Fuel Cell Modeling

In AMESim

IMAGINE Specific Thermodynamic Applications 04/2006

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Introduction

- Fuel Cells are complex multi-domain dynamic systems
  - Electrical, electrochemical, fluidic, thermal phenomena are coupled
  - Controlling such systems is a challenge to ensure efficiency and reliability
- Modelling fuel cells systems implies
  - Interoperability
  - Multi-disciplinary and dynamic simulation environment

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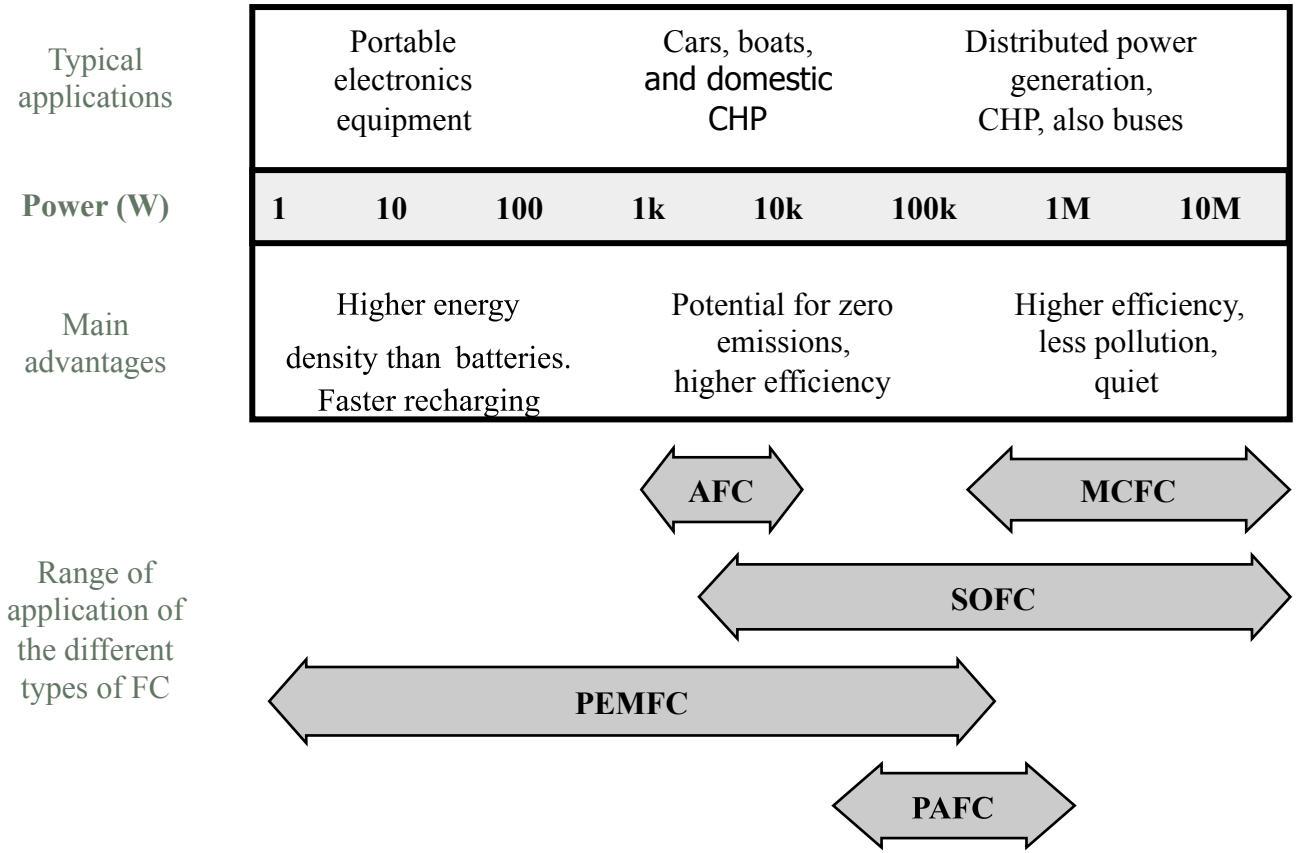
Power Based Fuel Cell Applications



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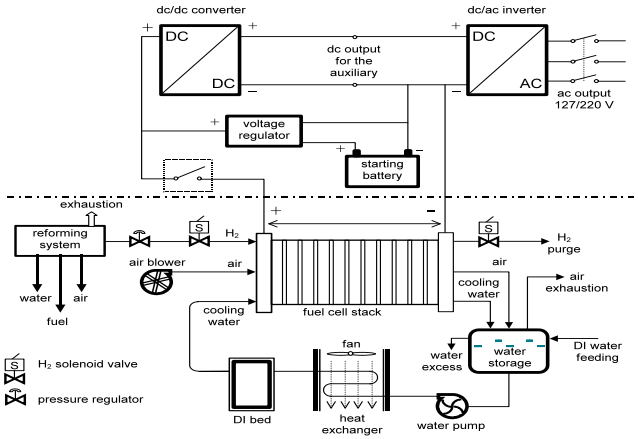
Typical Fuel Cell PEM Control System



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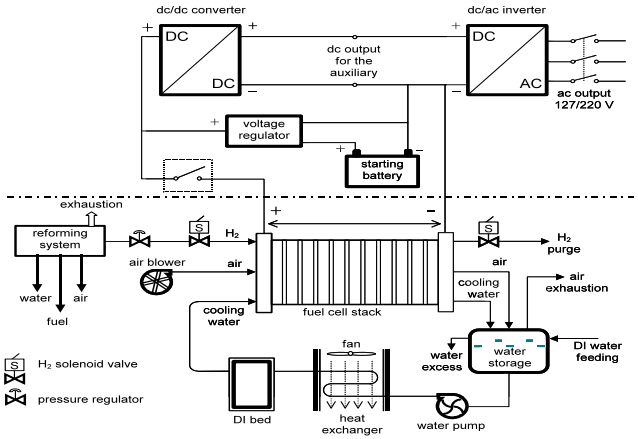

ELECTRICAL SUB-SYSTEM

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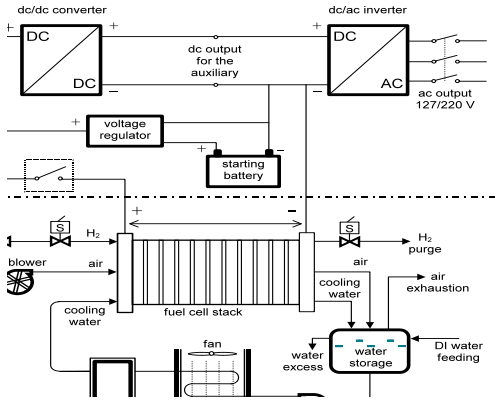

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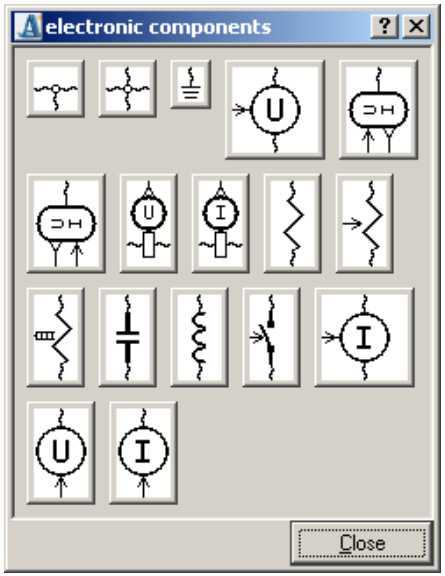

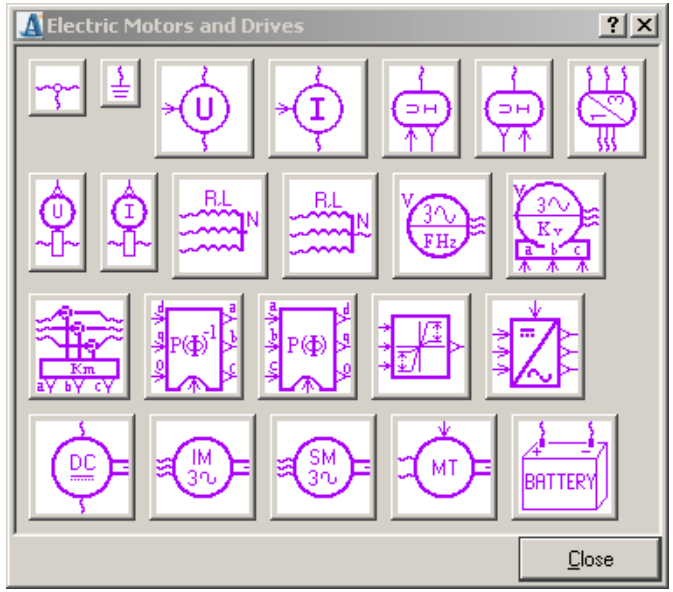

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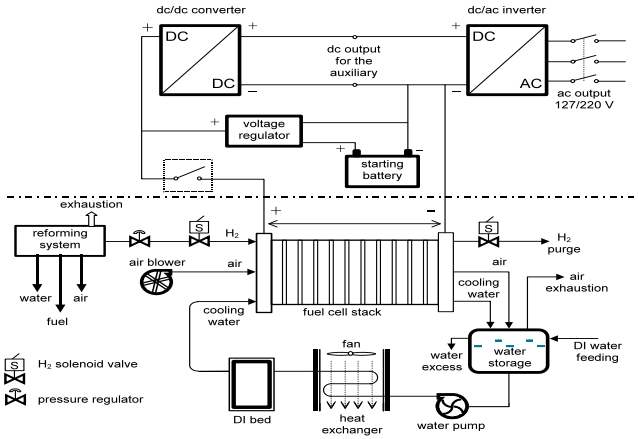

PNEUMATIC SYSTEM

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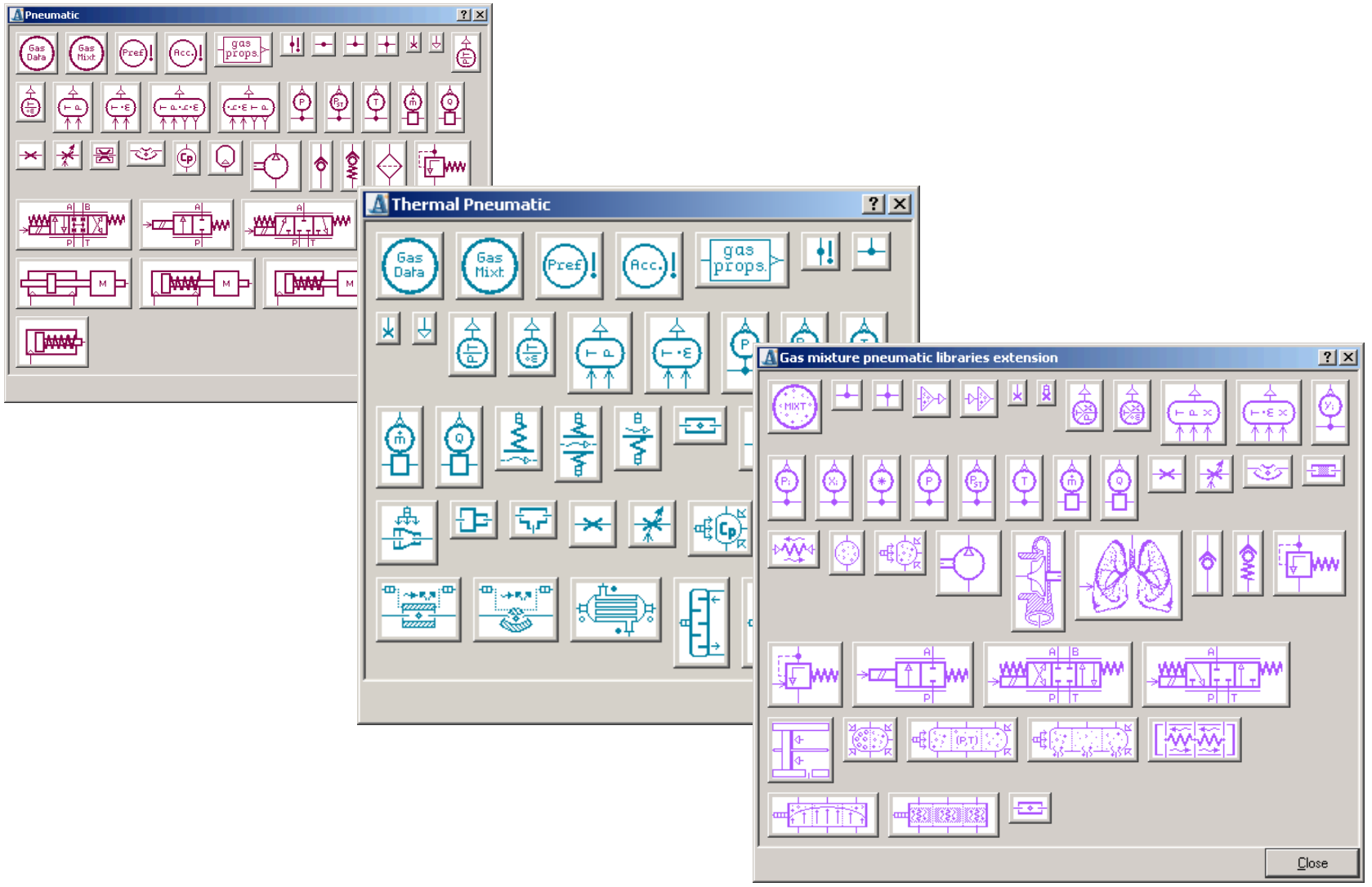
Typical Fuel Cell PEM Control System



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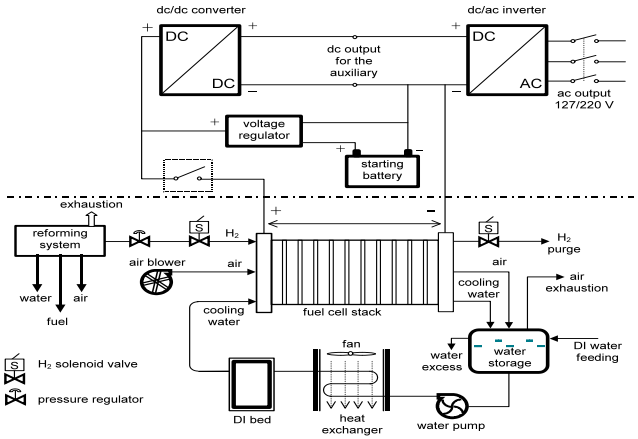
Typical Fuel Cell PEM Control System



COOLING SYSTEM

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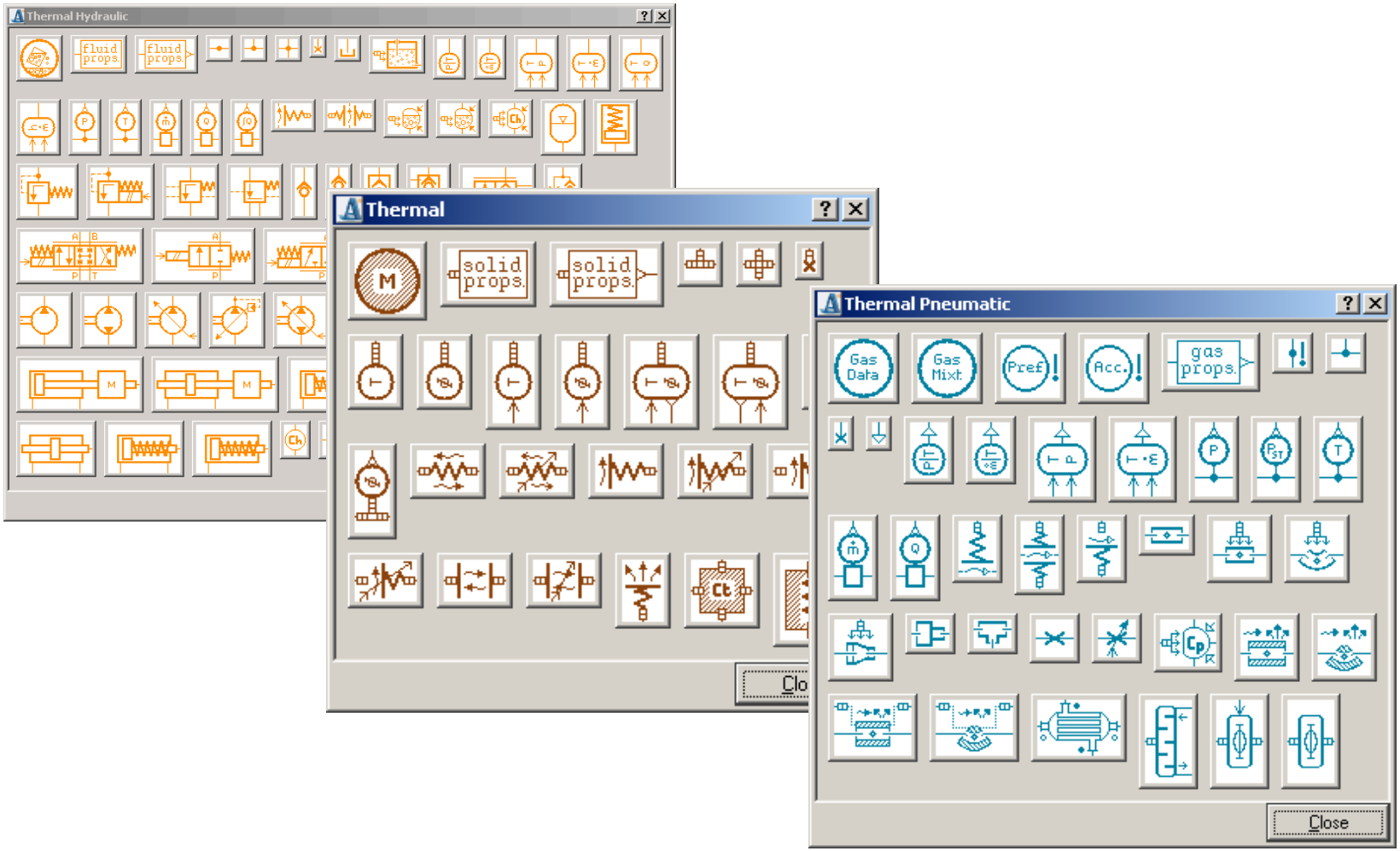
Typical Fuel Cell PEM Control System



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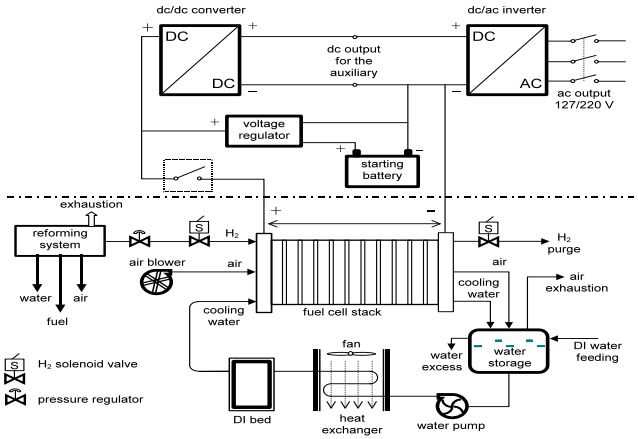
Typical Fuel Cell PEM Control System



STACK SYSTEM

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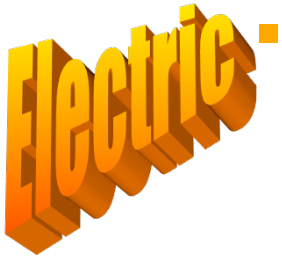
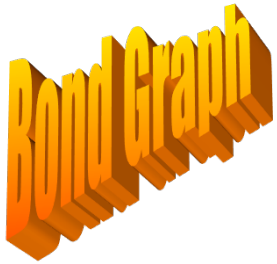
Introduction

- State of the art of PEMFC stack numerical models



  - Dynamic model of analogic electrical equivalent system
    - Pneumatics and chemicals are modelled with equivalent electric elements

  - Quasi-steady state model based on CFD code
    - Limited by boundary conditions
    - CPU cost: days on parallelized clusters



  - Bond-Graph model
    - Multi-domain (electrical/chemical/pneumatic)

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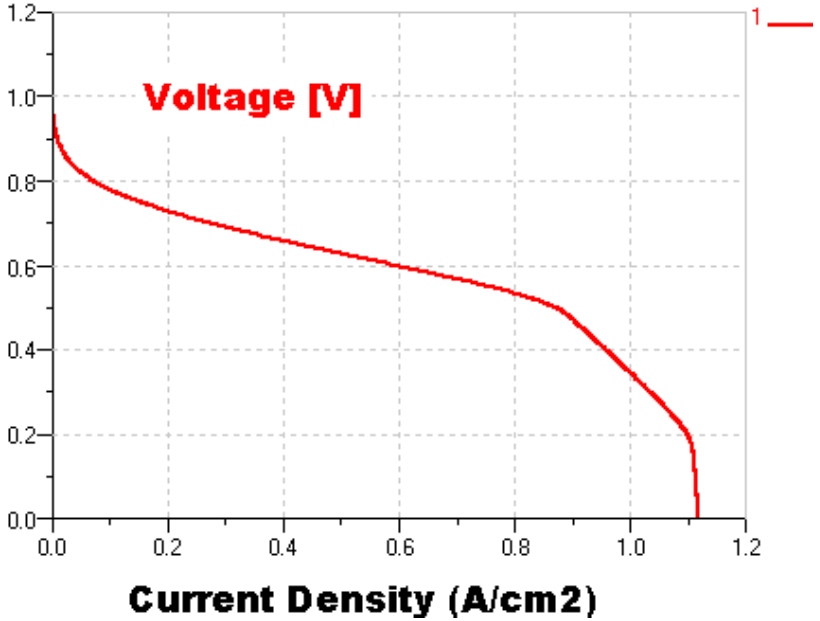
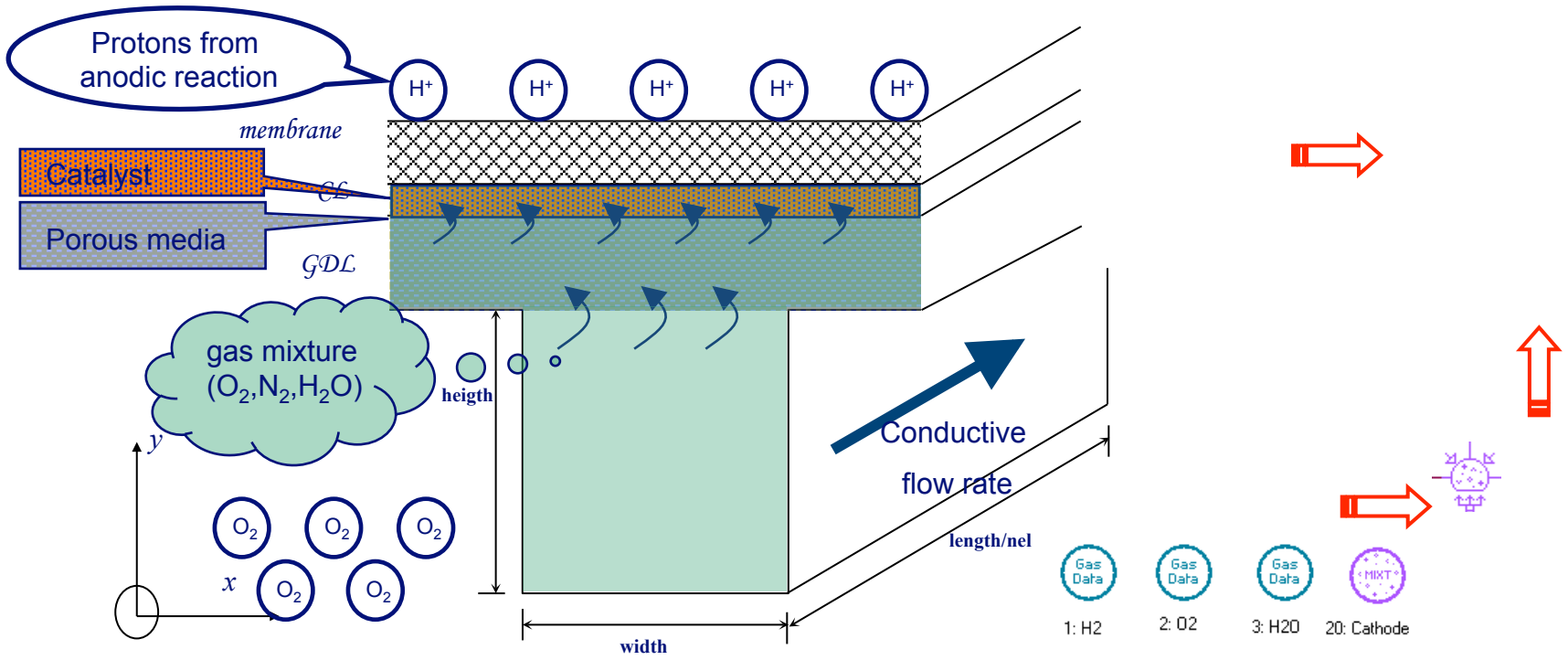
Stack System

- **AMESim Model** for stack modelling
  - Inspired from **Bond Graph**
  - **Physical model** of electrical, electrochemical, pneumatic and thermal phenomena
  - Stack design and optimization
  - **Dynamic modelling** of pneumatics, chemical reactions, etc…



PEM cell Model structure (Explanations)

Cathode side



Protonic resistance

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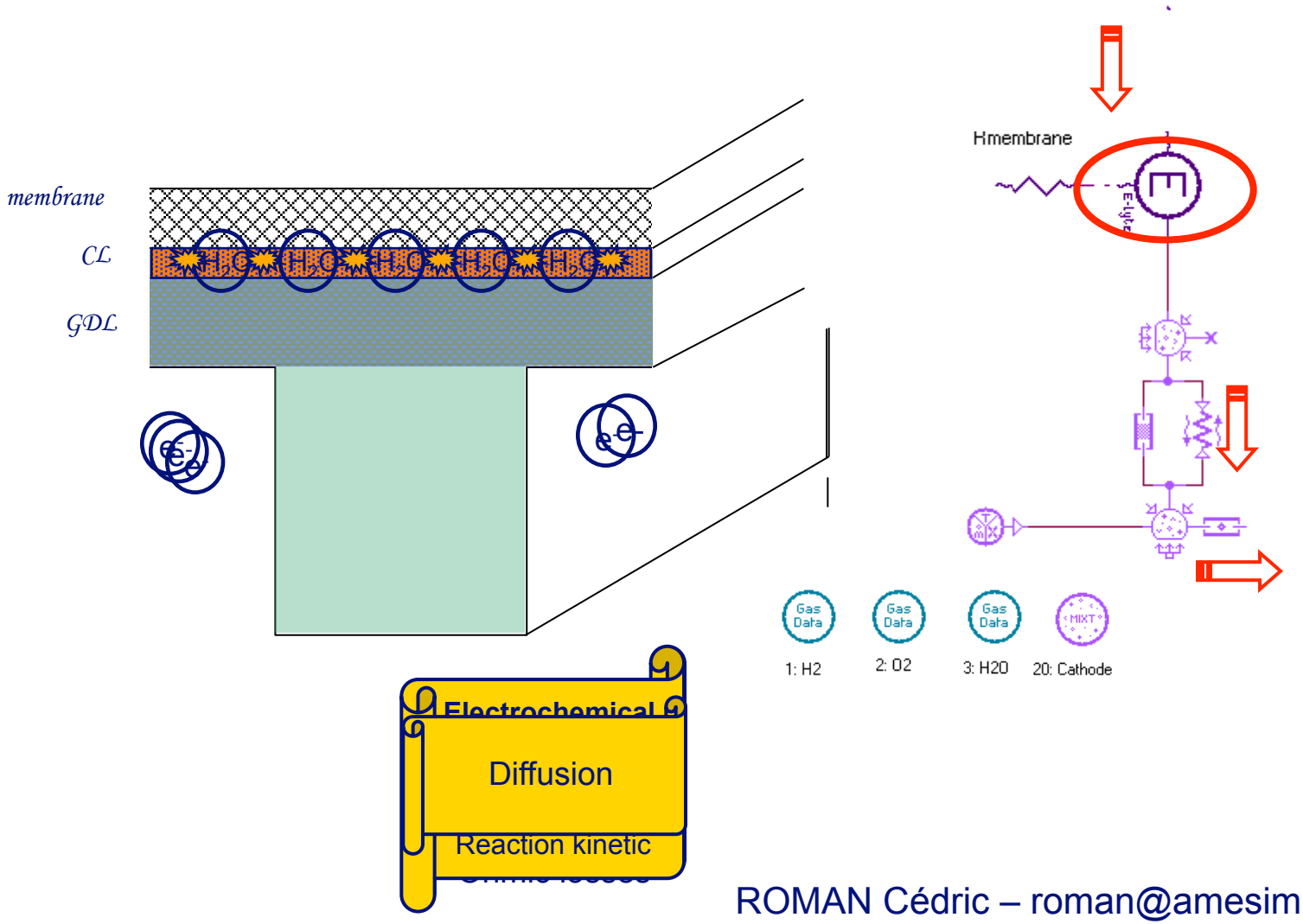
PEM cell Model structure (Explanations)



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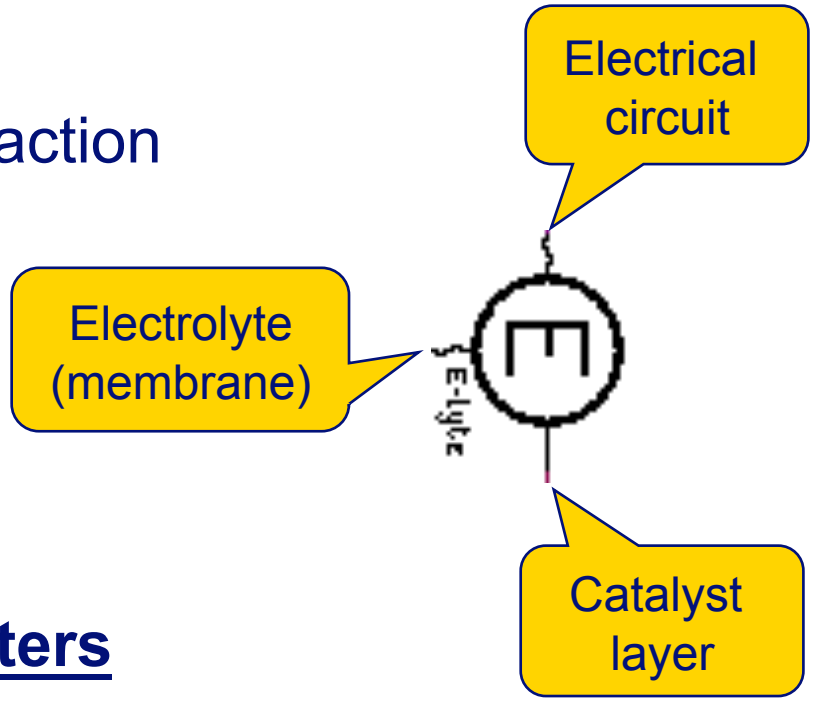
PEMFC Stack Model

- Core of model
  - electrochemical reaction
- Interfaces
  - Electrical circuit
  - Electrolyte
  - Catalyst layer
  - **Reaction parameters**
    - Stoechiometry in data file
      - Reference heat of formation, standard entropy
    - Kinetic parameters in data file
      - Partial orders, kinetic constant
    - Assymetry parameter



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PEMFC Stack model

- PEMFC cathode
  - Electrochemical reaction $O_2 + 4H^+ + 4e^- \Leftrightarrow 2H_2O$
  - Gas mixture equilibrium potential
    - Nernst equation $E_{rev} = E^o - \frac{RT}{4 \cdot F} ln\left(\frac{a_{H_2O}{}^2}{a_{O_2} \cdot a_{H^+}{}^4 \cdot a_{e^-}{}^4} \right)$
  - Overpotential
    - Activation Voltage
      – Equilibrium potential
    - = Disequilibrium $\eta = U - E_{rev}$
  - Reaction kinetic
    - Butler-Volmer equation $I = I_O \left[-exp\left(-\alpha_C n \frac{F\eta}{RT} \right) + exp\left(\alpha_A n \frac{F\eta}{RT} \right) \right]$

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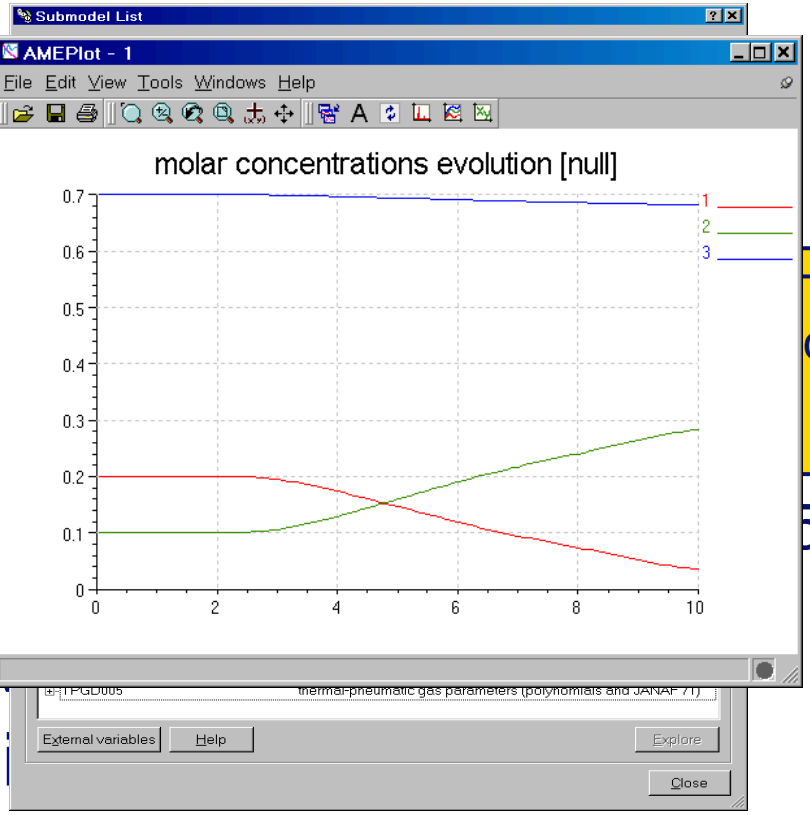
PEMFC Stack model

- Gas mixture description
  - Dyna
  - Mixtu
  - Perfe
    - Rea
  - Therr
    - JAN
      poly
      -
  - Diffusi
    - Binary coefficients / Wilke formula
  - Water condensation/vaporisation (to come…)



d

5 order

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PEMFC Stack model

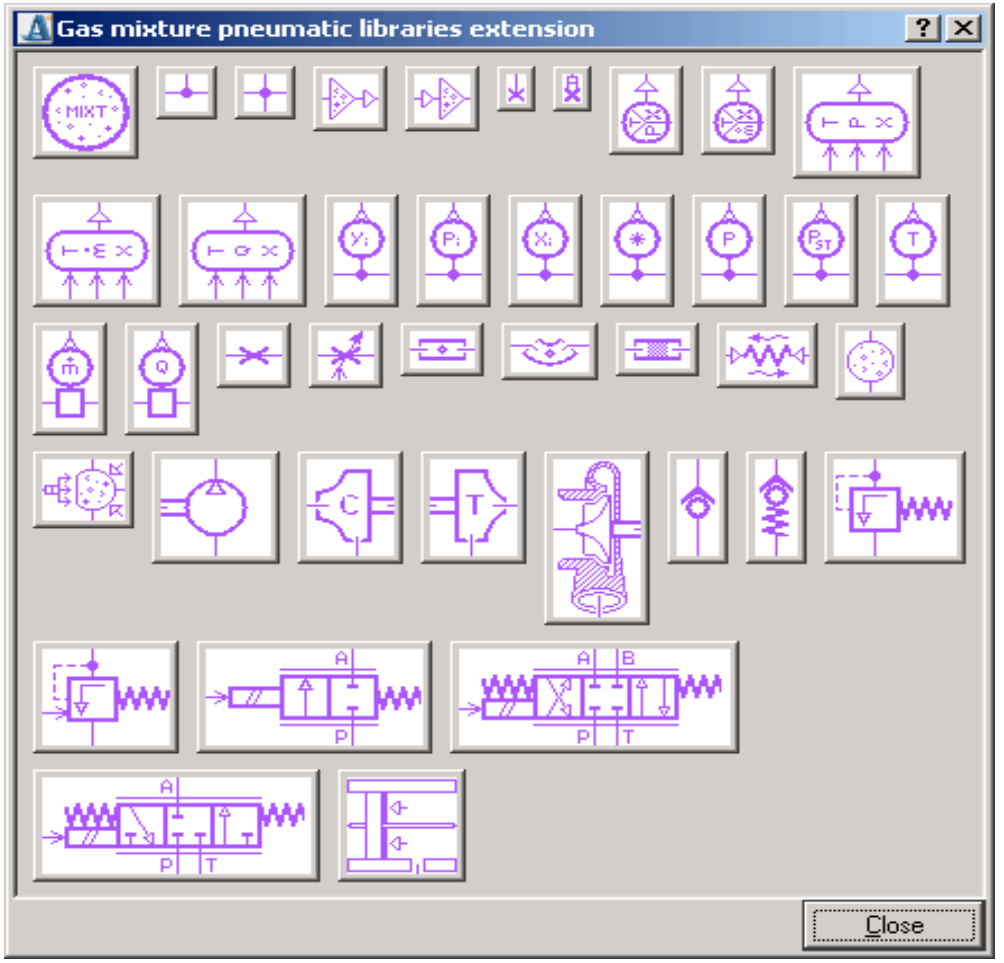
Add-on Gas Mixture

Basic Elements approach

Powerful features

Initialisation facility

Compatibility with PCD/PN/THPN



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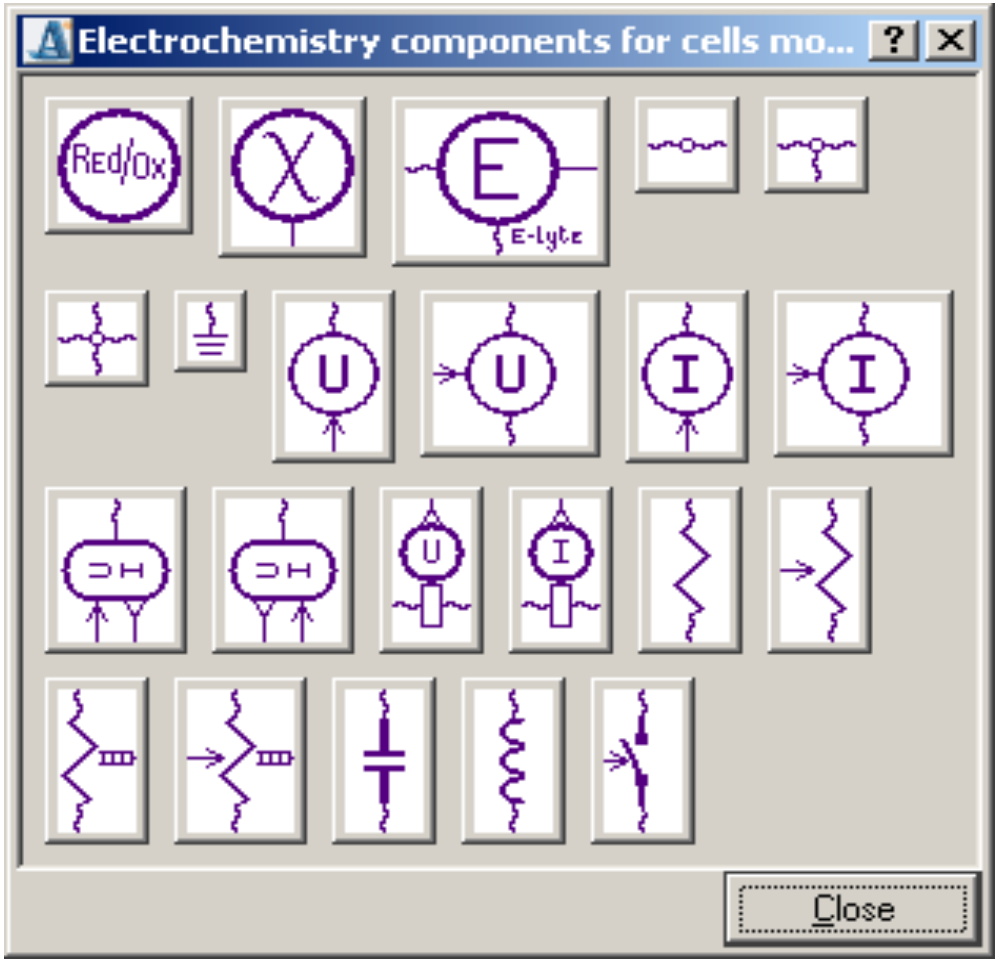
PEMFC Stack model

Add-on Fuel Cells

Basic Elements approach

Compatible with
Add-on Gas Mixture
Thermal libraries



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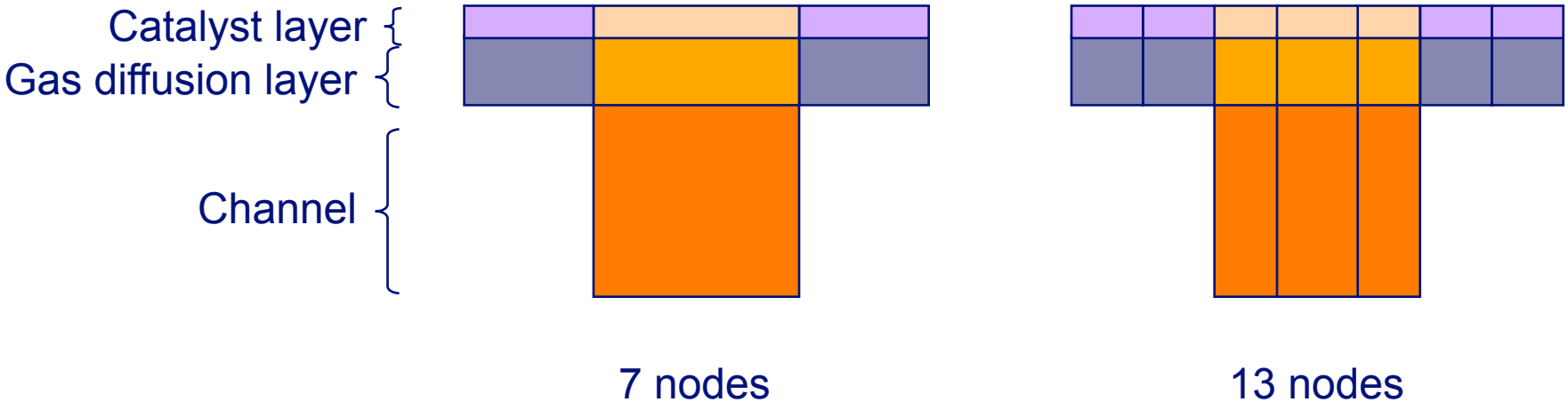
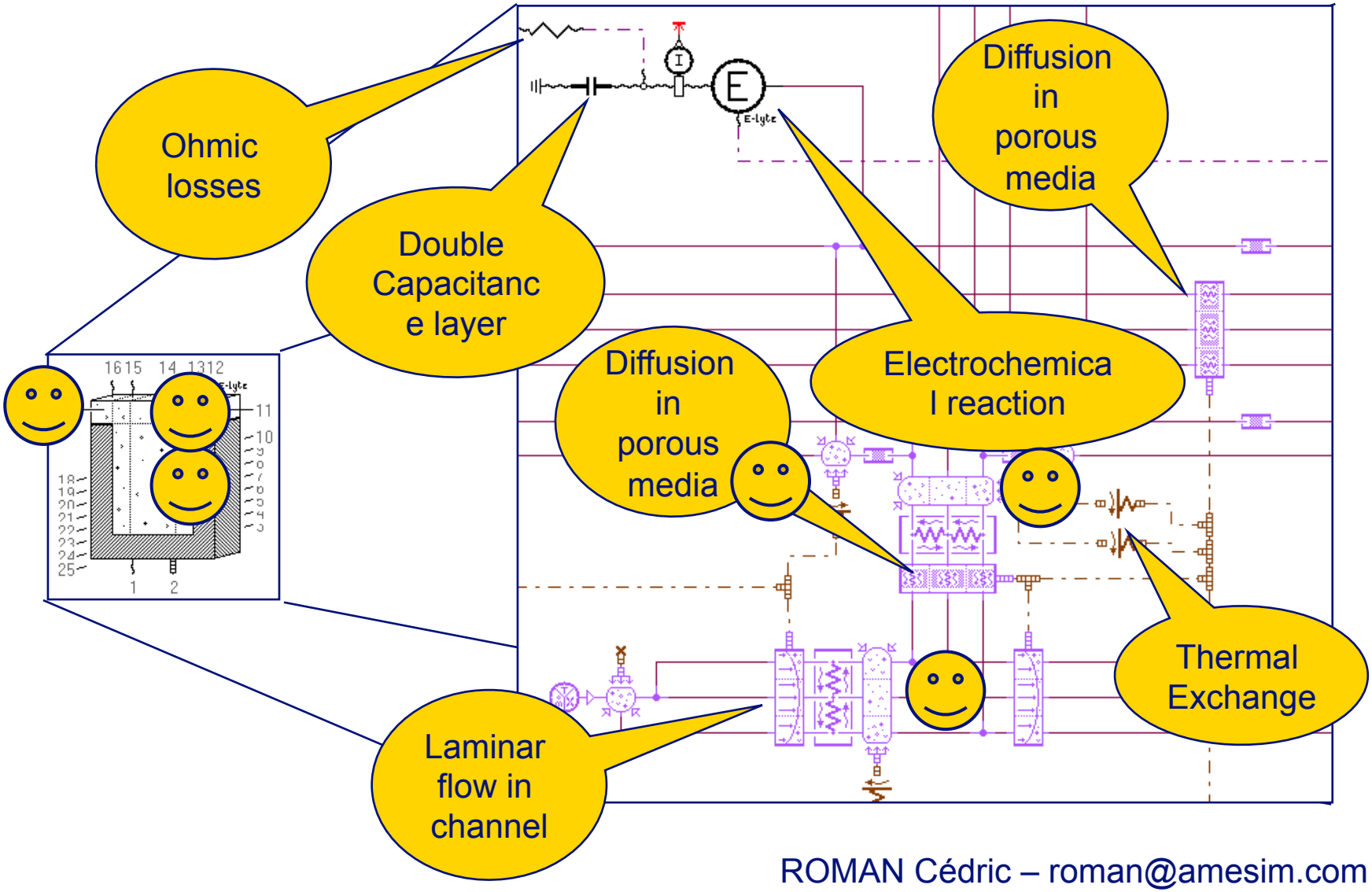
PEMFC Stack model

- Possible Discretizations



PEMFC Stack model



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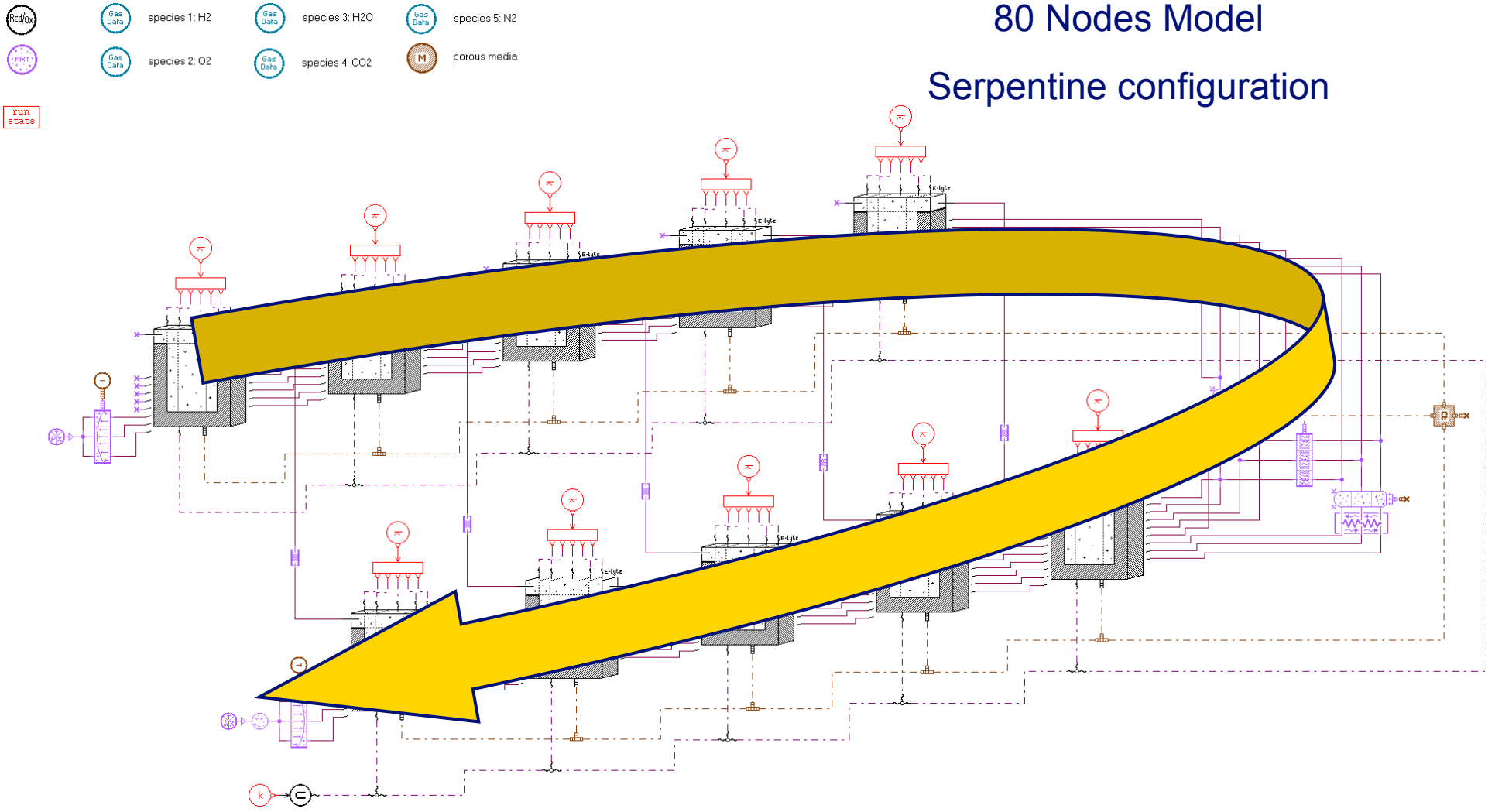

80 Nodes Model

Serpentine configuration

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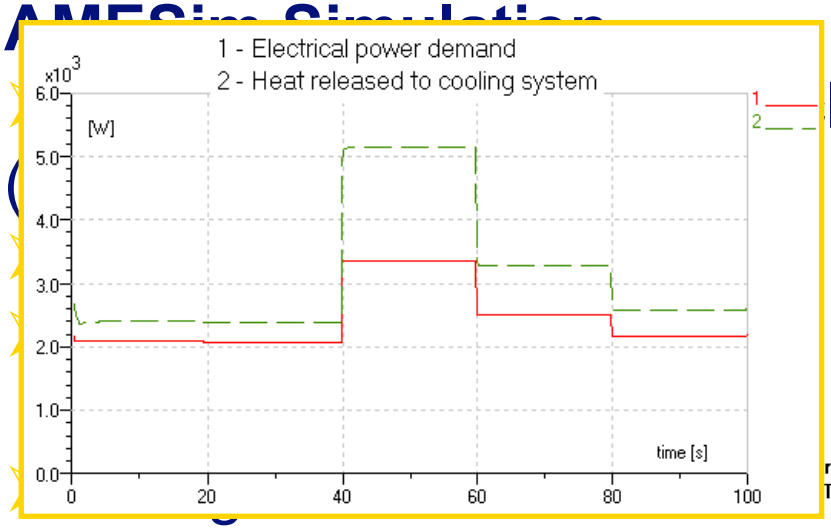
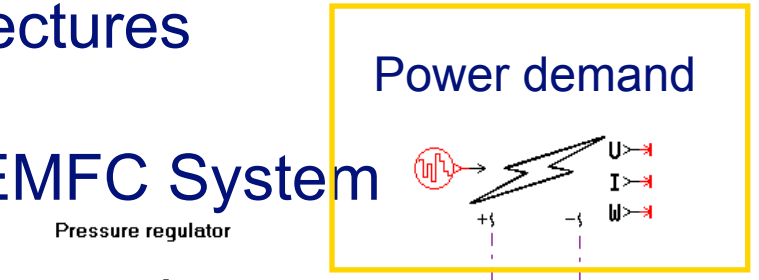
PEMFC system simulation

AMESim Simulation



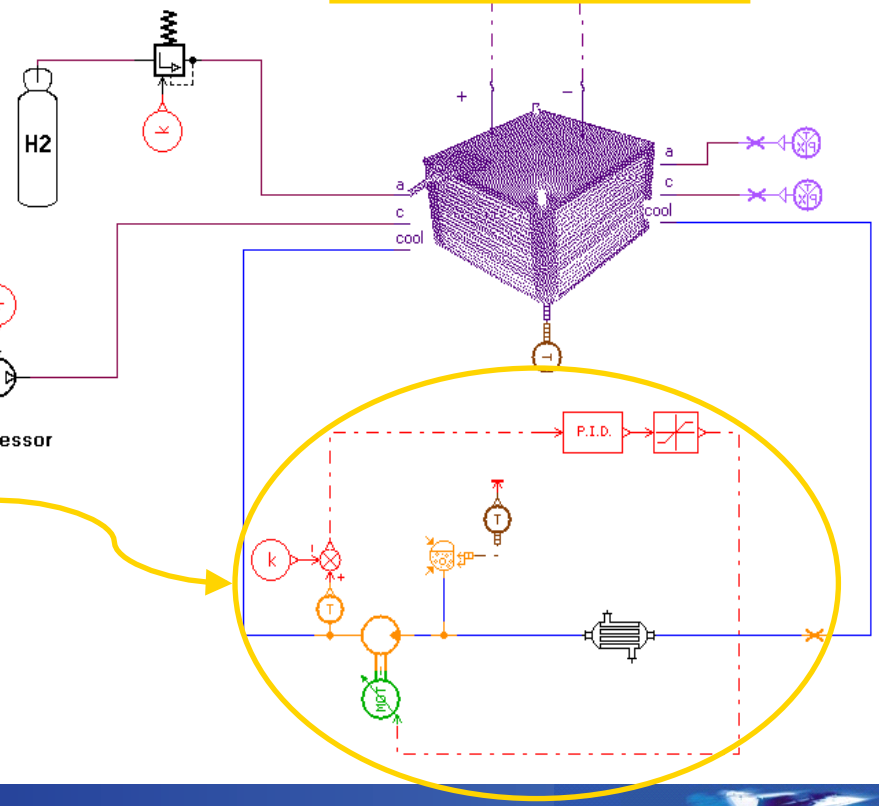
hitectures

PEMFC System



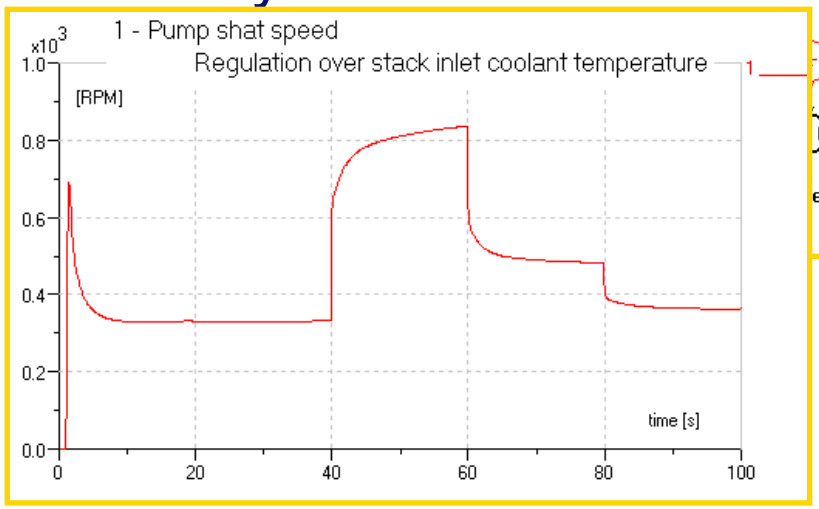
Pressure regulator

re
Tank



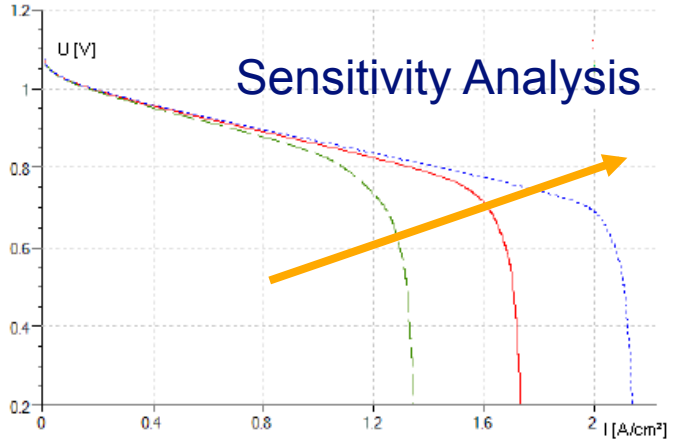
essor

➢ Drive cycle

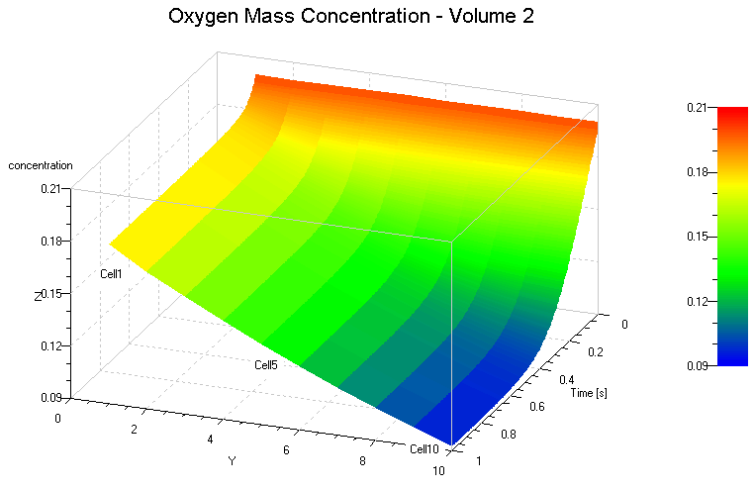


PEMFC AMESim model

- Allow quick results
  - Physical model
  - Transient behaviour
  - Gas diffusion efficiency
  - Thermal management



- Robustness & Risk analysis
  - AMESim features
    - Monte-Carlo simulation
    - Design of experiment
    - Optimization



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PEMFC AMESim model

- Gain Time & Performance

- Have a better understanding of physics
- Use all powerfuls AMESim applications
  - Compatible with standard libraries
  - Activity index
  - Linear analysis (Bode, Nyquist, Nichols,…)
  - Design of Experiment / Optimization
  - Real-time

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