ionic current is calculated as the sum of the charge carried by the Nernst-Planck ion fluxes:

$$i_l = F\Sigma(z_i N_i) \quad (3)$$

  Charge must be conserved across the solid and liquid phases. The divergence of current in the solid phase (σ) must perfectly equal the current entering the liquid phase via the Faradaic reaction:

$$\nabla \cdot (-\sigma_{\text{eff}} \nabla \Phi_s) = -j_F \quad (4)$$

$$\nabla \cdot i_l = j_F \quad (5)$$

- **Gas Transport (Fick's First Law)**
  Dissolved gases move through the liquid network purely via diffusion. Because the dissolved concentrations of hydrogen and oxygen within the liquid electrolyte remain strictly within the dilute limit, solute-solute interactions are negligible. Therefore, the complex multicomponent Maxwell-Stefan formulation is unnecessary, and transport is accurately governed by Fick's First Law, where each gas species diffuses independently through the dominant solvent medium:

$$N_{Dis,gas} = -D_{\text{eff}} \nabla c \quad (6)$$

- **Electrochemical Kinetics (Butler-Volmer Equation)**
  The volumetric reaction rate at any node in the catalyst layer is governed by the local activation overpotential:



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$$\eta = \Phi_s - \Phi_l - E_{eq} \quad (7)$$

This is the extra voltage required to overcome the sluggishness of the chemical reactions at the catalyst surfaces.

$$j_F = a_s i_0 [\, exp(\alpha n F \eta / RT) - exp(-(1-\alpha)\, n F \eta / RT) \,] \quad (8)$$

Note: $E_{eq}$ is calculated using the Nernst Equation, accounting for both the operating temperature and operational gas pressures (via Henry's Law).

- Two-Phase Flow & Bubble Penalties

  The model accounts for gas bubbles displacing the liquid electrolyte, which chokes ion transport.

  Supersaturation limit: Bubbles form when dissolved gas exceeds a critical threshold:

$$c_{th} = M_{sat} c_{eq} \quad (9)$$

  Transport penalty: The effective transport properties (diffusion coefficients) are penalized by both the solid structure and the bubble presence ($\beta$ is the Penetration Exponent):

$$D_{eff} = D_{bulk} (\varepsilon / \tau) \left(1 - S_g\right)^{\beta} \quad (10)$$

  Here $S_g$ is the fraction of pore space filled by bubbles. The bubble volume grows as the applied current increases, until it hits a maximum limit.



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## 3.2. Results

To verify the physical consistency of the AEL model prior to experimental validation, a parametric sensitivity analysis was performed across a standard load range. The following simulations isolate specific degradation mechanisms to demonstrate the models' theoretical response.

### AEL Gas Crossover vs. Load:

The gas crossover fractions (HTO and OTH) display a theoretically expected asymptotic decline. This behaviour is the direct result of the mathematical intersection between mass transport and electrochemical kinetics. The diffusive crossover of dissolved gases through the liquid separator is governed by Fick's First Law and remains relatively constant, as it is driven by steady concentration gradients [Newman & Thomas-Alyea, 2012]. However, the bulk production of gas at the electrodes, governed by Faraday's Law, scales linearly with the applied current. Therefore, as the current density increases, the constant diffusive crossover flux becomes increasingly diluted by the rapidly growing volume of bulk gas generation, resulting in the classic inverse (1/x) asymptotic curve universally observed in electrolyzer literature [Trinke et al., 2018].

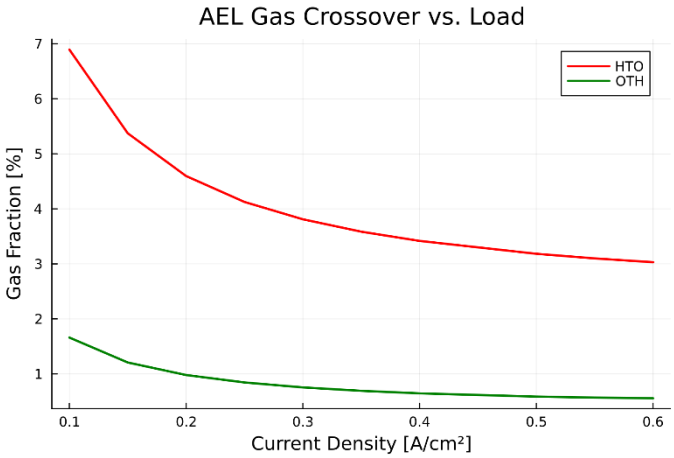



*Figure 2: Gas crossover at varying loads for AEL.*

### Impact of Degraded Conductivity:

Decreasing the effective separator conductivity from 31.0 S/m to 25.0 S/m simulates the effect of separator degradation, such as pore clogging or structural wear. This response is a direct macroscopic manifestation of the Nernst-Planck equation [Newman & Thomas-Alyea, 2012]. As the effective ionic diffusion coefficients ($D_{\text{eff}}$) are mathematically scaled down, the model requires a steeper liquid potential gradient ($\nabla \Phi_l$) to drive the required migratory ion flux. Because this required potential gradient scales proportionally with the applied current, the restricted ion mobility mathematically steepens the slope of the polarization curve.



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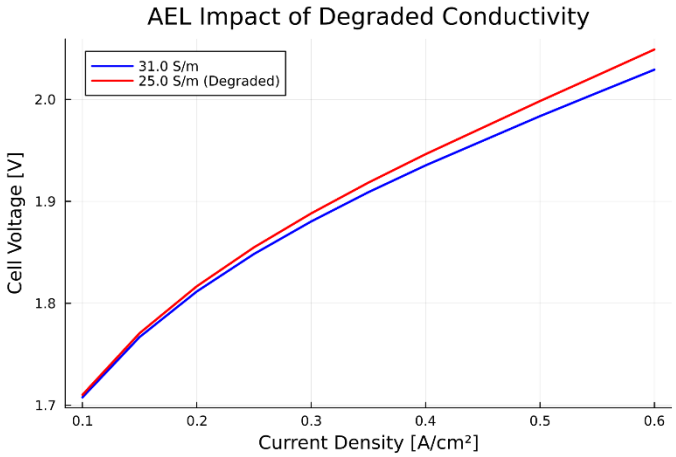



*Figure 3: Impact of degraded separator on AEL performance.*

### Impact of Degraded Exchange Current (Kinetic Activity):

Simulating electrode degradation, such as catalyst poisoning or loss of active area by lowering the exchange current density results in a parallel upward shift of the entire polarization curve. This response aligns with Butler-Volmer kinetics operating in the Tafel regime [Bard & Faulkner, 2001]. Because the activation overpotential scales logarithmically with the exchange current, any reduction in catalytic activity mathematically manifests as a constant, uniform voltage penalty across all operating loads.

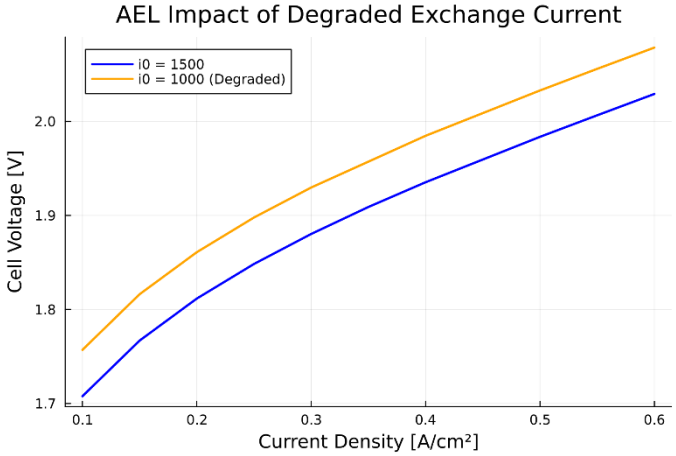



*Figure 4: Impact of degraded electrode on AEL performance.*

## 3.3.Conclusion

The parametric sensitivity analysis demonstrates that the AEL model produces reasonable, physically expected trends that align with established electrochemical literature. Crucially, this physical fidelity is achieved without any loss of computational speed. Each full simulation run executes in approximately 1.5 seconds. This rapid execution time confirms that the 1D model is suitable for the larger scope of the DELYCIOUS project, specifically for seamless, real-time coupling with dynamic diagnostic algorithms without creating a computational bottleneck



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# 4. PEM

## 4.1.Mathematical Model & Governing Physics

We developed a 1D macro-homogeneous porous electrode model designed to simulate the internal physics of a PEM electrolyzer. The physical laws are expressed as a system of time-dependent partial differential equations (PDEs) that track the conservation of mass (dissolved gases) and charge (electrons and protonic potential) across the various layers of the cell (Cathode PTL -> Cathode Catalyst Layer -> Membrane -> Anode Catalyst Layer -> Anode PTL).

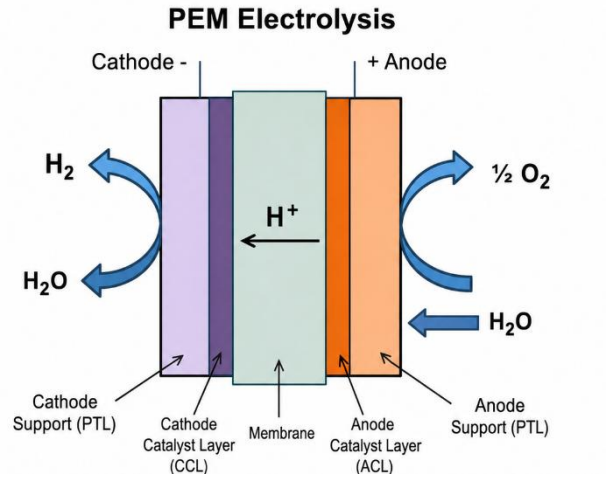



*Figure 5: Schematic of PEM.*

The 1D space across these five layers is discretized into microscopic finite volumes. The model calculates the transport fluxes crossing the boundaries of each volume. Because the governing equations are highly coupled, the robust DASKR differential-algebraic solver in the Julia programming language is utilized to step the transient system through time until it converges on a steady-state solution.

### 4.1.1. Primary State Variables

The model iteratively solves for 5 primary variables at every spatial node:

- $c_{H2}$: $Dissolved\ hydrogen\ gas\ concentration\ \in\ the\ liquid\ phase\ (mol/m^3)$
- $c_{O2}$: $Dissolved\ oxygen\ gas\ concentration\ \in\ the\ liquid\ phase\ (mol/m^3)$
- $\Phi_l$: $Liquid\ electrolyte\ potential\ (V)$
- $\Phi_{s,c}$ : $Solid\ phase\ electrical\ potential\ \in\ the\ cathode\ (V)$
- $\Phi_{s,a}$: $Solid\ phase\ electrical\ potential\ \in\ the\ anode\ (V)$

### 4.1.2. Governing Equations

The solver forces these variables to satisfy the following physical laws simultaneously:

- Charge Conservation (Ionic & Electronic Current)



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The charge must be conserved across the solid and liquid phases. The divergence of current in the solid phase (σ) must perfectly equal the current entering the liquid phase via the Faradaic reaction:

$$\nabla \cdot (-\sigma_{eff} \nabla \Phi_s) = -j_F \quad (11)$$

$$\nabla \cdot (-k_{eff} \nabla \Phi_l) = j_F \quad (12)$$

Unlike AEL, the PEM model does not calculate ionic (proton) mass transport. Because electroneutrality locks the proton concentration to the fixed charges in the solid polymer, transport is strictly driven by migration and is entirely accounted for by Ohmic charge conservation.

- **Gas Transport**
  Dissolved gases move through the liquid network purely via diffusion:
  $$N_{Dis,gas} = -D_{eff} \nabla c \quad (13)$$

- **Electrochemical Kinetics (Butler-Volmer Equation)**
  The volumetric reaction rate at any node in the catalyst layer is governed by the local activation overpotential:

  $$\eta = \Phi_s - \Phi_l - E_{eq} \quad (14)$$

  $$j_F = a_s i_0 [\, exp(\alpha n F \eta / RT) - exp(-(1-\alpha) n F \eta / RT)] \quad (15)$$

  *Note:* $E_{eq}$ is calculated using the Nernst Equation, accounting for both the operating temperature and local gas saturation limits via Henry's Law.

- **Two-Phase Flow & Bubble Penalties**
  The model accounts for gas bubbles displacing the liquid electrolyte, which chokes dissolved gas and ion transport.

  Supersaturation limit: Bubbles form when dissolved gas exceeds a critical threshold:

  $$c_{th} = M_{sat} c_{eq} \quad (16)$$

  Transport penalty: The effective transport properties (diffusion coefficients) are penalized by both the solid structure and the bubble presence ($\beta$ is the Penetration Exponent):

  $$D_{eff} = D_{bulk} (\varepsilon / \tau) \left(1 - S_g\right)^{\beta} \quad (17)$$

  Here $S_g$ is the fraction of pore space filled by bubbles. The bubble volume increases by increasing current density, until the maximum limit is reached.



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## 4.2. Results

To verify the physical consistency of the PEM model, a parametric sensitivity analysis was performed across the expected load range. The following simulations isolate specific degradation mechanisms to demonstrate the model's theoretical response.

### PEM Gas Crossover vs. Load:

Similar to AEL model, the gas crossover fractions in PEM also exhibit the inverse asymptotic decline. The diffusive crossover of dissolved gases through the solid polymer membrane is driven by steady concentration gradients and remains relatively independent of the applied load [Newman & Thomas-Alyea, 2012]. Conversely, the bulk gas production at the catalyst layers is governed by Faraday's Law and scales linearly with the applied current. Consequently, as the current density increases, the steady diffusive crossover flux is increasingly diluted by the massive volume of generated bulk gas, resulting in the classic inverse curve widely documented in PEM literature [Schalenbach et al., 2013].

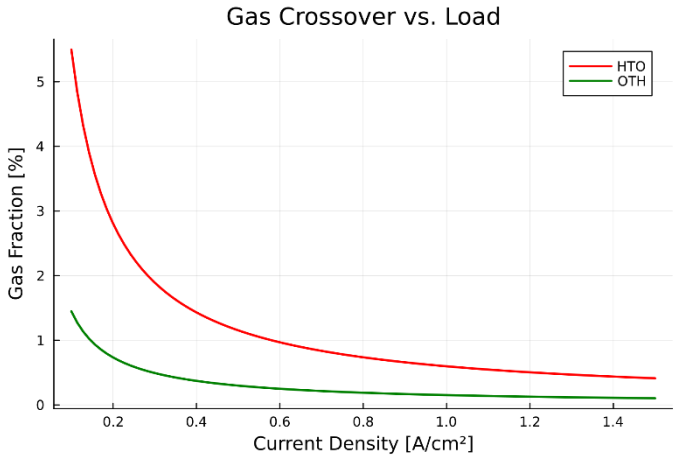



*Figure 6: Gas crossover with varying load for PEM.*

### Impact of Degraded Conductivity:

Decreasing the effective membrane conductivity from 14.4 S/m to 10.0 S/m simulates the effect of ohmic degradation, such as membrane dehydration or structural thinning. This response is a macroscopic manifestation of Ohm's Law for ionic conductors [Newman & Thomas-Alyea, 2012].

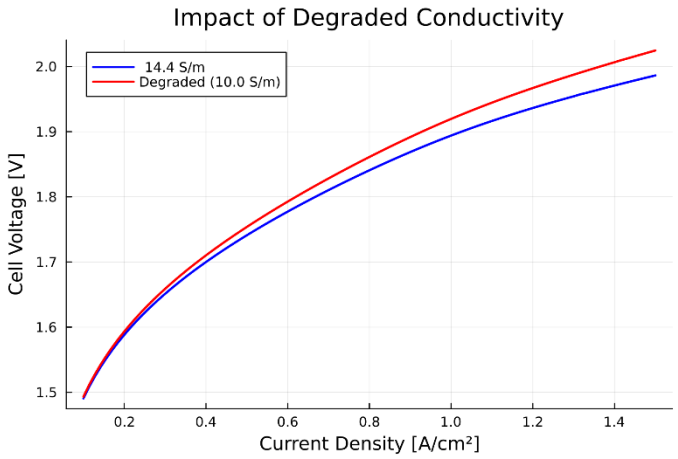



*Figure 7: Impact of degraded membrane of PEM performance.*



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As the effective ionic conductivity is reduced, the local area-specific resistance of the membrane increases. Because the ohmic overpotential is directly proportional to the applied current density ($V_{ohm} = I \cdot R_{ASR}$), the model translates this resistance increase into a steeper slope in the polarization curve. This compounding voltage penalty at higher operating loads confirms that the model captures the theoretically expected ohmic behavior without relying on empirical linear approximations.

**Impact of Degraded Exchange Current (Kinetic Activity):**

Simulating electrode degradation, such as catalyst poisoning or loss of active electrochemical surface area by lowering the exchange current density results in a parallel upward shift of the entire polarization curve. Much like AEL, this response also aligns with Butler-Volmer kinetics operating in the Tafel regime [Bard & Faulkner, 2001]. Because these electrolyzers typically operate at activation overpotentials large enough to render the reverse reaction negligible, the activation overpotential ($\eta$) scales logarithmically with the exchange current density. Consequently, any reduction in catalytic activity manifests as a constant, uniform voltage penalty across all operating loads.

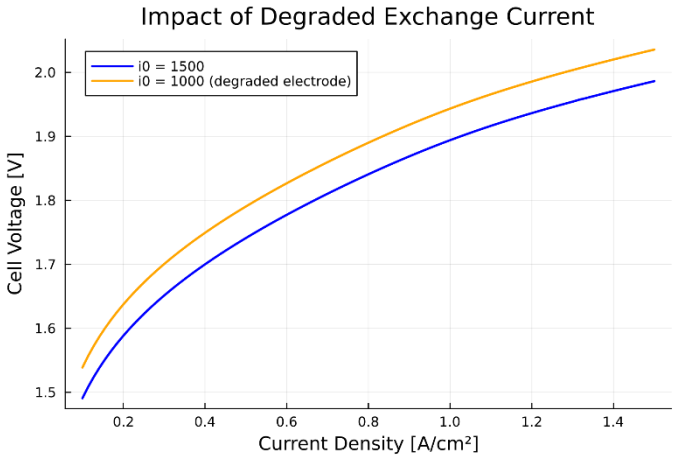



*Figure 8: Impact of degraded electrode of PEM cell performance.*

## 4.3. Conclusion

The parametric sensitivity analysis demonstrates that the PEM model produces reasonable, physically expected trends that align with established electrochemical literature. By successfully capturing macroscopic behaviors such as the inverse asymptotic decline of gas crossover through the solid polymer and the linear ohmic penalty of the ionomer, the model proves its thermodynamic reliability. Crucially, this physical fidelity is achieved without any loss of computational speed. Each full simulation run executes in approximately 1.5 seconds. This rapid execution time confirms that the 1D PEM model is suitable for real-time coupling with dynamic diagnostic algorithms without creating a computational bottleneck.



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# 5. SOEC

## 5.1. Mathematical Model & Governing Physics

We developed a 1D macro-homogeneous porous electrode model designed to simulate the internal physics of a high-temperature SOEC. The physical laws are expressed as a system of PDEs that track the conservation of mass (multiphase gas transport) and charge (electrons and solid-state oxygen ions) across the functional layers of the cell (Fuel Electrode -> Solid Electrolyte -> Oxygen Electrode).

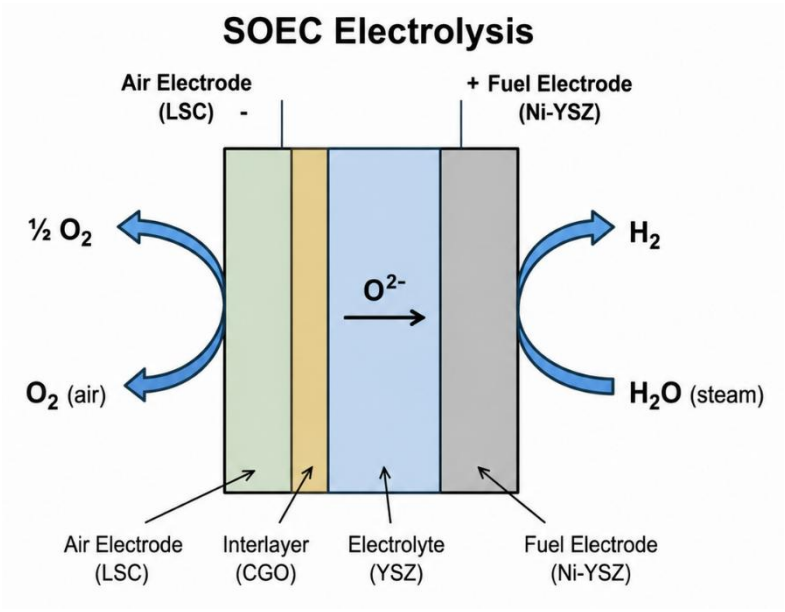



*Figure 9: Schematic of SOEC.*

The 1D spatial domain is discretized into microscopic finite volumes, calculating the transport fluxes crossing the boundaries of each node. Because the governing equations are highly coupled and computationally demanding, the model is implemented in C++ and leverages the PETSc framework for parallelization. PETSc's robust suite of scalable nonlinear solvers (employing Newton-Krylov methods) is utilized to efficiently resolve the stiff system and drive to a converged steady-state solution.

### 5.1.1. Primary State Variables

The primary state variables the nonlinear solver iterates to find at every spatial node are:

- $c_{H2}$: $Hydrogen\ gas\ concentration\ \in\ the\ porous\ fuel\ electrode\ (mol/m^3)$
- $c_{O2}$: $Oxygen\ gas\ concentration\ \in\ the\ porous\ air\ electrode\ (mol/m^3)$
- $c_{N2}$: $Nitrogen\ gas\ concentration\ \in\ the\ porous\ air\ electrode\ (mol/m^3)$
- $c_{H2O}$: $Steam\ (water\ vapor)\ concentration\ \in\ the\ porous\ fuel\ electrode\ (mol/m^3)$
- $\Phi_{ionic}$: $Ionic\ potential\ within\ the\ solid\ electrolyte\ phases\ (V)$
- $\Phi_{electronic}$ : $Solid\ phase\ electrical\ potential\ (V)$



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### 5.1.2. Governing Equations

The solver forces these variables to satisfy the following physical laws simultaneously:

- **Charge Conservation (Ionic & Electronic Current)**
  The charge must be conserved across the solid electron-conducting phase and the solid ion-conducting phase. The migration of electrons and oxygen vacancies is governed by macroscopic Ohm's law.

$$\nabla \cdot (-\sigma_{eff} \nabla \Phi_{electronic}) = -j_F \quad (18)$$

$$\nabla \cdot (-k_{eff} \nabla \Phi_{ionic}) = j_F \quad (19)$$

- **Gas Transport (Dusty Gas Model)**
  The gases move through the porous electrode structures via a combination of molecular diffusion (gas-gas collisions) and Knudsen diffusion (gas-wall collisions). The explicit molar flux ($N_i$) of each gas species is calculated at every spatial node using the combined gradients of concentration (c) and dynamically derived pressure (p):

$$N_i = -\sum_j D_{ij}^{DGM} \nabla c_j - \left(\sum_j D_{ij}^{DGM} \frac{c_j}{D_{j,K}^{eff}}\right) \frac{B_g}{\mu} \nabla p \quad (20)$$

  For the SOEC's multicomponent mixture, the effective diffusion matrix is calculated dynamically at each node by summing gas-wall (Knudsen) and gas-gas (molecular) flow resistances into a friction matrix (H), which is then inverted to yield the final conductance:

$$H_{ii} = \frac{1}{D_{i,K}^{eff}} + \sum_{i \neq j} \frac{X_j}{D_{ij}^{eff}} \quad (21)$$

$$H_{ij} = \frac{X_j}{D_{ij}^{eff}} \quad (22)$$

$$D^{DGM} = H^{-1} \quad (23)$$

- **Electrochemical Kinetics (Butler-Volmer Equation)**
  The volumetric reaction rate at any node in the catalyst layer is governed by the local activation overpotential:



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$$\eta = \Phi_s - \Phi_l - E_{eq} \quad (24)$$

$$j_F = i_{vol}[\, exp(\alpha nF\eta/RT) - exp(-(1-\alpha)nF\eta/RT)\, ] \quad (25)$$

## 5.2. Results

To verify the physical consistency of the SOEC model, a parametric sensitivity analysis was performed across the operating voltage range. The following simulations isolate specific degradation mechanisms to demonstrate the models' theoretical response.

### Impact of Degraded Conductivity:

Decreasing the effective electrolyte conductivity scaling factor from 1.0 to 0.75 simulates the effect of ohmic degradation, such as solid electrolyte aging, microstructural decay, or impurity segregation at grain boundaries. This macroscopic response is governed by Ohm's Law for solid-state ionic conductors [Newman & Thomas-Alyea, 2012]. As the effective ionic conductivity for oxygen ion transport is mathematically scaled down, the local area-specific resistance of the solid electrolyte increases. Because the ohmic overpotential is directly proportional to the applied current density, the model translates this resistance increase into a steeper slope in the polarization curve.

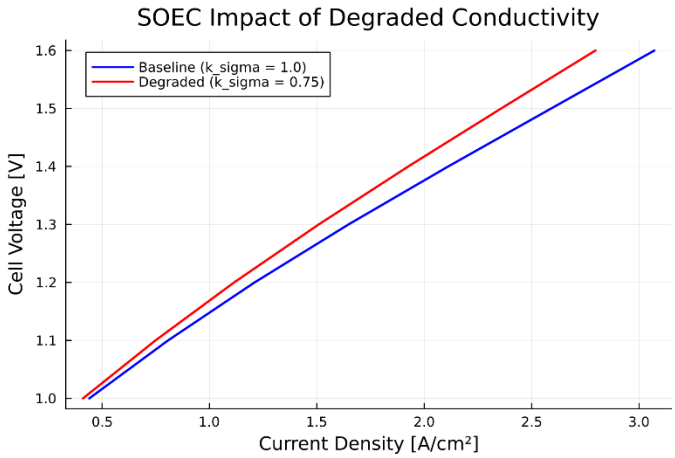



*Figure 10: Impact of degraded solid electrolyte on SOEC performance.*

### Impact of Degraded Electrodes:

Decreasing the exchange current density scaling factor from 1.0 to 0.5 to simulate catalyst degradation results in a steeper polarization curve, rather than a parallel shift. This behaviour is characteristic of high-temperature SOEC operation, where rapid kinetics keep activation overpotentials small. Consequently, the Butler-Volmer equation reduces to its linear approximation [Bard & Faulkner, 2001].



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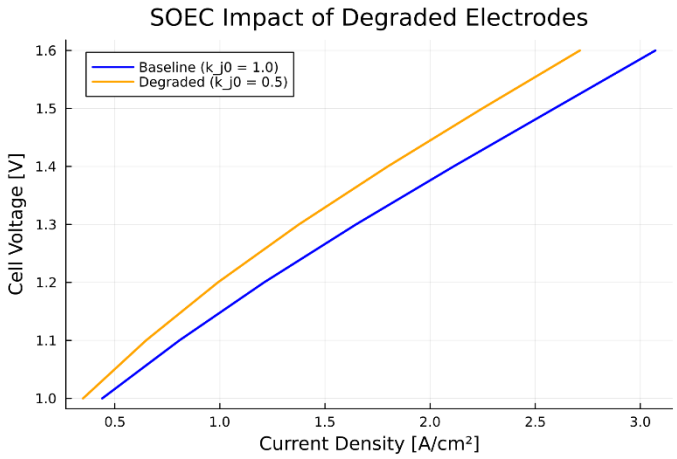



*Figure 11: Impact of degraded electrode on SOEC performance.*

In this regime, the exchange current density acts as an effective kinetic resistance. Halving $i_0$ doubles this resistance, producing a voltage penalty that scales linearly with current.

### 5.3. Conclusion

The parametric sensitivity analysis demonstrates that the SOEC model produces reasonable physical trends that align with established solid-state electrochemical literature. By successfully capturing macroscopic behaviours specific to high-temperature systems such as the linear compounding of oxygen ion ohmic resistance and the linear kinetic approximation of the Butler-Volmer equation, the model proves its thermodynamic reliability. Crucially, by leveraging a robust C++ and PETSc parallelized framework, this physical fidelity is achieved without any loss of computational speed. Each full transient simulation executes in approximately 1.5 ms. This rapid makes the 1D SOEC model suitable for real-time coupling with dynamic diagnostic algorithms without creating a computational bottleneck.

# 6. Outlook

The development of the 1D macro-homogeneous models for AEL, PEM, and SOEC establishes a rigorous, thermodynamically reliable baseline for the DELYCIOUS project. Across all three technologies, parametric analyses confirm that the models exhibit the thermodynamic, mass transport, and degradation trends explained in literature. Crucially, by leveraging robust computational frameworks (Julia/DASKR and C++/PETSc), this high physical fidelity is achieved with rapid execution speeds.



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Because the mathematical boundaries of the models are stable and physically constrained, they are uniquely primed to be coupled with dynamic condition-monitoring algorithms, such as Extended Kalman filters. This will allow the models to continuously ingest real-world operational and diagnostic data to map the physical aging of the cells. The immediate next step in this progression will be detailed in Deliverable (D6.1), which will provide a comprehensive quantitative validation of these models against experimental data. Finally, capitalizing on its computational efficiency, the rapid AEL model will serve as the foundational building block to scale up the simulation and predict full stack-scale behaviour within the Delycious project.

# 7. Literature


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