EMR’25, Lille (France)

http://emrwebsite.org

« EMR-BASED MODEL OF AN ELECTROLIZER»

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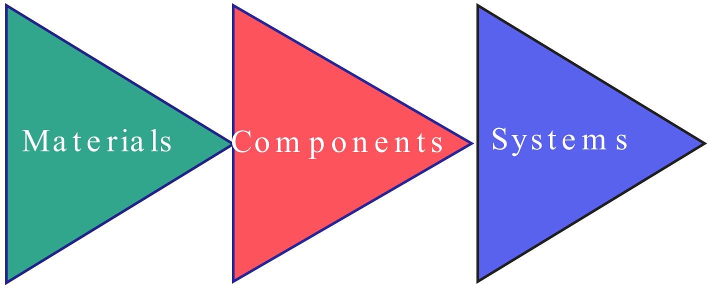
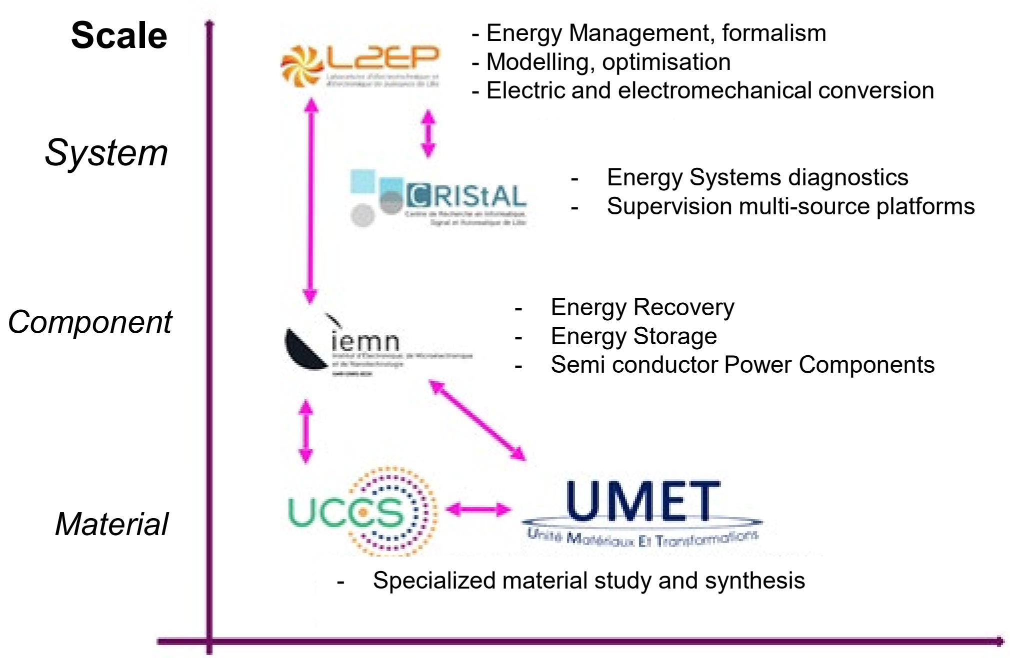
- Outline -

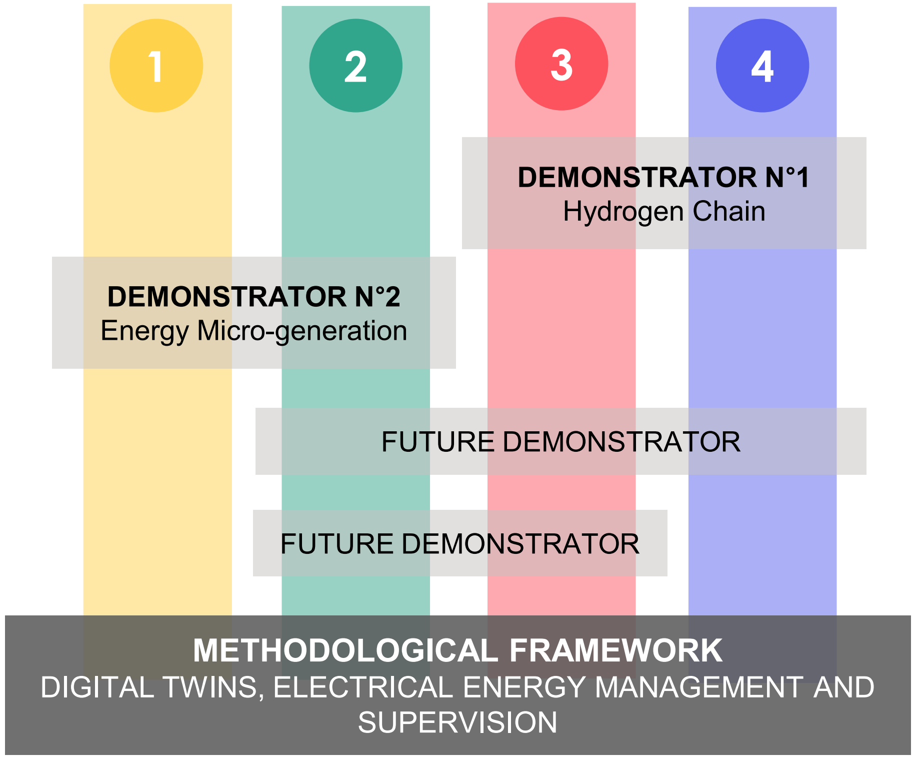
1. Introduction

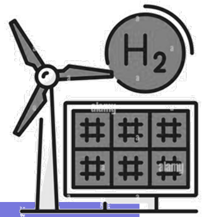
EMR-Based Model of an Electrolyzer

Context: COMASYS / University of Lille









Electrolysis + RE helps produce H2 without CO2 emissions

Research in electrolysis can help reducing the cost and impact of renewable H2

Objective:

- Develop a modular, scalable energy simulation model with EMR.
- Validate the model using experimental tests

Future applications:

- Deduce the control using model inversion
- Use the system for simulations of different use cases and control strategies
- Improve the model to be applicable in other setups

2. Studied system

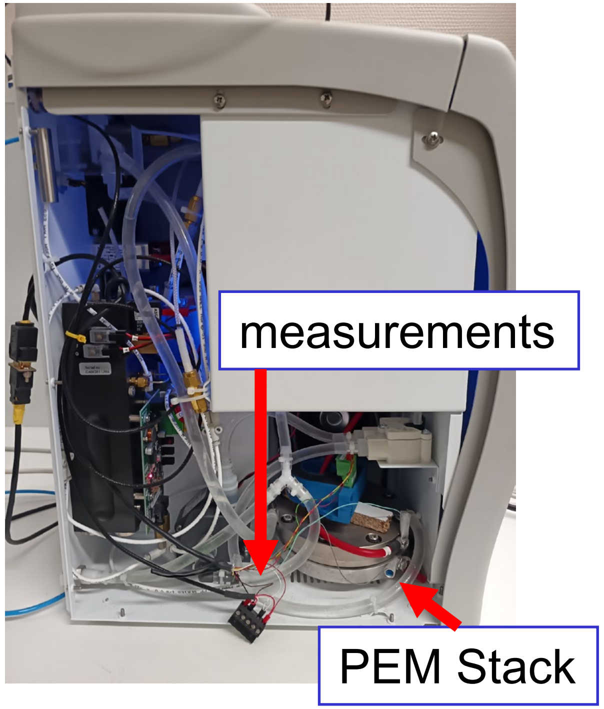
- Green Hydrogen Platform at Polytech Lille -

Platform:

- Installed at Polytech by CRIStAL
- Connected to wind and solar generators (incl. power controllers)

Hydrogen production:

- Single-cell PEM Electrolyzer stack
- Output flow stored in H2 tank
- Bond-Graph based model for supervision with RT link to Matlab
- Allows RT measurements of cell current, temperature, voltage and output H_2 flow

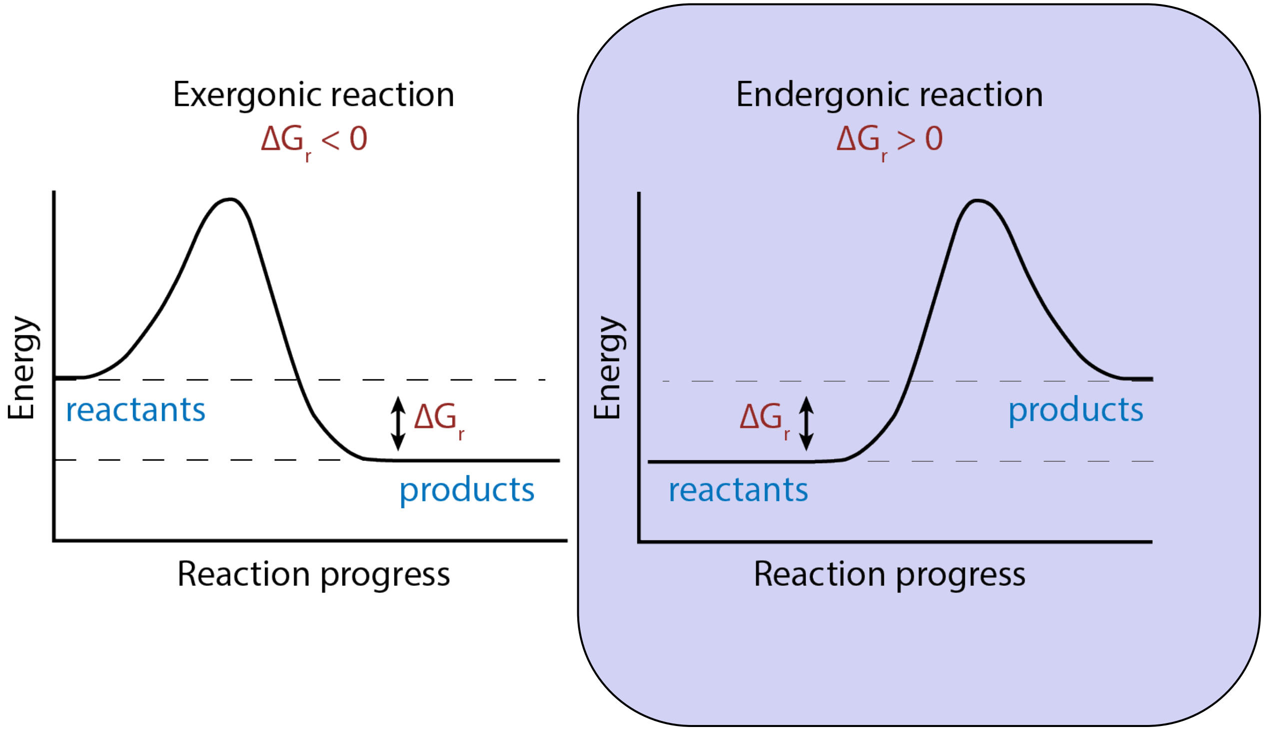


Assumptions for analysis and EMR

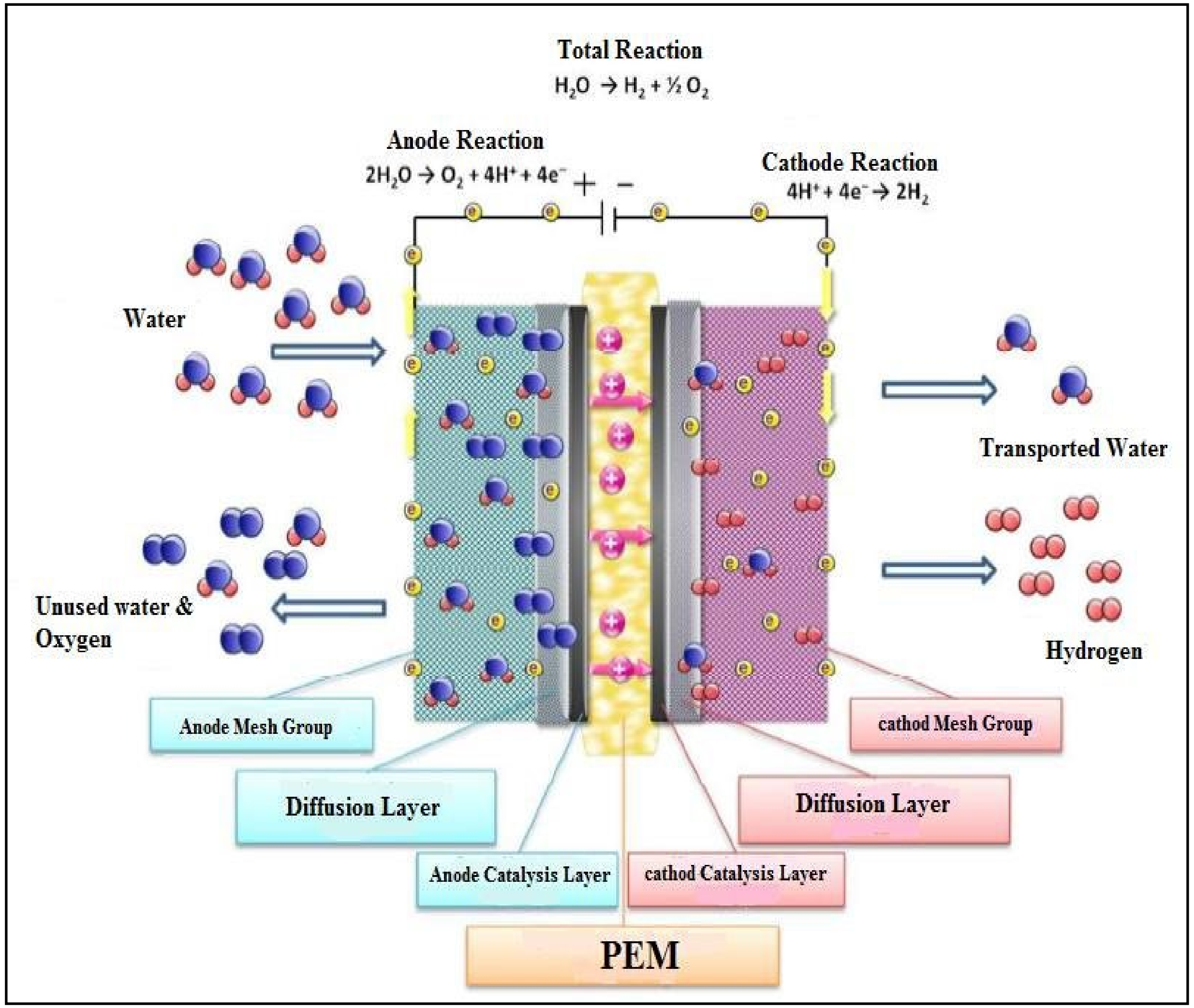
- Model does not deal with control of external sub-systems such as pumps, compressors and separators
- Model focuses on the relation of the current to the temperature and its effects in H2 production
- Single cell electrolyser operated within specifications
- Ideal power converter (no losses)
- Fluid dynamics are simplified, as they are considered quick with regards to the thermal dynamics
- Infinite permeability for hydrogen at the membrane
- Pressure losses at the membrane are considered

3. From Electrolysis Model to EMR

Electrolysis: The principle



- liquid water (H_2O) is more stable and has a lower Gibbs free energy than the separate gases H_2 and O_2.
- Electricity increases energy and breaks water into H_2 and O_2 (electrolysis).
- Separating them requires energy
- Recombining them releases energy (fuel cell).
- PEM uses a membrane to support the reaction.



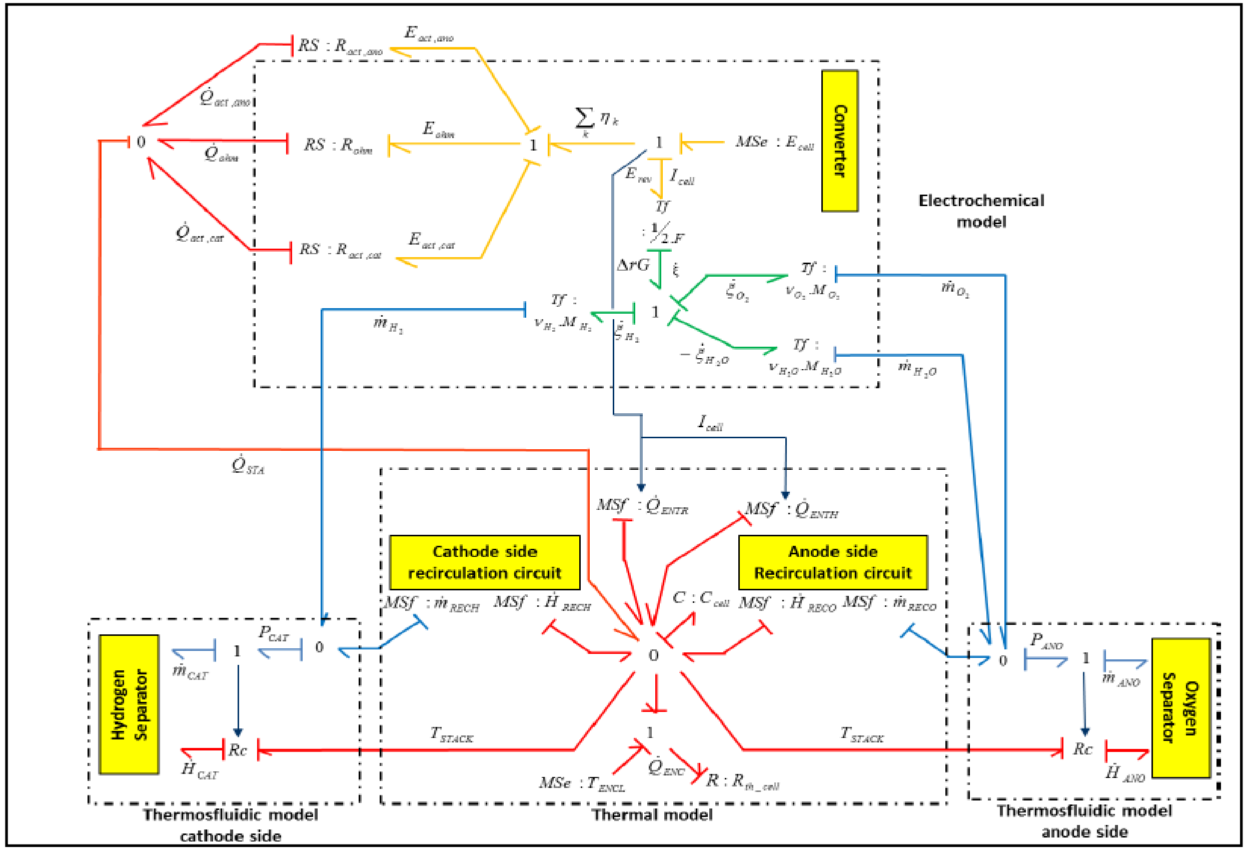
Electrolysis breaks down water (H_2O) into hydrogen (H_2) and oxygen (O_2) using an electric current.

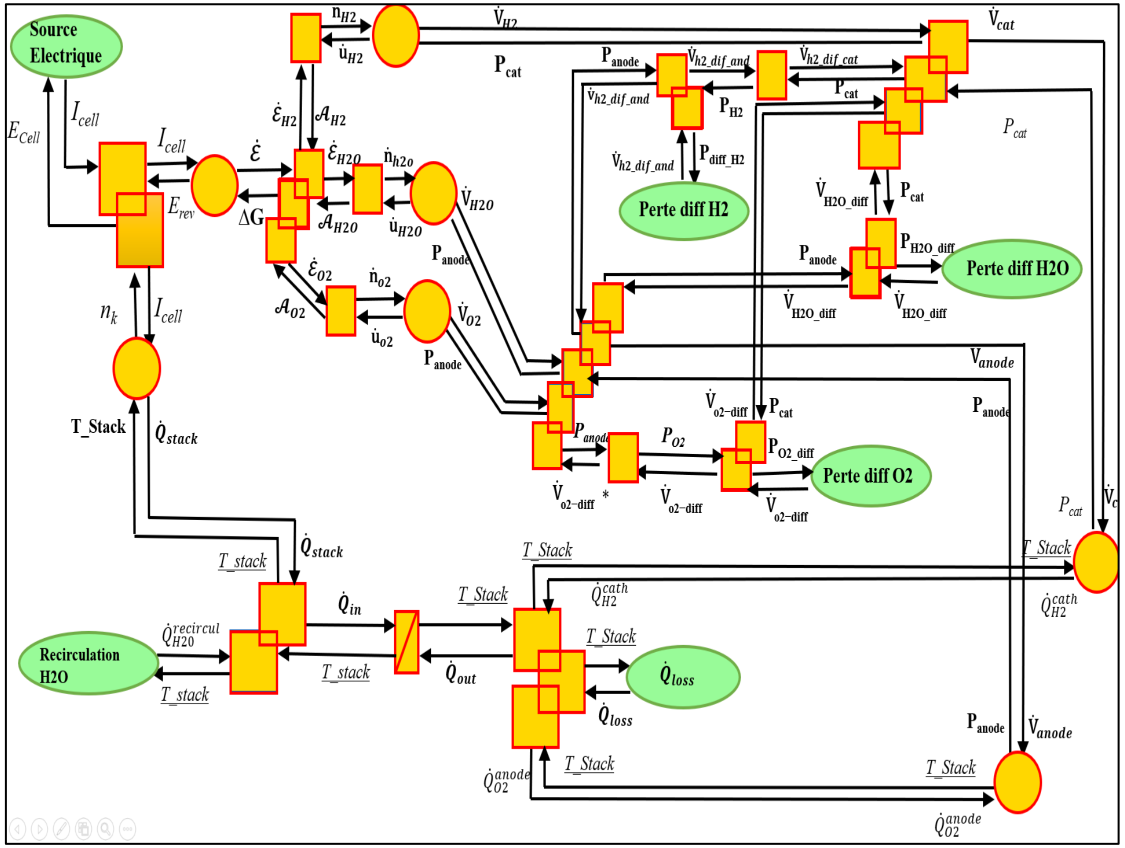
Cathode (–): hydrogen is produced.
Anode (+): oxygen is produced.

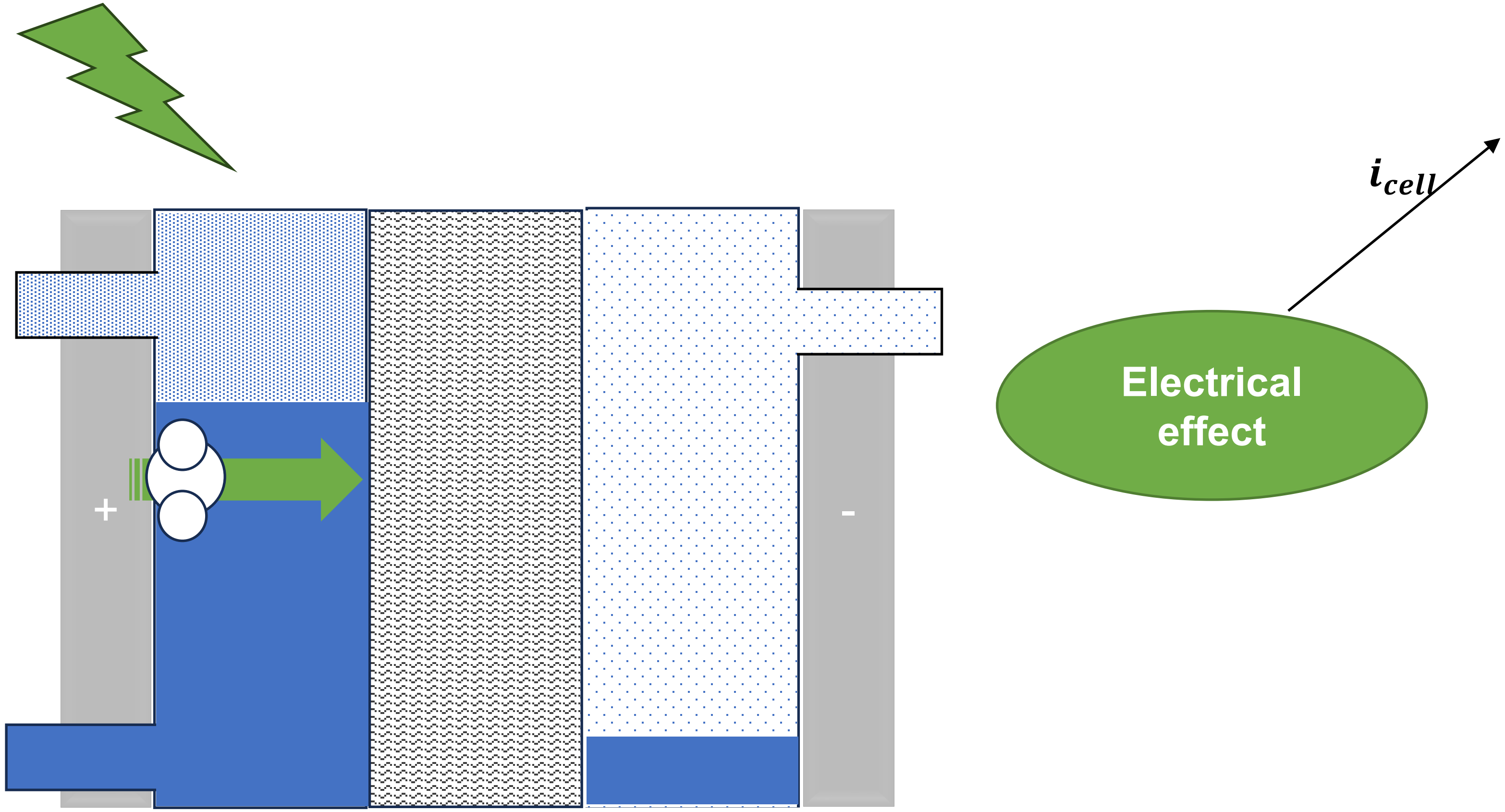
Structure of a cell:
Two electrodes, a membrane, active layers, bipolar plates (with channels), and current collectors.

A **Stack** connects many cells in series, helping improve current density

Model to EMR

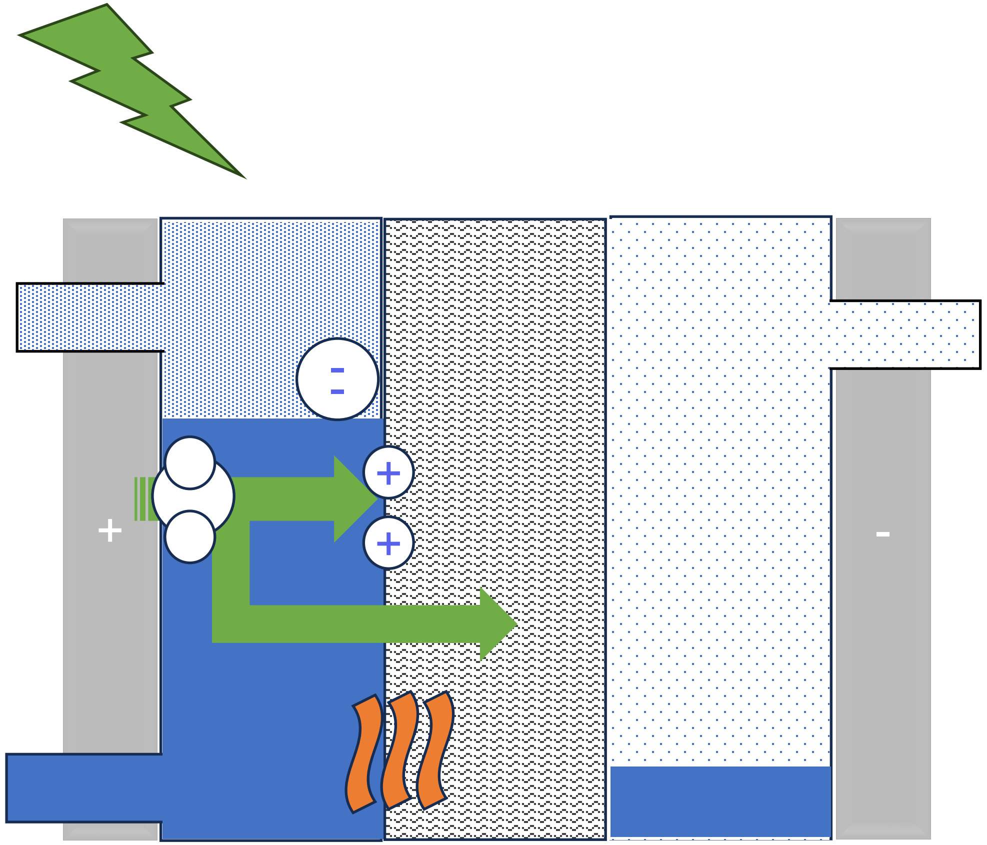

Converter
Electrochemical model
Cathode side recirculation circuit
Anode side Recirculation circuit
Hydrogen Separator
Oxygen Separator
Thermosfluidic model cathode side
Thermal model
Thermosfluidic model anode side

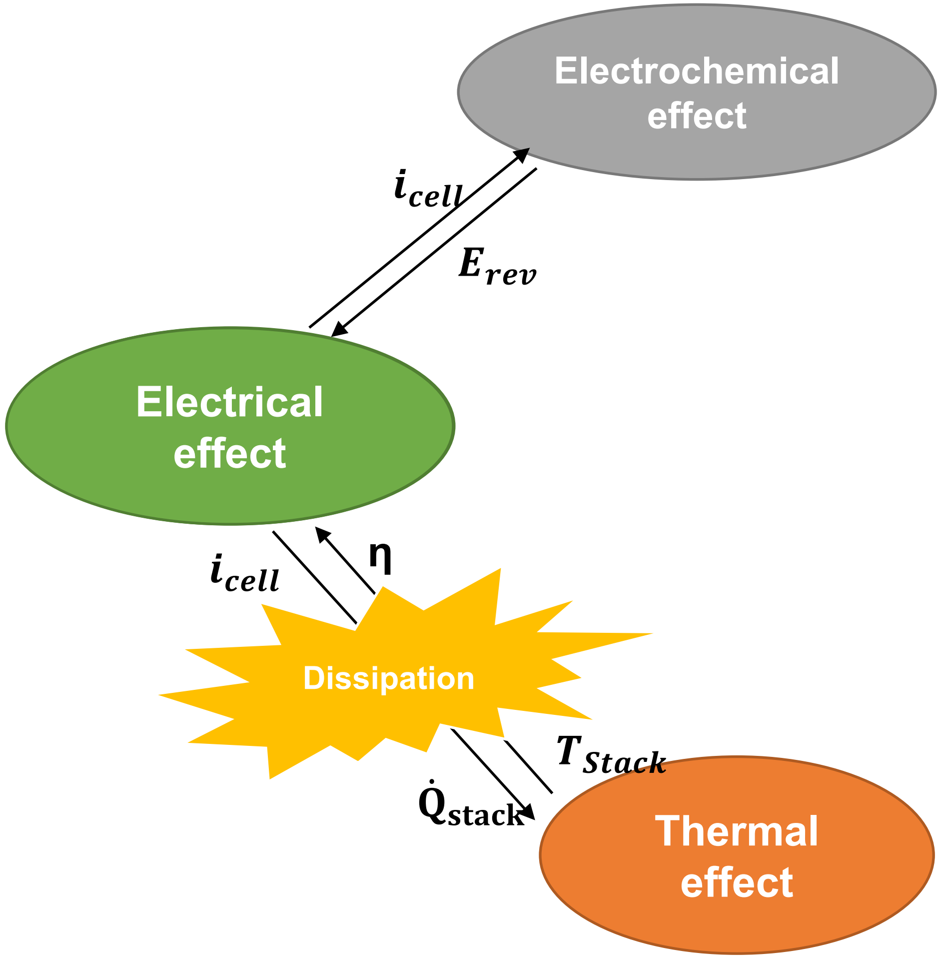

Source Electrique
Perte diff H2
Perte diff H2O
Perte diff O2
Recirculation H2O
T_Stack
T_stack


+
-
i_{cell}
Electrical effect

EMR-Based Model of an Electrolyzer

Multi-physical sub-system modelling approach



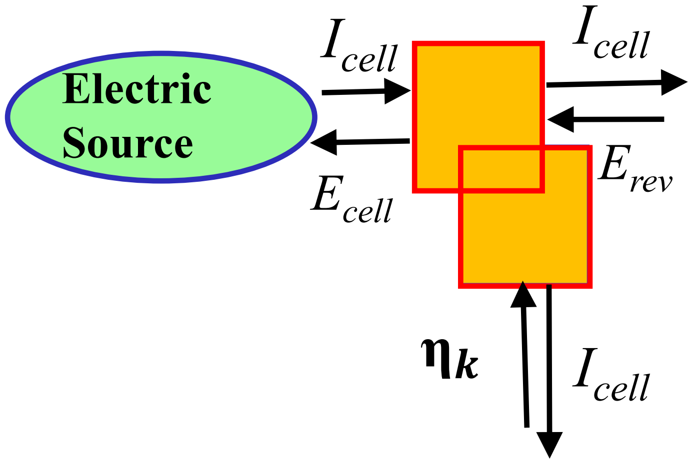


•The electrolyser is fed: E.S. **imposes the current I_{cell}**

•This current triggers two separate effects:

a. **Production of Hydrogen and Oxygen gases** (electrochemical reaction).
b. **Thermal dissipation**

$$E_{cell} = E_{rev} + \eta_k$$

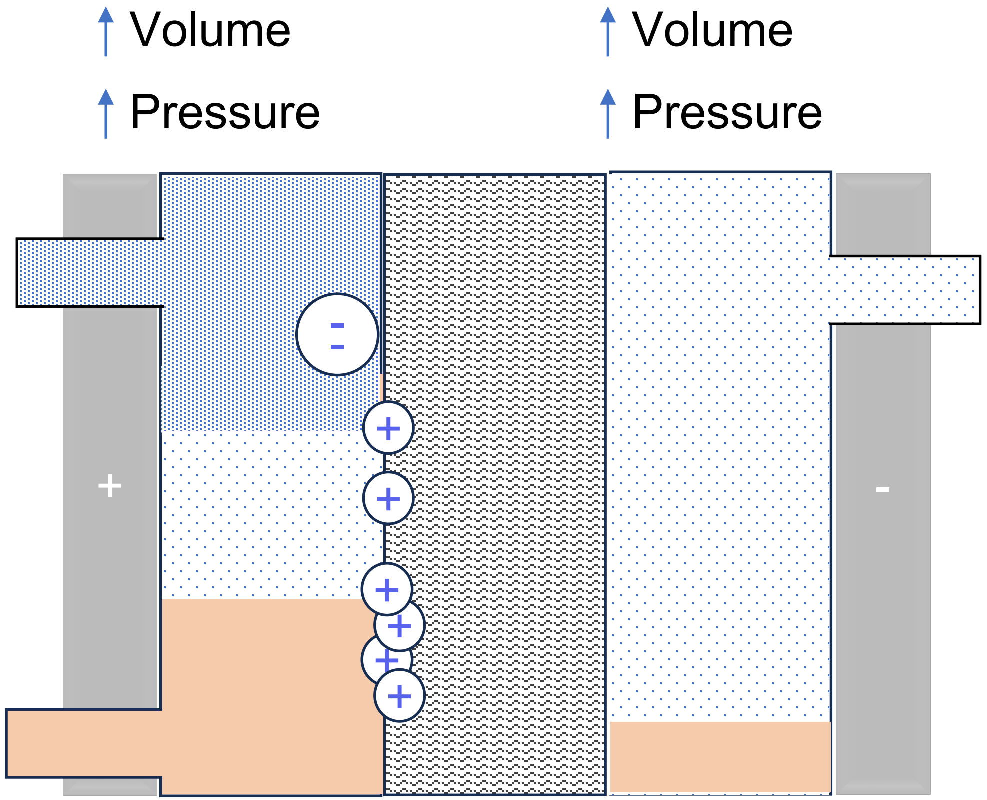


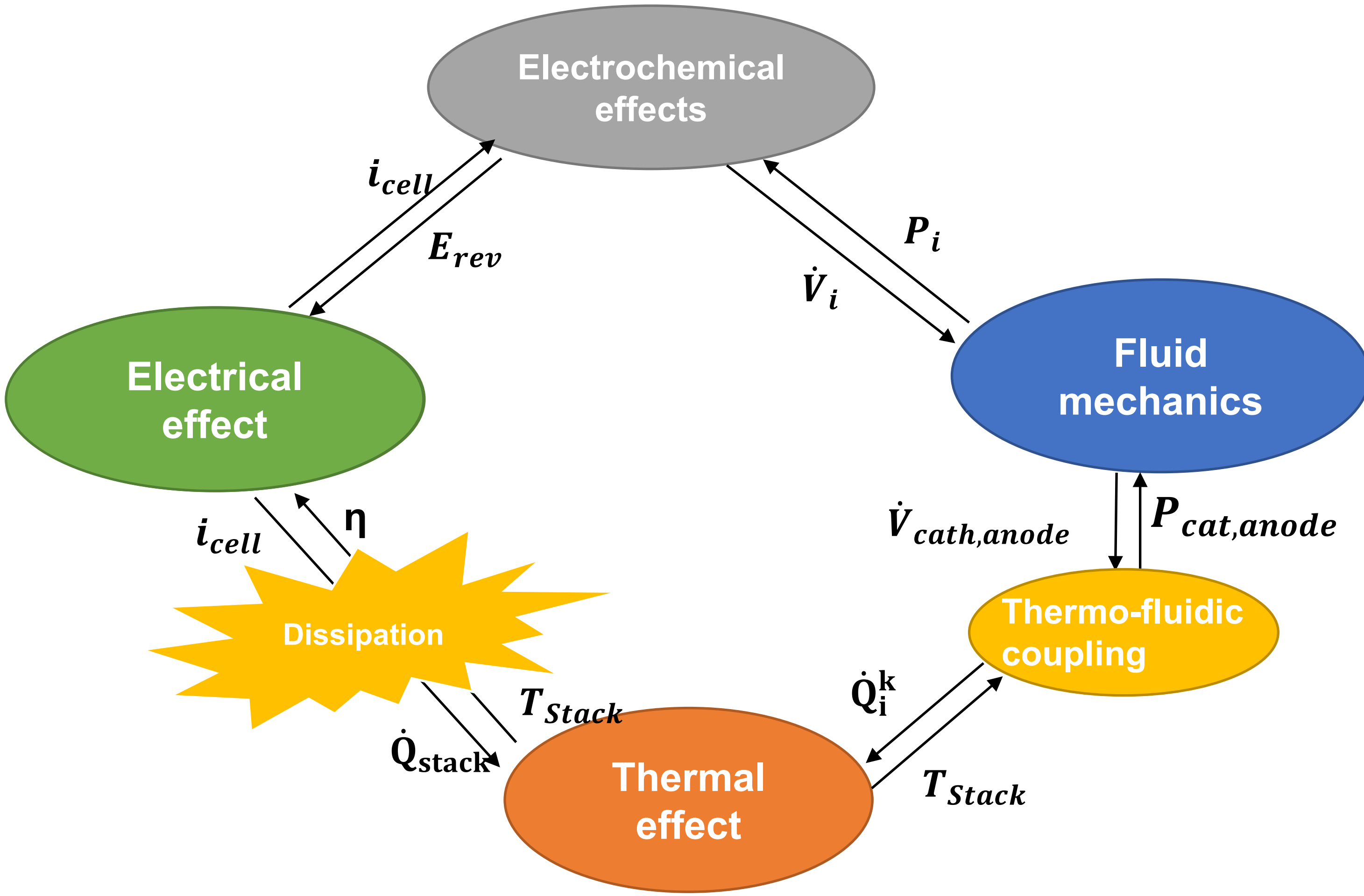
Variable	Description	Unit
E_{cell}	Cell voltage	V
η_k	Overvoltage	V
I_{cell}	Cell current	A
E_{rev}	Reversible voltage	V

EMR-Based Model of an Electrolyzer

Multi-physical sub-system modelling approach

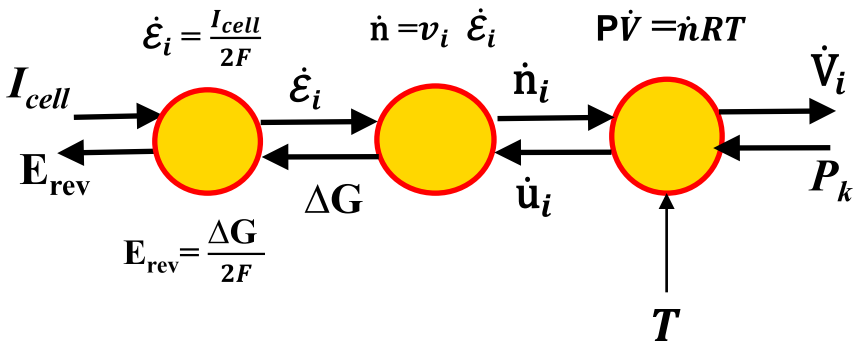
EMR'25, Lille, July 2025





- The electric current determines the **quantity of matter** produced in moles via **Faraday's law**, then converted into **volumetric flow** by the **ideal gas law**.

- The dissociation of H_2O requires **a free energy (ΔG)**, supplied by the current and carried by the chemical potential of the species.



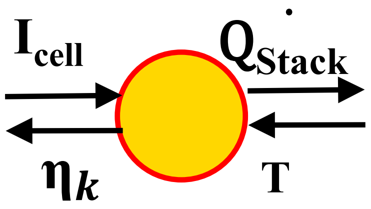
Variable	Description	Unit
$\dot{n}_i$	Molar flux	mol/s
$\dot{u}_i$	Chemical potential	J/mol
P_k	Pressure	Pascal
$\dot{V}_i$	Volumetric flux	m^3/s
R	Ideal gas constant	$J \cdot K^{-1} \cdot mol^{-1}$
T	Stack temperature	Kelvin
F	Faraday constant	C/mol

- The passage of current through the membrane produces energy losses in the form of heat Q_{stack}.
- For the reaction to remain possible despite these losses, one must apply a higher voltage than the equilibrium voltage E_{rev} .
- This additional voltage corresponds to:

η_{ohm} : Ohmic overvoltage

η_{act} : Activation overvoltage

Variable	Description	Unit
$\dot{Q}_{stack}$	Entropy flux	W/K
η_k	Overvoltage	V
J_{cell}	Current density	A/m^2
A_{ohm}	Membrane surface	m^2
L_{PEM}	Membrane thickness	m



Equations:

$$\eta_k = E_{act,K} + E_{ohm}$$

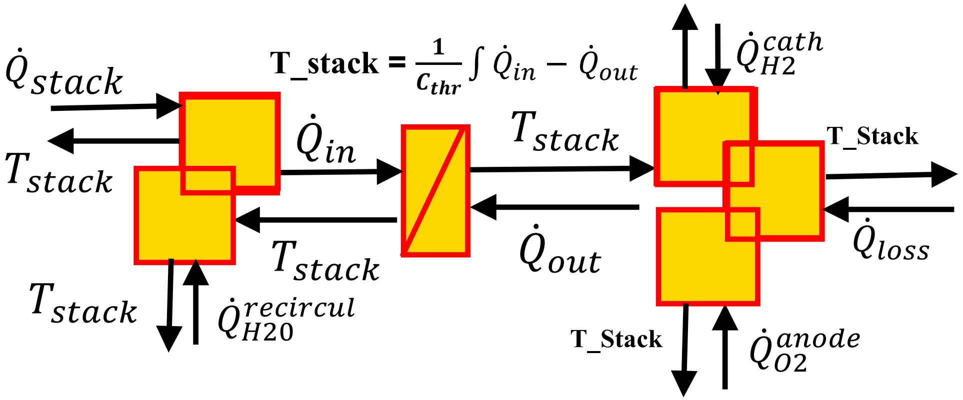
$$E_{act,K} = \frac{R\ Tstack}{F} sinh^{-1}\left(\frac{J_{cell}}{2.J_k}\right)$$

$$I_{cell} = \frac{E_{ohm}}{R_{ohm}}$$

$$R_{ohm} = \frac{L_{PEM}}{\sigma_{ohm} A_{ohm}} + R_{others}$$

Thermal effect (2)

- The cell produces heat in the form of an enthropy flux $\dot{Q}_{stack}$ when the current is applied
- The entering heat flow from the water recirculation $\dot{Q}_{H20}^{recircul}$ is also taken into account
- Part of this heat is evacuated by the gas $\dot{Q}_{H2}^{cath}, \dot{Q}_{O2}^{anode}$ and lost to the environment $\dot{Q}_{loss}$
- The heat difference is cumulated in the stack



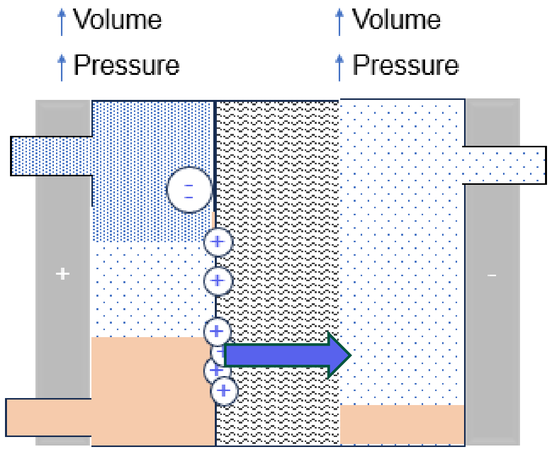
Equations:

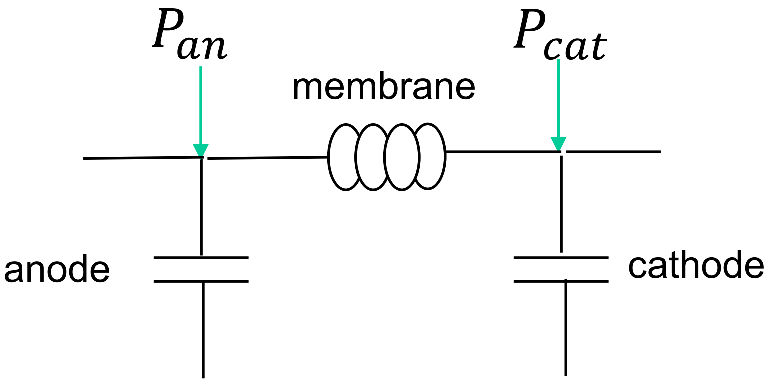
$$\dot{Q}_{in} = \dot{Q}_{stack} + \dot{Q}_{H20}^{recircul}$$

$$\dot{Q}_{out} = \dot{Q}_{loss} + \dot{Q}_{H2}^{cath} + \dot{Q}_{O2}^{anode}$$

$$T_{stack} = T_0 e^{\frac{1}{C} \int \dot{Q}_{out} - \dot{Q}_{in} dt}$$

- At the anode, a discrepancy between the inlet and outlet volumetric flow rates, and the conversion of water into gas induces a localized accumulation of fluid, thus an increase in pressure.
- Across the membrane, a pressure differential between the anode and cathode drives a transmembrane volumetric flux. This flux depends on the permeability of the membrane
- This inlet of hydrogen gas causes a localized accumulation of fluid, thus an increase in pressure.

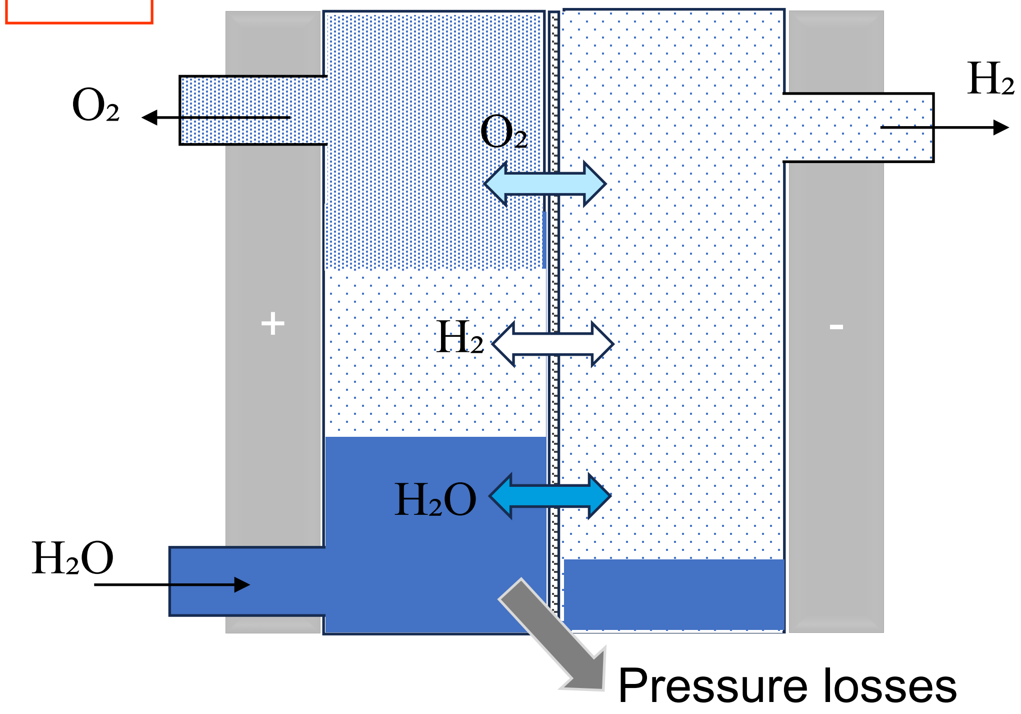


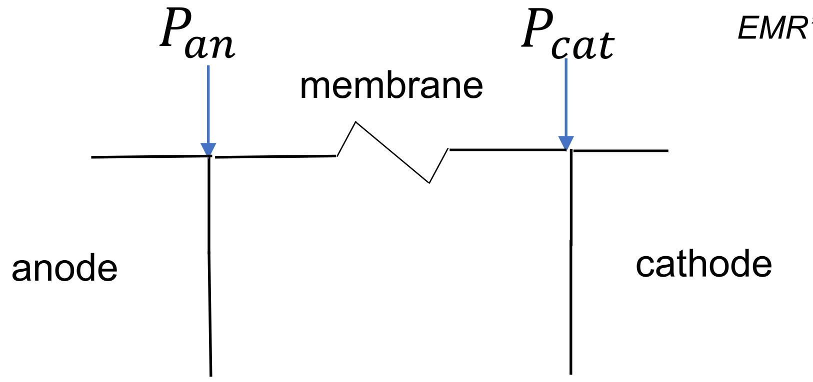


The model relies on parameters that are non-linear, time-varying, and exhibit hysteresis, making them particularly challenging to identify. To simplify the model while preserving its accuracy, a series of assumptions were validated.

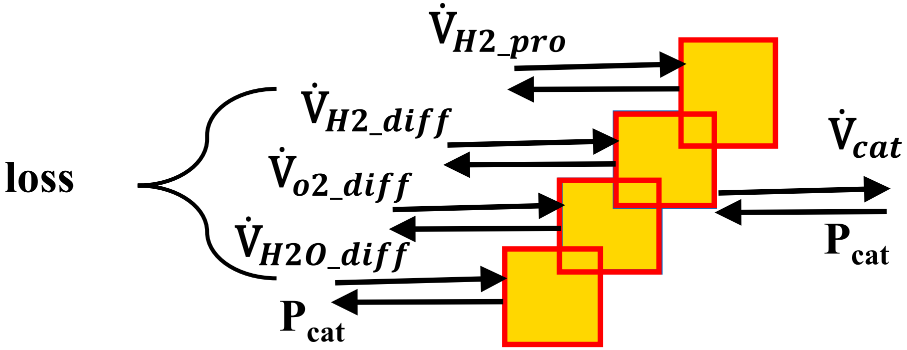
EMR-Based Model of an Electrolyzer

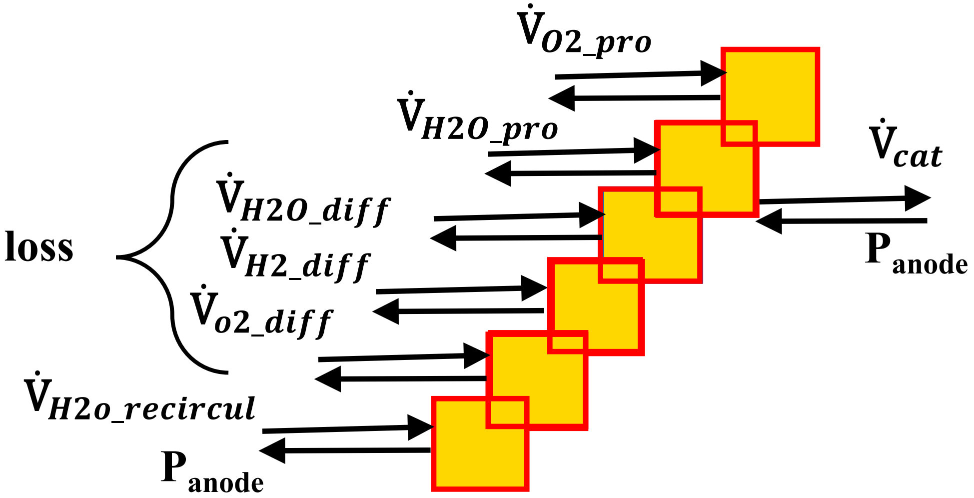
Fluid mechanics

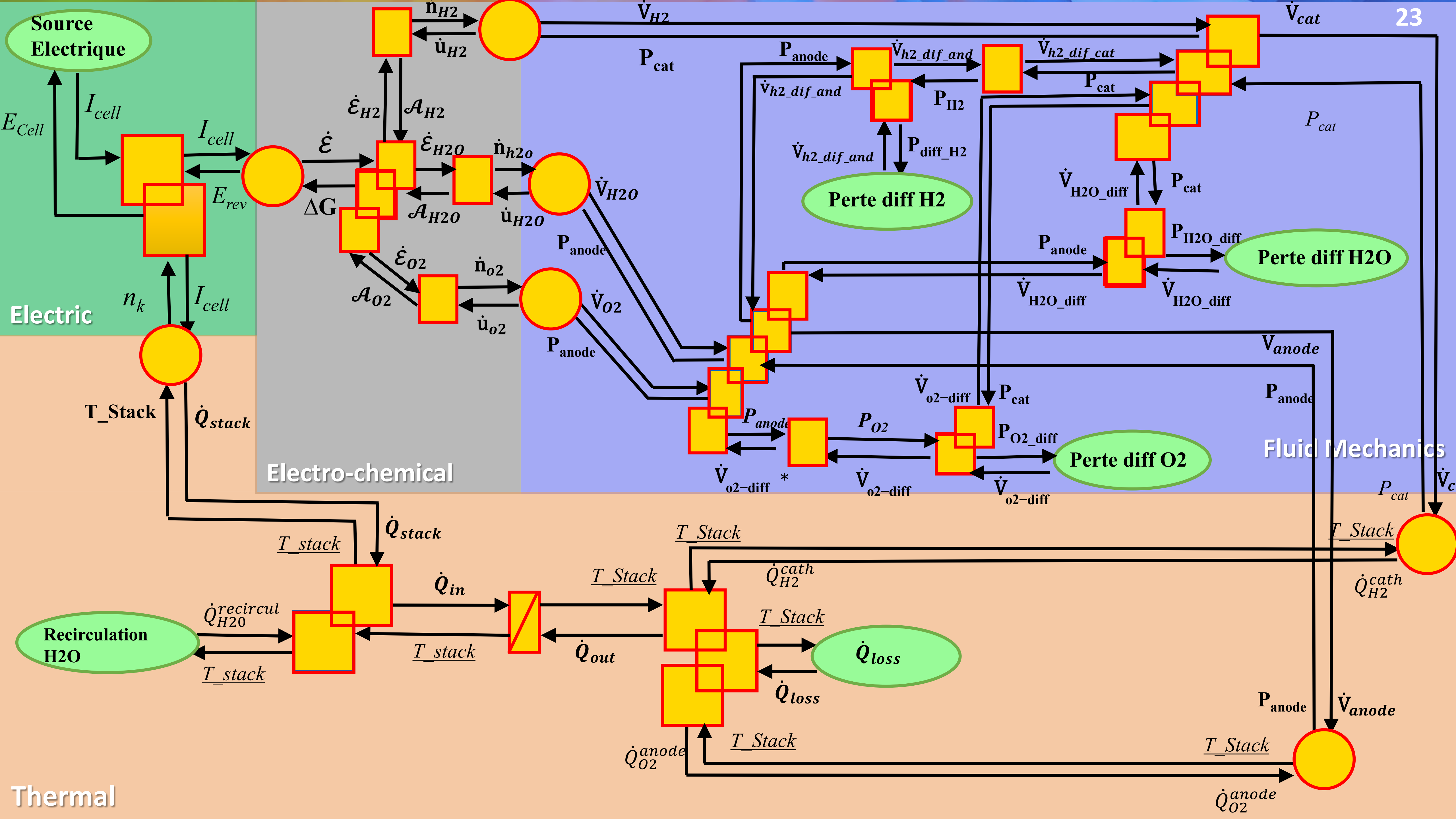




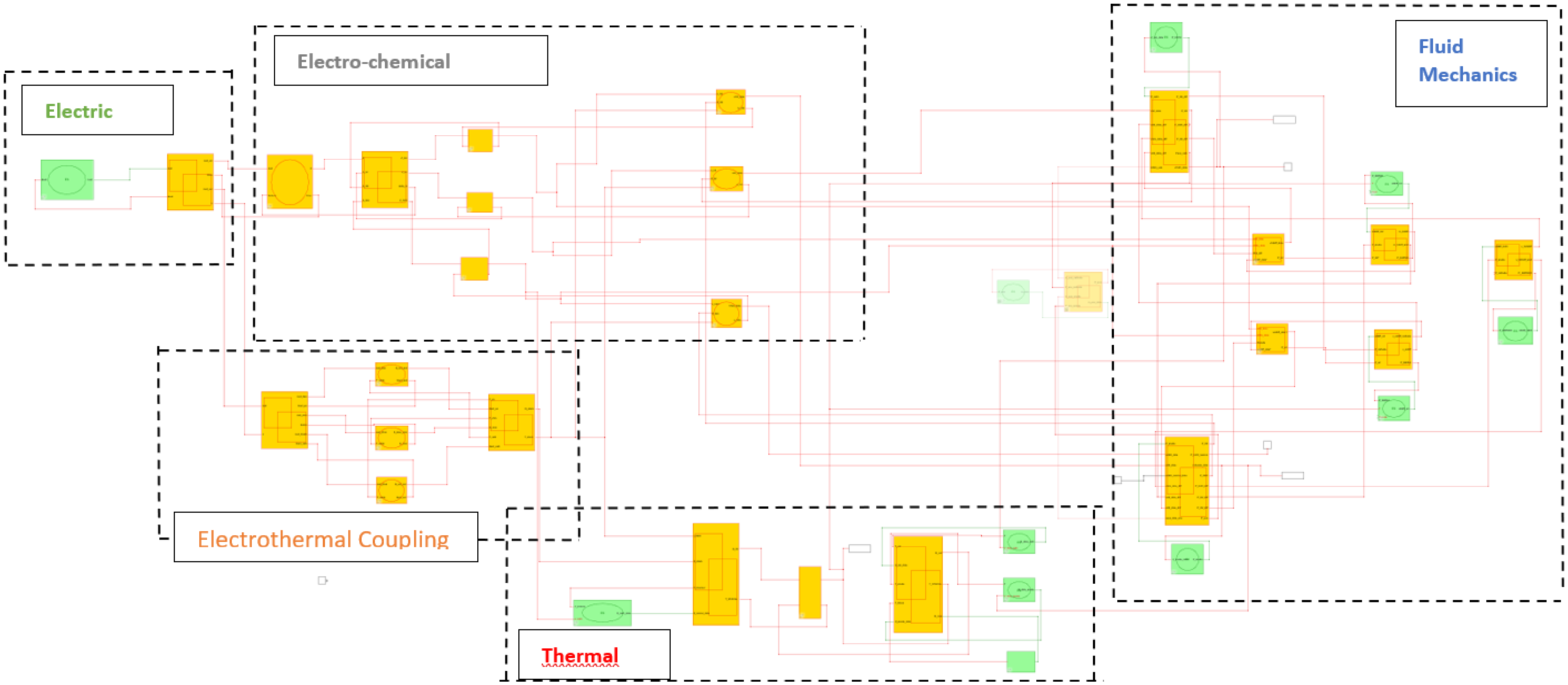
We model the system as a simple tube, with an infinitly permeable membrane for H2, which has pressure losses



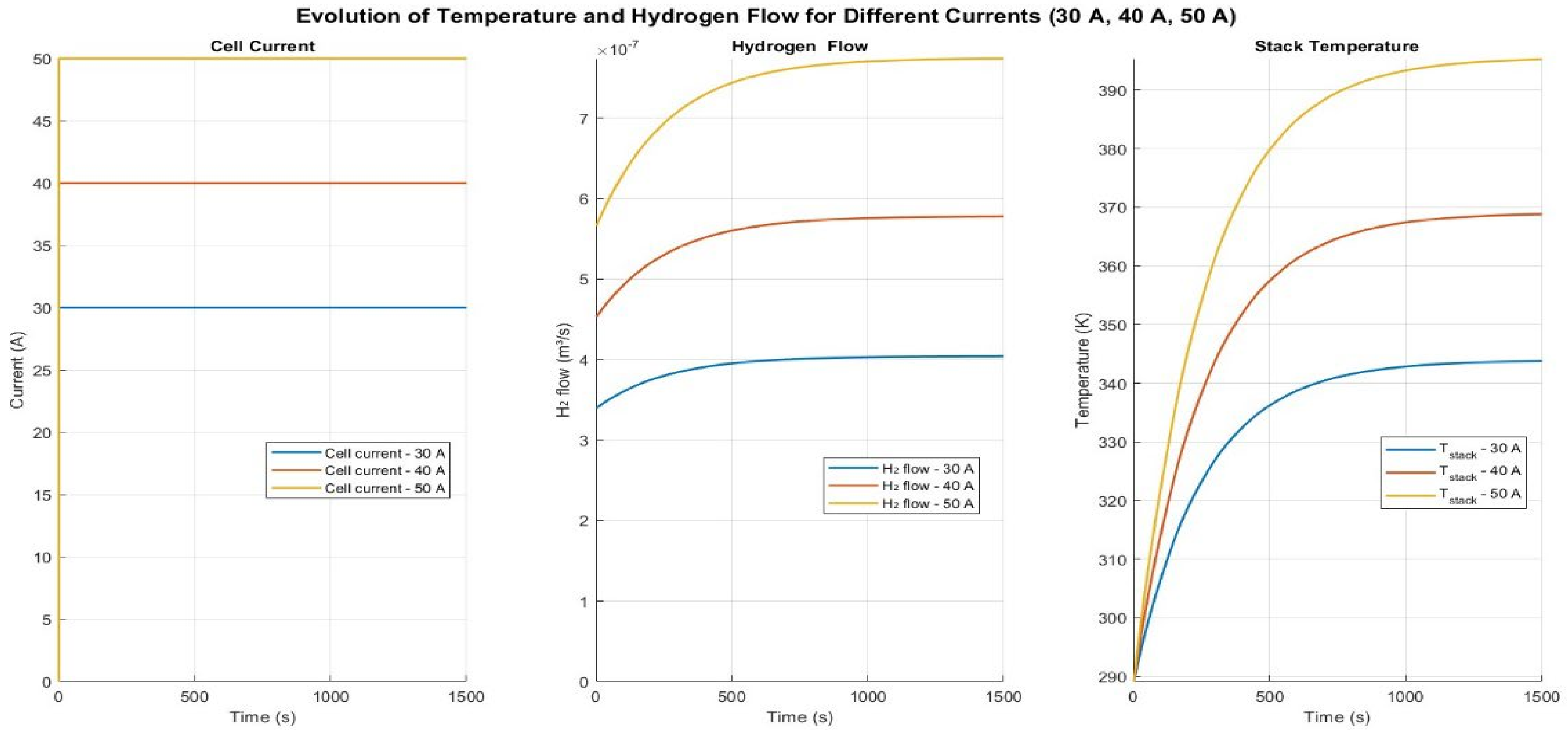



Source Electrique
Electric
Electro-chemical
Fluid Mechanics
Thermal
Perte diff H2
Perte diff H2O
Perte diff O2
Recirculation H2O
E_{Cell}
I_{cell}
E_{rev}
n_k
$\dot{\mathcal{E}}$
ΔG
$\dot{n}_{H2}$
$\dot{u}_{H2}$
$\dot{\mathcal{E}}_{H2}$
$\mathcal{A}_{H2}$
$\dot{\mathcal{E}}_{H2O}$
$\dot{n}_{h2o}$
$\mathcal{A}_{H2O}$
$\dot{u}_{H2O}$
$\dot{\mathcal{E}}_{O2}$
$\dot{n}_{o2}$
$\mathcal{A}_{O2}$
$\dot{u}_{o2}$
$\dot{V}_{H2}$
$\dot{V}_{cat}$
P_{cat}
P_{anode}
$\dot{V}_{h2\_dif\_and}$
$\dot{V}_{h2\_dif\_cat}$
P_{H2}
P_{diff_H2}
$\dot{V}_{H2O}$
$\dot{V}_{H2O\_diff}$
P_{H2O_diff}
$\dot{V}_{O2}$
$\dot{V}_{o2-diff}$
P_{O2}
P_{O2_diff}
V_{anode}
$\dot{V}_{anode}$
T_Stack
$\dot{Q}_{stack}$
T_stack
$\dot{Q}_{in}$
$\dot{Q}_{out}$
$\dot{Q}^{recircul}_{H2O}$
$\dot{Q}^{cath}_{H2}$
$\dot{Q}_{loss}$
$\dot{Q}^{anode}_{O2}$

4. Preliminary results



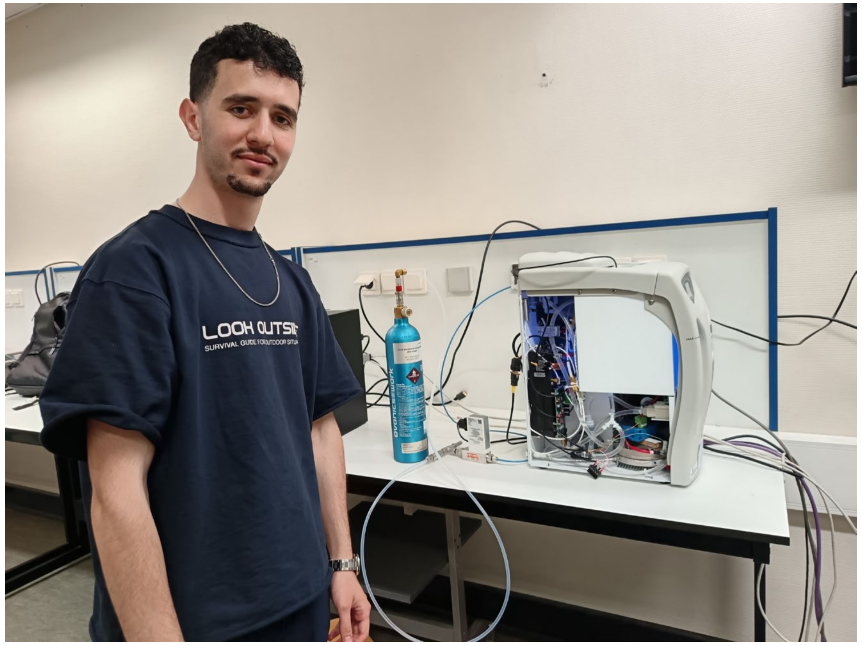
Electric
Electro-chemical
Fluid Mechanics
Electrothermal Coupling
Thermal

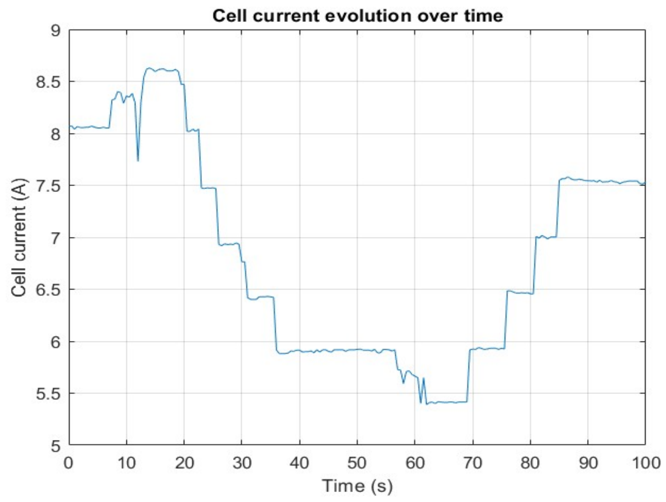


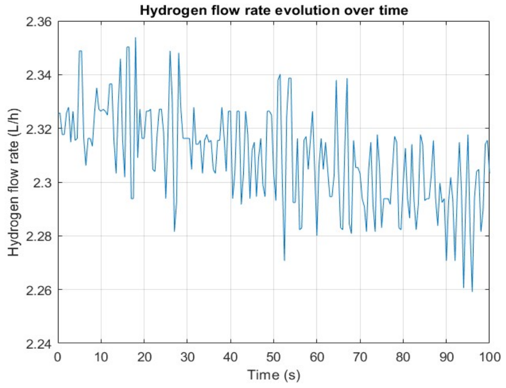
Evolution of Temperature and Hydrogen Flow for Different Currents (30 A, 40 A, 50 A)
Cell Current
Current (A)
Time (s)
Cell current - 30 A
Cell current - 40 A
Cell current - 50 A
Hydrogen Flow
×10^-7
H2 flow (m³/s)
Time (s)
H2 flow - 30 A
H2 flow - 40 A
H2 flow - 50 A
Stack Temperature
Temperature (K)
Time (s)
T stack - 30 A
T stack - 40 A
T stack - 50 A

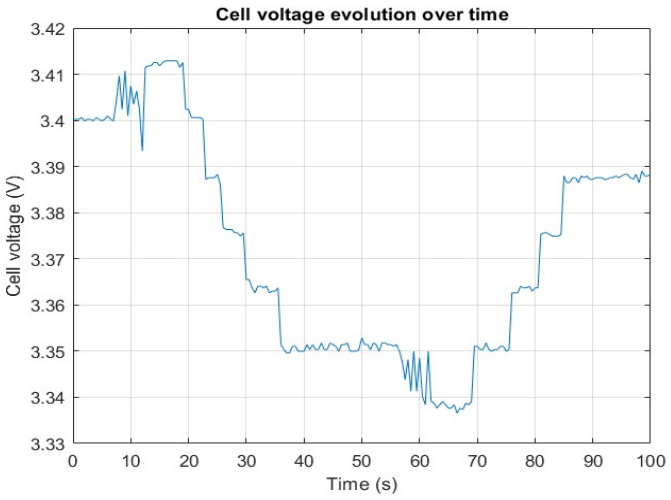
EMR-Based Model of an Electrolyzer

Work on the H2 platform

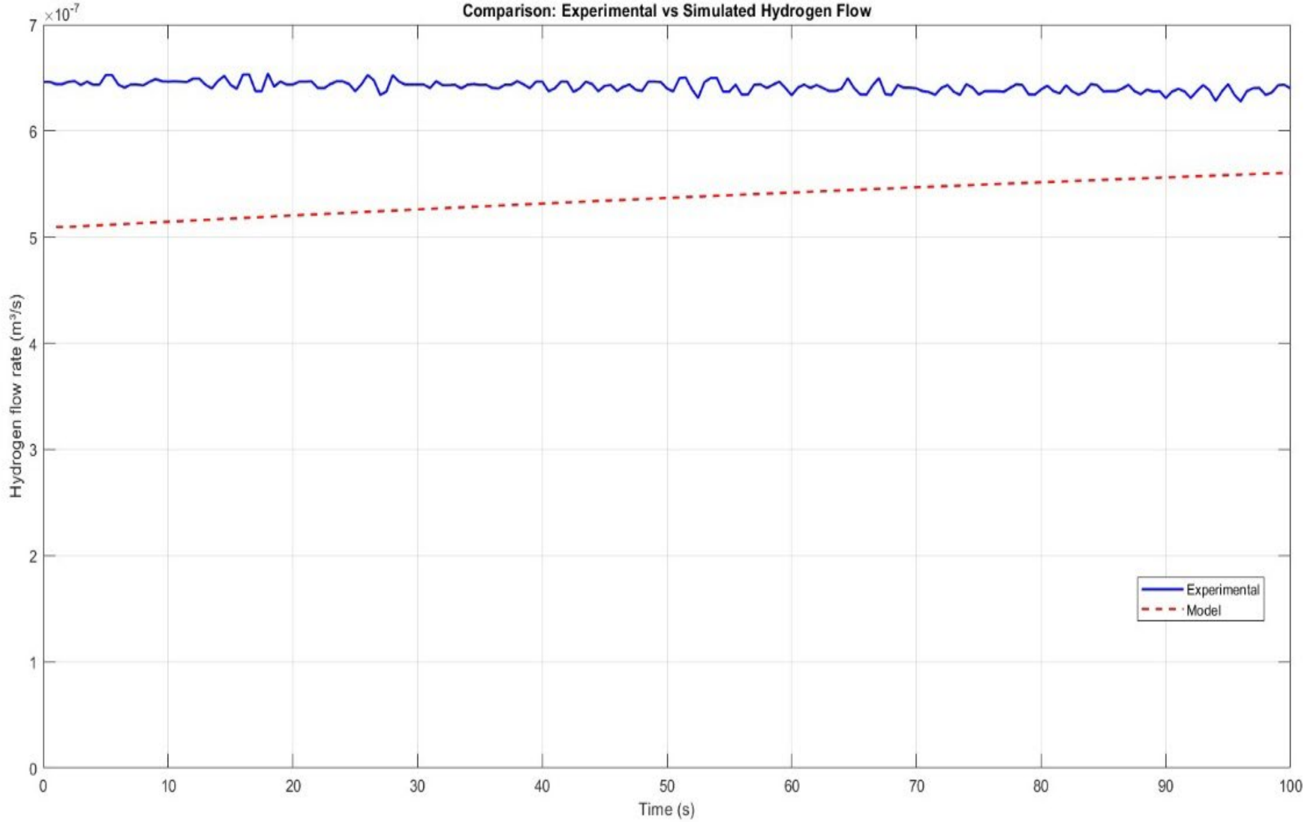






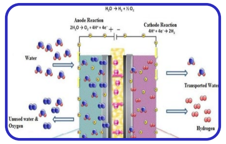


Parameter verification (work in progress)

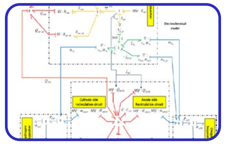


5. Conclusions and next steps

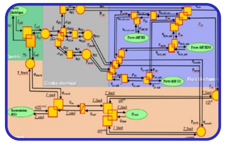
Conclusions and next steps



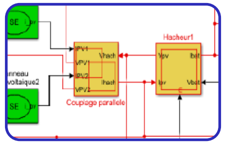
Studied PEM electrolysis modelling and causality



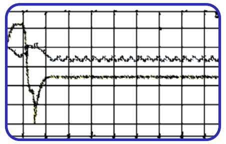
Understood Bond Graph representation of PEM EZ



Created EMR of the model



Created Simulink model



First simulations

First measurements in H2 platform

This Project **NEXT STEPS**

- Use measurements in H2 platform to refine parameters of the model
- Change testing conditions to validate model
- Develop SMC and simulate different operation cases

Future research

- Extend the model including electro-osmothic effect
- Try the inclusion of cumulative elements in the fluidic model
- Take into account the endothermic aspect of reactions

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[2] **Sumit SOOD** ,Multiphysics modelling for online diagnosis and efficiency tracking: Application to green H2 production,2021 Centre de Recherche en Informatique, Signal et Automatique de Lille ,Université de Lille 1.

[3] **Kréhi Serge AGBLI** , Modélisation multiphysique des flux énergétiques d'un Couplage Photovoltaïque-Electrolyseur PEM–Pile à Combustible PEM en vue d'une application stationnaire , 2012 , Université de Franche-Comté.

[4] **Loïc Boulon**,Modélisation multiphysique des éléments de stockage et de conversion d'énergie pour les véhicules électriques hybrides. Approche systémique pour la gestion d'énergie,2009,Université de Franche-Comté.

[5] **Samer Rabih** Contribution à la modélisation de systèmes réversibles de types électrolyseur et pile à hydrogène en vue de leur couplage aux générateurs photovoltaïques,2008,l'institut national polytechnique de Toulouse.

[6] Marcelo Carmo, *A comprehensive review on PEM water electrolysis*, 2013, Chair for Fuel Cells, RWTH Aachen University, Germany.

[7] Kazuo Onda, Performance Analysis of Polymer-Electrolyte Water Electrolysis Cell at a Small-Unit Test Cell and Performance Prediction of Large Stacked Cell, 2002, Journal of The Electrochemical Society, Department of Electrical and Electronic Engineering, Toyohashi University of Technology, Japan.