



Universidad
del País Vasco

Euskal Herriko
Unibertsitatea

Development of a Multiphysics model for an aqueous organic redox flow battery

HIGREEW Workshop II

Aitor Beloki Arrondo

16/05/2023

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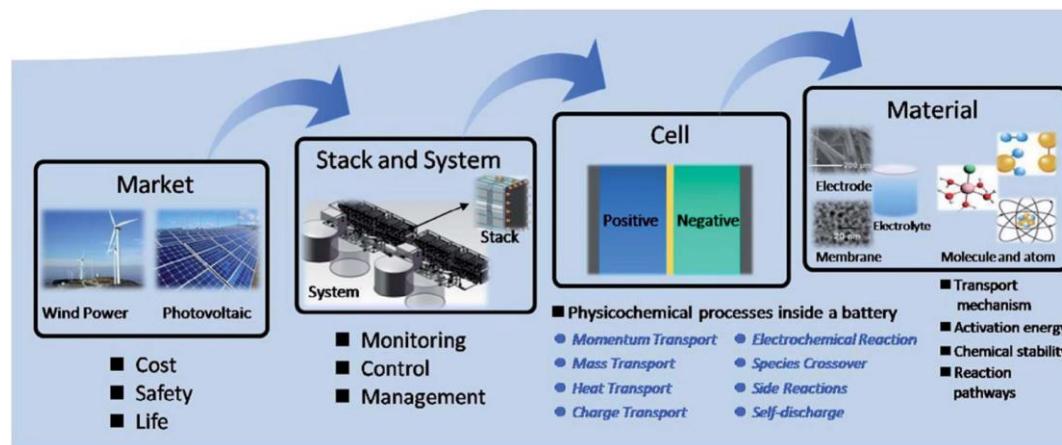
MEMBER OF BASQUE RESEARCH
& TECHNOLOGY ALLIANCE

> Multiphysics Modelling of an AORFB

THESIS OVERVIEW

“Design Optimization of Redox Flow Batteries by means of 3-D Multiphysics Computational Simulation”

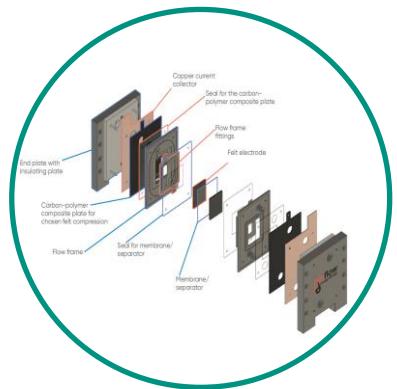
- **Multiphysics** → Coupled Fluid-dynamic, Electrochemical and Thermal Model. (Collaboration EES-TES)
- Model oriented to aqueous organic RFBs. (**TEMPO-Viologen** system)
- Model based on Computational Fluid Dynamics (CFD). Model implementation in **ANSYS Fluent**.
- Experimental validation in a **20 cm² single cell lab test rig**.



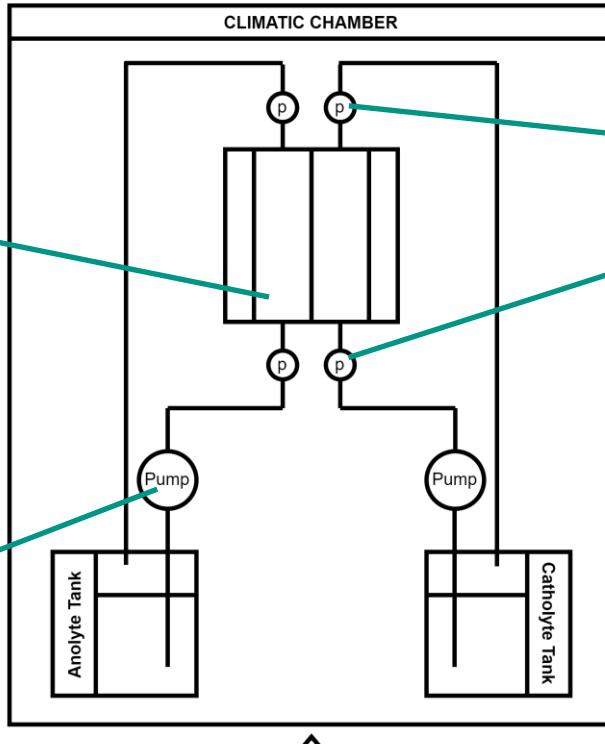
Fluid-Dynamic Model of an Aqueous Organic Redox Flow Battery

> Multiphysics Modelling of an AORFB

EXPERIMENTAL SET-UP



PinFlow 20cm² Cell



Iwaki Centrifugal Pumps



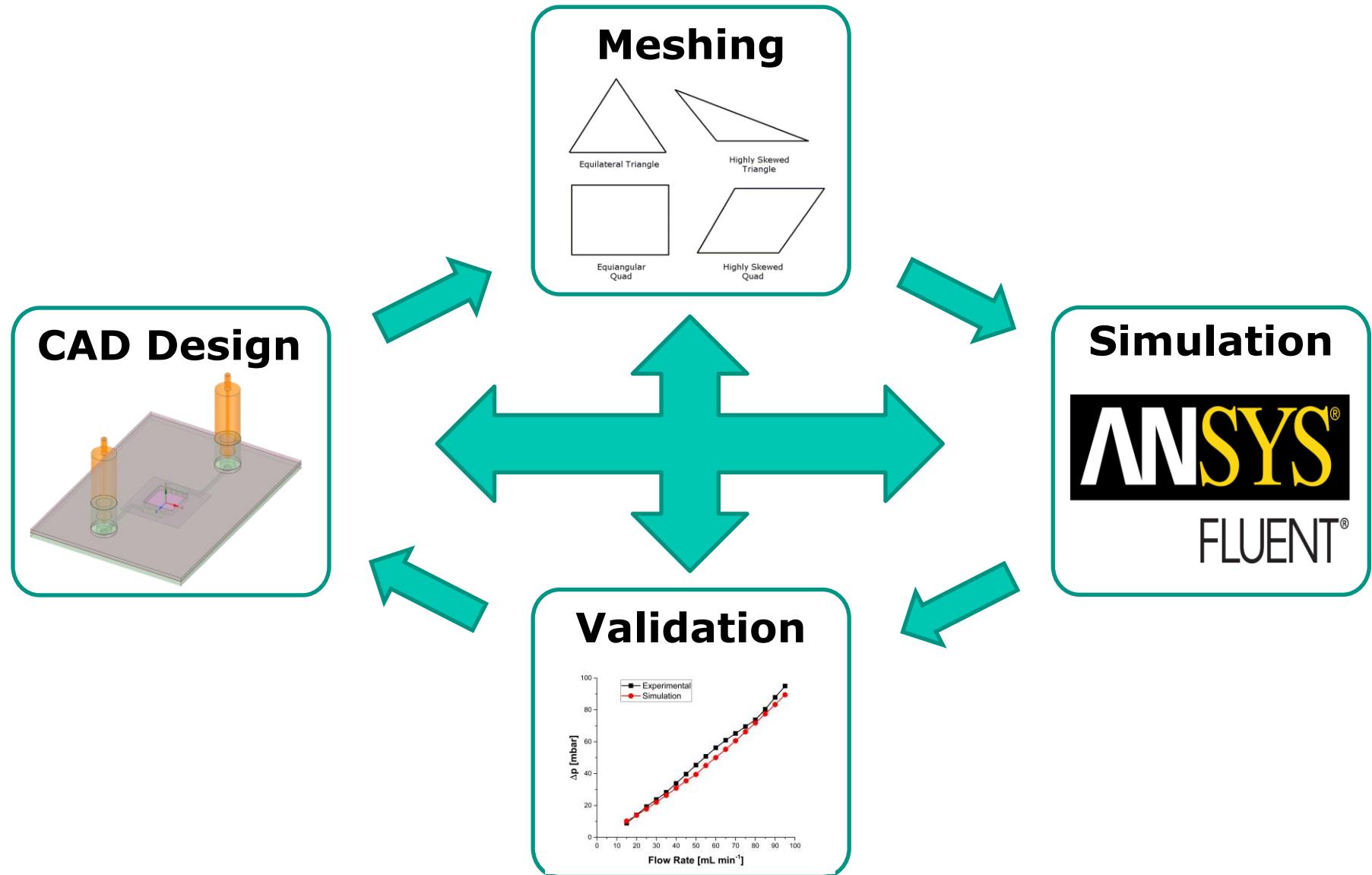
Huba Control Pressure sensors



PTC + Data Module

> Multiphysics Modelling of an AORFB

MODELLING & SIMULATION PROCESS

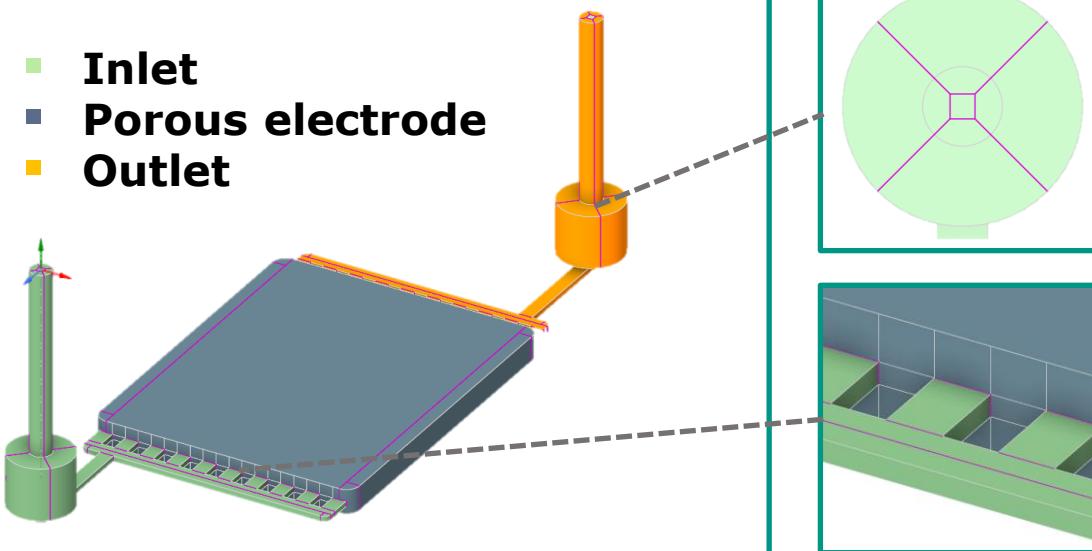


> 3D Fluid-Dynamic Model of an AORFB

CAD DESIGN

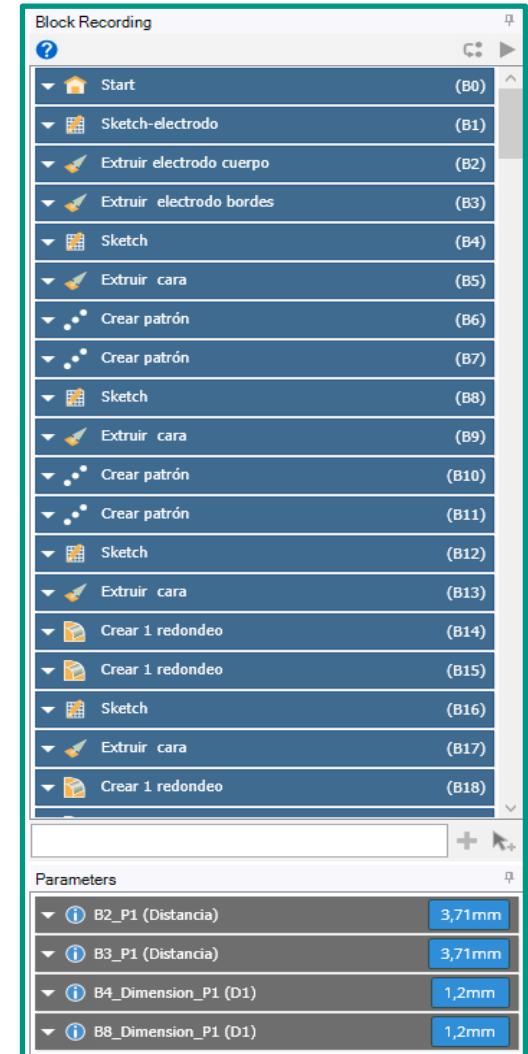
Control Volume

- Inlet
- Porous electrode
- Outlet



- Geometry Simplifications
- Control Volume Partitioning
- Surface Printing

CAD Design adaptation for mesh optimization



> Fluid-Dynamic Model of an AORFB

MESHING

Simulation Accuracy

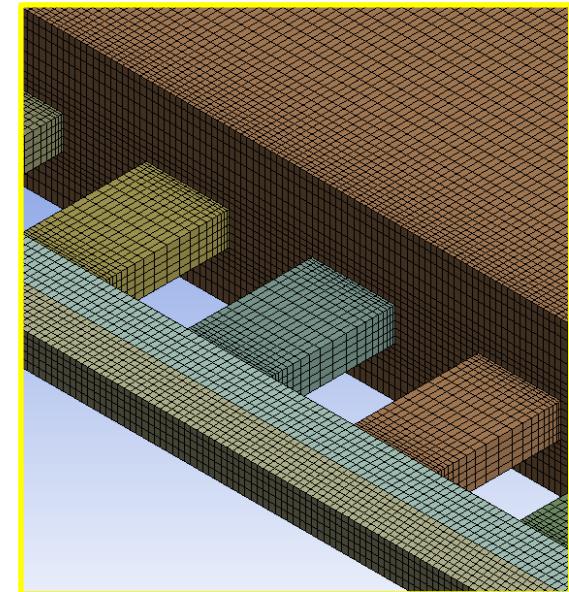


Computational Cost

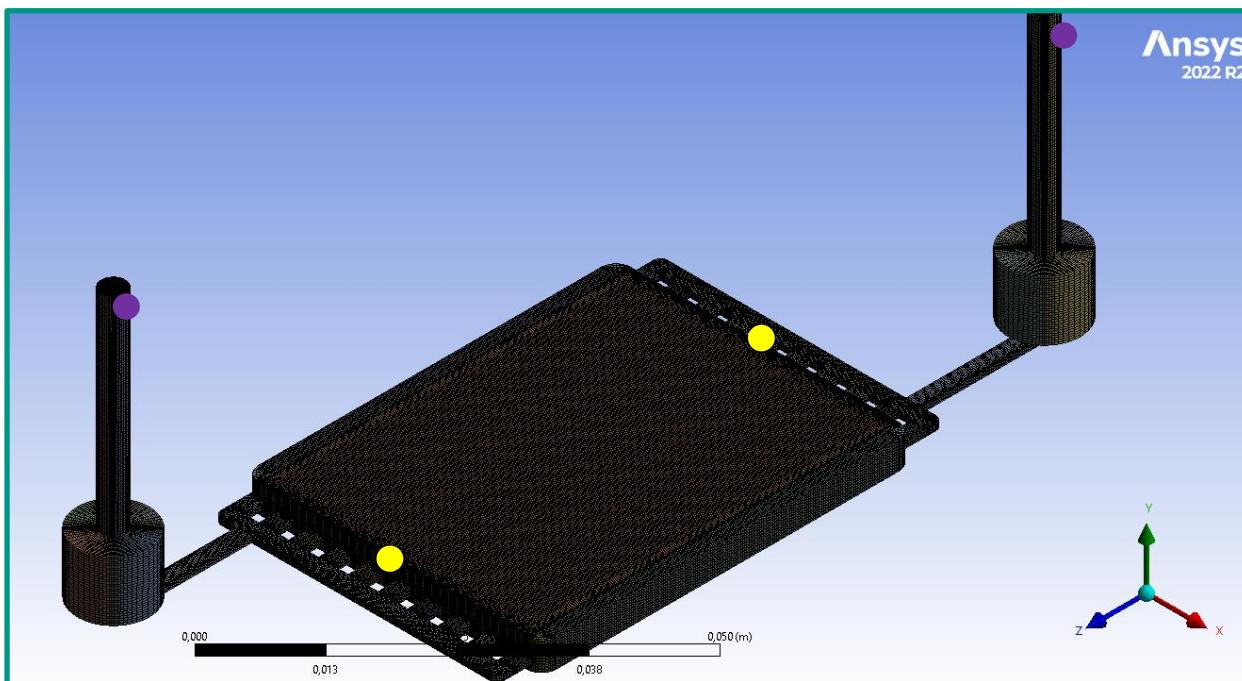
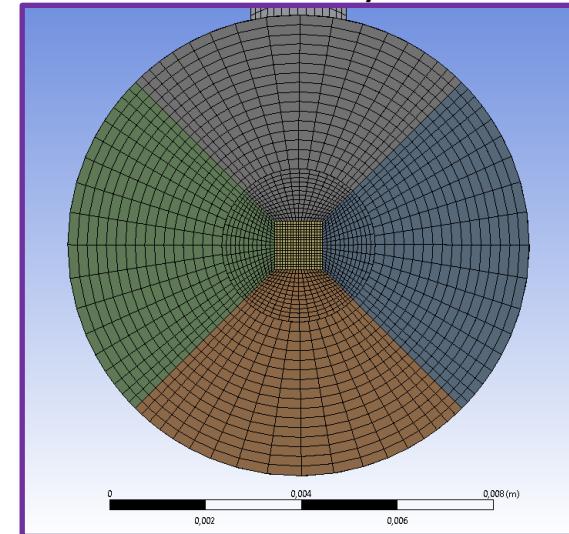


Hexahedral Mesh

Channel-Electrode Interface



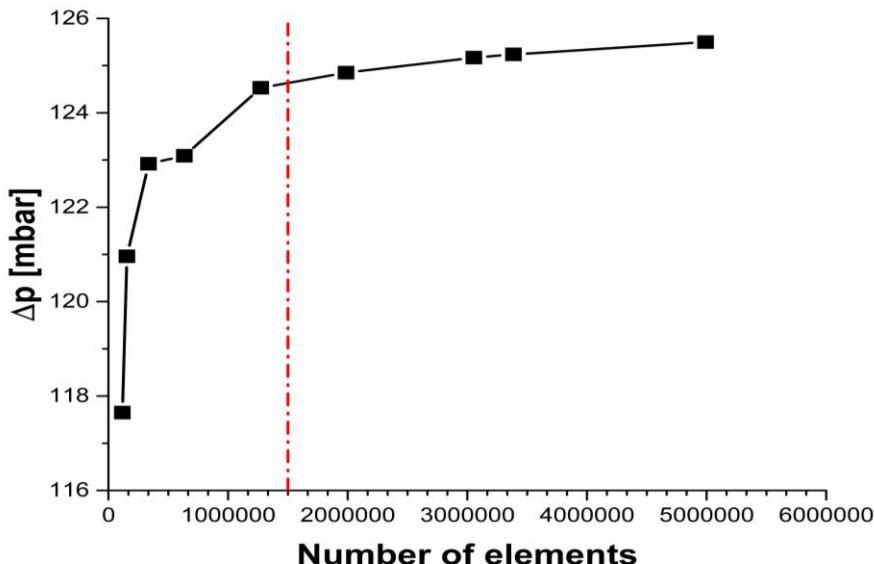
Flow Frame Inlet/Outlet



> Fluid-Dynamic Model of an AORFB

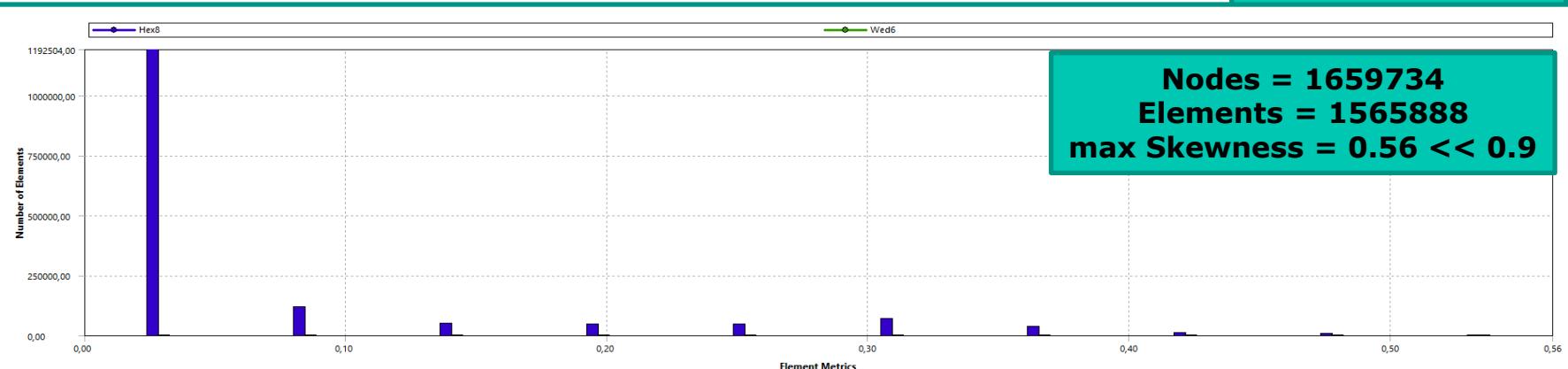
MESHING

Mesh Independence Study



For the fluid-dynamic model does not make any sense to go over $1,5 \cdot 10^6$ elements in the mesh

Mesh Quality

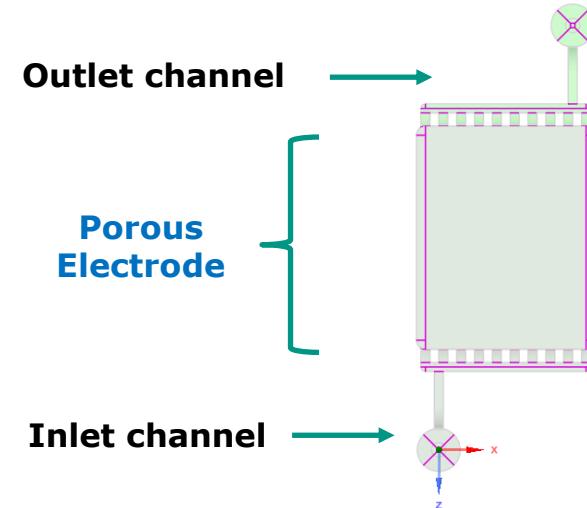


> 3D Fluid-Dynamic Model of an AORFB

MATHEMATICAL MODEL

Hypothesis:

- Incompressible fluid
- Laminar flow rate
- Viscous losses >> Inertial losses → **Darcy's Law**
- Isotropic porous media
- Physical velocity: $u_{superficial} = \varepsilon_c \cdot u_{physical}$



Inlet/Outlet channels

Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{u}) = 0$$

Navier-Stokes Equations

Momentum conservation equation:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla \left(\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F}$$

Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{u}) = 0$$

Porous Media Model

Momentum conservation equation:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon} \right) = -\nabla p + \mu(\nabla^2 \mathbf{u}) - \varepsilon \frac{\mu}{k} \mathbf{u}$$

> Fluid Dynamic Model AORFB

ELECTRODE CHARACTERIZATION

GFD 4.65EA

$$k = \frac{d_f^2 \varepsilon_c^3}{K_{KC} (1 - \varepsilon_c)^2}$$



Permeability estimation by Kozeny-Carman's model

- Open Porosity – MIP**

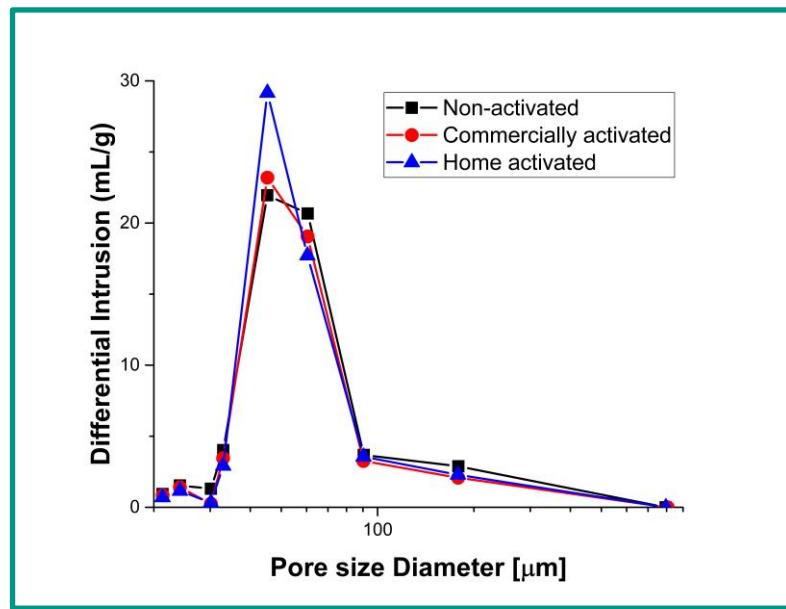
$\varepsilon_{NA} = 0.924$

$\varepsilon_{CA} = 0.9151$

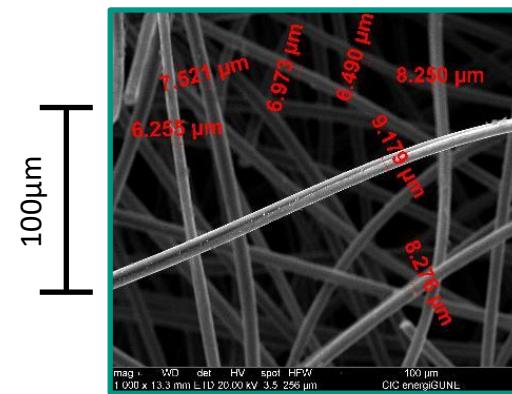
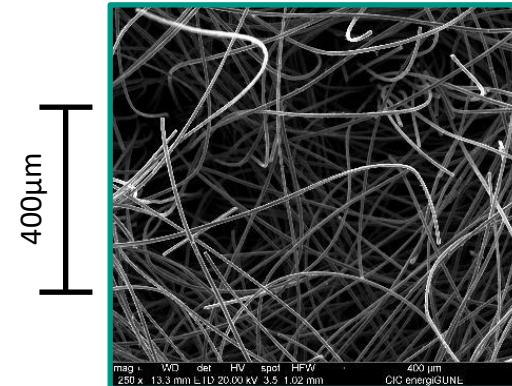
$\varepsilon_{HA} = 0.926$ (400°C 30h)

$\varepsilon = 0.92 \pm 0.5$

($\varepsilon_{Ref} = 0.94$)



- Fiber diameter - SEM**



$d_f = 9.2 \mu\text{m}$

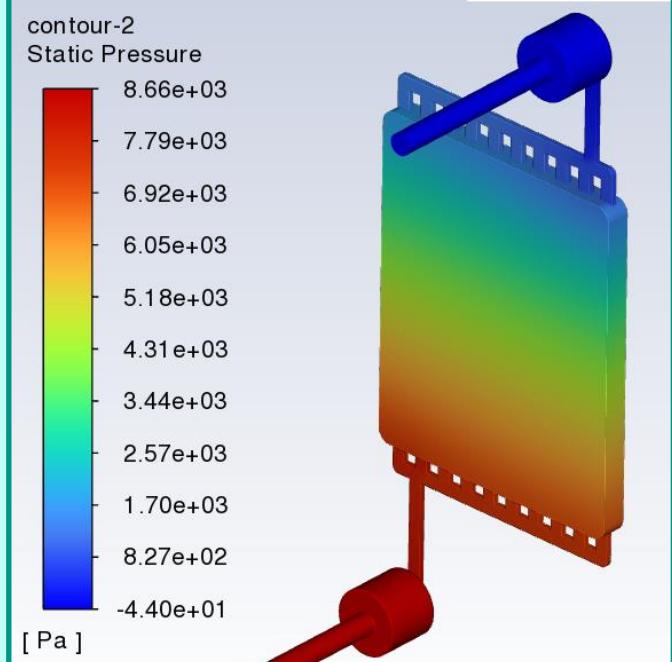
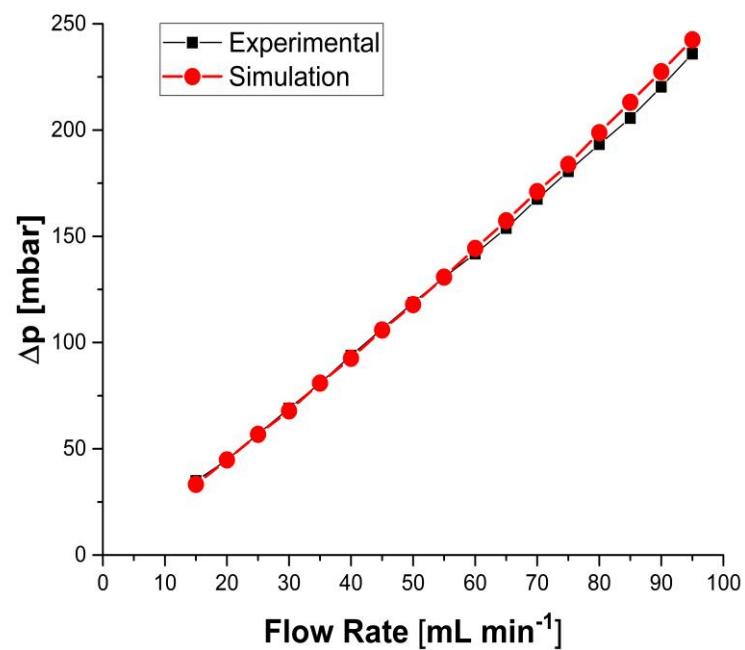
> Fluid Dynamic Model AORFB

ELECTRODE PERMEABILITY

Experiment

Analysis

Validation

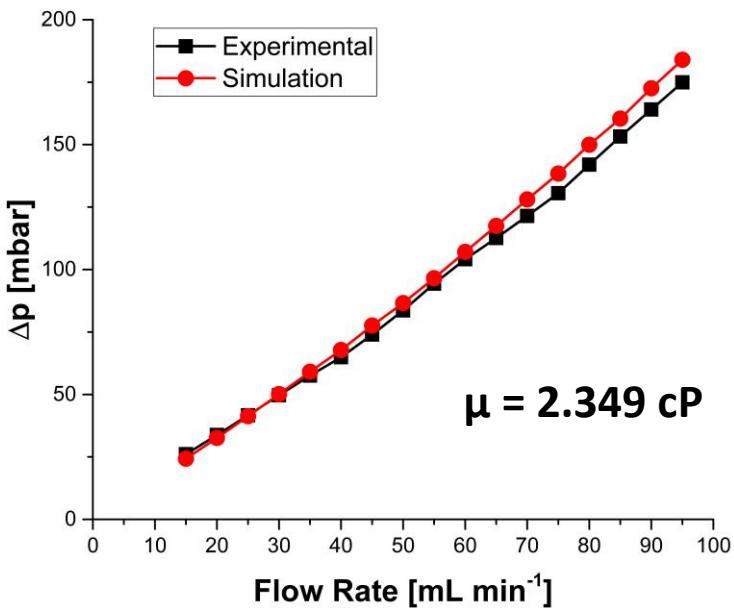


> Fluid Dynamic Model AORFB

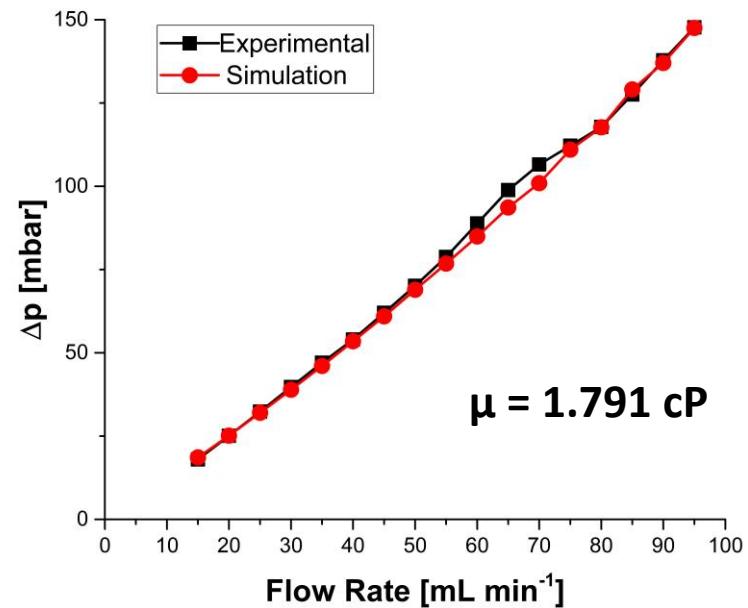
MODEL VALIDATION

Permeability, $\kappa = 1.156 \text{ e}^{-10} \text{ m}^2$

30% Glycerin



20% Glycerin



> Multiphysics modelling of an AORFB

CONCLUSIONS & FUTURE WORK

Fluid-dynamic Model:

- A high-quality mesh (**max skewness = 0.56**) has been obtained, providing robust simulations within acceptable computational times.
- The model correlates **accurately** the simulation results to the experimental measurements at **low flow rates**.
- Model validation for half-cell configurations with different CRs.

Electrochemical Model:

- Current challenge → Modelling the charge balance equation in the electrode-electrolyte interface.

> Acknowledgements

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GRACIAS · THANK YOU · ESKERRIK ASKO

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