cea liten

Modeling, simulation and digital twins in the development of new energy technologies

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OUTLINE

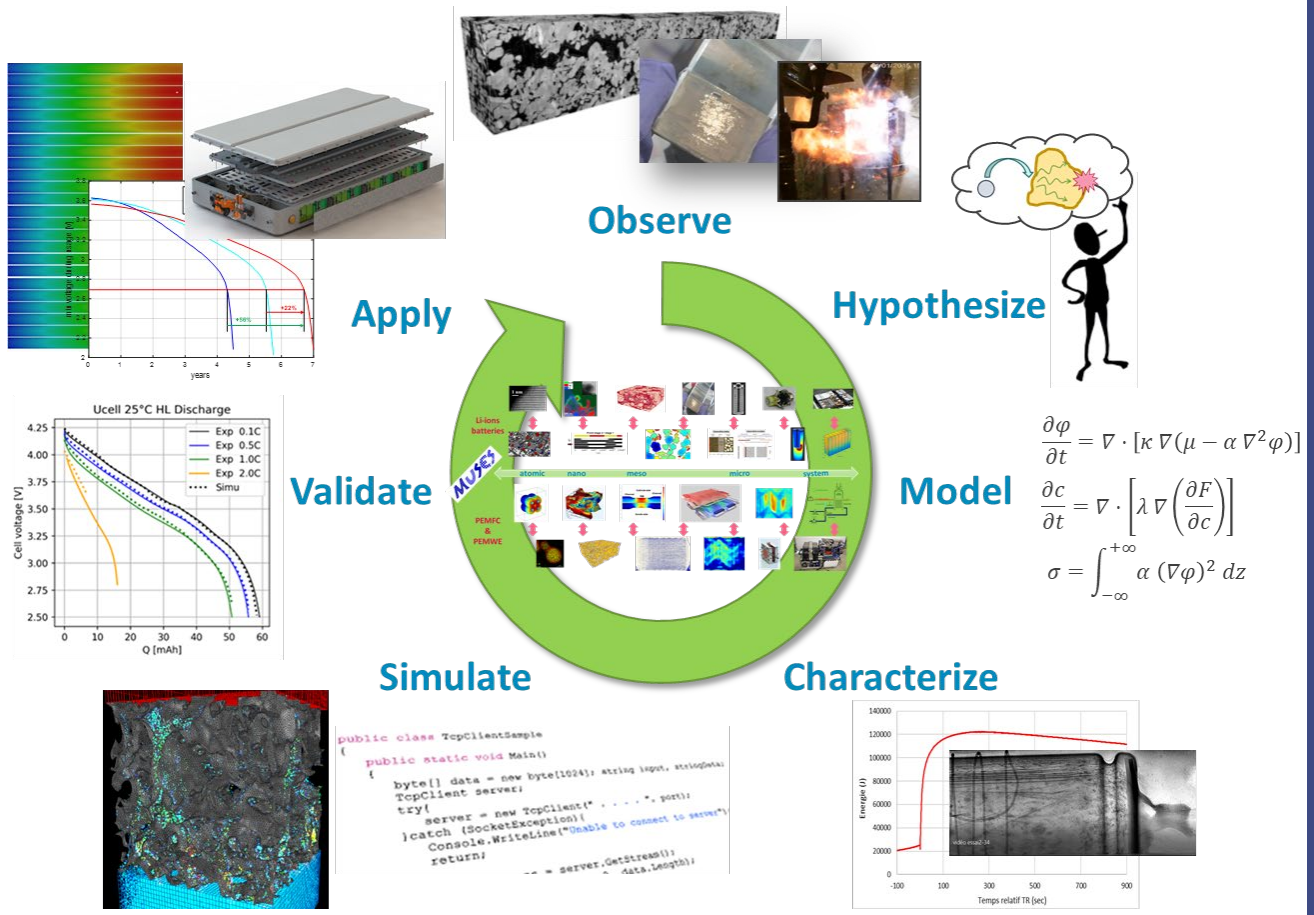
1. **Why modeling & simulation at Liten?**

2. **Modeling & simulation to support the development of key technologies**

3. **Accelerate the deployment of these key technologies in the applications**

The simulation approach at Liten

From experimental observation to predictive simulation



Modeling and simulation and **experimentation** are complementary and closely bonded

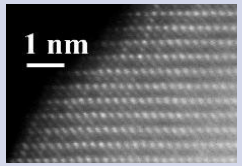
The MUSES platform

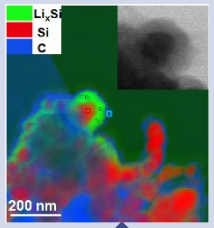
A common multi-scale and multi-physics simulation platform for batteries and fuel cells

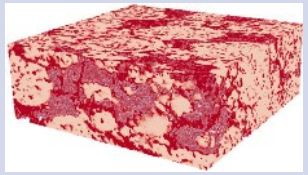
Experimentation

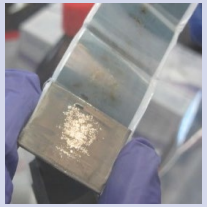
Modeling & simulation

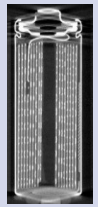
Experimentation

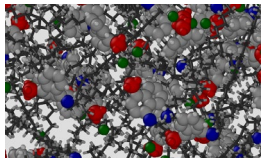


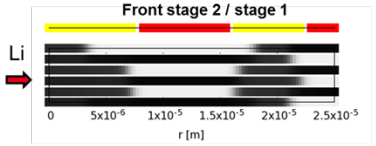


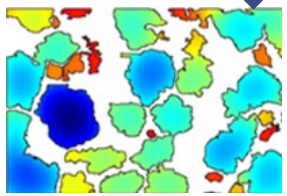


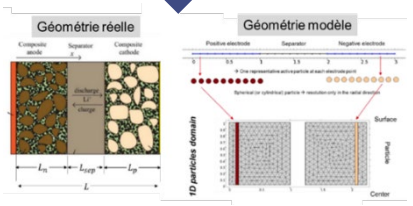


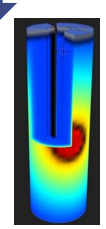


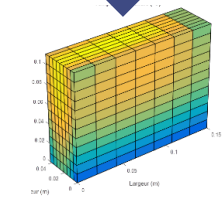




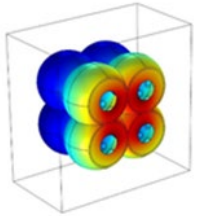


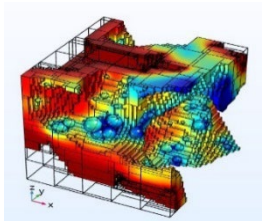


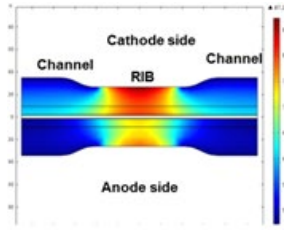


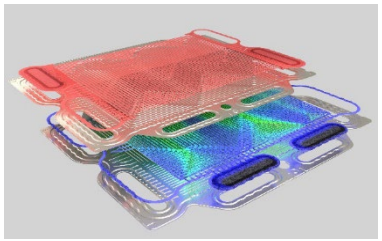


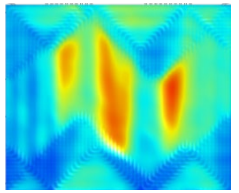
atomic nano meso micro system

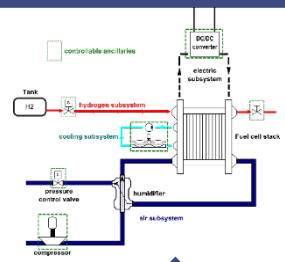


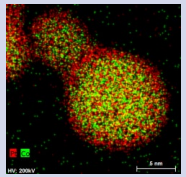


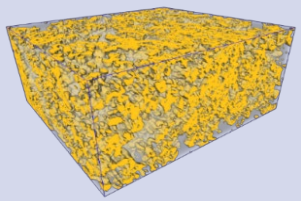


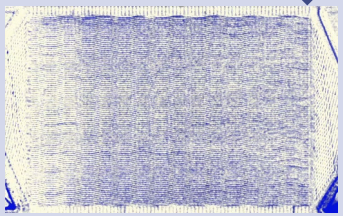


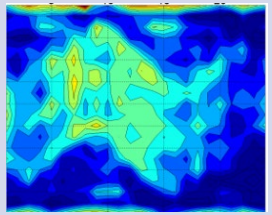










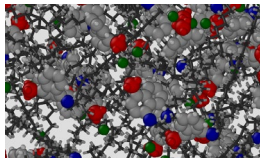


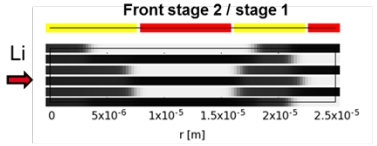
The MUSES platform

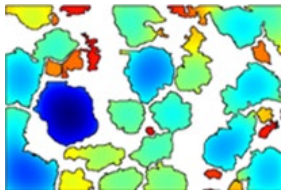
Model development

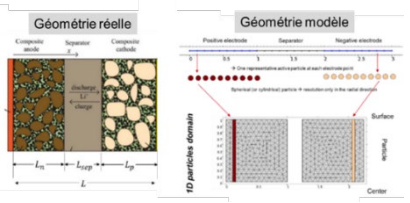
Software development

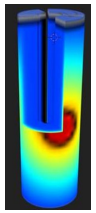
- Identify the dominant phenomena and the relevant scales for specific needs
- Adapt the approach to meet the need

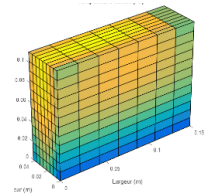




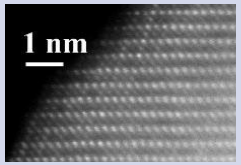


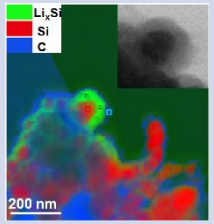


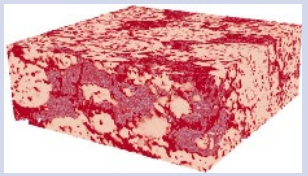


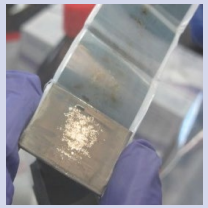


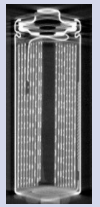
atomic | **nano** | **meso** | **micro** | **system**











Advanced experimental characterizations

Database management

- Specific and adapted models through acquiring the relevant parameters
- Best experimental techniques to guarantee the level of validation of the models

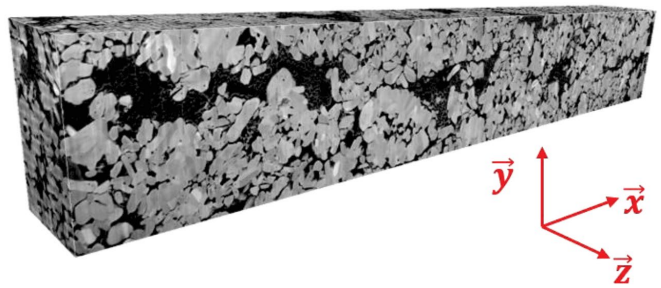
Example of application on Li-ion batteries

Reference simulation

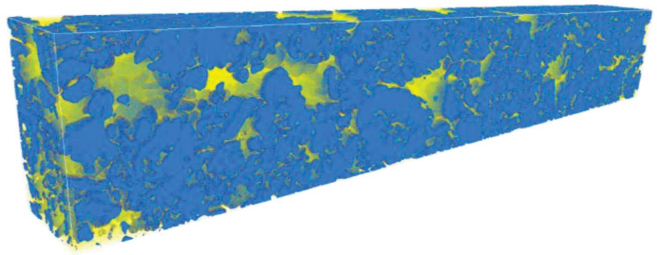
Battery discharge at the scale of the electrode microstructure

atomic | nano | **meso** | micro | system

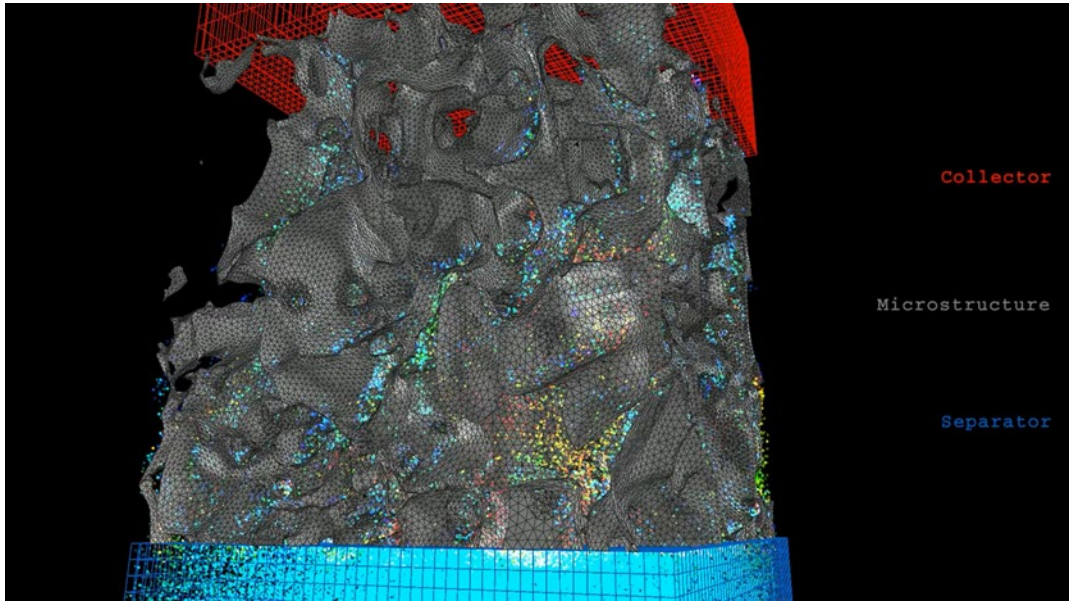
a.



b.



3D real microstructures
Virtual electrodes possible



Example of application on Li-ion batteries

Reference simulation

Battery discharge at the scale of the electrode microstructure

atomic | nano | **meso** | micro | system

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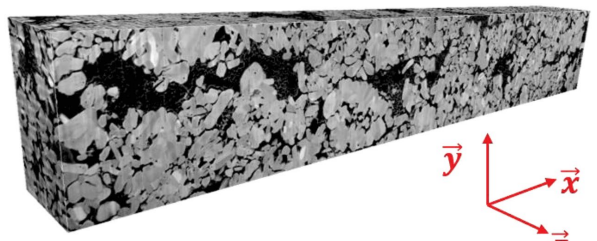
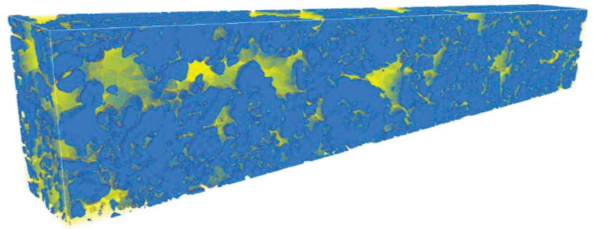
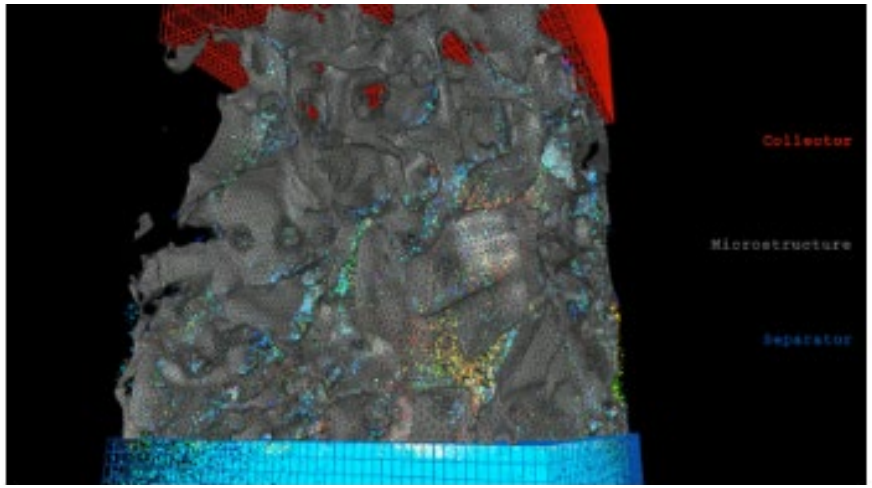


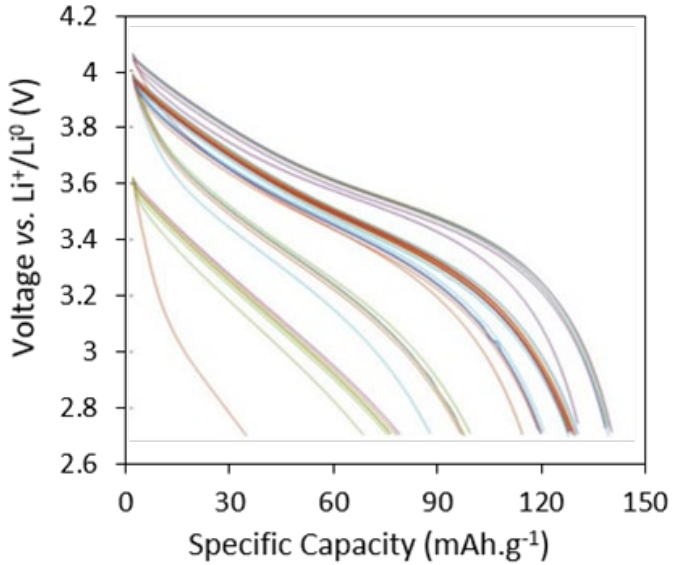
b.



3D real microstructures
Virtual electrodes possible



Access to local conditions
Not possible experimentally
Crucial for ageing understanding



Access to electrochemical performances
Dependence on materials properties

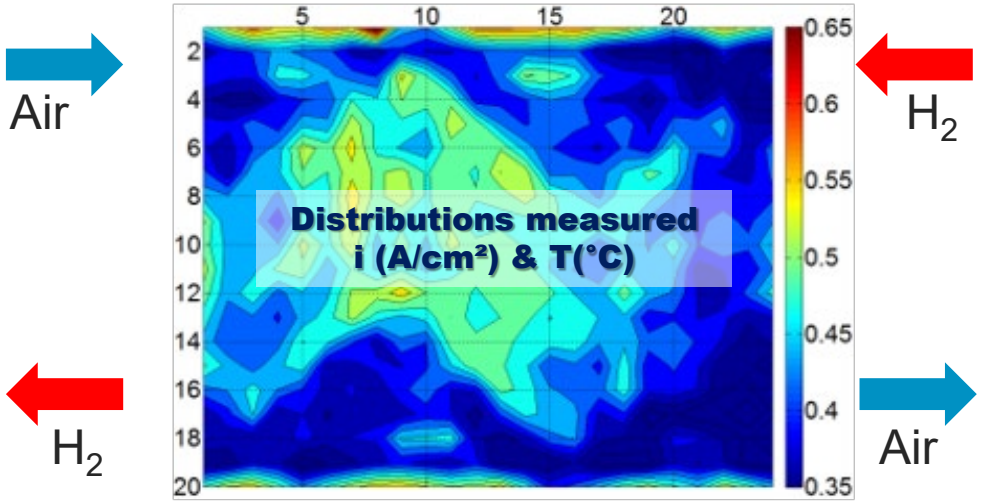
Example of application on PEM fuel cell

Development acceleration

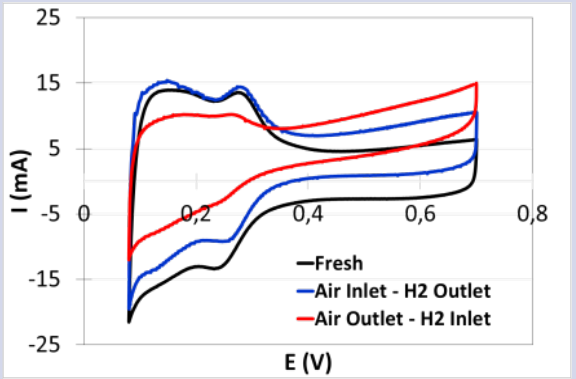
Optimization of MEA surface structure to optimize the PEMFC durability

atomic | nano | meso | **micro** | system

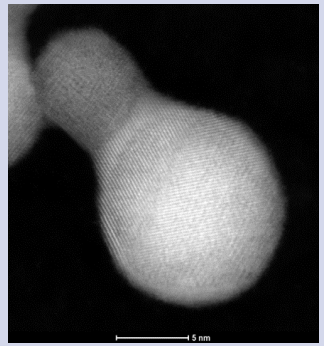
In situ & ex situ experimental analyses at end of life

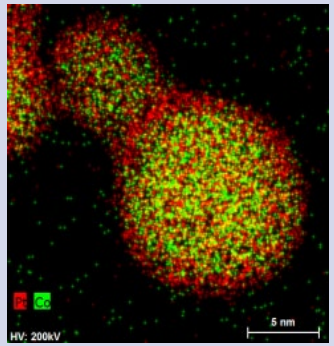


Electrochemistry



Electronic microscopy





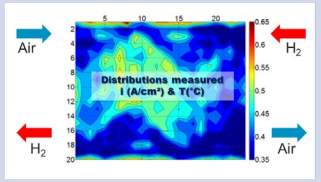
How CO possibly present in H_2 degrades the performance of PEMFC and how to limit this degradation?

Example of application on PEM fuel cell

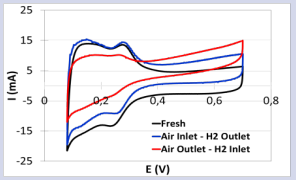
Development acceleration

Optimization of MEA surface structure to optimize the PEMFC durability

In situ & ex situ experimental analyses



Electrochemistry



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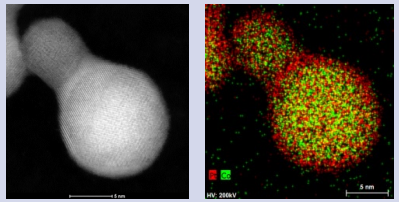
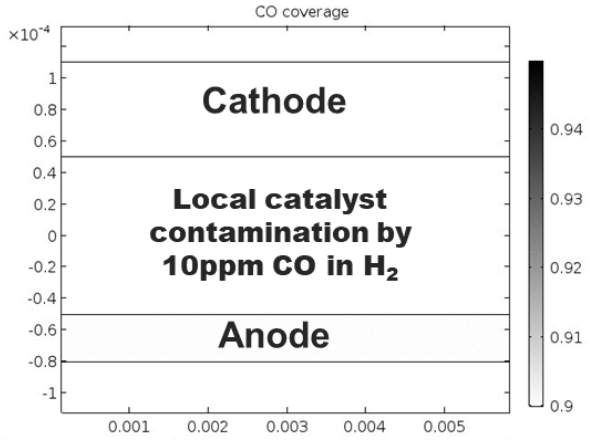
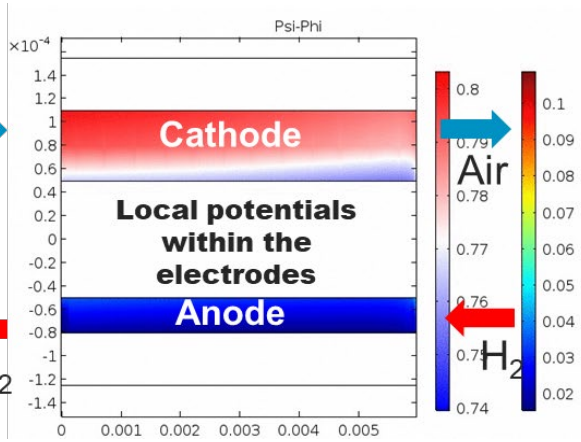
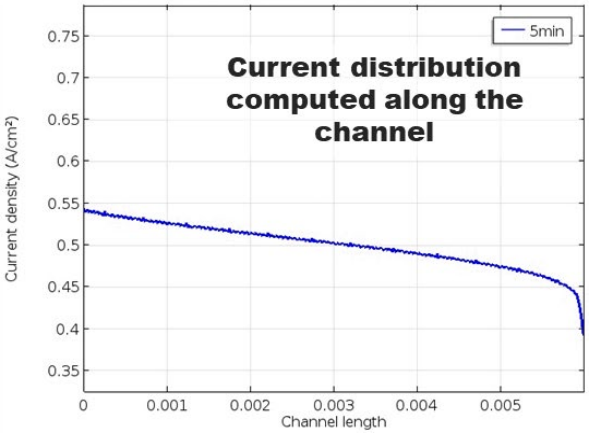


2D transient simulation







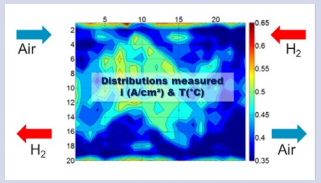
Complementary information provided by the model

Example of application on PEM fuel cell

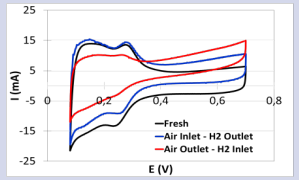
Development acceleration

Optimization of MEA surface structure to optimize the PEMFC durability

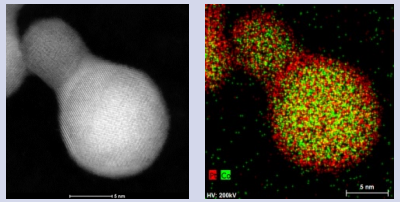
In situ & ex situ experimental analyses



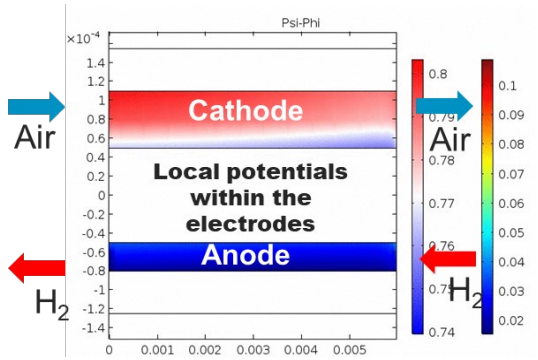
Electrochemistry

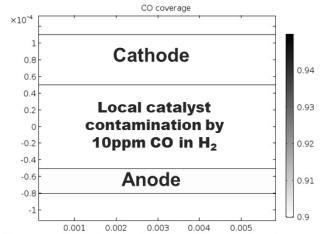


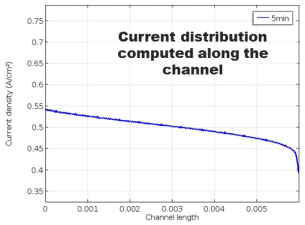
Electronic microscopy



2D transient simulation

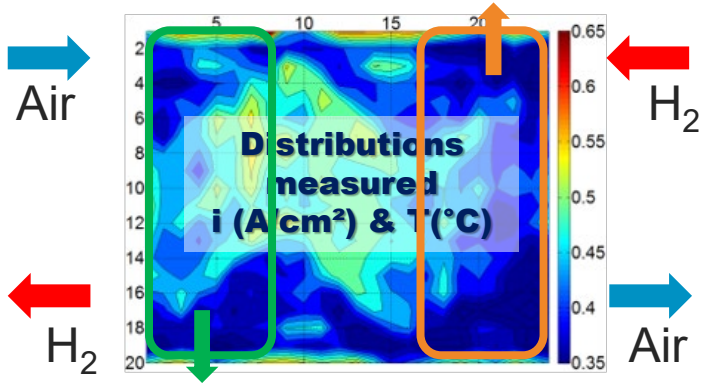






Explanation of local mechanisms

Co dissolution & ionomer contamination



Ru dissolution
Decrease of tolerance to CO

Example of application on PEM fuel cell

Development acceleration

Optimization of MEA surface structure to optimize the PEMFC durability

atomic | nano | meso | **micro** | system

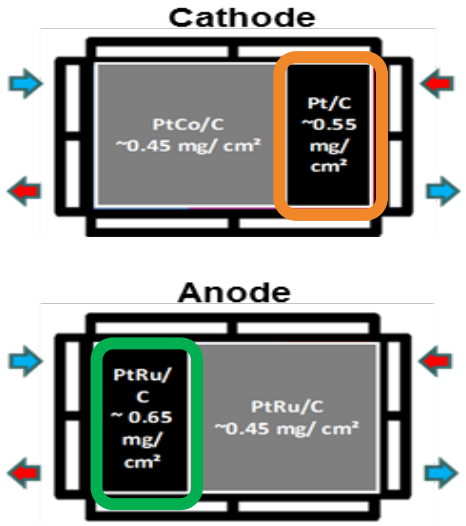
In situ & ex situ experimental analyses

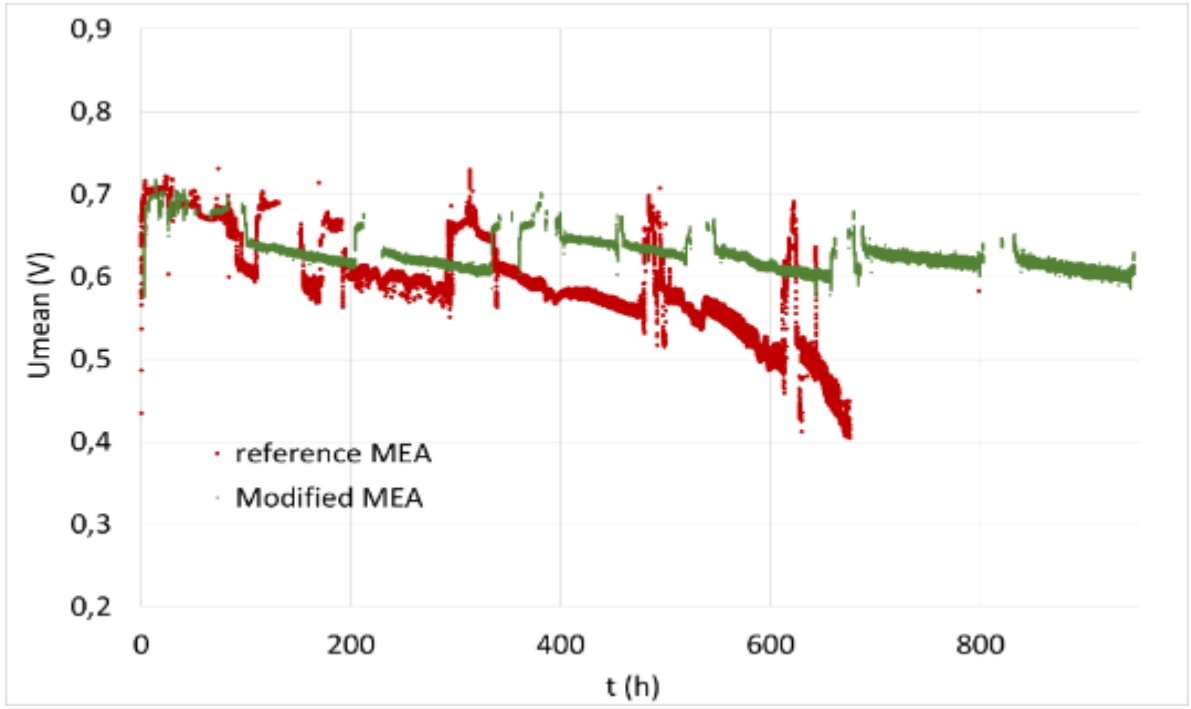
+

2D transient simulation

Explanation of local mechanisms

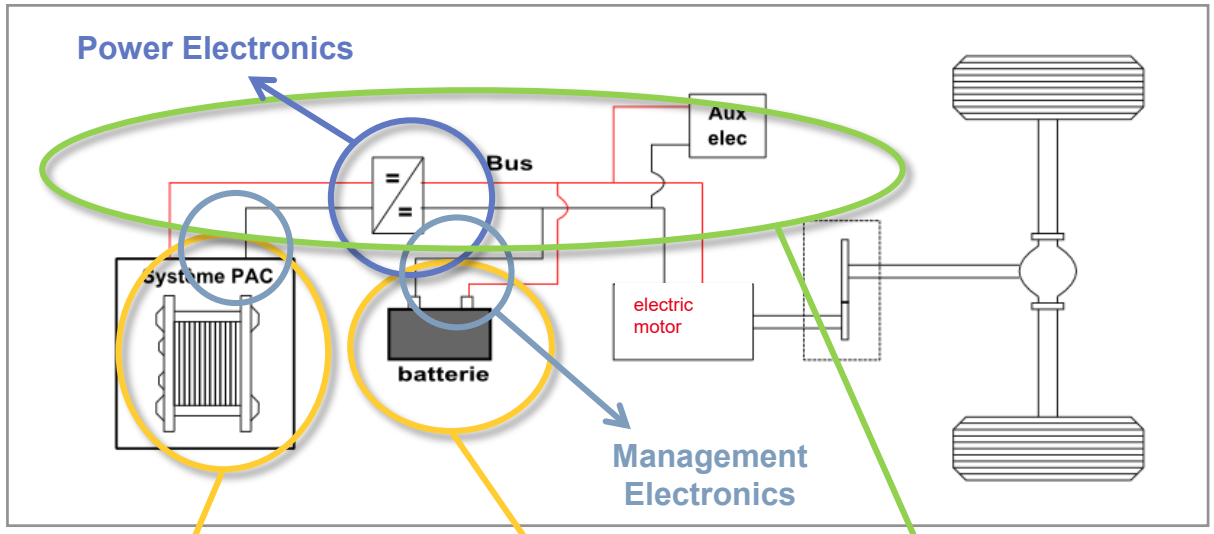
Solution → Local adaptation of the composition of the electrodes

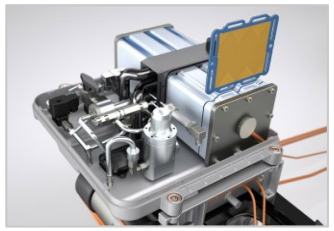




Improvement of the performance stability

Optimal usage of the technologies in applications





Technology development from material to system

atomic | nano | meso | micro | system

Simulation to accelerate the design

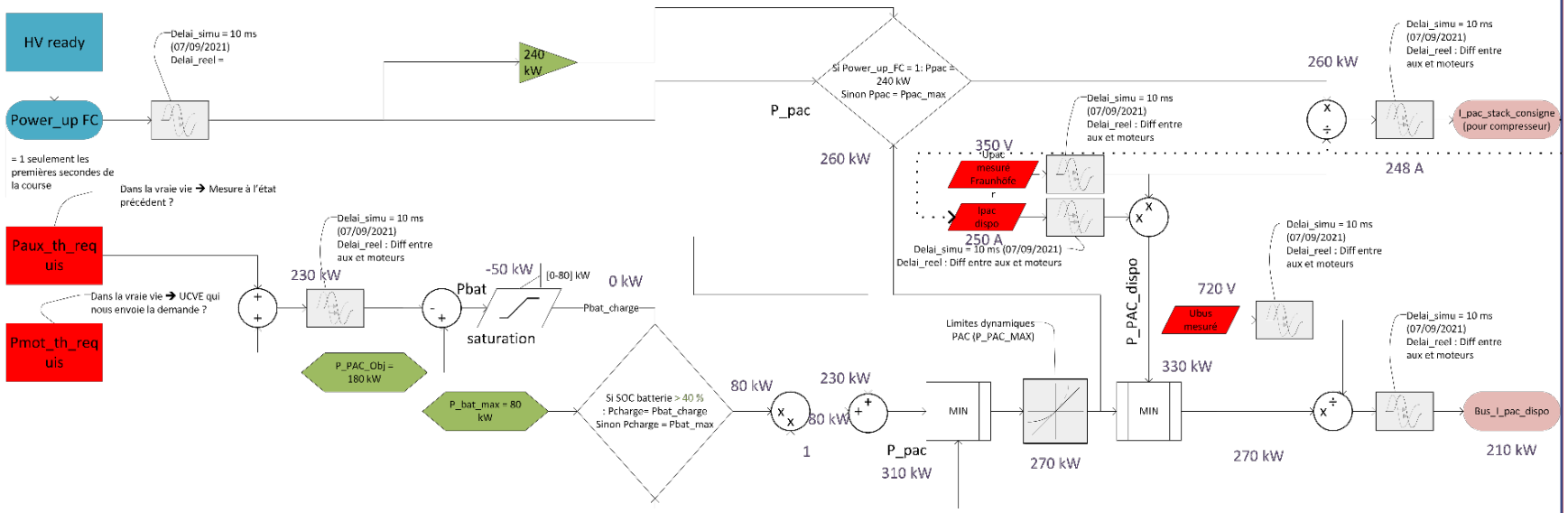
- Which best electric sources?
- Which sizing of each sub-system?
- Which optimal architecture?
- Which optimal management strategy of the different sub-systems?

Energy system model

Digital twin to validate the sizing and the energy management strategies

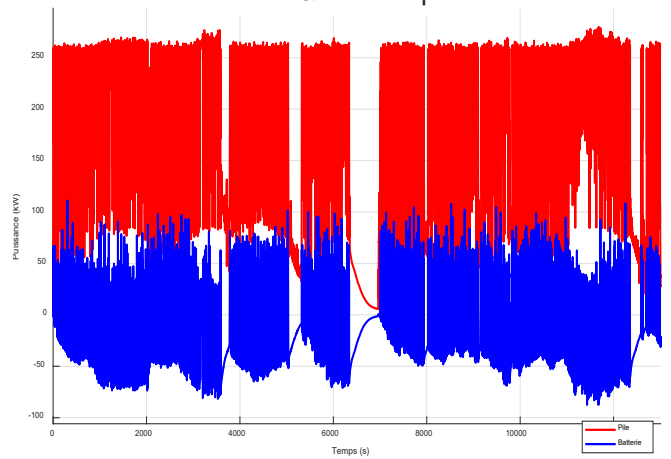
Digital twin of hybrid electrical systems

Digital Twin

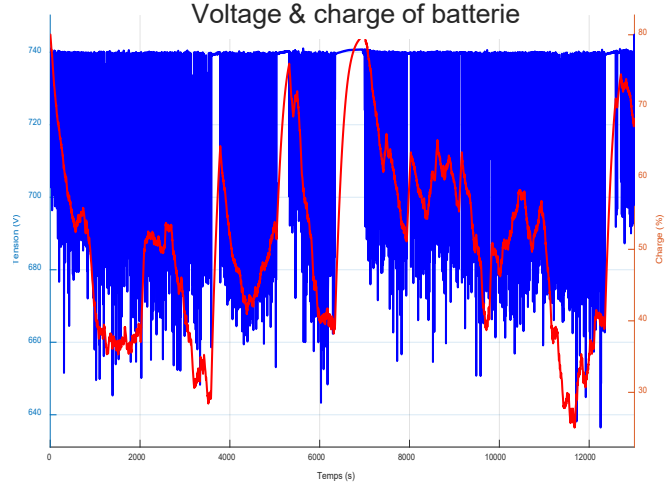


Results

Batteries & fuel cell power



Voltage & charge of batterie



Optimization of the power-management strategy during the design phase

Digital twin of hybrid electrical systems

Get predictive models that interact in real-time with physical systems

Accelerate and “derisk” the hardware developments through fast prototyping

Digital twin of hybrid electrical systems

Get predictive models that interact in real-time with physical systems

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Get a complete and coherent software / hardware approach

Digital twin of hybrid electrical systems

Get predictive models that interact in real-time with physical systems

Accelerate and “derisk” the hardware developments through fast prototyping

Get a complete and coherent software / hardware approach

Towards providing more services through a software / hardware symbiosis

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Thank's for your attention