Multi-objective adjoint optimization tool for electro-chemical systems applied to membrane-less electrolyzer

Wiebke Schrader[1] | David Mueller[1] | Pooria Hadikhani[2] | Alexander Stroh[1]

[1]Institute of Fluid Mechanics (ISTM), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
[2]Institute for Applied Materials – Electrochemical Technologies (IAM-ET), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Abstract

A multi-objective optimization tool based on adjoint sensitivity analysis [1] to model a simplified electrolysis cell is proposed. One major design challenge for membrane-less electrolyzers is achieving a high hydrogen purity while maintaining its efficiency, representing contradictory objectives for the optimization. By modelling the topology of the simplified electrolysis cell with the Immersed Boundary Method (IBM), it is used as the design variable for the adjoint method. The multiphase system is modeled using a single-fluid approach, considering mixture fluid properties.

The Adjoint Method

- gradient based
- design variable: distance $\Psi \rightarrow$ indicator Φ
- sensitive to inital conditions
- based on penalty methods
- unknown derivatives $\rightarrow$ adjoint operator $\mathcal{L}^*$:

$$\int_\Omega u_i\,\mathcal{L}\,v_i\,dV = \langle u_i, \mathcal{L}\,v_i\rangle = \langle v_i, \mathcal{L}^*\,u_i\rangle = \int_\Omega v_i\,\mathcal{L}^*\,u_i\,dV$$

Application

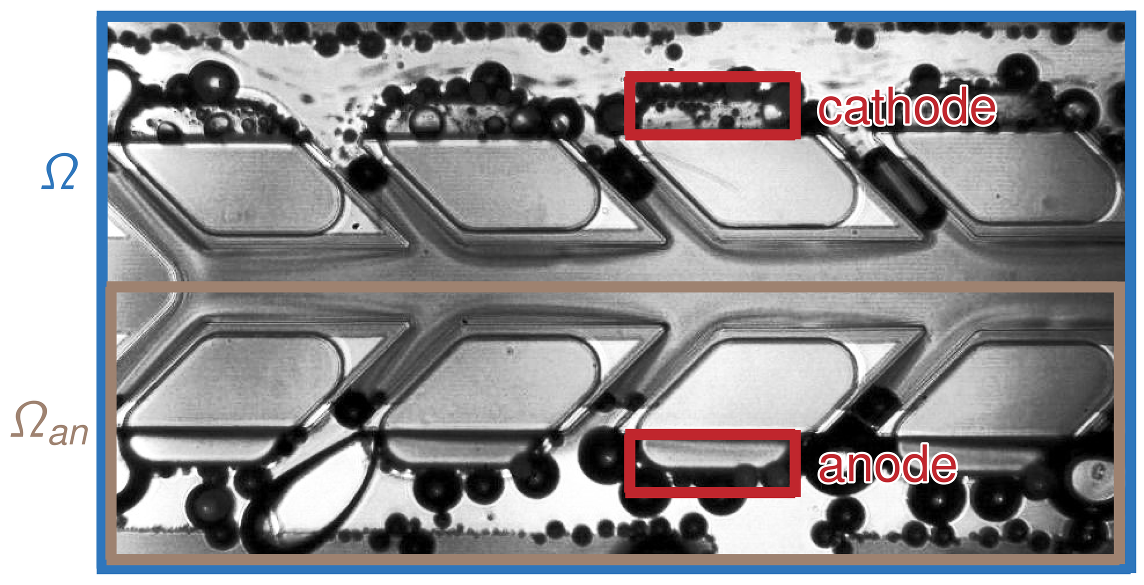
Optimization of electrolysis cell for

- increased efficiency $\rightarrow$ high mixing
- increased hydrogen (H_2) purity

Formulation of objective functions

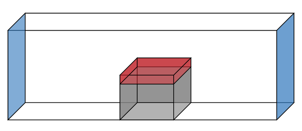
- indicator functions for evaluations

$\rightarrow$ increase H_2 production in Ω
$\rightarrow$ decrease H_2 concentration in Ω_{an}



Experimental setup of membrane-less electrolyzer [3]

Primal Set-up



$$R_i^v = \frac{\partial(\bar\rho\,v_i)}{\partial t} + \frac{\partial(\bar\rho\,v_i\,v_j)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\bar\rho\,\bar{\mathfrak{D}}\frac{\partial v_i}{\partial x_j}\right] + \frac{\partial(\bar\rho\,p)}{\partial x_i} + \Phi\,\eta\,v_i + (1-\Phi)\,m_{v,i}$$

$$R^{\alpha^k} = \frac{\partial(\bar\rho\alpha^k)}{\partial t} + v_j\frac{\partial(\bar\rho\alpha^k)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\left(\Phi\,\mathfrak{D}_s^k + (1-\Phi)\,\mathfrak{D}_f^k\right)\bar\rho\frac{\partial\alpha^k}{\partial x_j}\right] + (1-\Phi)\,w^k + \Phi_{cat}\,\dot S^k$$

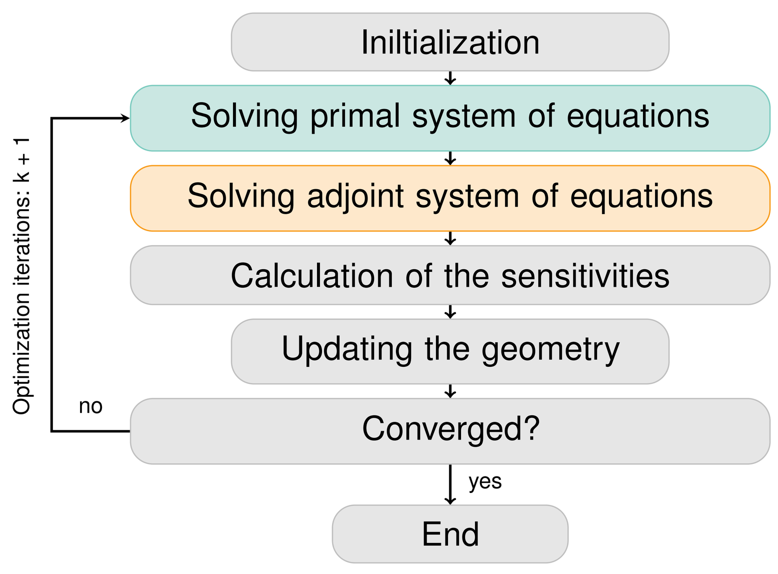
$$R_i^m = \bar\rho\int_\Omega(1-\Phi)\,(v_i - V_b)\,dV\,,\quad R^{w^k} = \int_\Omega(1-\Phi)\left(\alpha^k - C_b^k\right)dV$$

multiphase system
- mixture fluid properties
- depending on α^k

solid
- solid indicator Φ
- represented by IBM

inlet/outlet
- periodic boundaries
- sources $m_{v,i}$ and w^k

Sensitivities for adjoint optimization



Adjoint Set-up

Lagrange Equation with Adjoint variables

- based on time averages

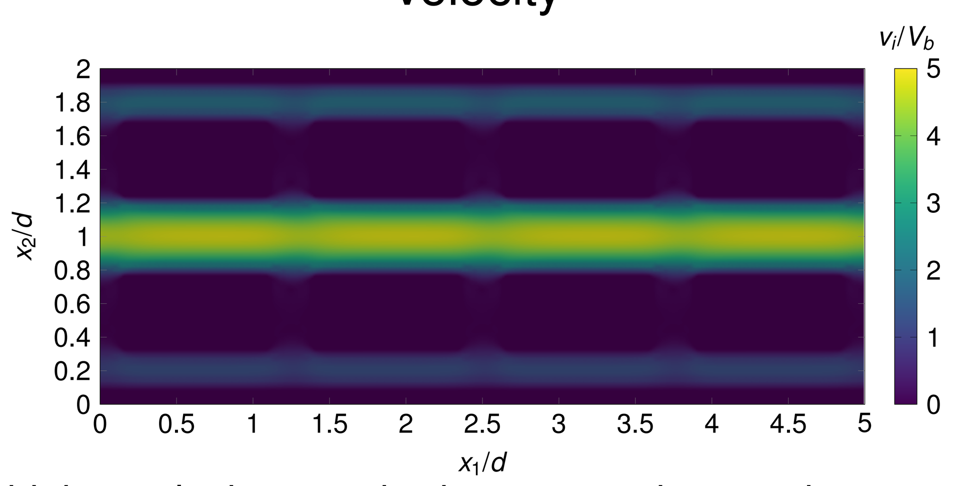
$$L = J + \sum_{j=1}^{m}\int_\Omega \mu_j R^j\,dV = J + \lambda_i^m\overline{R_i^m} + \lambda^{w^k}\overline{R^{w^k}} + \int_\Omega q\overline{R^p}dV + \int_\Omega u_i\overline{R_i^v}dV + \int_\Omega \omega^k\overline{R^{\alpha^k}}dV$$

Objective Functions

$$J^{eff} = \int_\Omega(1-\Phi)\left(\alpha^{H_2} - C_b^{H_2}\right)dV \qquad J^{H_2,pur} = -\int_{\Omega_{an}}(1-\Phi_{an})\left(\alpha^{H_2} - C_{an}^{H_2}\right)dV$$

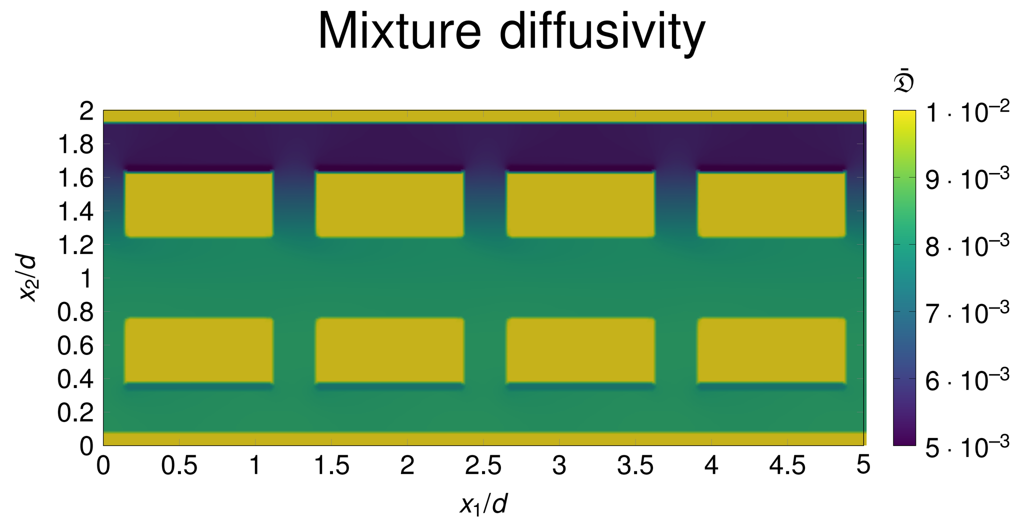
Results

Velocity



- higher velocity at cathode compared to anode
- main channel provides the electrolyte
- steady recirculation areas
- no convective flow from the outer to the inner channel

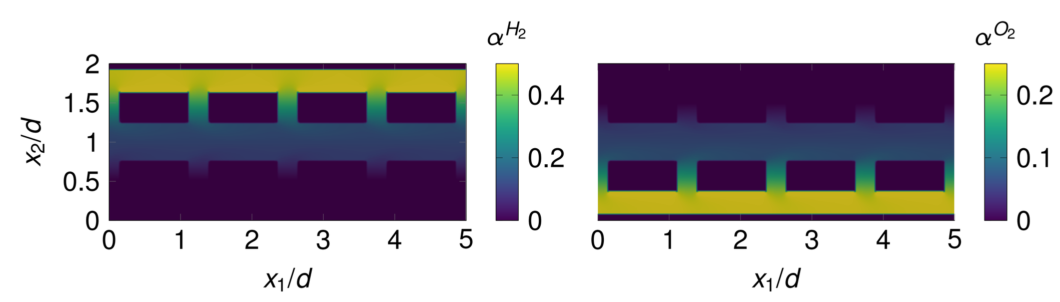
Mixture diffusivity



- mixture diffusivity results from void fractions:

$$\bar{\mathfrak{D}} = \sum_{k=1}^{n}\left(\alpha^k\mathfrak{D}^k\right) + \left(1 - \sum_{k=1}^{n}\alpha^k\right)\mathfrak{D}^{liquid}$$

Void fractions



- constant void fraction at the catalysts
- low gas transport to the inner channel
- accumulation at the catalysts

$\rightarrow$ high purity, low efficieny

Conclusion and Outlook

- simulation of the electrochemical system with simplified equations
- derivation of an adjoint framework for multi-objective optimization
- validation of the simplified model with experimental results
- optimization of the simplified model with weighted objectives
- extension of the adjoint framework for more complex models

References

1. Papoutsis-Kiachagias et al. (2016) Continuous adjoint methods for turbulent flows, applied to shape and topology optimization: industrial applications. Archives of Computational Methods in Engineering, 23.2
2. Y. Kametani et al. (2020) A new framework for design and validation of complex heat transfer surfaces based on adjoint optimization and rapid prototyping technologies. Journal of Thermal Science and Technology 15.2
3. P. Hadikhani et al. (2021) A membrane-less electrolyzer with porous walls for high throughput and pure hydrogen production. Sustainable Energy & Fuels 5.9, 2419-2432.

ICE 2023
4th International Conference on Electrolysis