Electrochemical Computational Fluid Dynamic (CFD) Modelling of Ethylene Oxide

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Introduction

The UK's commitment to achieving net zero by 2050 necessitates innovative strategies to decarbonize industries and advance sustainable chemical processes. Computational fluid dynamics (CFD) provides an effective approach to optimizing electrochemical reactors for high-volume chemical products. Ethylene oxide production *via* the chlorine evolution reaction (CER) is an ideal candidate (**Figure 1.**) which offers a sustainable and alternative to traditional fossil-fuel-based methods, while reducing greenhouse gas emissions.

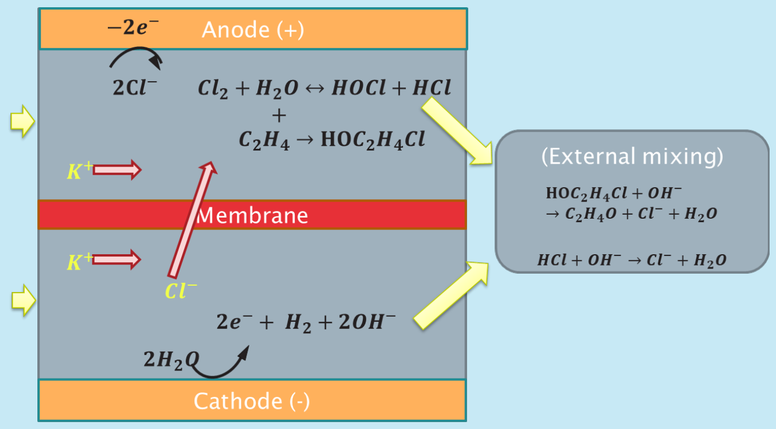

Figure 1. Reaction mechanism of the chlorine mediated electrosynthesis of ethylene oxide.

Aims and Objectives

- Contribute to sustainable chemical manufacturing while supporting the UK's decarbonization goals.
- Develop advanced CFD models of electrochemical reactors for ethylene oxide production.
- Enhancing reactor design and improving process efficiency.
- Investigating mass and heat transfer in the CER to reduce energy consumption and maximise yield.

Methods

- Computational simulations of the electrochemical reactor (**Figure 2.**) – with an active surface area of 16 cm^2, performed in ANSYS Fluent (2024 R2).
- A grid dependency study was conducted to ensure that the results were independent of the mesh size **(Figure 3.).**

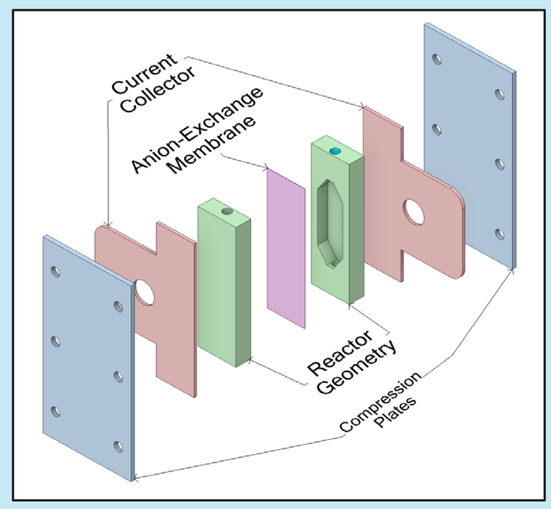

Figure 2. Exploded schematic diagram of the electrochemical reactor. Only the fluid volume of the reactor geometry and AEM were simulated.

Results and Discussion

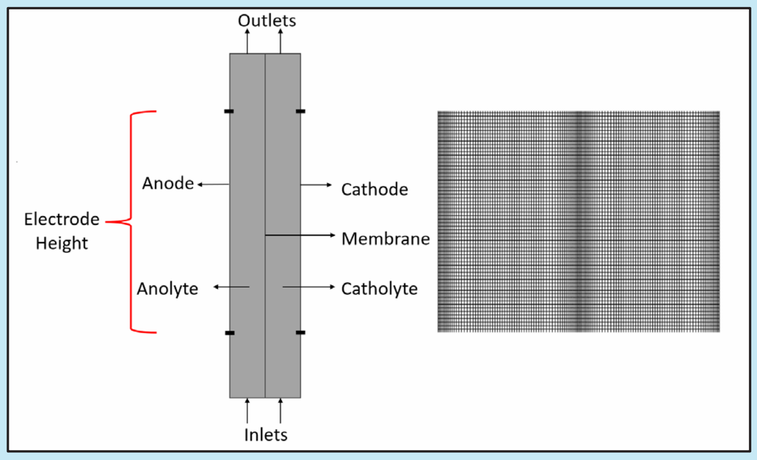

Figure 3. Computational domain and mesh used within the simulations.

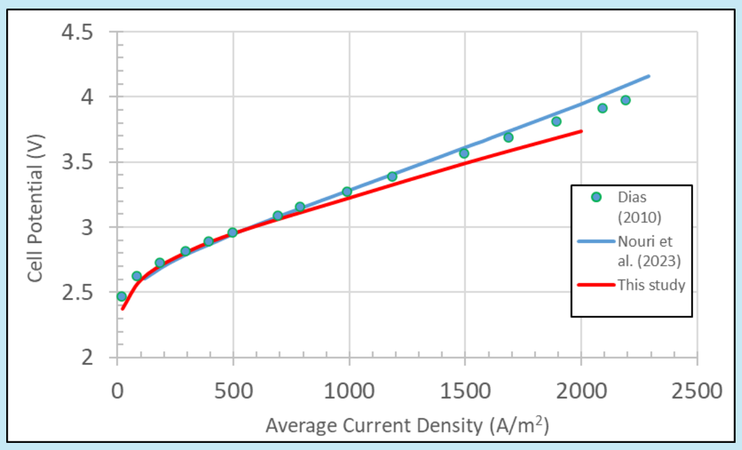

Figure 4. Validation of computational model against Dias (2010) [2], and Nouri *et al.* (2023) [3].

- The UK shipping industry consumes 7 MT/year of LNG fuel, equating to approx. 26 $MT_{(CO2e)}$ of GGE [1].
- To facilitate the shipping industries energy requirement using H_2, annual production must exceed 2.42 MT/year.
- Initial validation of the CFD model was achieved by comparing the cell potential at varied current densities against experimental and numerical literature values (**Figure 4.**).
- Outlet concentrations of Cl_2 and H_2 were taken and used to determine scale-up requirements (**Figure 5.**).
- Applying a scale-up factor of 62,500 to the simulation allows a pathway to achieve production demands (**Figure 6.**).

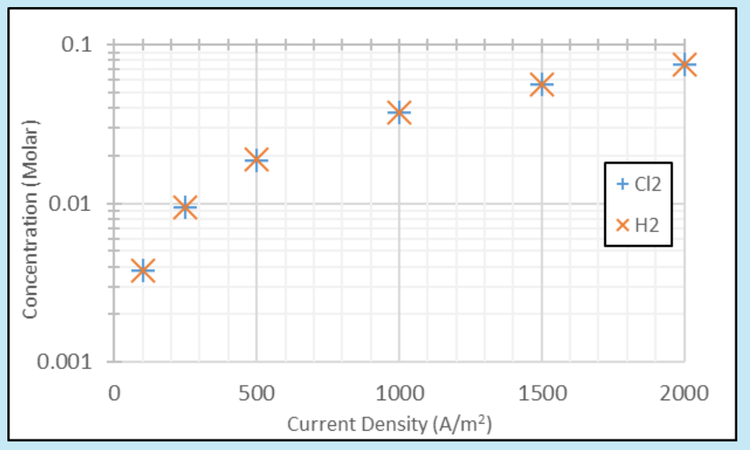

Figure 5. Chlorine and hydrogen concentrations at the outlets, current density range of 20-2000 A/m^2.

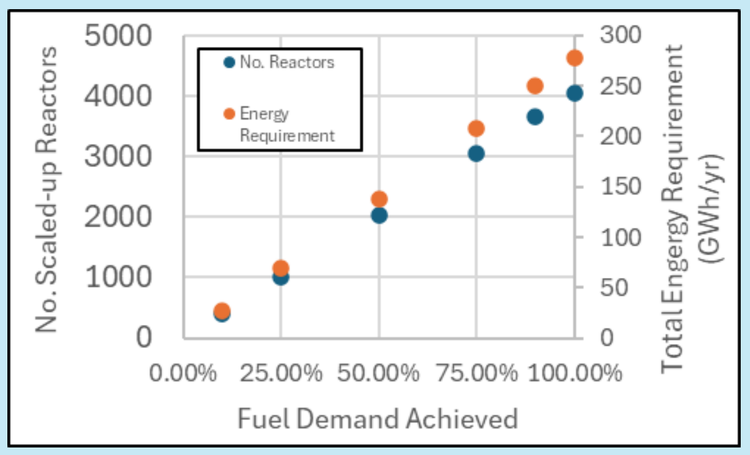

Figure 6. Scale-up of reactor to 2 m^2, with 50 to a stack. Total scale up factor equals $6.25x10^4$.

Future Work & Conclusion

The implementation of a more robust kinetic model for determining the extent of chlorine hydrolysis equilibrium at elevated ionic strengths will be crucial for improving model accuracy.

Validation will be achieved using UV-Vis spectroscopy experiments. Furthermore, a parametric study will be undertaken to optimise process conditions.

References

[1] Transport & Environment (January 2024); *Long, loud and legal: the case for zero-emission UK shipping;* Accessed (15/12/2024).

[2] de Bastos Vidal Dias, A. C., Mendes, A. M. M., de Magalhães, F. D. de M. B. M. & Araújo, P. A. P. Chlor-Alkali Membrane Cell Process: Study and Characterization. *PQDT - Global* (Portugal, 2010).

[3] Nouri, F., Habibzadeh, S. & Norouzi, H. R. Tertiary current distribution of a chlorine-evolving electrochemical system: A comprehensive computational study. Int J Heat Mass Transf 205, 123887 (2023).

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