DIGITAL CFD MULTIPHASE MODELLING FOR CO_2 ELECTROREDUCTION DESIGN

Myles Bentley

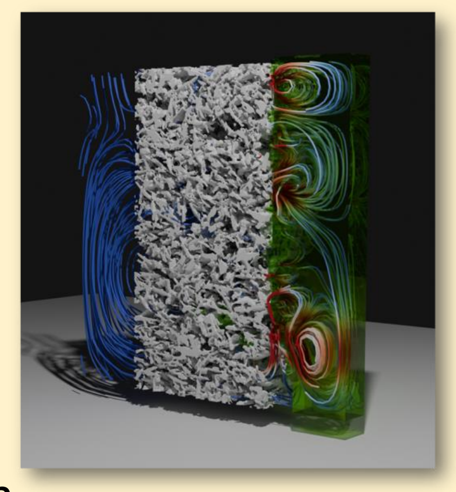
Priority Topic Area: **Digitalisation and Artificial Intelligence**

Background

- Johnson Matthey aims to convert CO_2 from a harmful pollutant into a carbon-negative chemical feedstock for the future.
- To achieve this, CO_2 is electrocatalytically reduced using a porous CuO/Nafion electrode in 1M $KHCO_3$.
- However, to be economically viable the efficiency must be improved; therefore, by applying CFD modelling the key physical parameters of the system can be optimised.
- Collaboration with **'Electrochemical Transformation'** team to understand the effect of inlet gas flow rate, contact angle, pore size and pressure distribution.

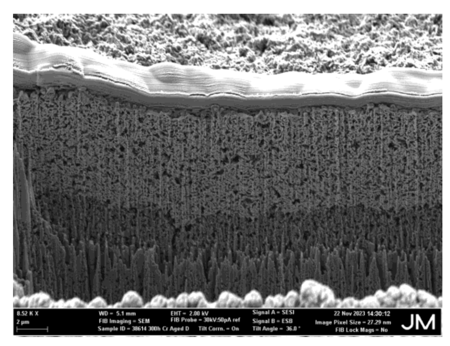
Conclusion

- Increasing CO_2 flow rate draws more electrolyte into pores, which may limit catalytic reaction sites.
- Higher contact angles suppress electrolyte intrusion.
- Contact angle strongly influences interphase geometry, indicating wettability is a key design variable for gas-liquid distribution.
- Optimising wettability and flow conditions is essential for improving CO_2 transport and achieving economically viable electroreduction.



Simulation Method

- **FiB-SEM** (Focused Ion Beam-Scanning Electron Microscope) and digitalisation into **STL** (Stereo Lithography) for real CuO/Nafion porous catalyst structure.
- Geometry preparation and mesh generation to build simple electrolyser structure (schematic on right).
- **OpenFOAM** with **interFoam** multiphase solver.



Real CuO/Nafion catalyst layer generated using FiB-SEM and converted to STL for CFD model

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OpenFOAM CFD software used with interFoam multiphase solver

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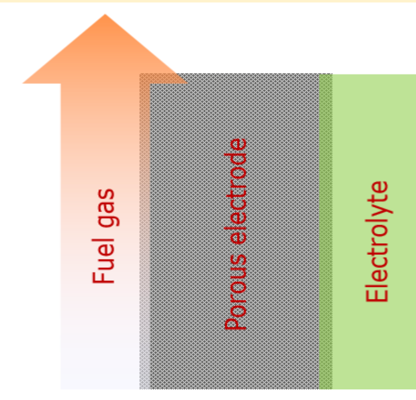


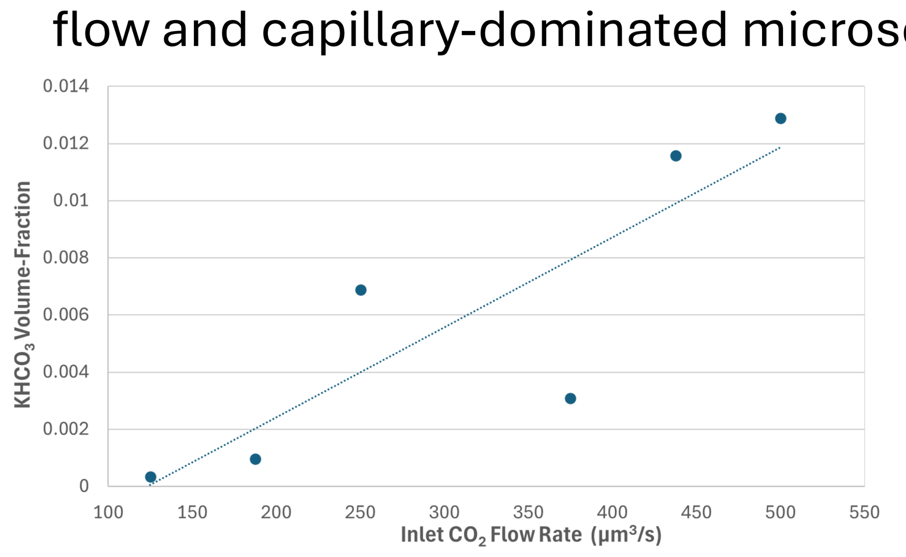
Schematic representation of electrolyser

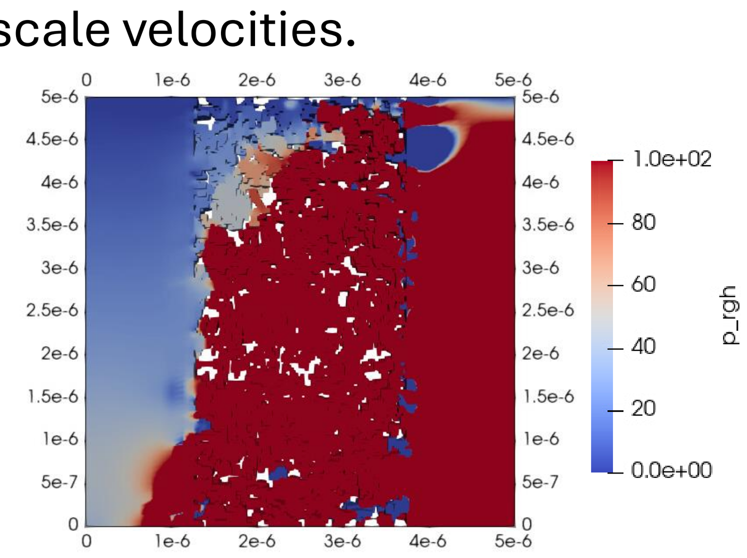
Results

- CFD sensitivity analysis to observe how experimental parameters influence multiphase transport in porous catalyst structure.

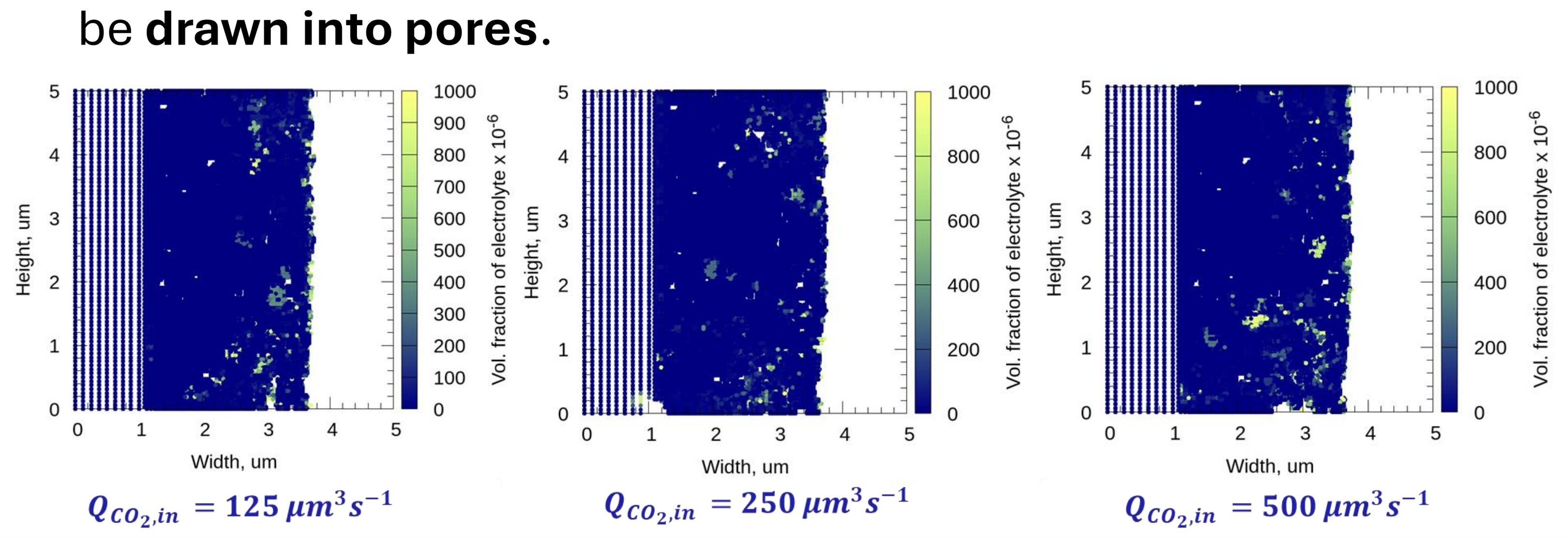
Inlet Gas Flow Rate Study:

- **Transient**, **multiphase** flow regime forming fingering, channelised flow and capillary-dominated microscale velocities.

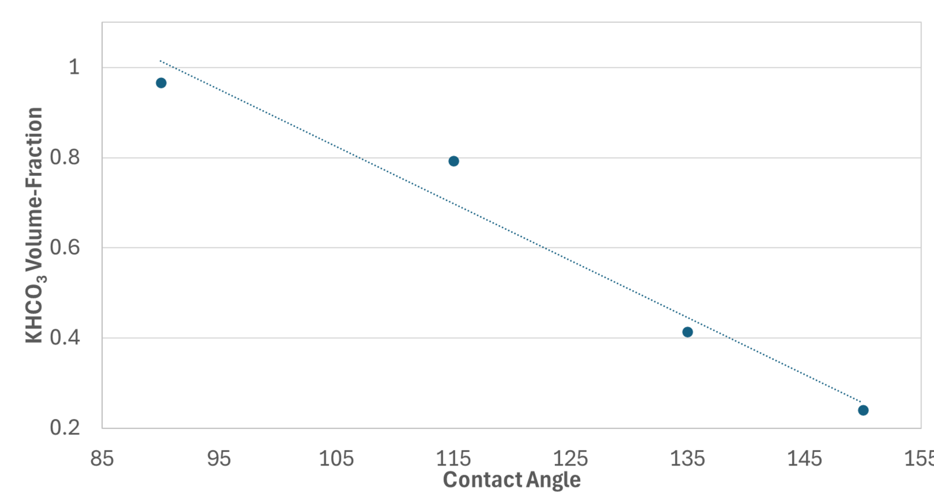




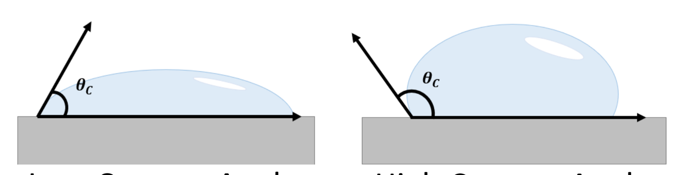
- Increasing the inlet gas flow rate decreases pressure along gas channel (**Bernoulli's principle**).
- $\Delta p_{(liquid \rightarrow gas)} = p_l - p_g$ is **positive** which causes electrolyte to be **drawn into pores**.



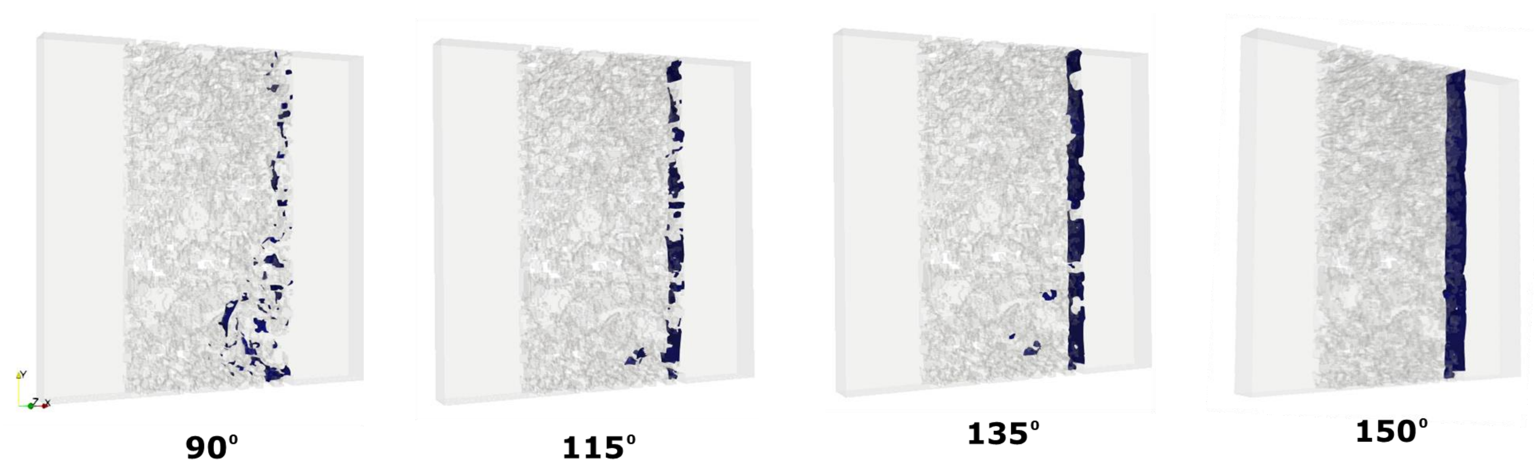
Contact Angle Study:



- **Angle** formed at intersection between **liquid**, **gas** and **solid**.



- **Increasing** contact angle **decreases** electrolyte concentration at electrolyte-pore interface.
- At **lower** contact angles, electrolyte appears **dispersed**, implying greater penetration of electrolyte.
- At **higher** contact angles, electrolyte intrusion into the pores is **suppressed**, shown by a **continuous band** at the interface.



Benefit to Society

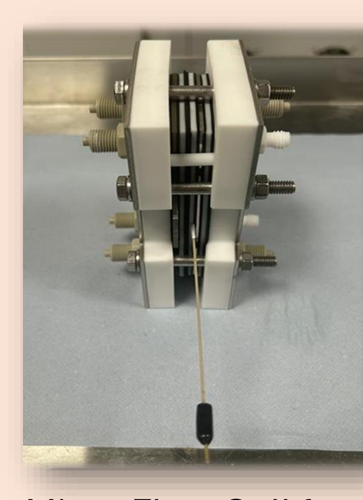
- This project adds value to society by accelerating the development of low-carbon, electrified CO_2-to-ethylene technology through advanced digital modelling.
- This enables cleaner chemical production, circular carbon use and faster progress toward net-zero industrial processes.

Bridging the Gap

- **eCO_2 electroreduction** rig used to **reduce** CO_2 into a range of products, primarily **ethylene**.
- **Faradaic efficiency** can be calculated for catalyst layer and describes the overall **selectivity** of the electrochemical process:

$$Faradaic\ Efficiency = \frac{Charge\ consumed\ to\ form\ product}{Total\ charge} \times 100$$

- **Electrochemical Transformation** team can use CFD model to observe **bulk trends** and the effect of key operating parameters.
- Next step: to compare CFD results for **~40%** and **~70%** Faradaic-efficiency layers to identify the **causes** of the efficiency **differences**.



Micro Flow Cell from ElectroCell

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Electrochemical Transformation Group

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