UNIVERSITY OF LJUBLJANA | FS Faculty of Mechanical Engineering

Virtualna zaznavala in napredni kiber-fizikalni sistemi vodikovih tehnologij

Andraž Kravos, Tomaž Katrašnik in ekipa LICeM

University of Ljubljana

Faculty of Mechanical Engineering

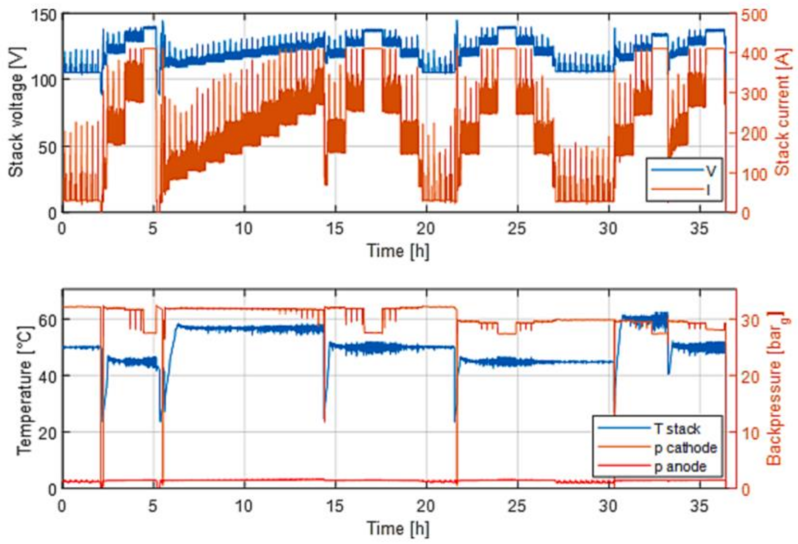
Laboratory for Internal combustion engines and electromobility

http://lab.fs.uni-lj.si/LICeM/

Introduction

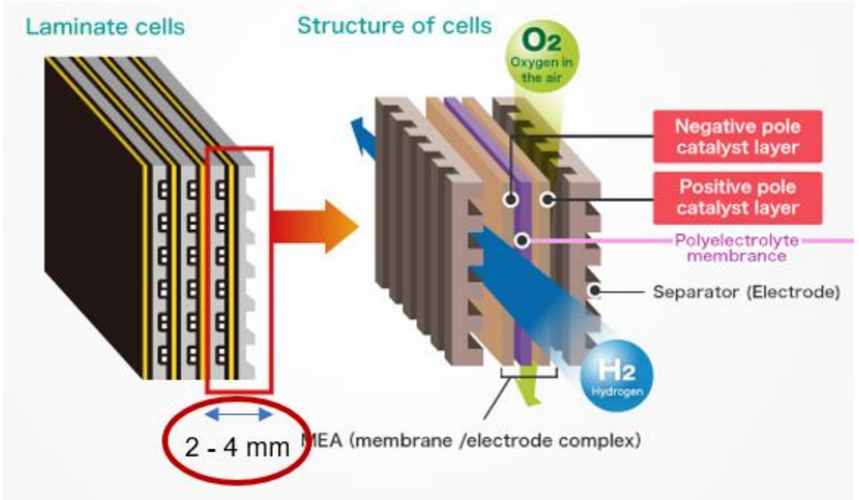
Highly dynamic operation of the EC in grid stabilization applications

Optimisation of efficiency and expected lifetime

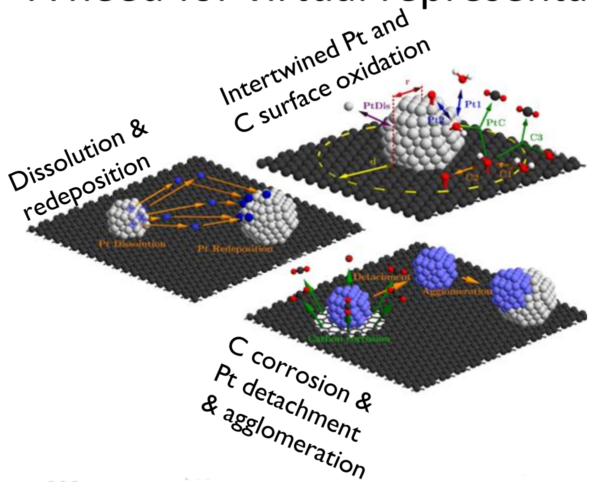


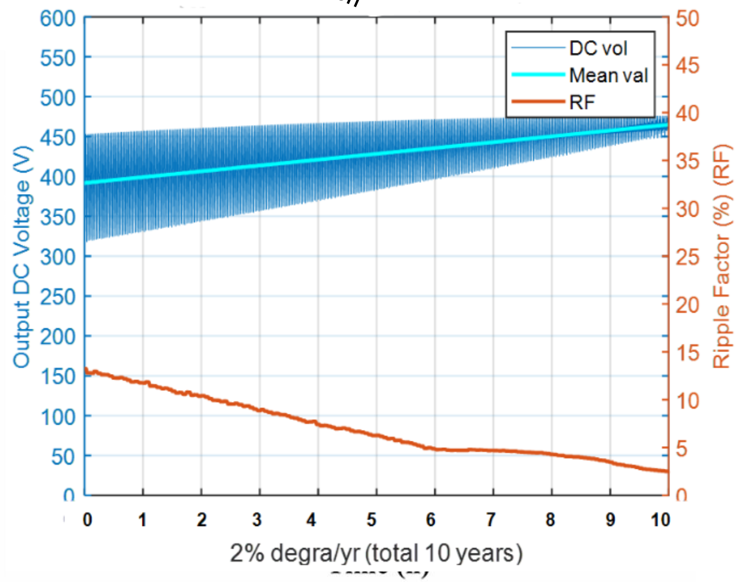
Elena Crespi et.al, Energy conversion and management, 2023

No space for efficient sensor placement



A need for virtual representation





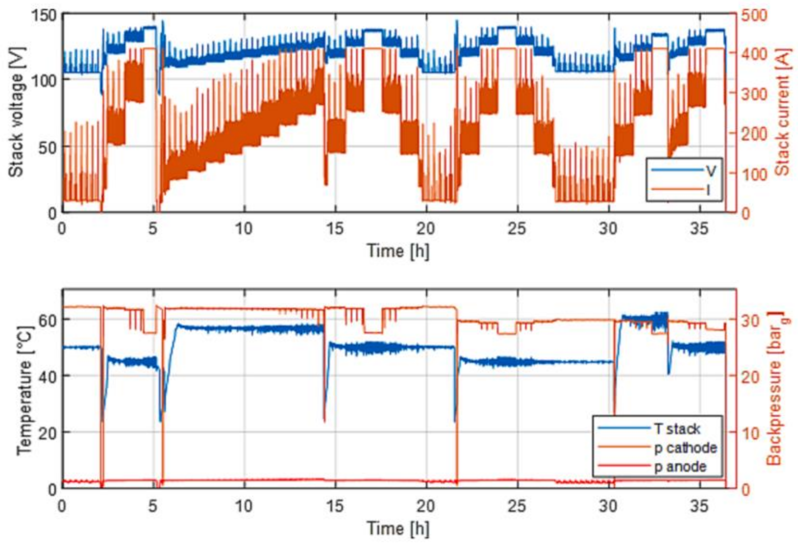
Jian Zuo et.al, Applied Energy, Volume 281, 2021

Introduction

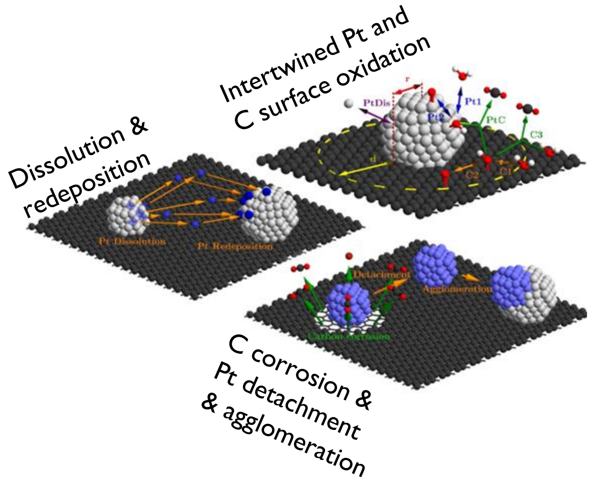
Highly dynamic operation of the EC in grid stabilization applications

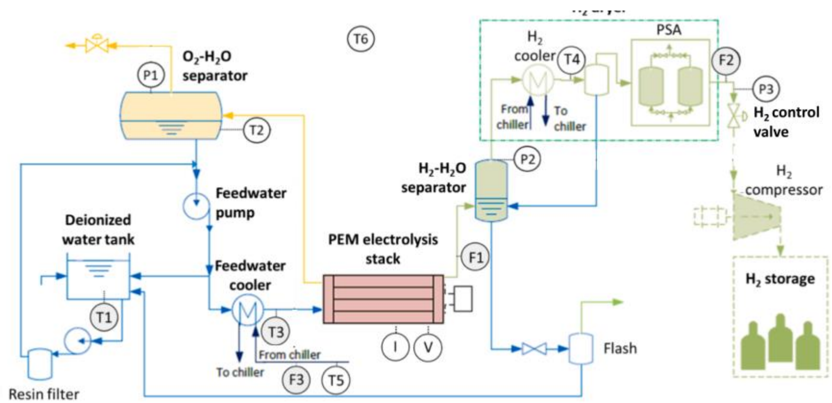
Optimisation of efficiency and expected lifetime

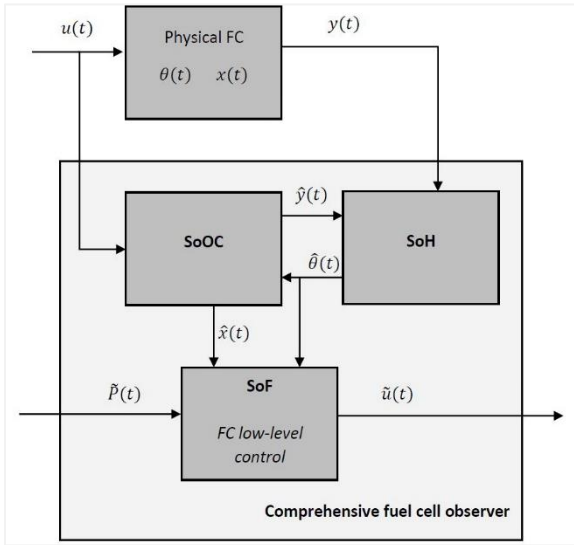
Online monitoring and control solutions



Elena Crespi et.al, Energy conversion and management, 2023



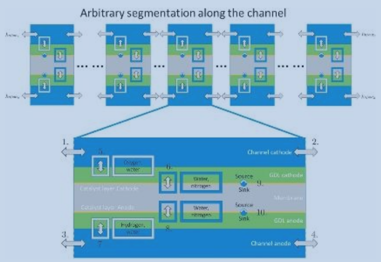




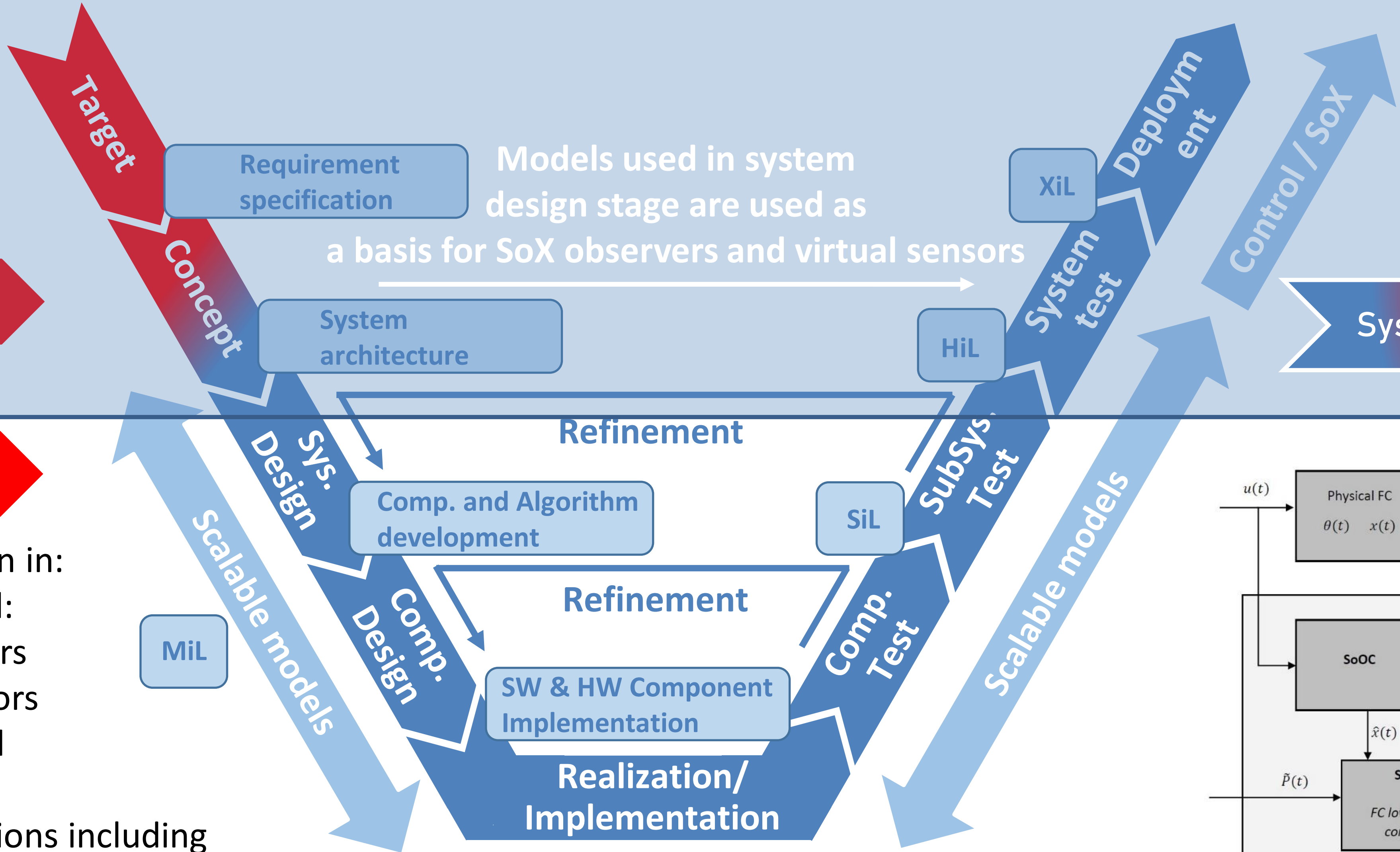
UNIVERSITY OF LJUBLJANA | FS Faculty of Mechanical Engineering

V-development process

LICeM



System design

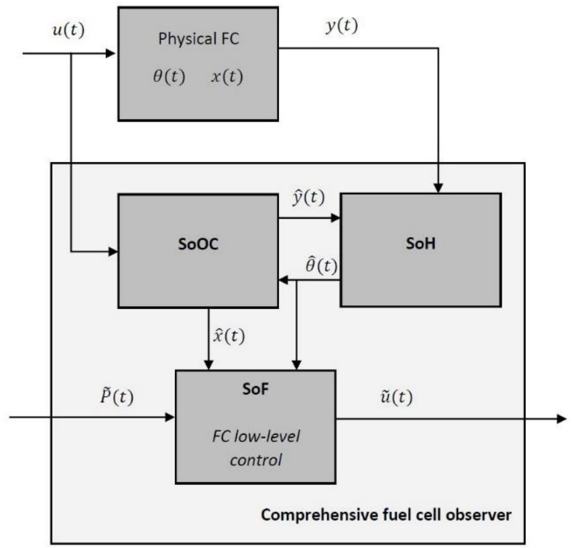


System testing

Beyond SotA

Models for utilization in:

- Spatially resolved:
  - SoX observers
  - Virtual sensors
- Advanced control functionalities
- Digital twin solutions including model-based fault detection and predictive maintenance



Framework of SoX observers

SoOC

- Voltage
- Membrane water content
- Flooding occurrence
- Fuel/species (starvation) detection

SoH

Observable

- EASA
- Membrane conductivity
- GDLs transport properties

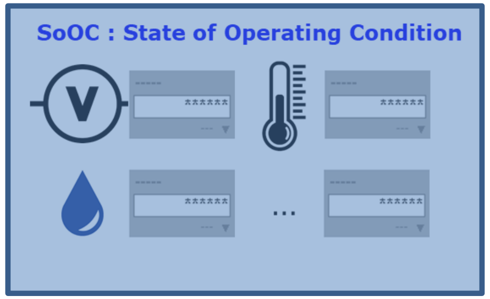
Virtual

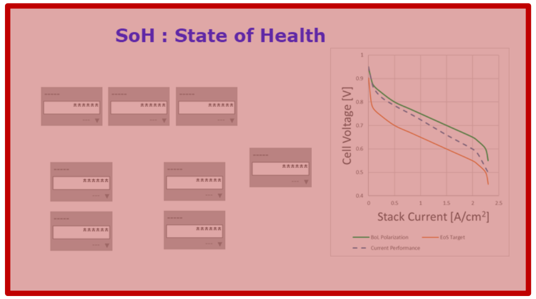
- Catalyst surface area
- Free surface (Pt coverage)
- Pt particle size (dissol., redep., Ostwald r. etc.)
- CO_2 emissions
- Fluoride emissions

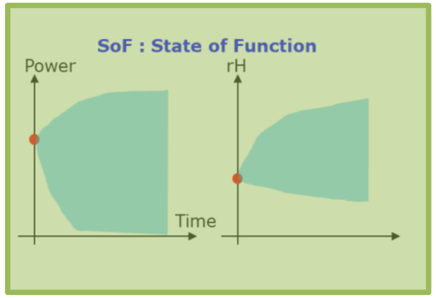
SoF

SoOC + SoH -> SoF: operating limits of the FC in imminent future:

- dP/dt the FC is capable of fulfilling
- P_{max}, i.e., turning point at current SoH and SoOC
- ΔRuL and ΔSoH for P and dP/dt







UNIVERSITY OF LJUBLJANA | FS Faculty of Mechanical Engineering

LICeM

Framework of SoX observers

SoOC

- Voltage
- Membrane water content
- Flooding occurrence
- Fuel/species (starvation) detection

SoH

Observable

- EASA
- Membrane conductivity
- GDLs transport properties

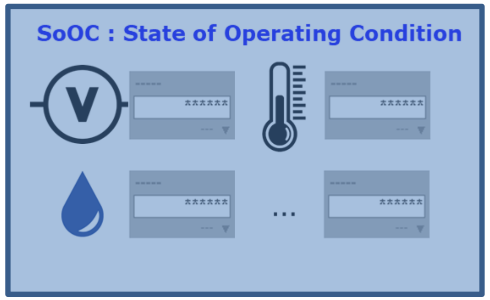
Virtual

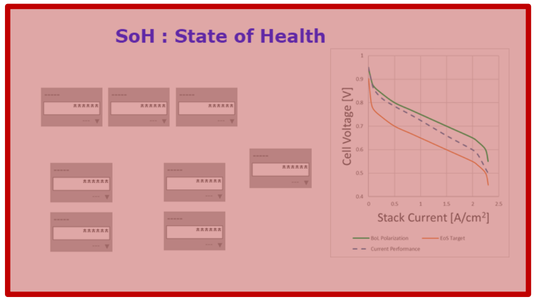
- Catalyst surface area
- Free surface (Pt coverage)
- Pt particle size (dissol., redep., Ostwald r. etc.)
- CO_2 emissions
- Fluoride emissions

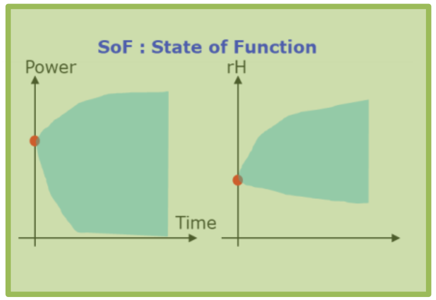
SoF

SoOC + SoH -> SoF: operating limits of the FC in imminent future:

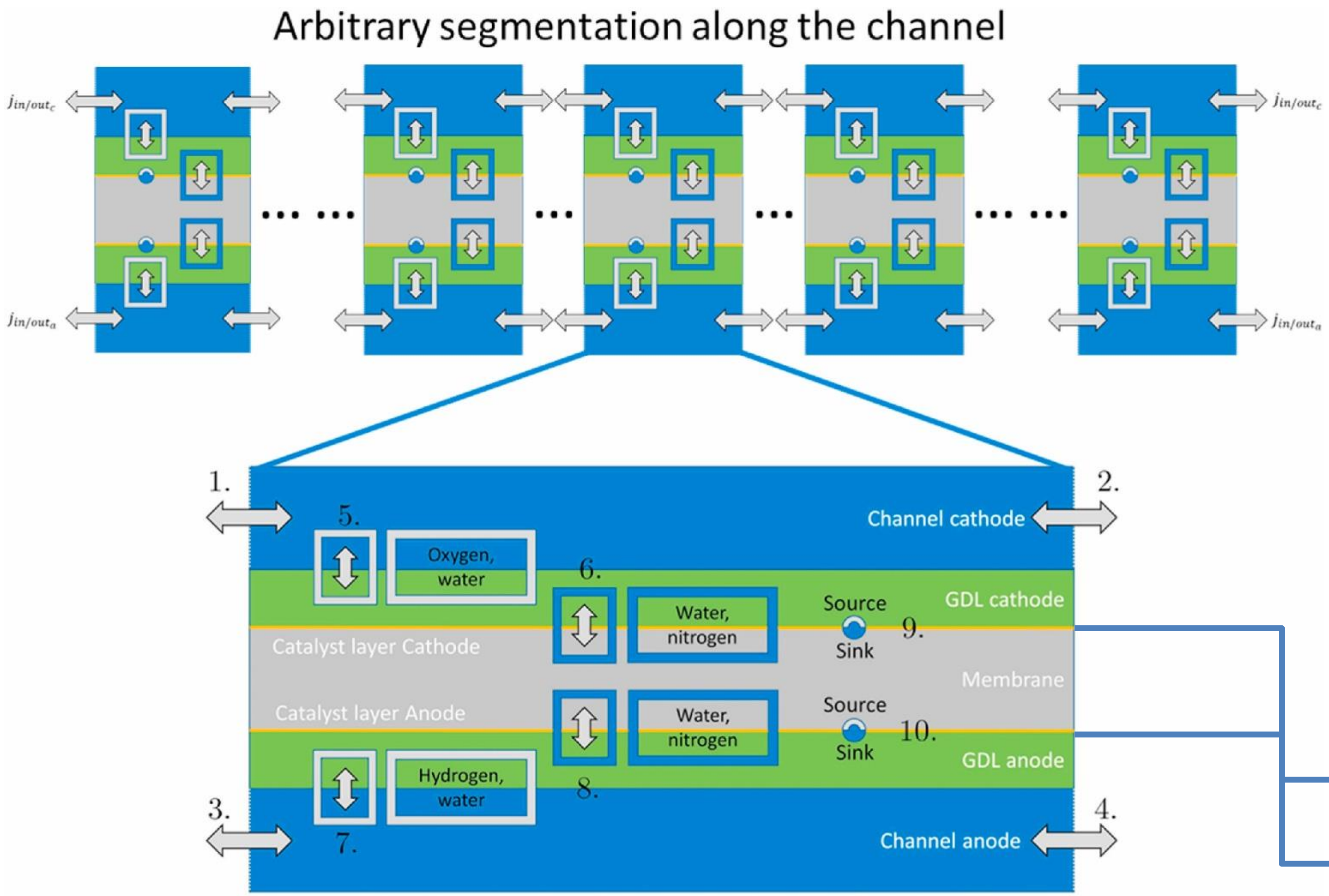
- dP/dt the FC is capable of fulfilling
- P_{max}, i.e., turning point at current SoH and SoOC
- ΔRuL and ΔSoH for P and dP/dt







Mechanistic model of EC/FC/RFC system



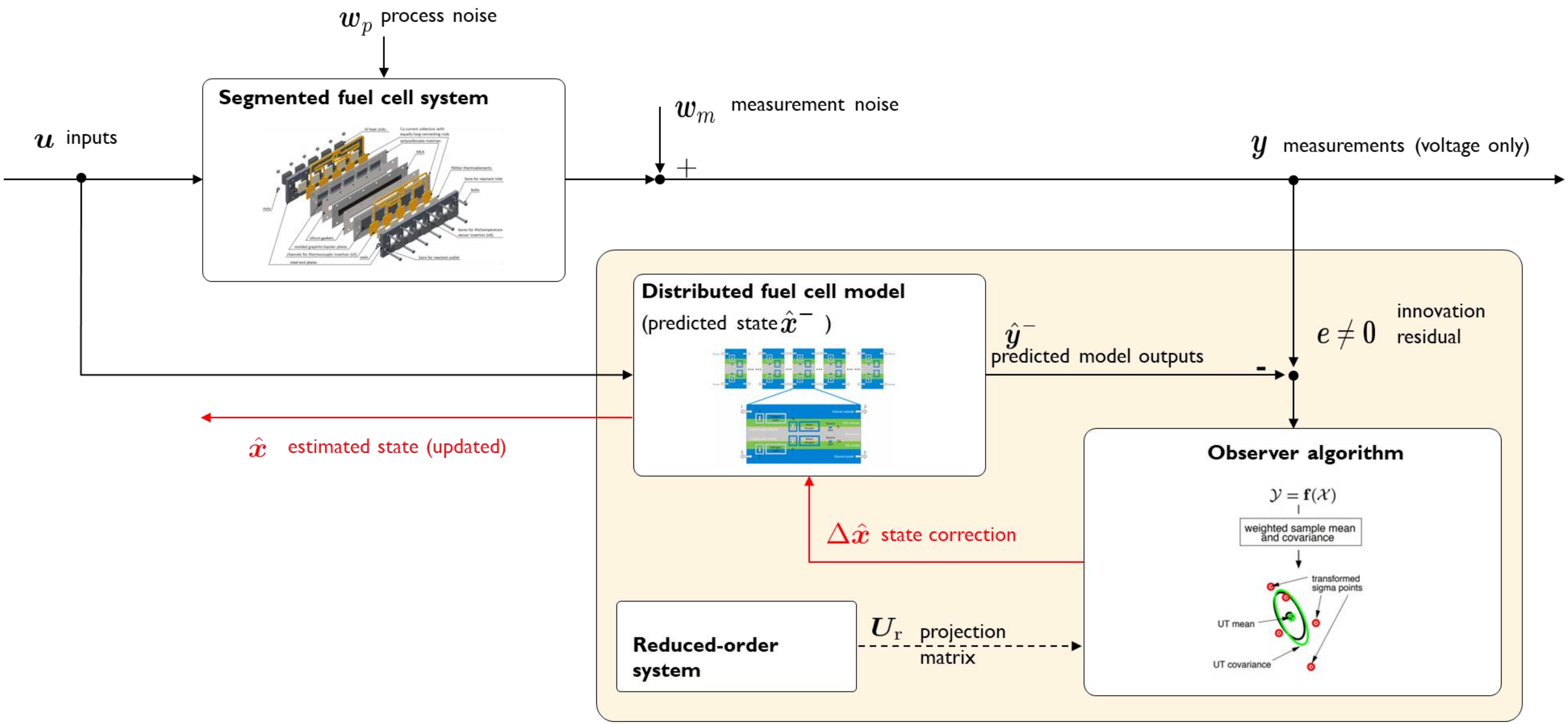
- Model configuration
  - 1D+1D
  - Arbitrary no. of slices

Main features/submodels

- Works with AC / DC signals
- Gaseous species transport
- Water phase change
- Liquid water phase transport
  - Capillary transport in GDL
  - Mechanistically based water droplet removal in channels
- Membrane water uptake
- Mixed potential change due to gas crossover effects with considering platinum band position and its effects
- 1D resolved catalyst layers

An interface to fully couple with degradation modelling framework

Advanced SoOC observer = Physicochemically consistent model + Observer



Framework of SoX observers

SoOC

- Voltage
- Membrane water content
- Flooding occurrence
- Fuel/species (starvation) detection

SoH

Observable

- EASA
- Membrane conductivity
- GDLs transport properties

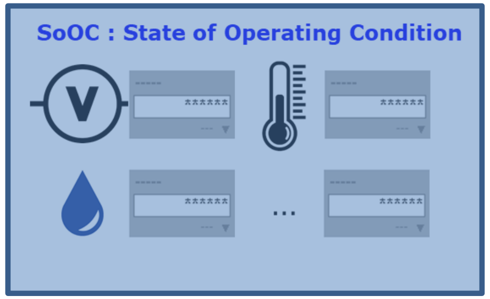
Virtual

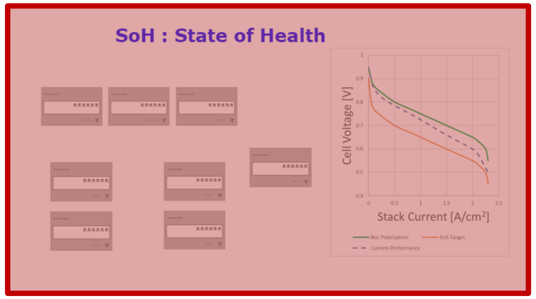
- Catalyst surface area
- Free surface (Pt coverage)
- Pt particle size (dissol., redep., Ostwald r. etc.)
- CO_2 emissions
- Fluoride emissions

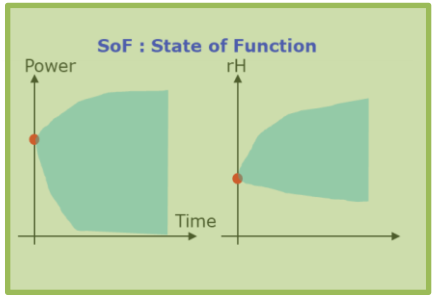
SoF

SoOC + SoH -> SoF: operating limits of the FC in imminent future:

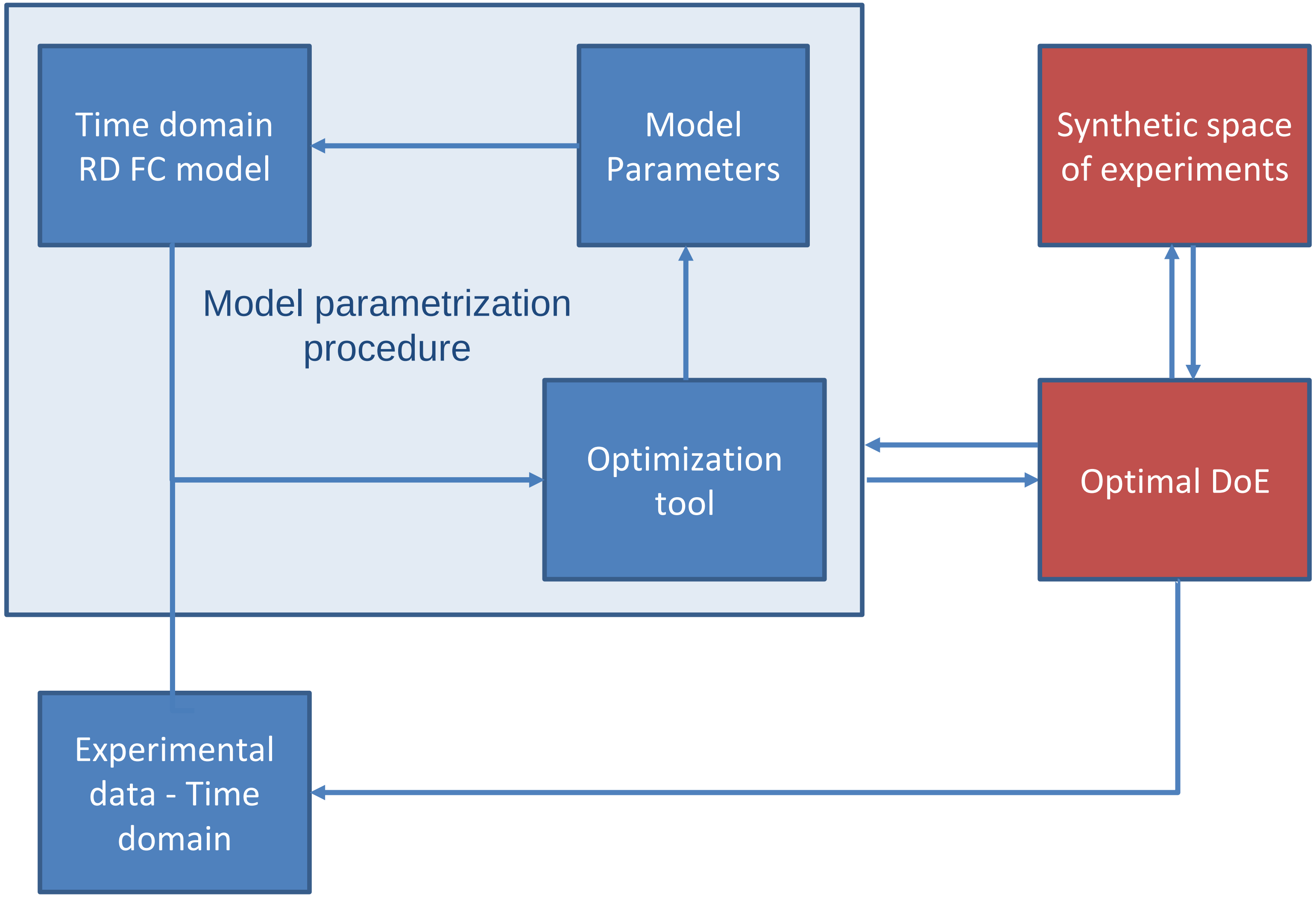
- dP/dt the FC is capable of fulfilling
- P_{max}, i.e., turning point at current SoH and SoOC
- ΔRuL and ΔSoH for P and dP/dt







Model parametrization and model-based DoE



[2] A. Kravos, D. Ritzberger, C. Hametner, S. Jakubek, T. Katrašnik, Methodology for efficient parametrisation of electrochemical PEMFC model for virtual observers: Model based optimal design of experiments supported by parameter sensitivity analysis, International Journal of Hydrogen Energy

Optimal design of experiments

Determination of smallest experimental data set for successful parametrization of the model.

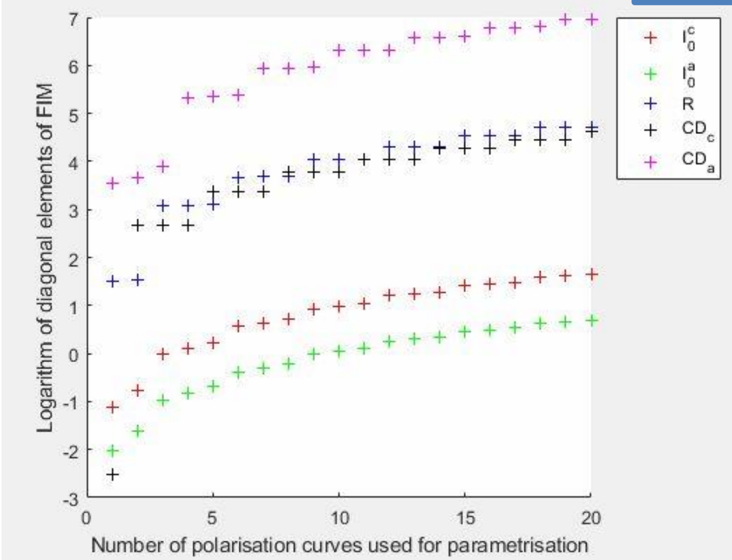
→

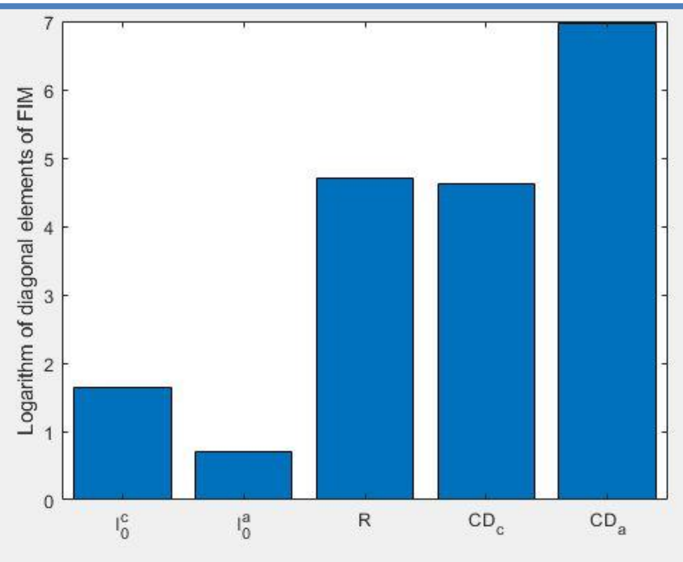
Synthetic experimental space with 9720 different operational conditions was created with already parametrized model.

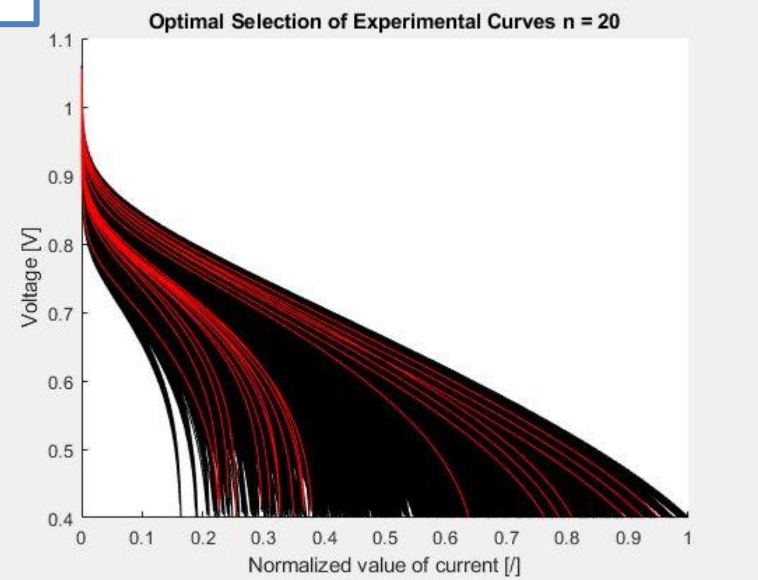
→

D-optimality was used to maximize the determinant of information matrix based on which optimal "experimental" points were selected.

Optimal selection of polarization curves





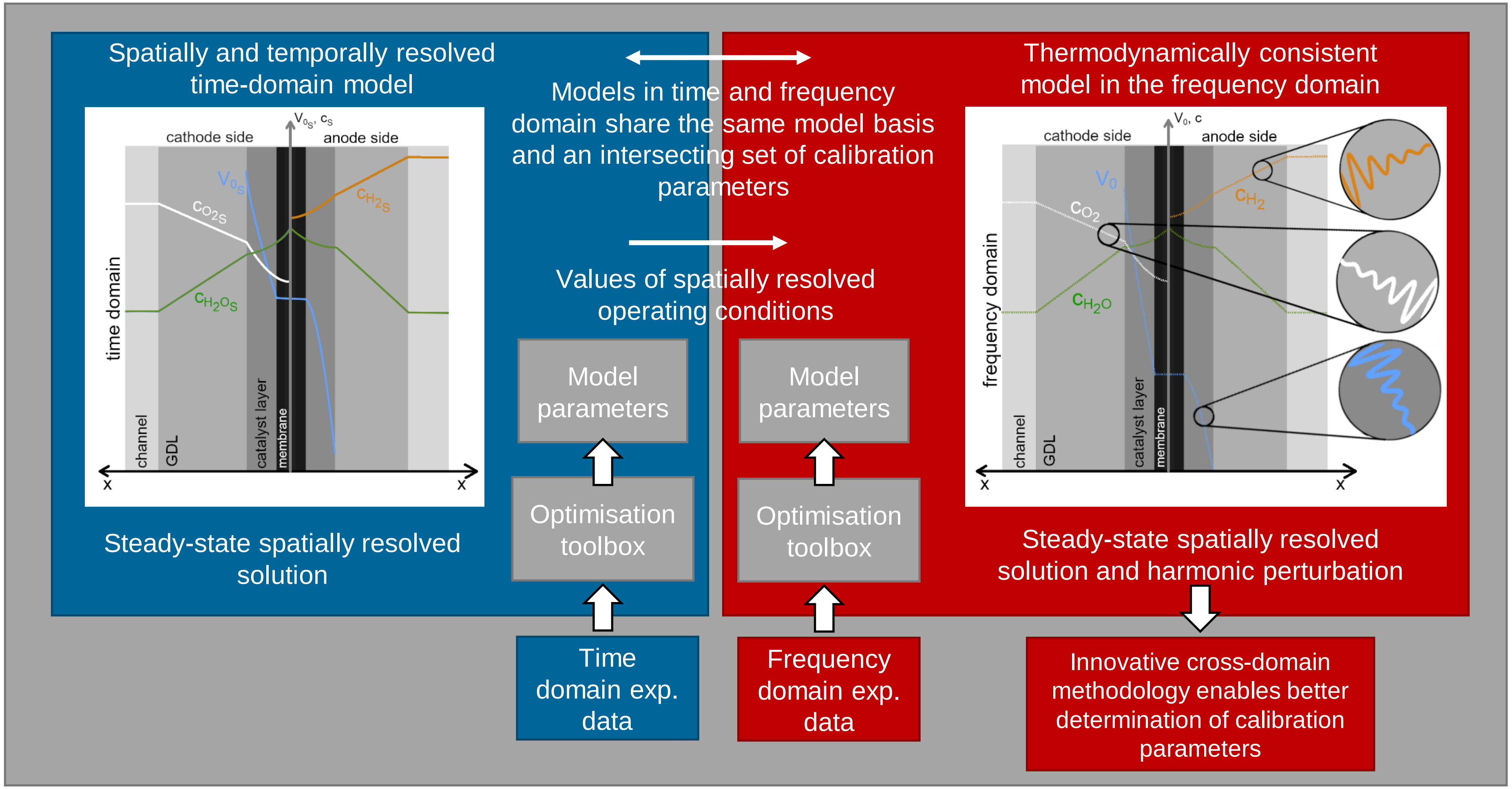


[2] A. Kravos, D. Ritzberger, C. Hametner, S. Jakubek, T. Katrašnik, Methodology for efficient parametrisation of electrochemical PEMFC model for virtual observers: Model based optimal design of experiments supported by parameter sensitivity analysis, International Journal of Hydrogen Energy

UNIVERSITY OF LJUBLJANA FS Faculty of Mechanical Engineering

Hybrid methodology for parametrisation

LICeM



Framework of SoX observers

SoOC

- Voltage
- Membrane water content
- Flooding occurrence
- Fuel/species (starvation) detection

SoH

Observable

- EASA
- Membrane conductivity
- GDLs transport properties

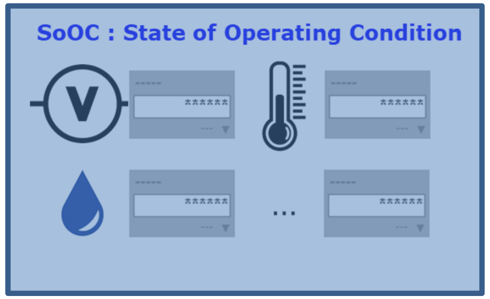
Virtual

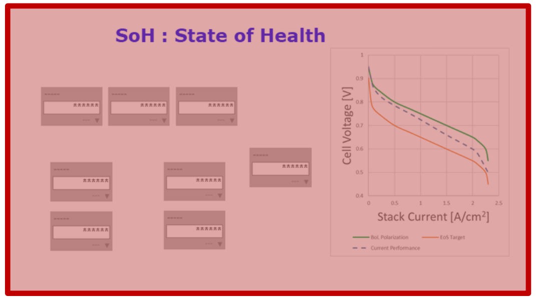
- Catalyst surface area
- Free surface (Pt coverage)
- Pt particle size (dissol., redep., Ostwald r. etc.)
- CO_2 emissions
- Fluoride emissions

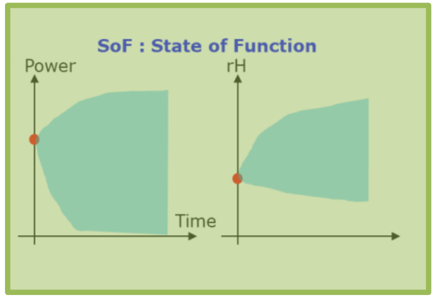
SoF

SoOC + SoH -> SoF: operating limits of the FC in imminent future:

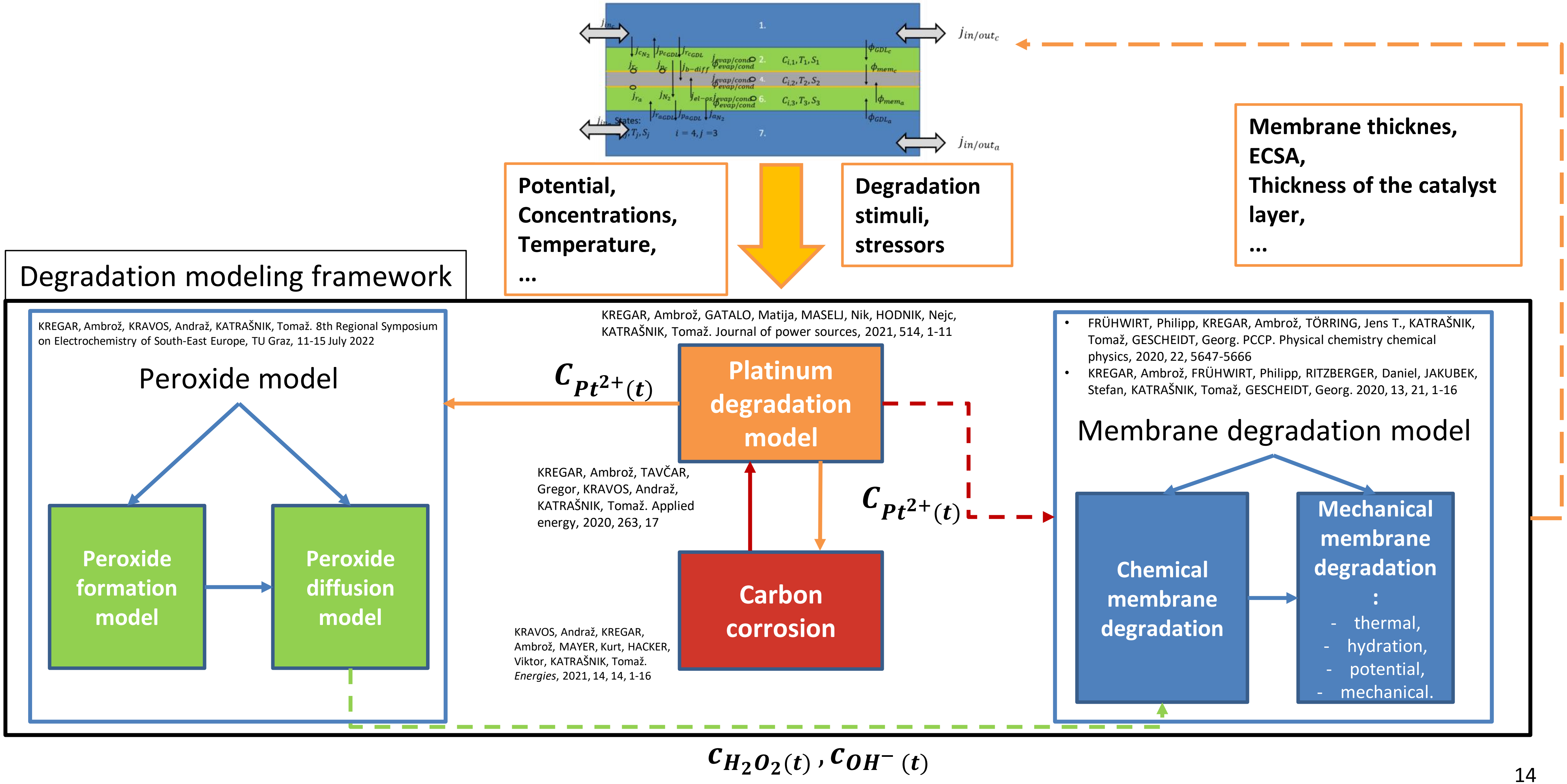
- dP/dt the FC is capable of fulfilling
- P_{max}, i.e., turning point at current SoH and SoOC
- ΔRuL and ΔSoH for P and dP/dt







Multi-scale interaction of performance and degradation models

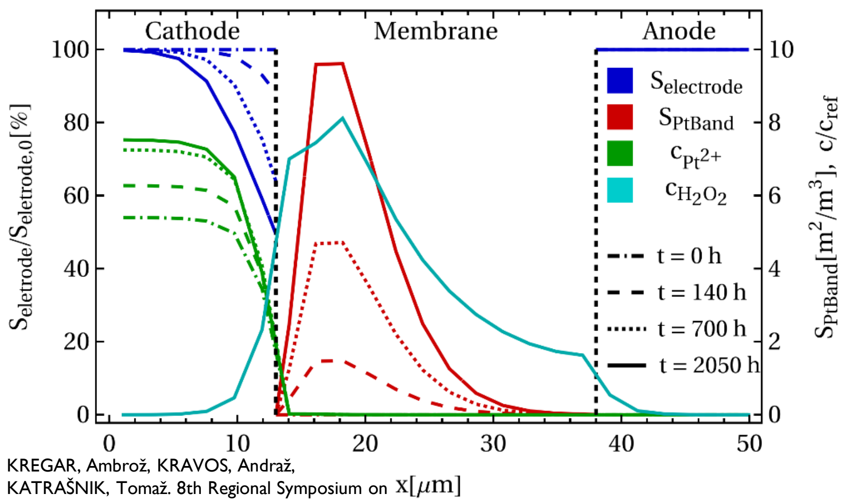


UNIVERSITY OF LJUBLJANA | FS Faculty of Mechanical Engineering

State of Health

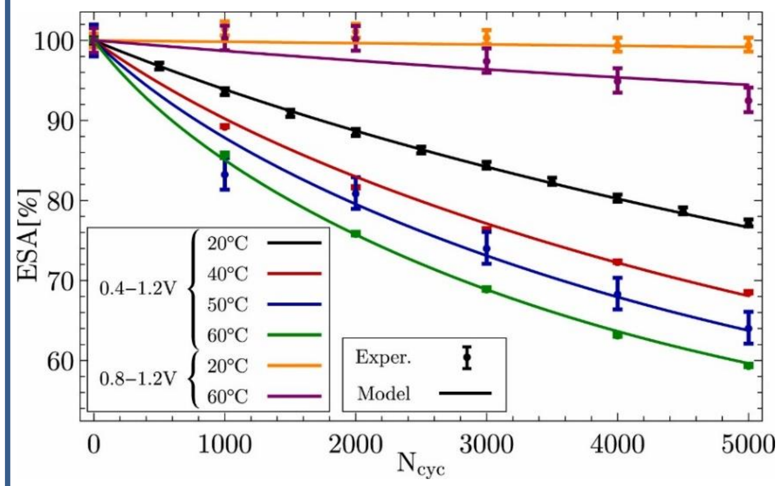
LICeM

Catalyst surface loss and hydrogen peroxide evolution at OCV.

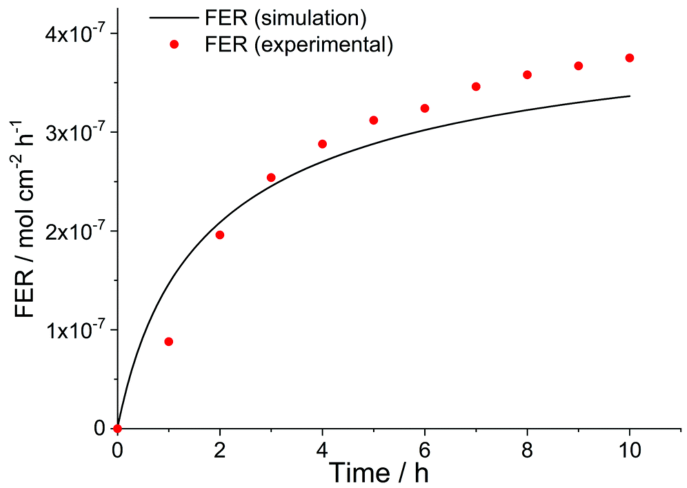


KREGAR, Ambrož, KRAVOS, Andraž, KATRAŠNIK, Tomaž. 8th Regional Symposium on Electrochemistry of South-East Europe, 2022

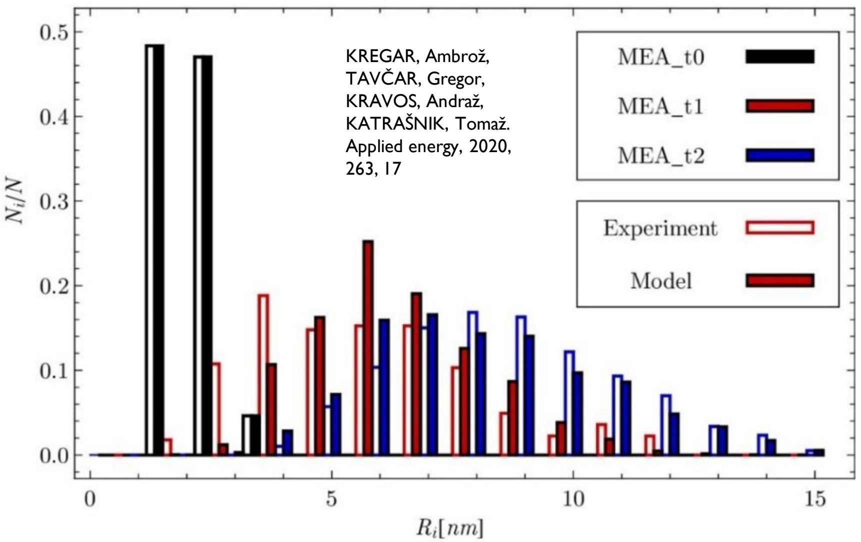
ESA during cycling for 6 different ASTs



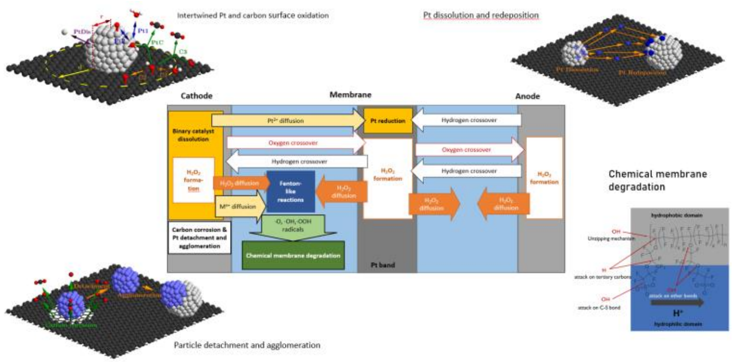
Time evolution of fluoride emission rate during an OCV hold test.



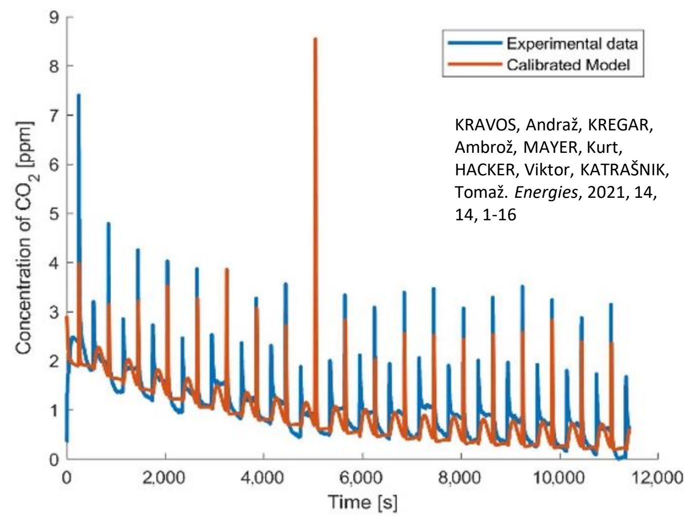
Experimental and modelled data of catalyst particle growth



Degradation modelling framework coupled to the performance model



Transient emissions of CO_2



Cyber-physical System – FC stack testbed

Testbed

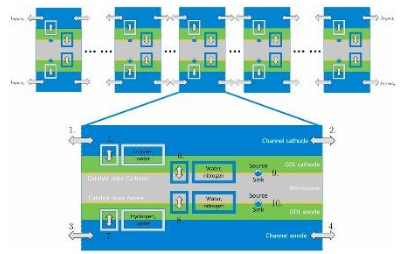
- **100:1 turndown** (max:min flow) on all Mass Flow Controllers (MFC)
- **Automatic contact humidification** module (up to 90C dew point, higher available)
- **Electric reheat module** (up to 110C inlet gas, higher temperatures available) - Nitrogen purge rotameter; software activated
- **Automatic back pressure control** module, independent anode/cathode (0-3 Barg) - Stack end-plate heater PID controllers (2x 220VAC-2A)
- **Programmable air cooled load bank.** Maximum: 1.4kW, 10V, 200A.
- **Emerald control and automation software** (allows 24/7 unattended dynamic operation)
- **H2 gas detector** (CE, ATEX, UL, CSA) for test station E-stop and warning
- Additional gas lines (e.g. to simulate reformate blends); select one for each of CO, CO2, N2, CH4, etc
- **Operating temperature**: 0-200°C
- **Control and integration of S++ Device**
    - start/stop measurements by the S++ device
    - control of measurement period
- **Gamry Reference 3000** + Gamry 30A Booster; Potentiostat/Galvanostat/ZRA fully integrated with Greenlight control and automation

Cyber-physical System – FC stack testbed

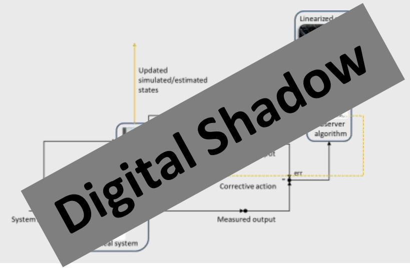
Testbed

Advanced SoX observers and virtual sensors

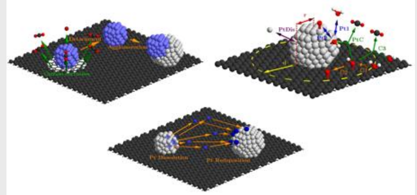
Mechanistic models



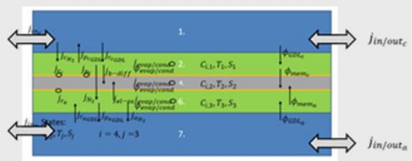
SoX observer methodology



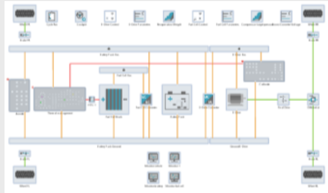
Material design



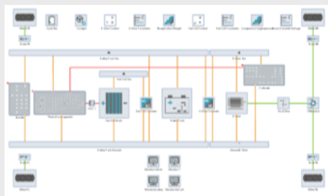
FC design



System design



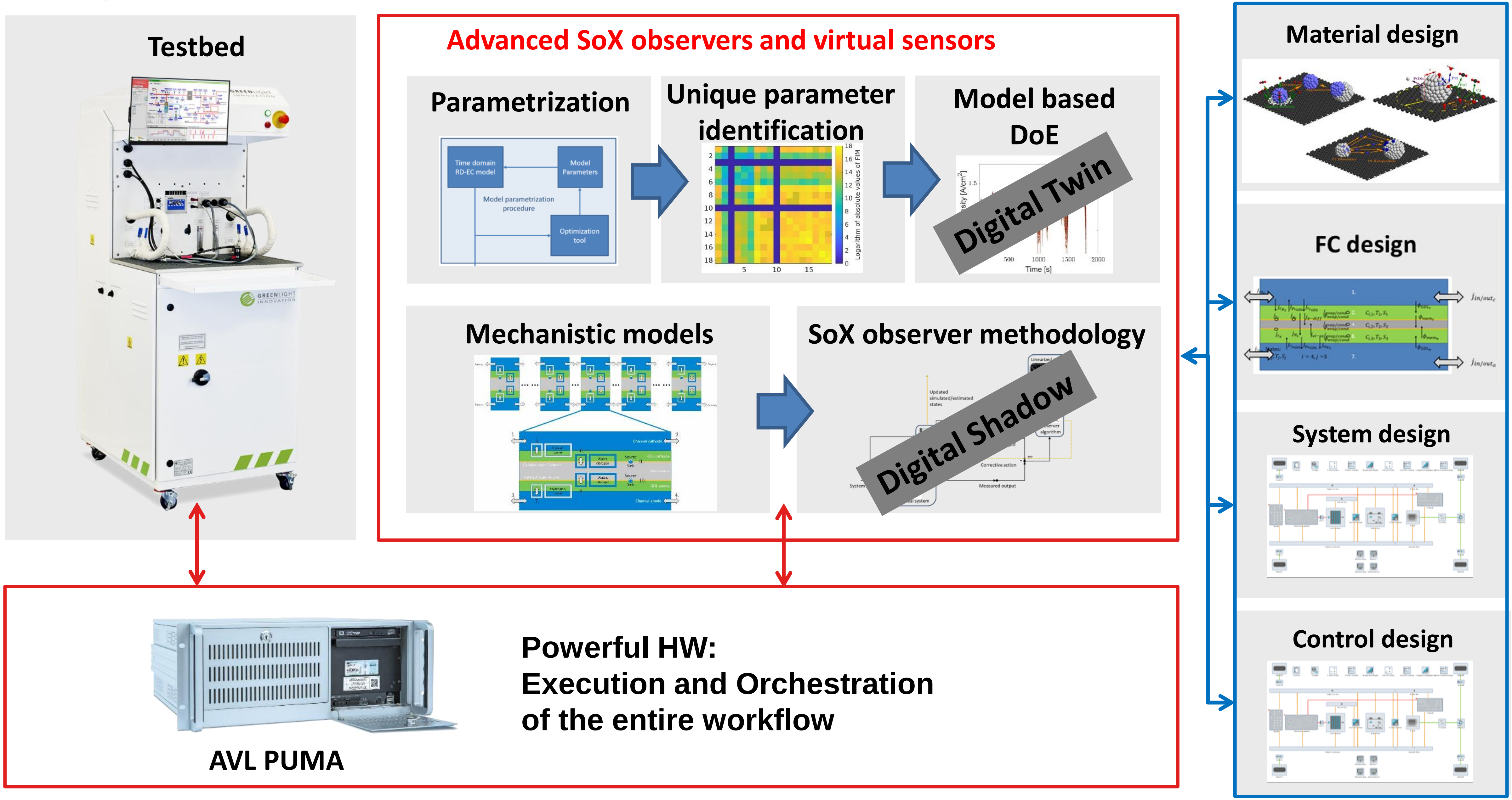
Control design



AVL PUMA

Powerful HW:
Execution and Orchestration
of the entire workflow

Cyber-physical System – FC stack testbed +



UNIVERSITY OF LJUBLJANA | FS Faculty of Mechanical Engineering

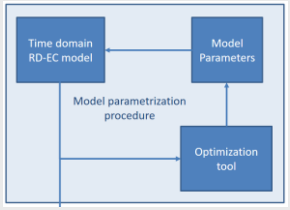
Cyber-physical System – FC stack testbed ++

LICeM

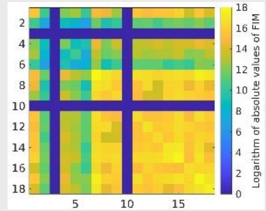
Testbed

Advanced SoX observers and virtual sensors

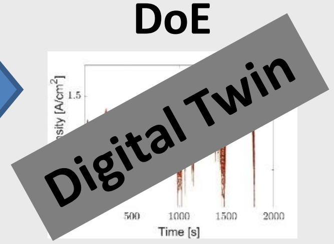
Parametrization



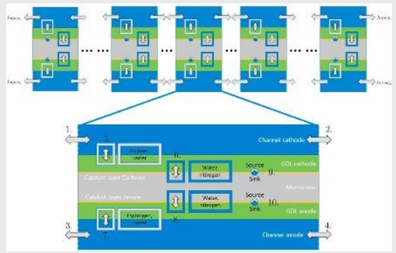
Unique parameter identification



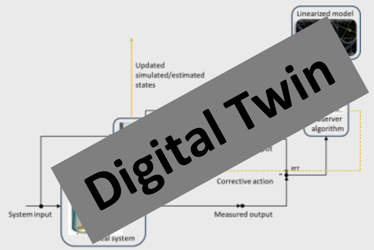
Model based DoE



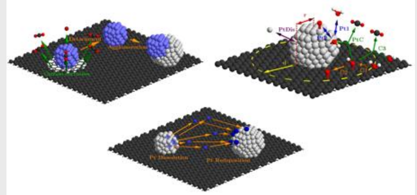
Mechanistic models



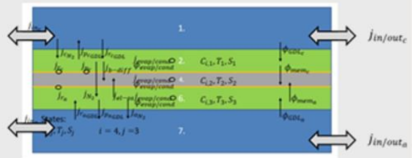
SoX observer methodology



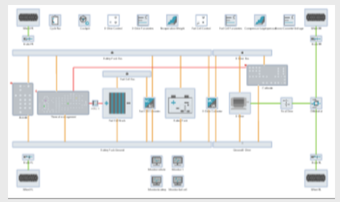
Material design



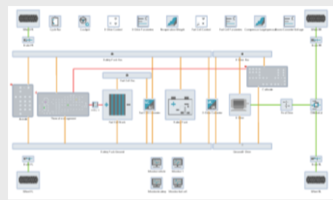
FC design



System design



Control design



AVL PUMA

Powerful HW:
Execution and Orchestration
of the entire workflow