6th Two-Day Meeting on Propulsion Simulations Using OpenFOAM Technology
11th – 12th March 2024

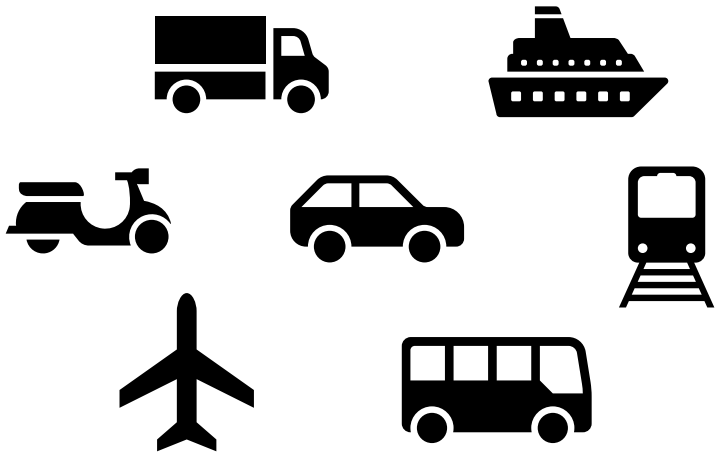
Application of a CFD methodology for the design of PEM fuel cells for propulsion applications

M. Bulgarini, A. Della Torre, A. Baricci, A. Grimaldi

Presentation outline

- Introduction
- Methodology
- Case study and validation
- Conclusions and next steps

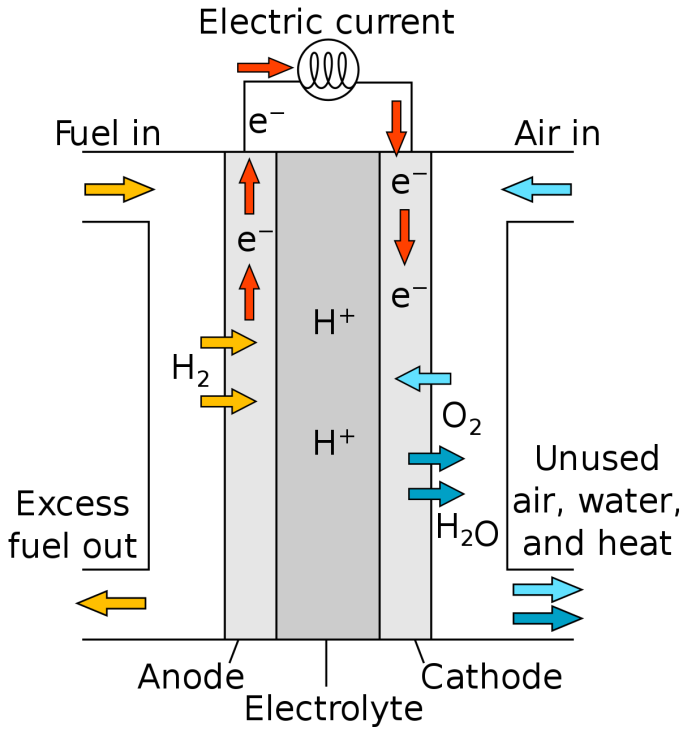
Propulsion scenario



- Mobility sector must guarantee **zero CO_2 emissions** within **2035**
- Different applications require different propulsion systems: ICE using alternative fuels, BEV, FCEV

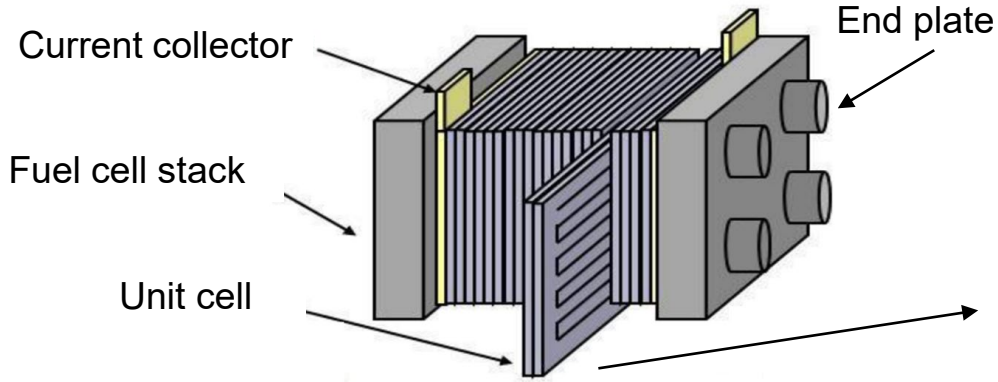
In this scenario **polymer electrolyte membrane (PEM) fuel cells** can play a crucial role in the decarbonization of the transport sector:

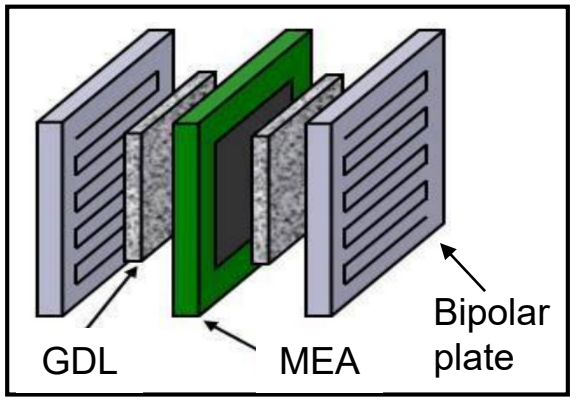
- Electrochemical conversion of H_2 and O_2 into H_2O, producing electric energy
- Zero direct CO_2 emissions, low temperature and high efficiency



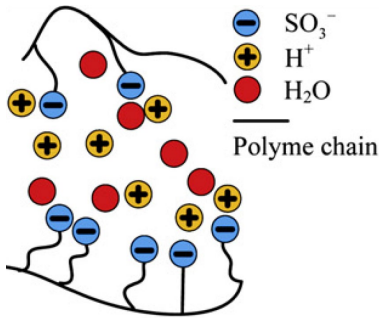
PEMFC: a multiscale modeling

The PEMFC operation is described through a **multiscale modeling** procedure.

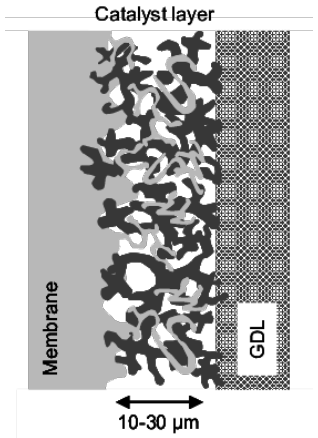




Å Nanoscale nm / µm Microscale mm / cm Macroscale m



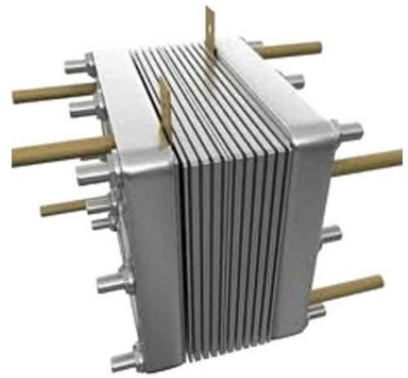
Membrane H_2O transport



Catalyst layer

Gas diffusion layer

Bipolar plate

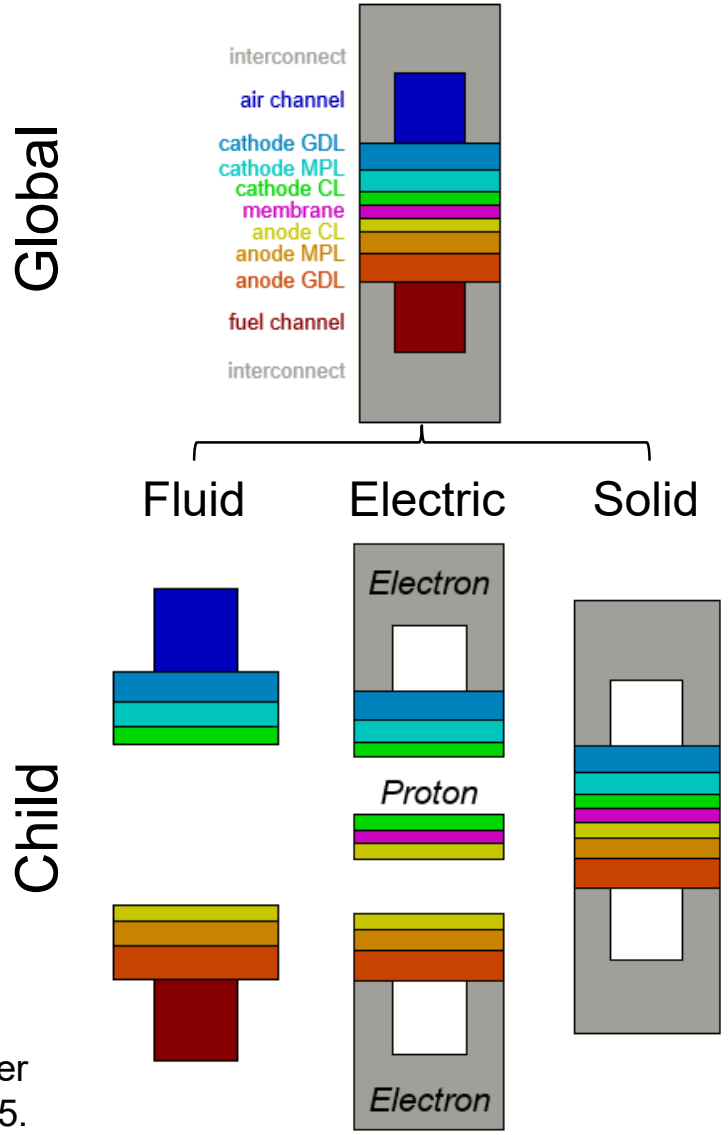


FC stack

- Introduction
- **Methodology**
- Case study and validation
- Conclusions and next steps

OpenFOAM methodology

- The PEMFC modeling is performed through the ***openFuelCell2*** **library** developed in [1] within the OpenFOAM code.
- The methodology is **multi-region** and **multi-physics**.
- Different **computational grids** are applied:
  - Global mesh: **energy conservation equation** is solved;
  - Child meshes (fluid, solid and electric): **specific governing equations** are solved to describe the major transport phenomena in the different regions of a PEMFC.



[1] S. Zhang et al, openFuelCell2: A New Computational Tool for Fuel Cells, Electrolysers, and Other Electrochemical Devices and Processes, SSRN Electron. J. (2023). https://doi.org/10.2139/ssrn.4540105.

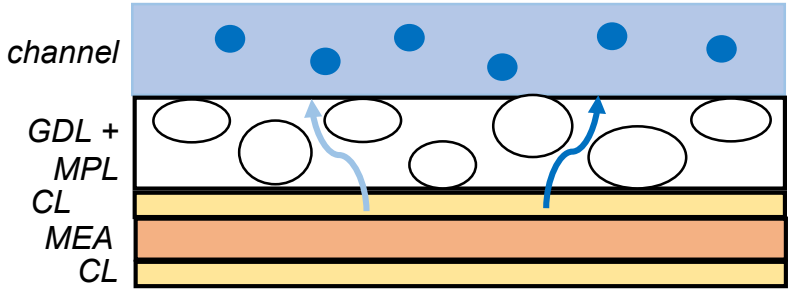
OpenFOAM methodology

On the child meshes **different physics** are solved:

Fluid region

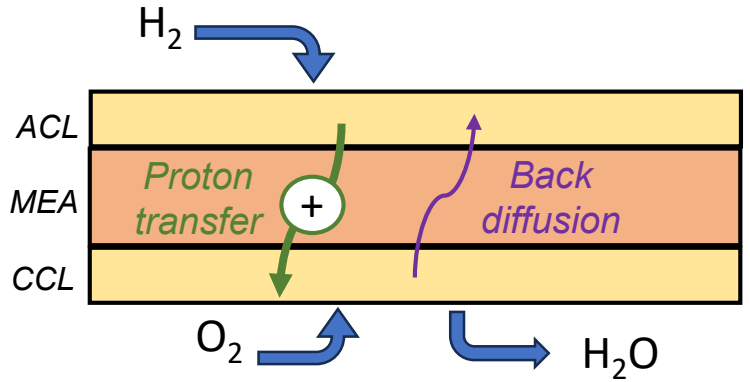
- **Multiphase flow** in air channel (Euleran-Euleran)
- **Water movement** in porous media is driven by capillarity pressure (Leverett function)
- **Mass transfer** in porous media considering the diffusion of **gas phase** only (Fick's law)

→ Diffusion coefficient accounts for pore blockage due to H_2O condensation



Electric region

- **Conservation** of electronic and protonic **charge** is imposed (Ohm's law)
- **Water cross-over** (λ phase) through membrane (**proton transfer** and **back diffusion**) is modelled
- **Electrochemical reactions** are solved



Solid region

- No governing equations are explicitly solved; **heat exchange** only is considered.

Electrochemical reaction kinetic

Electrochemical reactions:

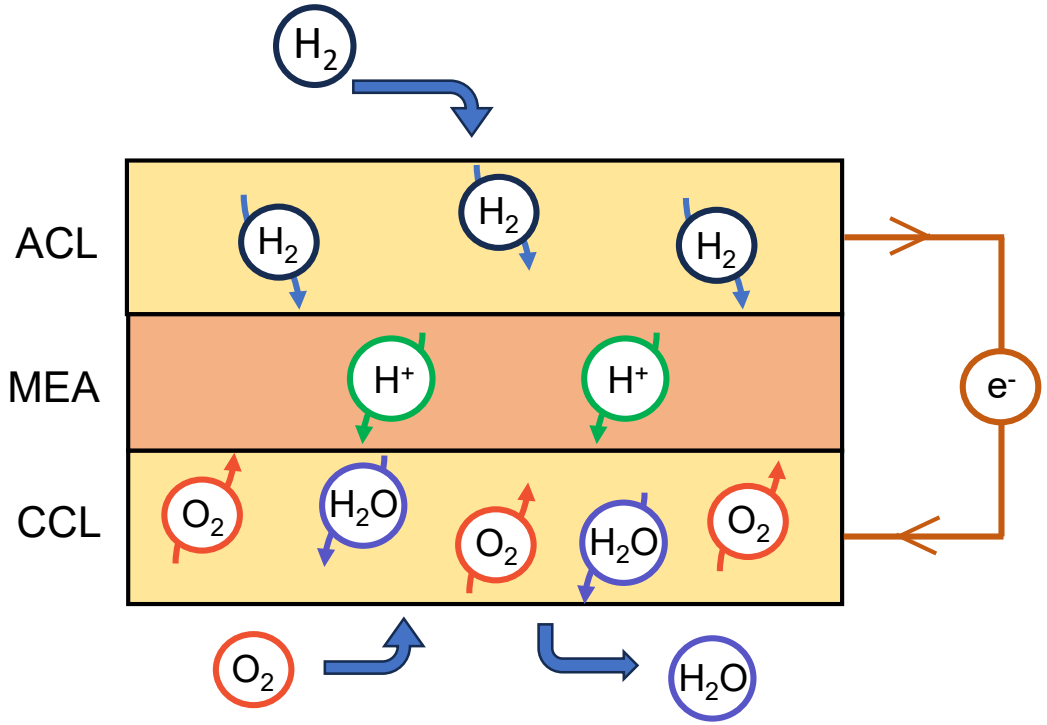
Anode $H_2 \rightarrow 2H^+ + 2e^-$ HOR

Cathode $1/2O_2 + 2H^+ + 2e^- \rightarrow H_2O$ ORR

Overall $H_2 + 1/2O_2 \rightarrow H_2O$

HOR = Hydrogen oxidation reaction

ORR = Oxygen reduction reaction



The electrochemical reactions are described by a kinetic expression as the **Butler-Volmer** equation:

$$j = j_{ref} \prod_i \left(\frac{C_i}{C_{ref}}\right)^{\xi} \left[\exp\left(\frac{-\alpha F \eta}{RT}\right) - \exp\left(\frac{(1-\alpha) F \eta}{RT}\right)\right]$$

j = produced current density [A/m^3]

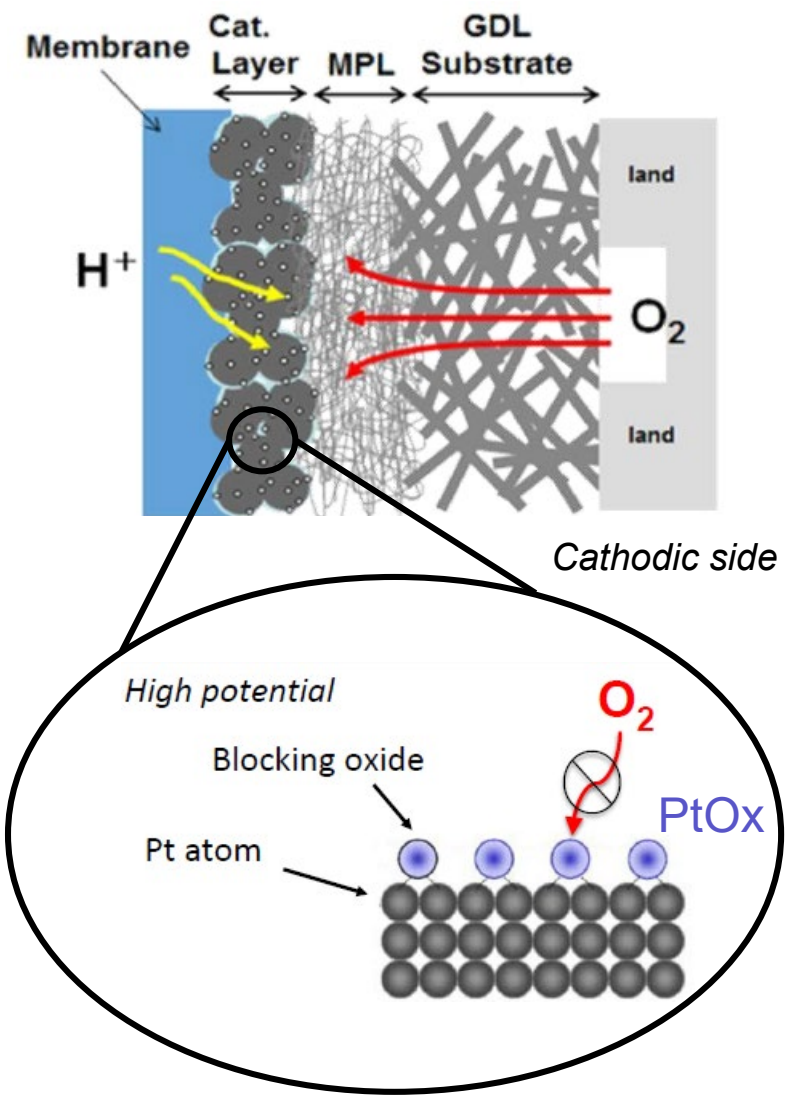
Implementation of PtOx formation

1. In presence of O_2 and above 0.8 V, **Pt particles** on cathodic catalyst layer can be **oxidized forming PtOx**.
2. Active **catalyst sites** are partially **blocked** (ECSA reduction), so **O_2 transport resistance** increases.
3. A **reduction of performance** with respect to theoretical Butler-Volmer law.

θ_{PtOx} = PtOx coverage ratio

$0 \leq \theta_{PtOx} \leq 1$

- $\theta_{PtOx} = 0$ Ideal kinetic
- $\theta_{PtOx} = 1$ Pt atoms fully covered



PtOx formation is governed by a Butler-Volmer equation:

$$\theta_{PtOx} = \frac{\exp\left(\frac{\alpha'_a F}{RT}\eta_{PtOx}\right)}{\exp\left(\frac{\alpha'_a F}{RT}\eta_{PtOx}\right) + \exp\left(\frac{-\alpha'_c F}{RT}\eta_{PtOx}\right)}$$

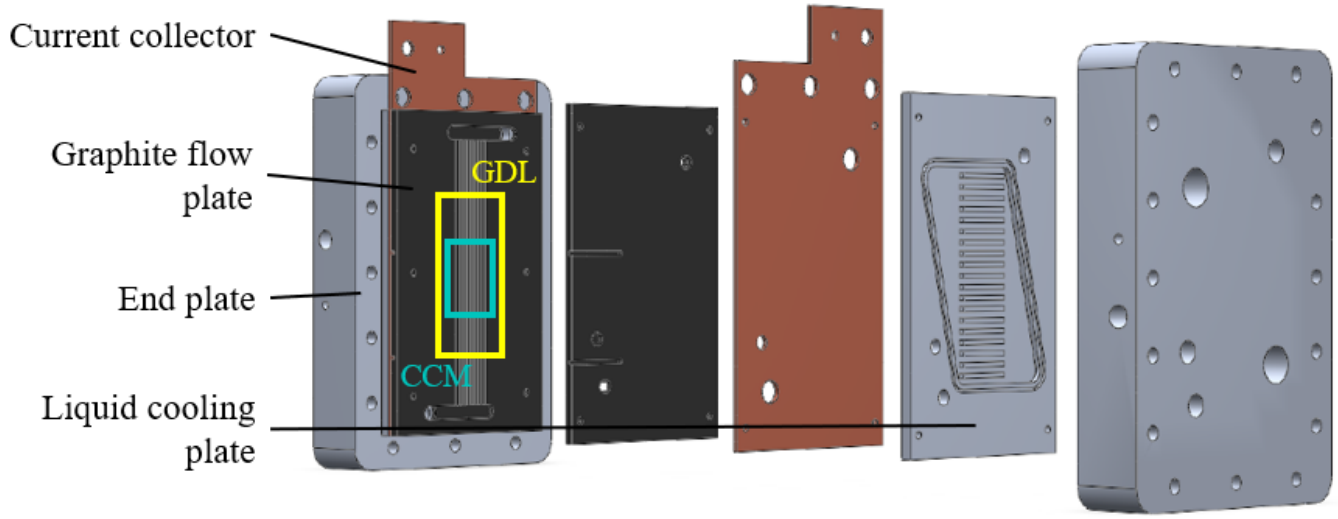
$$\eta_{PtOx} = U^{ORR} - U_{PtOx} + \eta_{act}^{ORR}$$

- Introduction
- Methodology
- **Case study and validation**
- Conclusions and next steps

Case study – Zero gradient cell hardware

- Cell hardware developed and tested at Politecnico di Milano (MRT Lab).

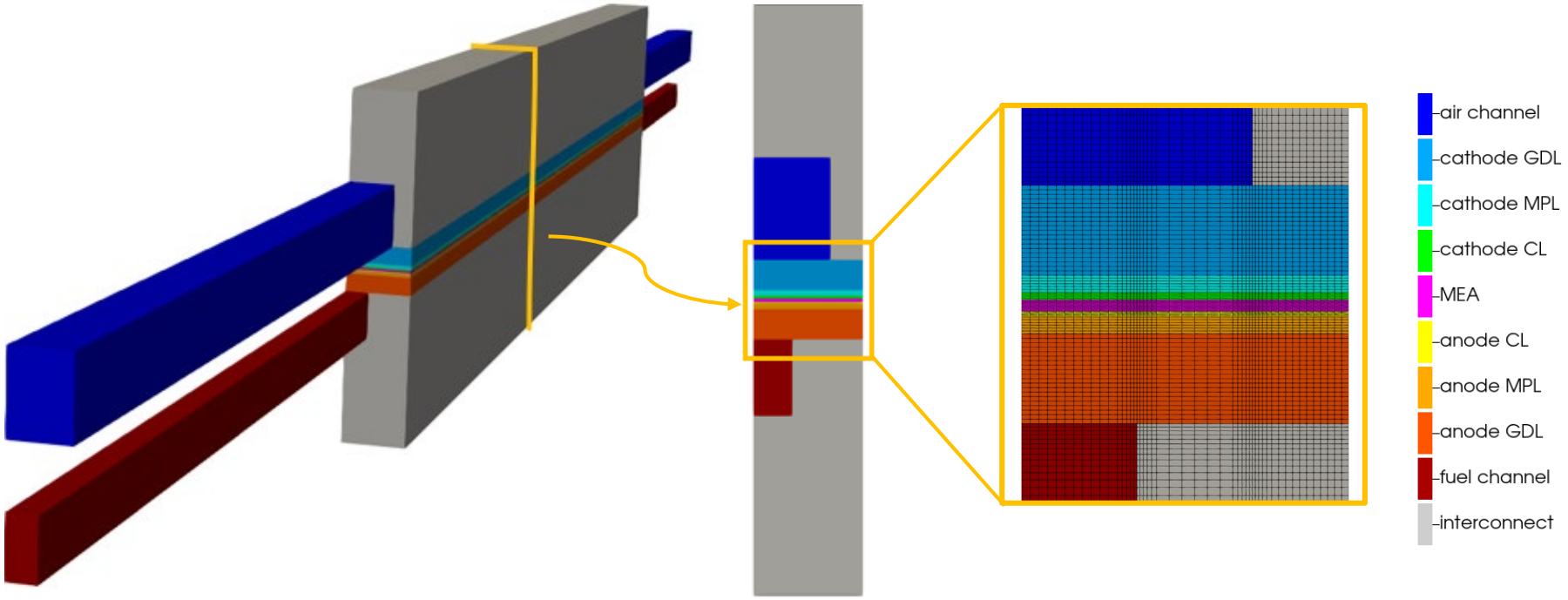
- It's a **parallel flow channels** configuration (24 channels at cathode and 25 at anode)



It's a **zero gradient cell hardware**:

- Designed with the purpose of obtaining almost **homogeneous operative conditions** in the channels from inlet to outlet and over the active surface area
- It minimizes the influence from testing hardware itself on results of performance and durability tests.

Case study – Computational domain



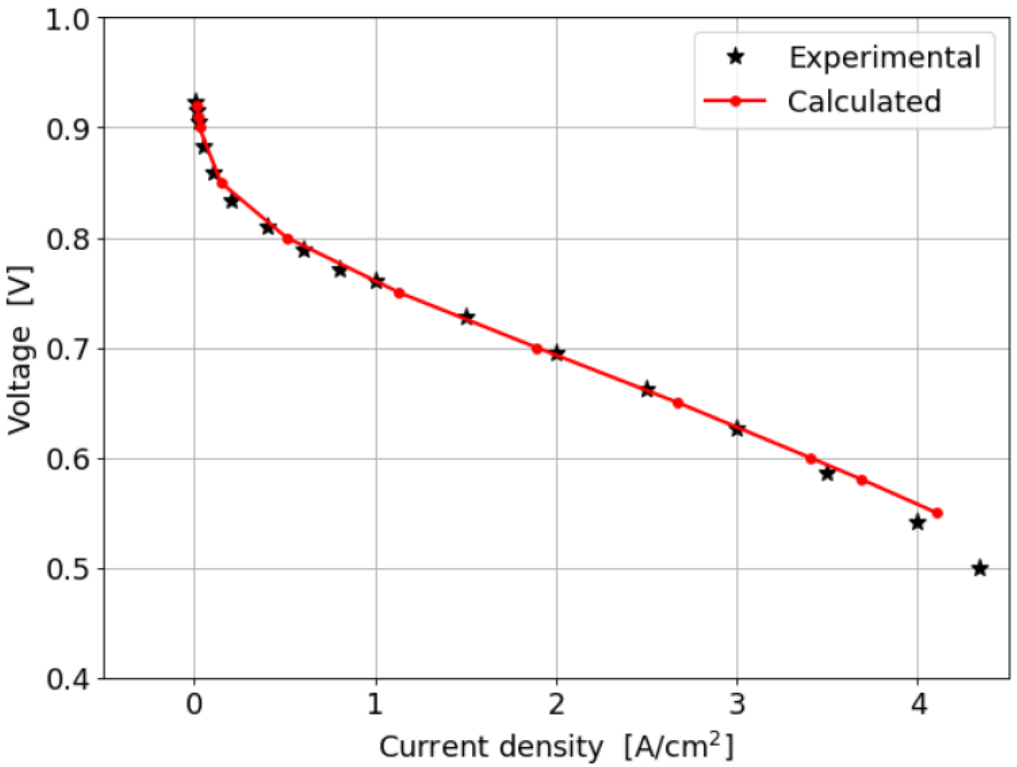
Computational domain:
$4.6 \cdot 10^5$ hexahedral cells

- The periodicity of the flow field is exploited, so only **half channel is simulated**.
- An ECSA of 4.25 mm^2 is simulated.
- **High stoichiometry factors** are used.

Operating conditions

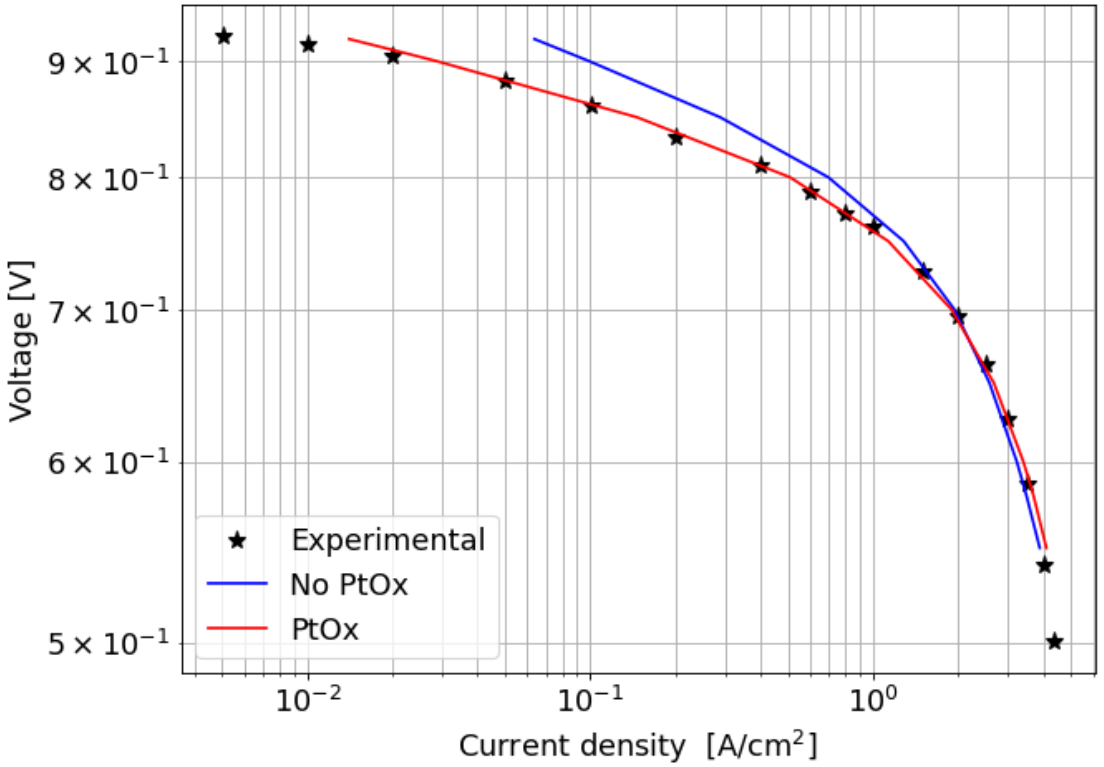
Anodic and cathodic RH in	100%	Operating temperature	80°C
Anode inlet pressure	2.5 bar	H_2 stoichiometry	8
Cathode inlet pressure	2.3 bar	O_2 stoichiometry	10

CFD model validation – Polarization curve



Log scale

High voltages

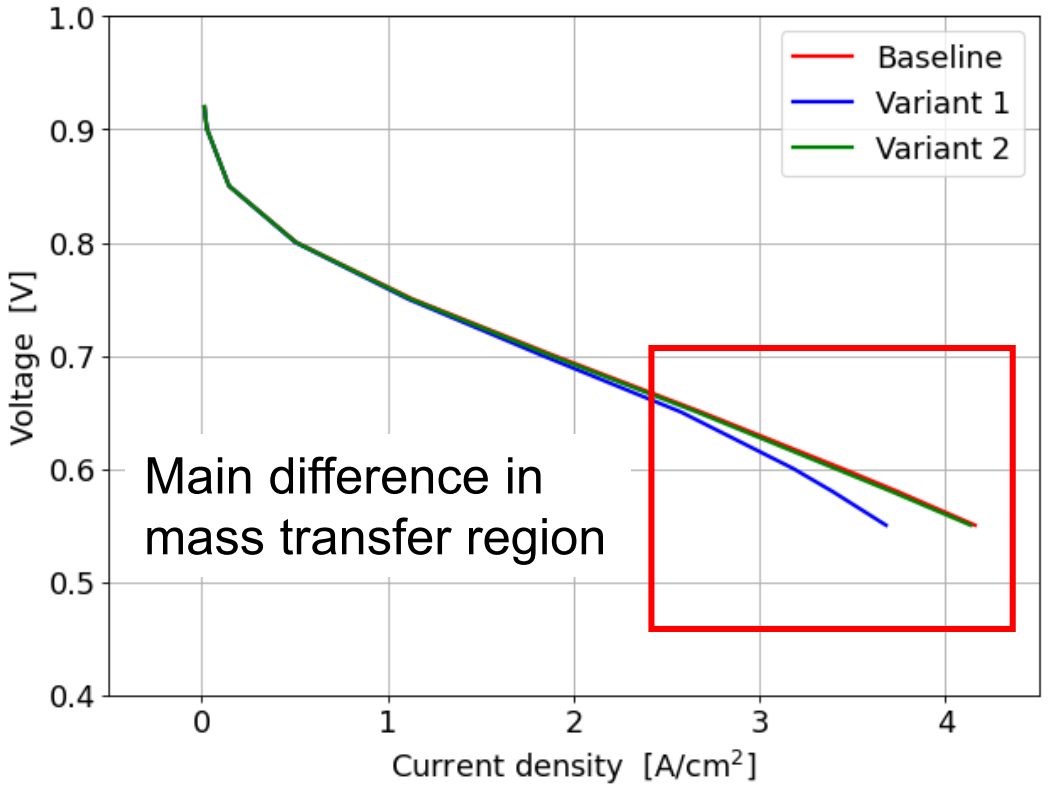


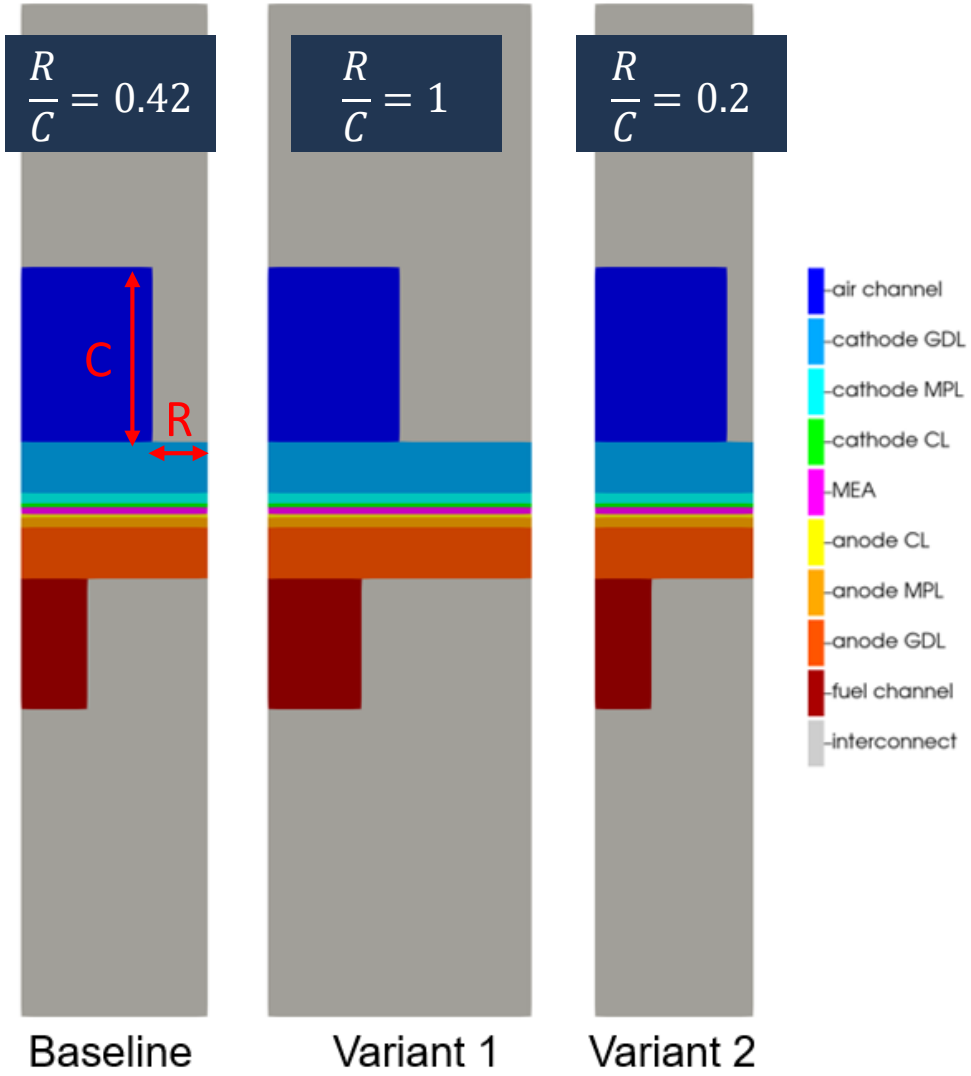
- A good agreement between numerical simulations and experiments is observed.
- The PtOx formation has a great impact on PEM performances at high voltages.

Parametric analysis – Variation of rib to channel ratio

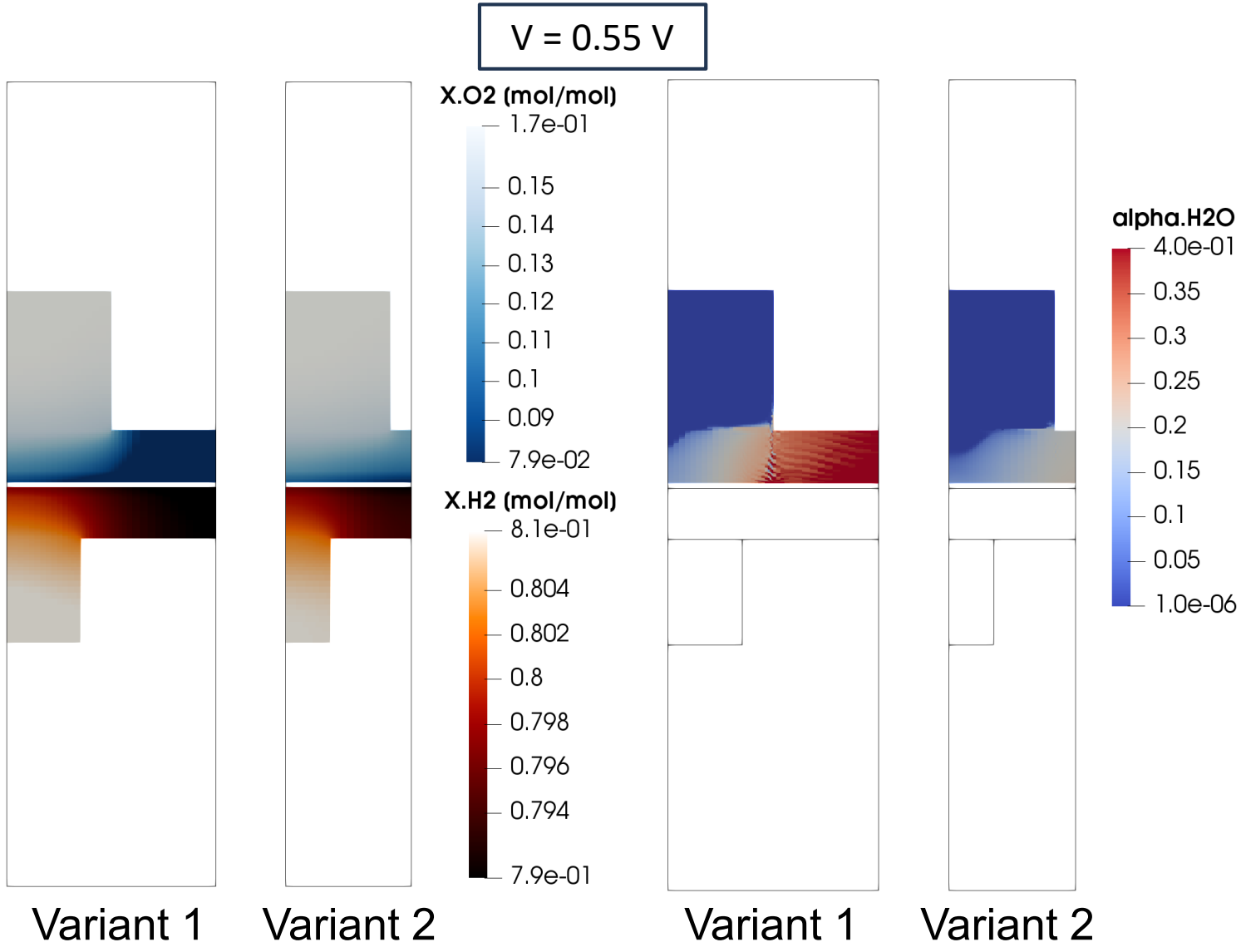
A variation of the rib to channel (R/C) ratio is imposed.

A comparison of performances with **constant reactants mass flow rate over the active surface area** is carried out.



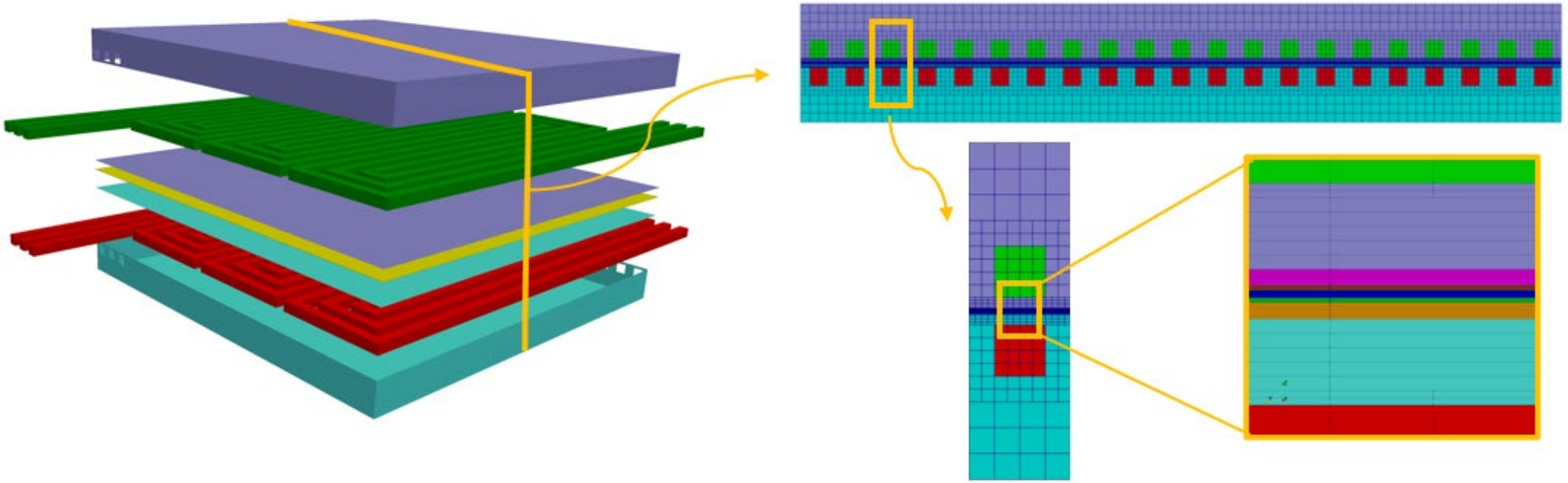


Parametric analysis – Diffusion of reactants



- Low O_2 **transport** in rib region for variant 1
- **Water management** issues arise for variant 1
- Trade-off between reactants diffusion and electron transport in GDL must be found.

Serpentine geometry



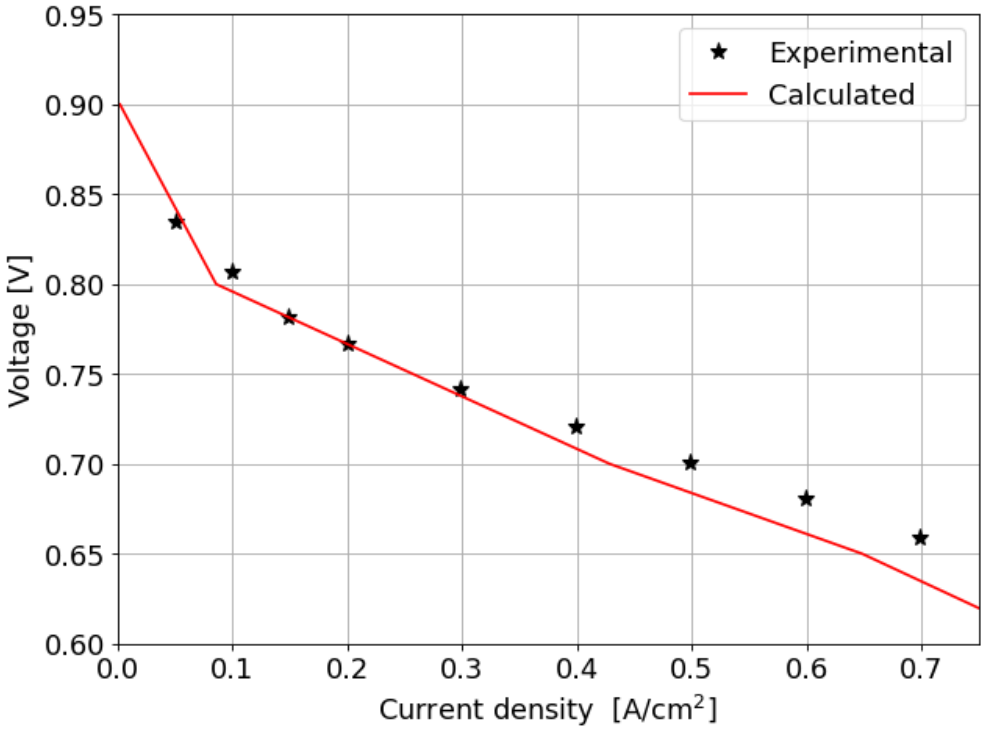
- It's a **serpentine flow field** configuration, featuring 3 channel each.
- An ECSA of 17.64 cm^2 is simulated.
- Single phase is assumed at cathode side.

Computational domain:
$2.3 \cdot 10^6$ polyhedral cells

Serpentine geometry

Operating conditions

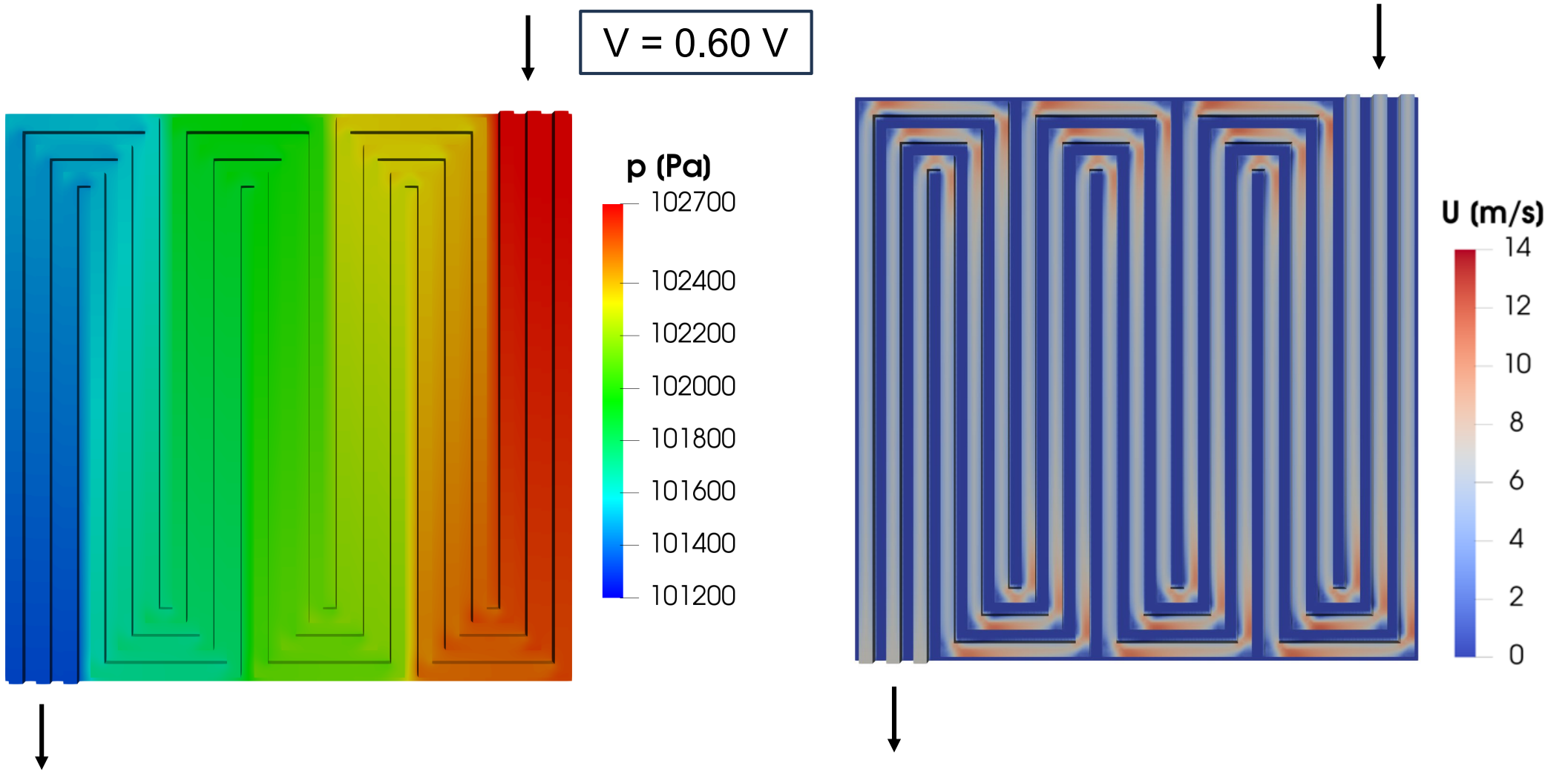
Anodic and cathodic RH in	90%
Anode inlet pressure	1 bar
Cathode inlet pressure	1 bar
Operating temperature	70°C
H_2 stoichiometry	1.2
O_2 stoichiometry	2.5



- **Low stoichiometries** are used for both anode and cathode sides.
- For low current densities, a good agreement between numerical simulations and experiments is observed.

Experimental data available in [2]: N. Weber, L. et al., Open-source Computational Model for Polymer Electrolyte Fuel Cells, OpenFOAM® J. 3 (2023) 26–48. https://doi.org/10.51560/ofj.v3.50.

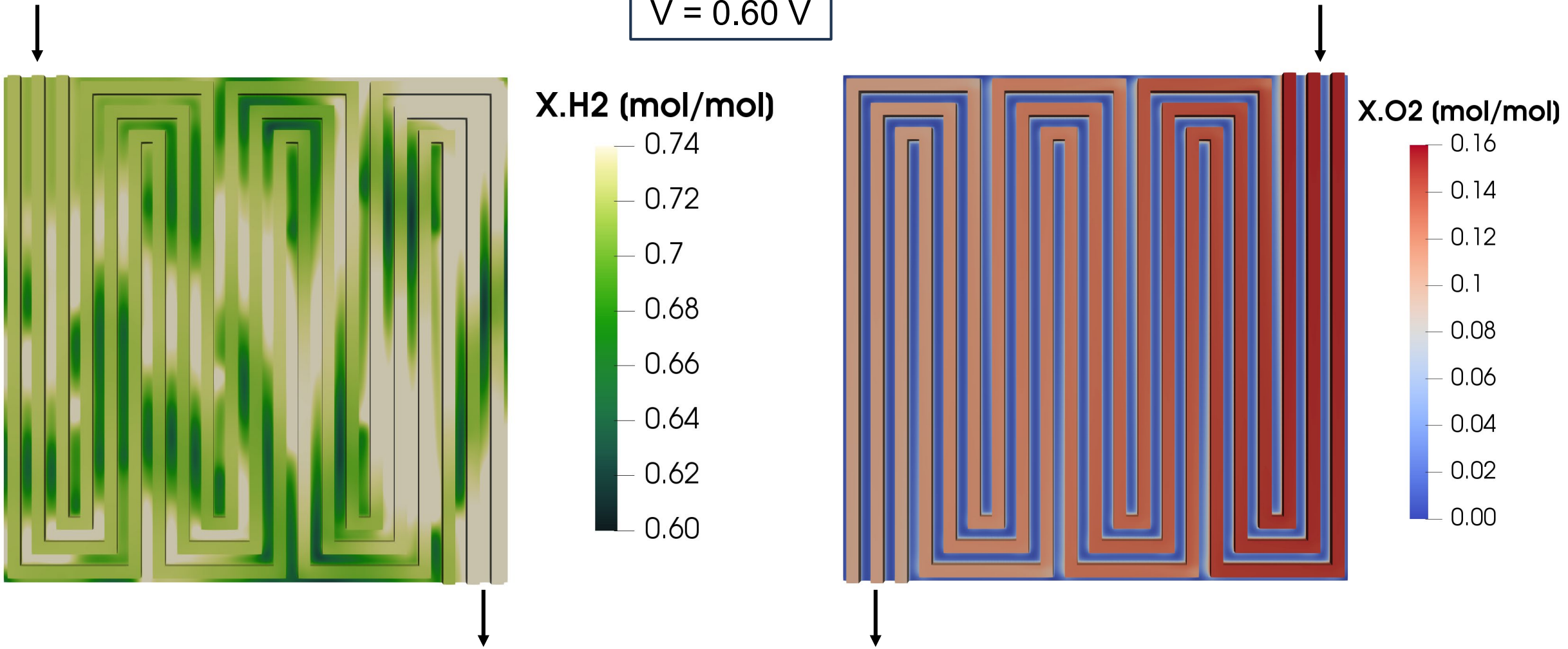
Pressure and velocity



Pressure and velocity of the cathodic channel

Reactants concentration

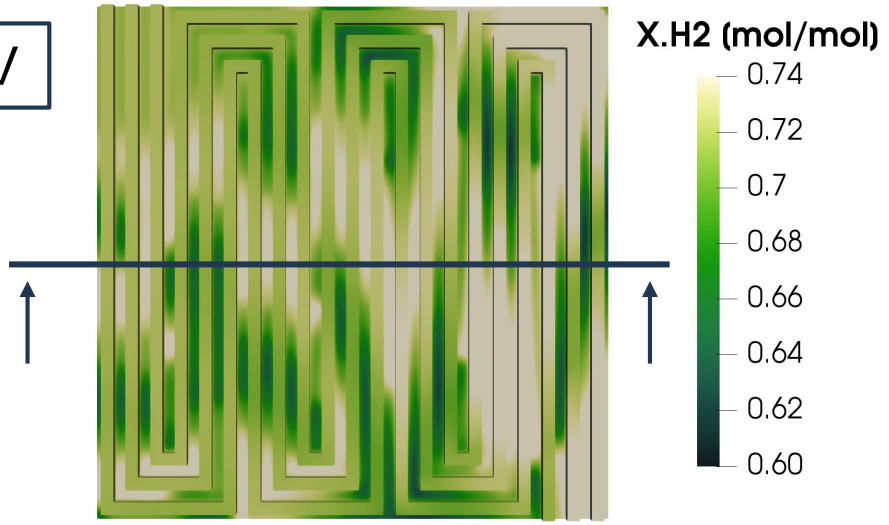
V = 0.60 V

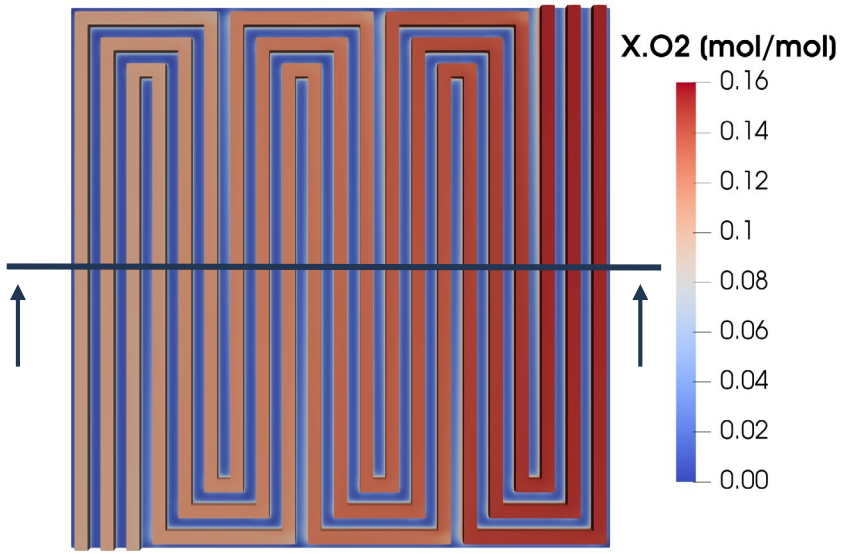


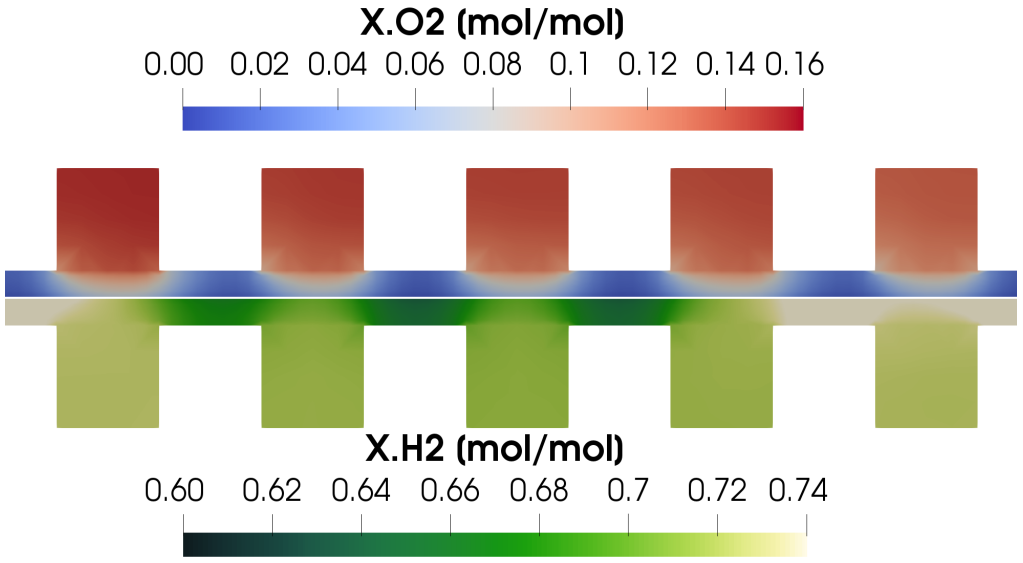
Hydrogen and oxygen concentrations in the anodic and cathodic channels

Reactants concentration

V = 0.60 V

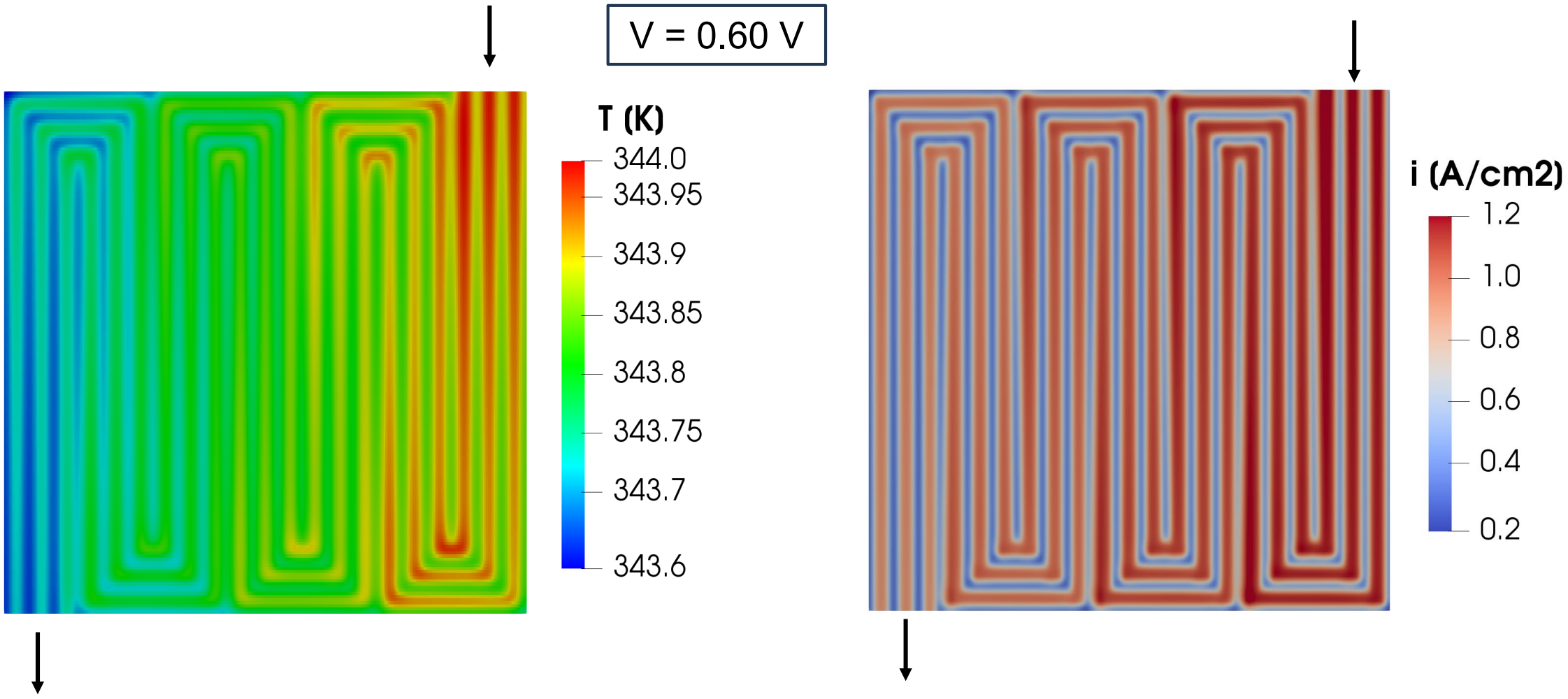






Diffusion of reactants in the porous media affects the PEMFC performances

Temperature and current density



Temperature and current density in the membrane

- Introduction
- Methodology
- Case study and validation
- **Conclusions and next steps**

Conclusion

An open-source code allows the **implementation** of the different **degradation mechanisms** that cause decrease of performances (e.g. PtOx formation)

PEMFC CFD modeling can be used to evaluate physical quantities **in-plane** and **through-plane distributions** that determine the component performances

The methodology can be adopted to **improve PEMFCs performances** and to reduce degradation

Next steps

Study of **new channel geometries** (wave shaped or tapered channels) to optimize reactants diffusion, water management will be carried out

Application of the methodology at the **device scale**

Contact info

Thanks for the attention!

Margherita Bulgarini | PhD student
Department of Energy, Politecnico di Milano
Via Lambruschini, 4a, 20156 Milano, Italy
margherita.bulgarini@polimi.it