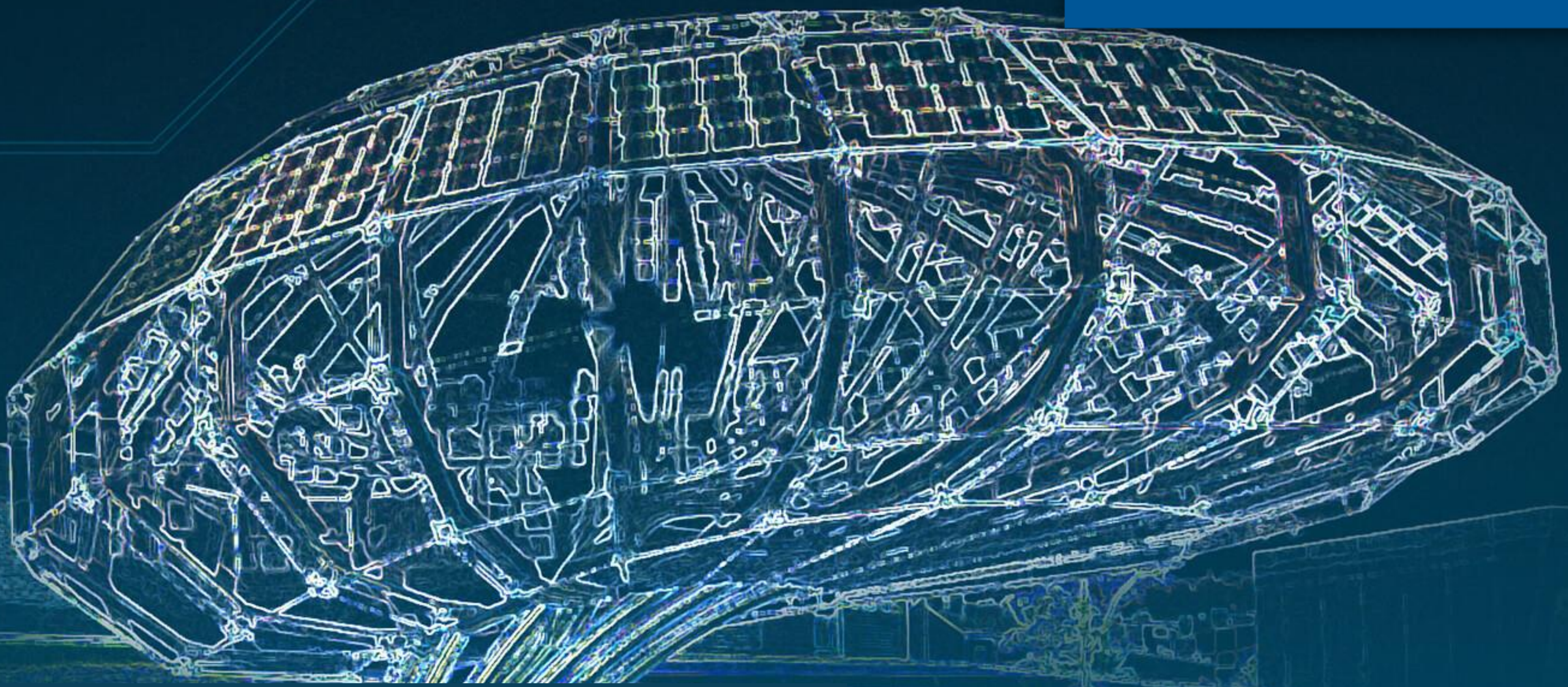


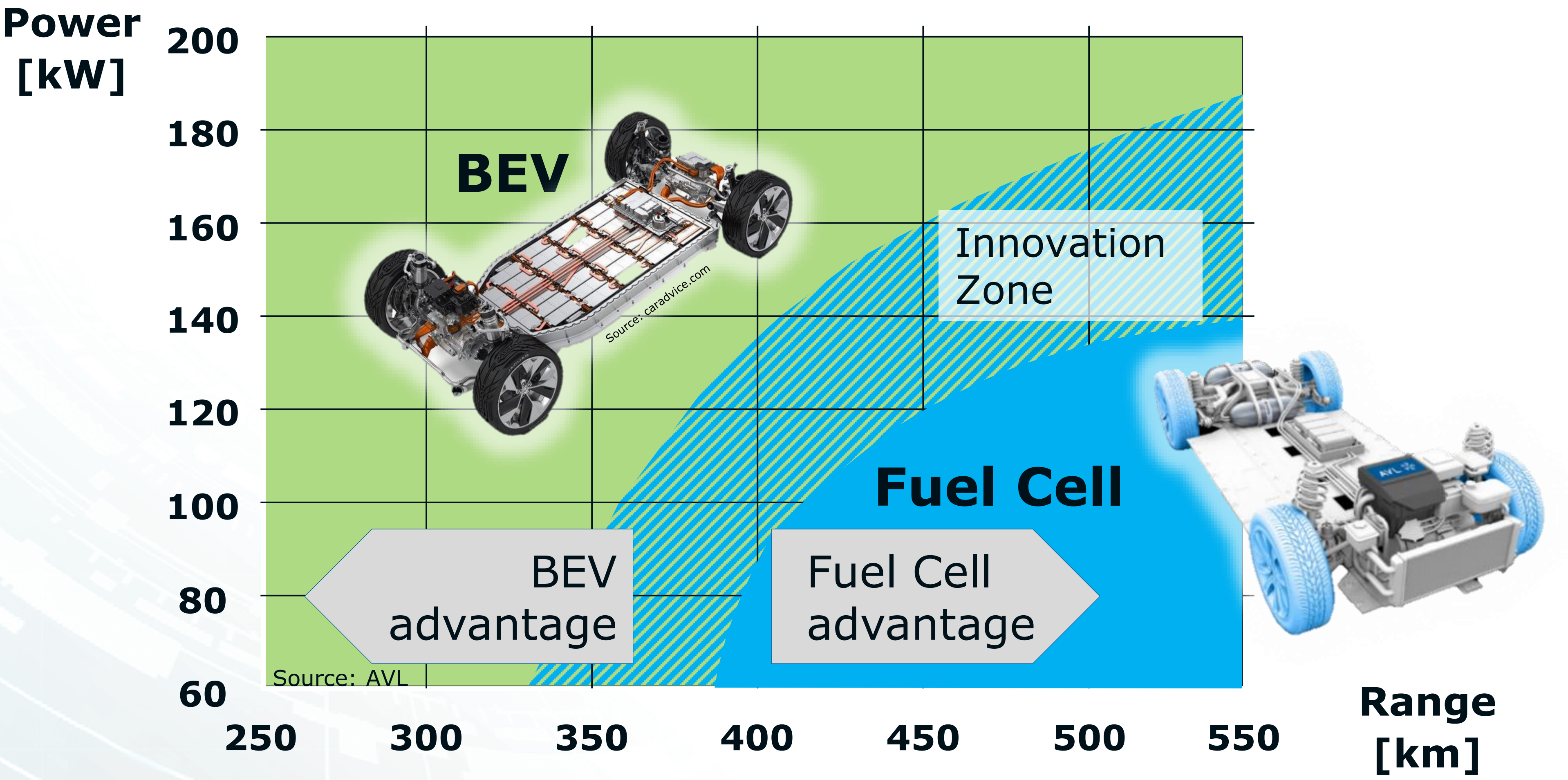
Fuel Cell Simulation

Virtual fuel cell performance and lifetime optimization from component to vehicle level

Juergen Schneider

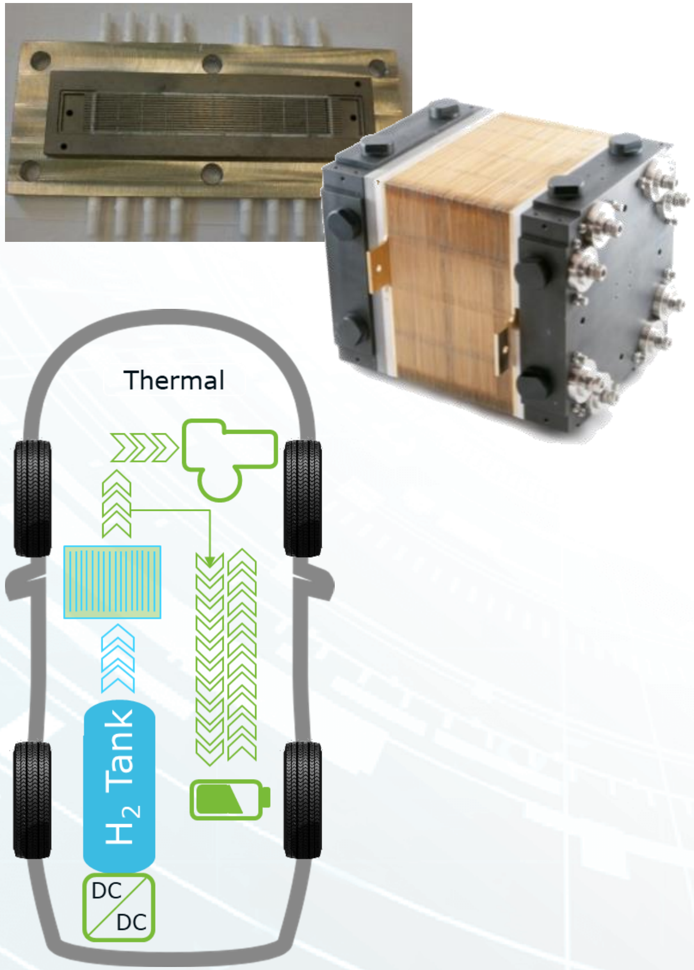
Public

Application Areas BEV vs. FCEV



For larger & long range vehicles, FCVs have a cost advantage compared to BEVs

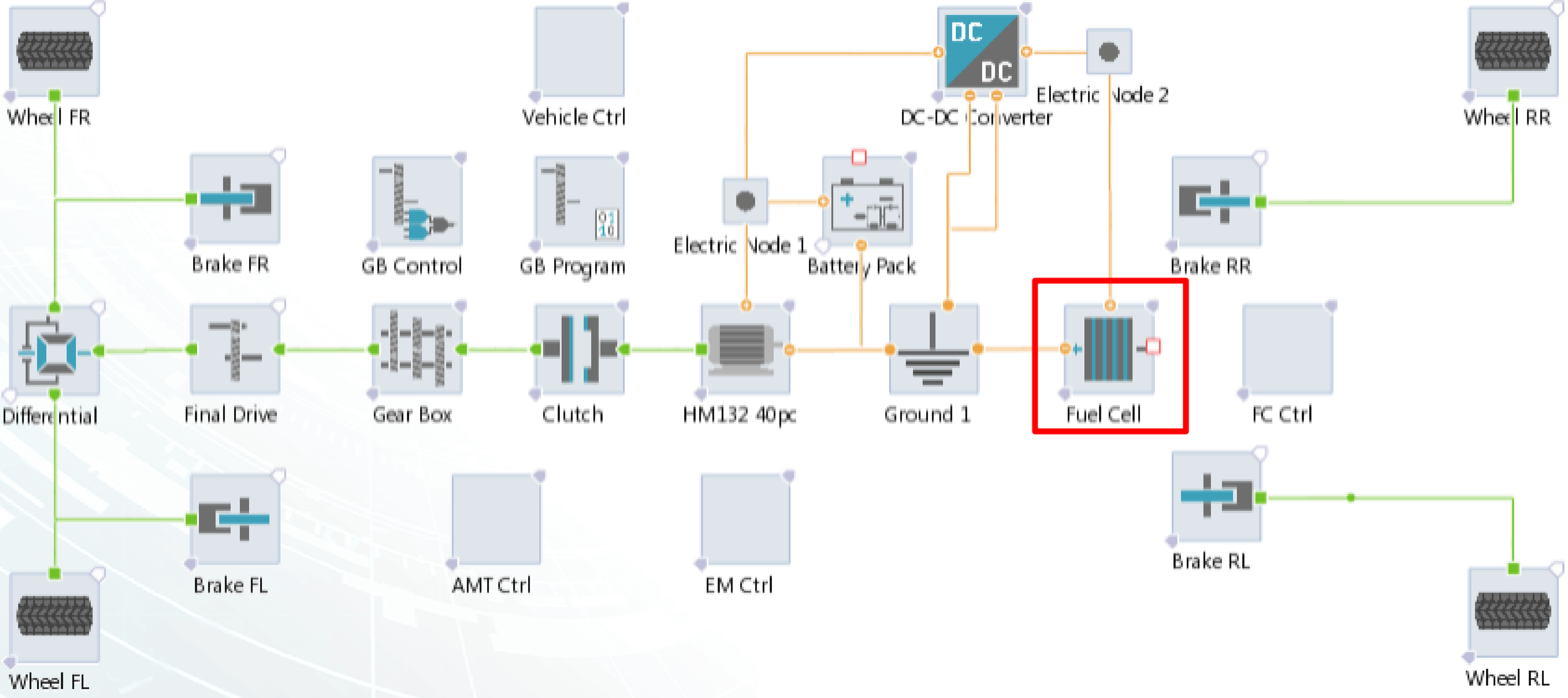
Technical Challenges



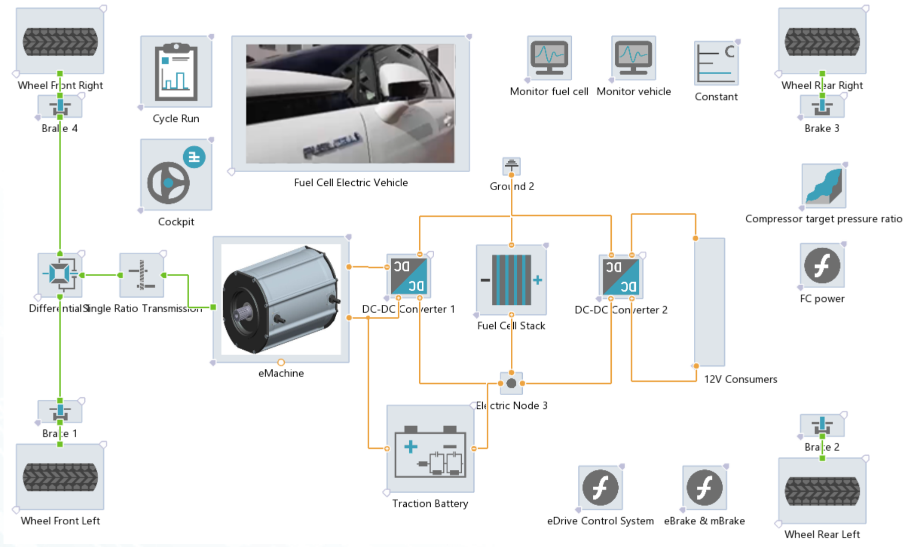
- **Maximize power density** for entire operating range
  - ⇒ Select proper design concept, e.g. bipolar plate, membrane-electrode-assembly (MEA), and media supply strategy
- **Eliminate critical locations**, e.g. hot spots, local water accumulation, fuel starvation
  - ⇒ Optimize flow field design and GDL/MPL properties to ensure proper fuel and oxidizer supply to catalyst layer
- **Avoid critical operating conditions**, e.g. excessive liquid water production, membrane drying, thermal issues
  - ⇒ Identify optimum media supply conditions (humidity, stoichiometry, pressure) and thermal operation parameters
- **Ensure efficient operation and highly dynamic response**
  - ⇒ Achieve proper and fast balance of hydrogen and air supply, fitting membrane humidification, fast heat up time
- **Minimize cell degradation**
  - ⇒ Identify degradation mechanisms and critical operating conditions

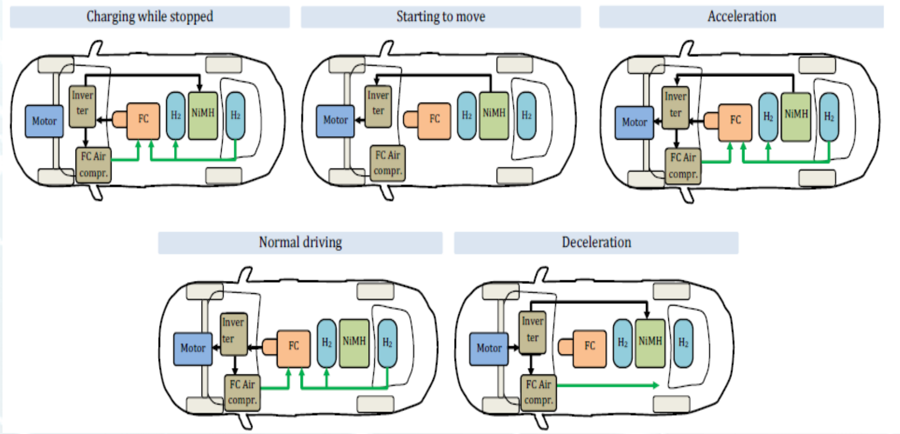
Fuel Cell – FCEV Concept Analysis

FC EV Development



FCEV Concept Definition

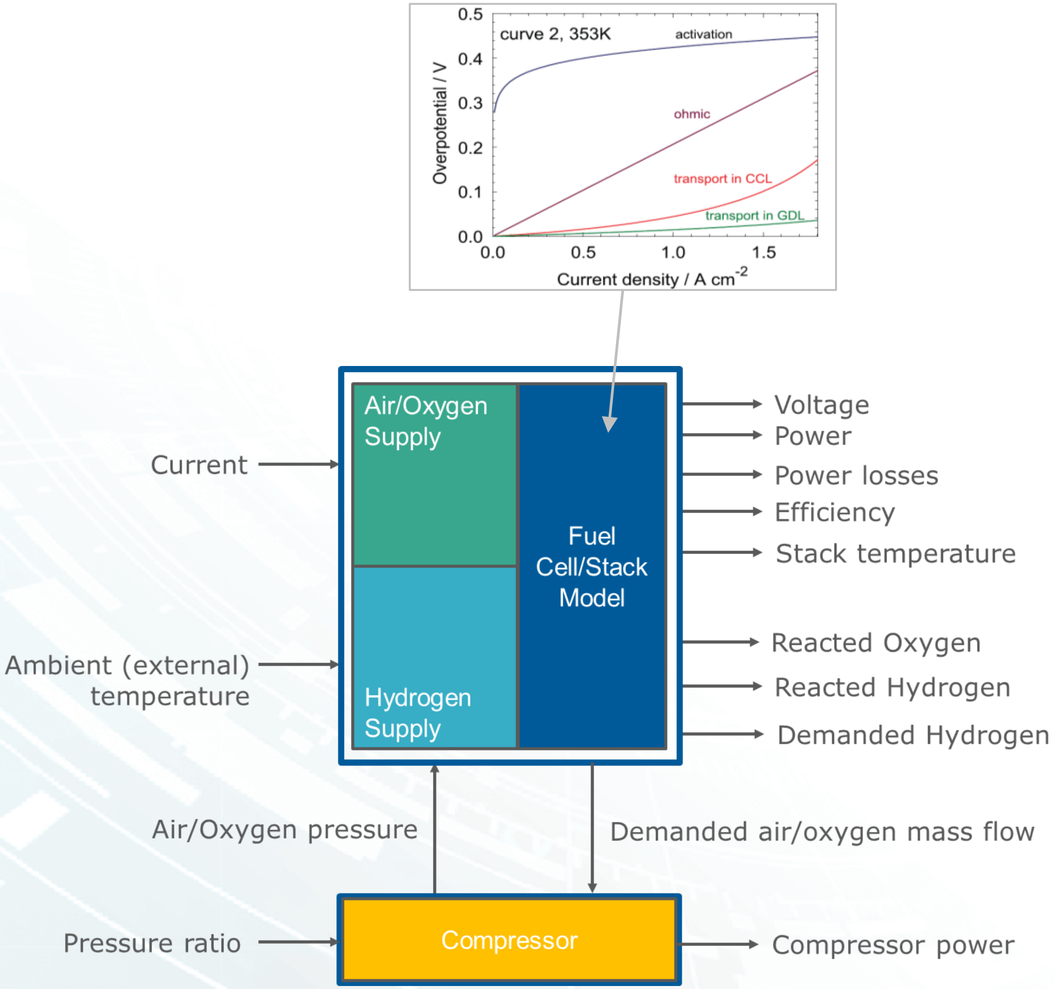




Application Scope

- Fuel Cell EV **concept definition**
- Powertrain systems and main **components sizing** e.g. battery / fuel cell size balancing
- Basic **control function** design related to **vehicle energy management**
- Generating **collective component loads** for detailed component design

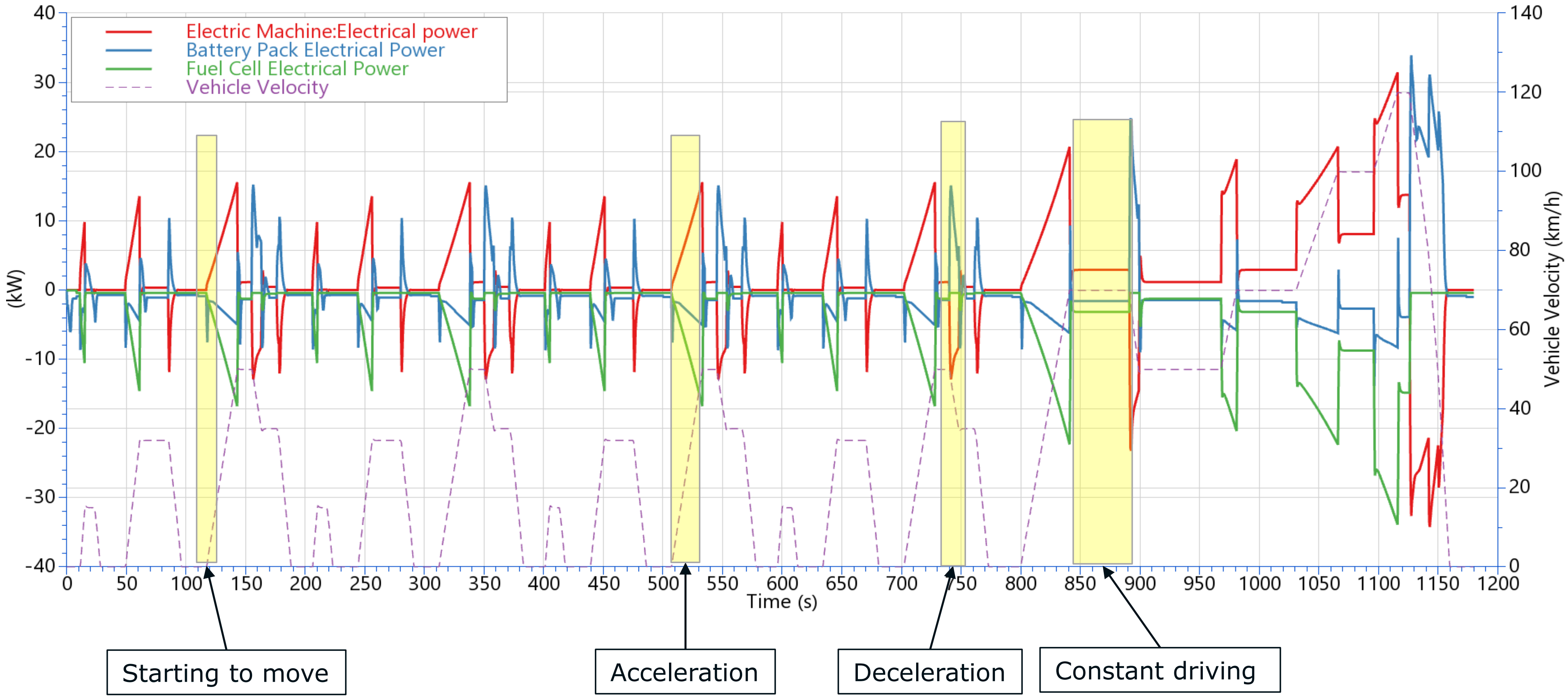
Functional Stack Modelling



Functional PEMFC Stack Model

- Model based on analytical equations acc. to **Kulikovski**
- Takes into account the **oxygen** and **proton transport losses** in the **CCL** and the **oxygen transport loss** in the **GDL**
- Input parameters can be obtained by **fitting the model equations to the polarization curves** of the fuel cell
- **Stationary** and **transient** FC behavior

FCEV Drive Cycle Results



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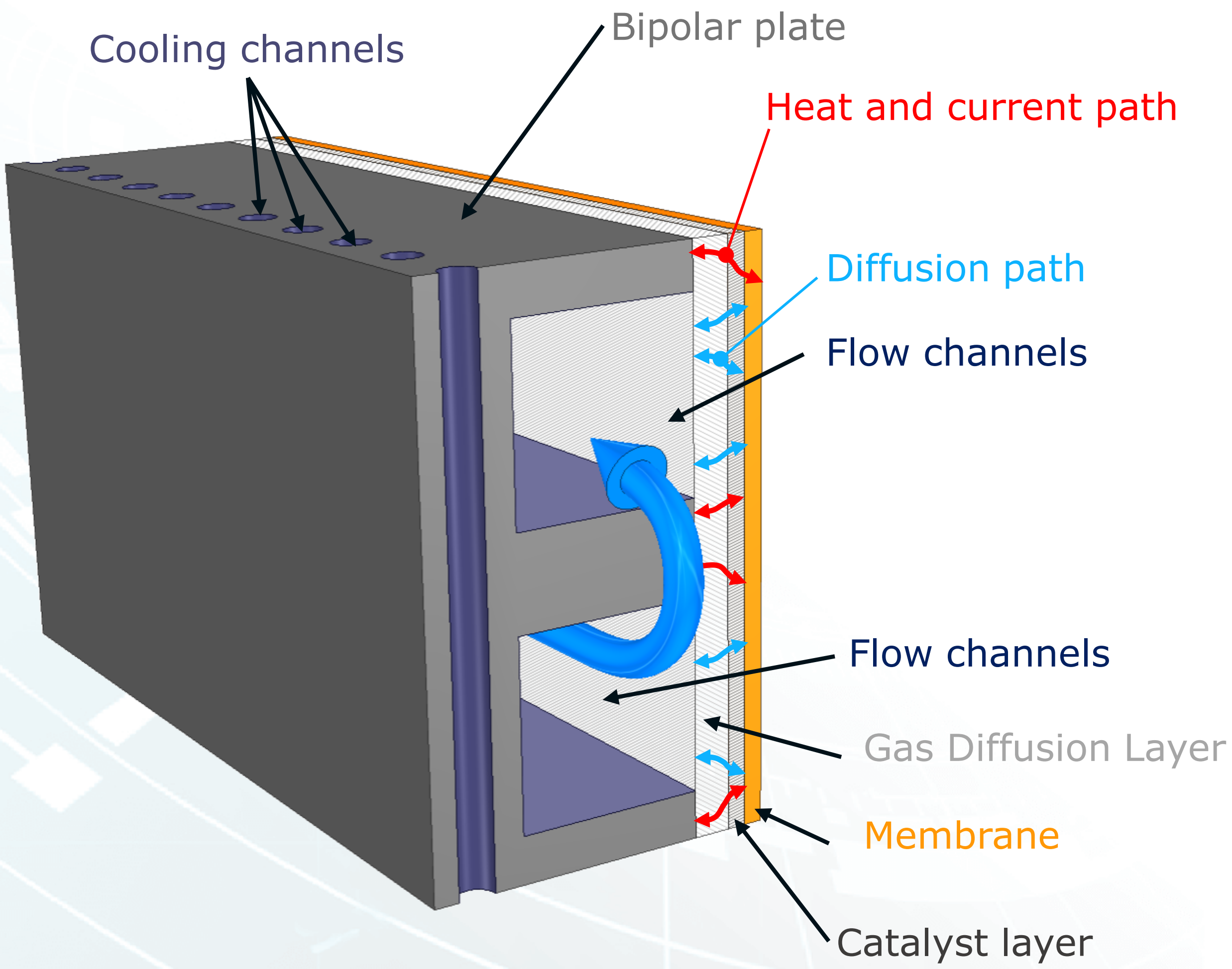
Detailed Component Development

E-Drive Component: Fuel Cell
Introduction: PEMFC Working principle

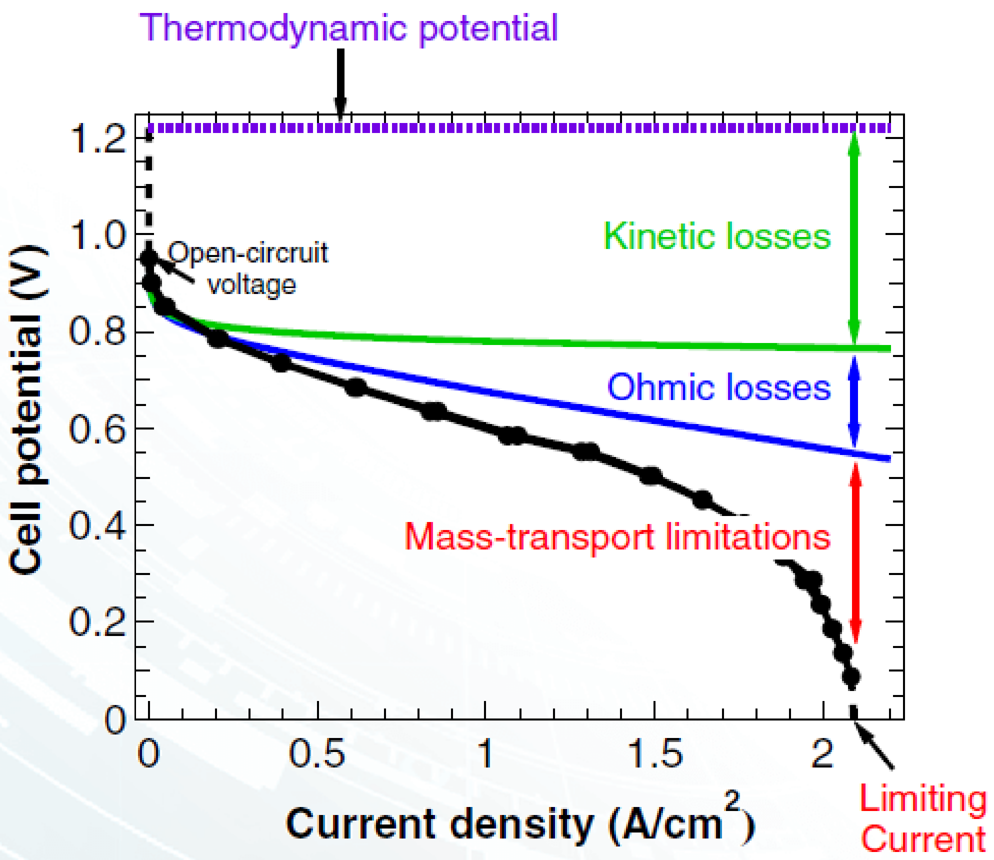


Transport and loss mechanism

Transport mechanisms

- Convection und diffusion
  in channels and porous layers
- Liquid water transport in porous structures
- Electric and thermal
  conduction in structures
- Ionic conduction in membrane and
  catalytic layer

E-Drive Component: Fuel Cell
Introduction: PEMFC Working principle



Transport and loss mechanism

Transport mechanisms

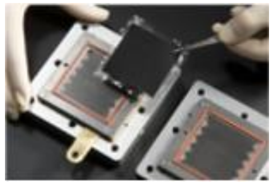
- Convection und diffusion in channels and porous layers
- Liquid water transport in porous structures
- Electric and thermal conduction in structures
- Ionic conduction in membrane and catalytic layer

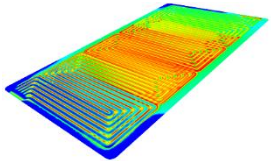
Loss mechanisms:

- Activation energy (kinetic energy of catalyst)
- Ohmic losses (ionic and electric conduction)
- Mass transport limitation (gas diffusion and liquid water transport)

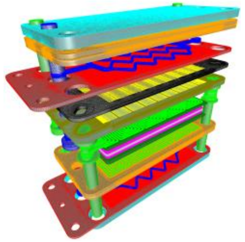
Multiphysics 3D-CFD Simulation

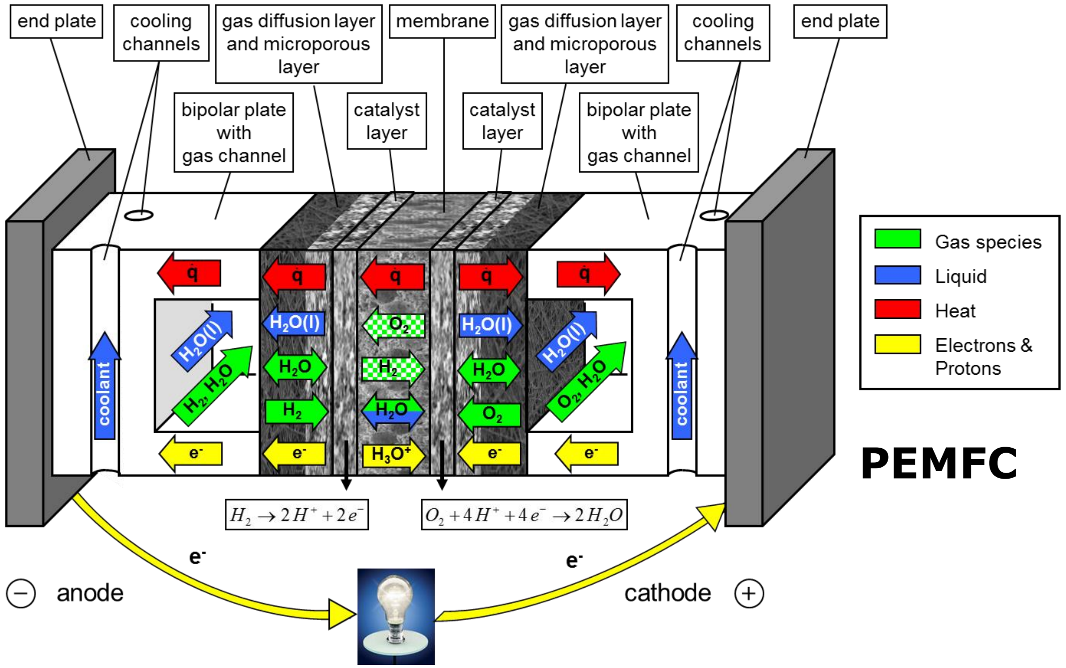
Cell level





Stack level





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- Identification of **critical** cell areas and **operating modes**
- Localization of **degradation** sensitive areas
- Easy assessment of **material parameter impact** on cell performance
- Identification of **membrane drying** and **liquid water** issues

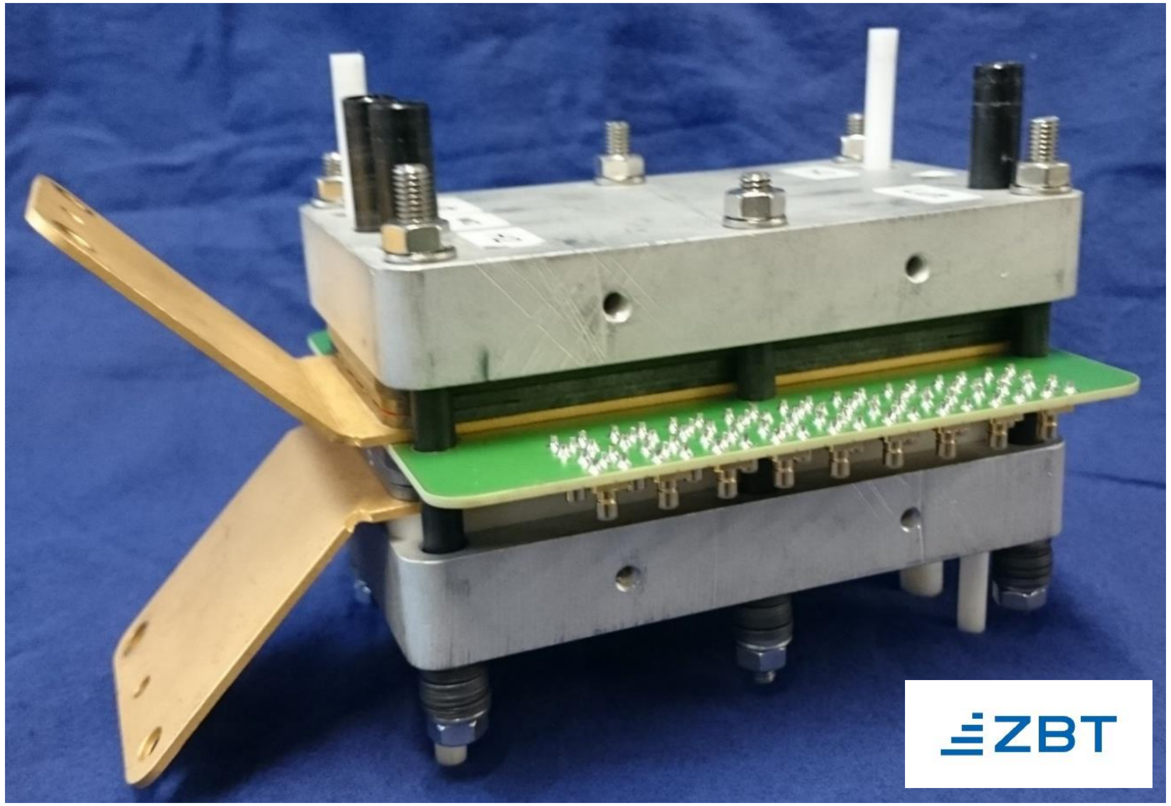
AVL FIRE™ Multiphysics PEMFC Simulation Module

Case Studies

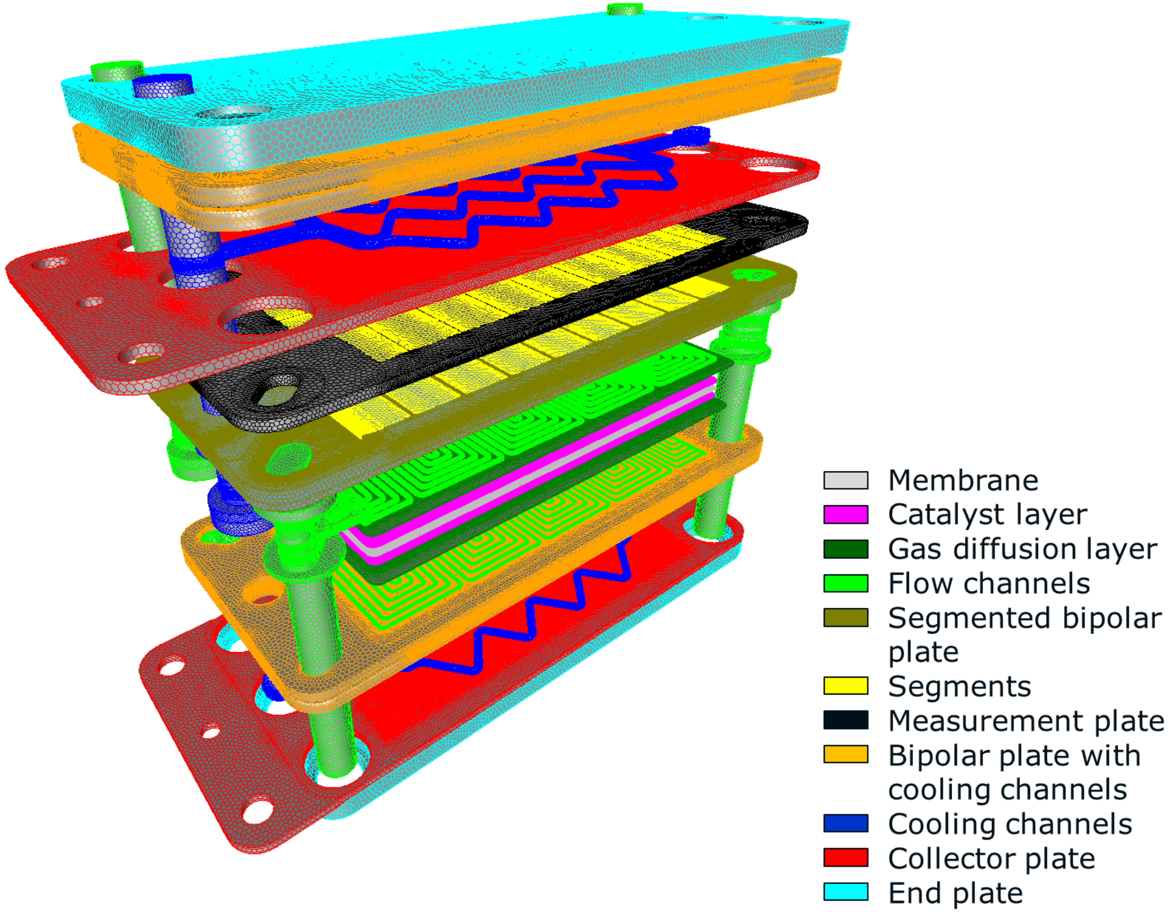
Detailed Performance Analysis

50 cm² serpentine flow field cell by ZBT

- Modeling of complete experimental setup

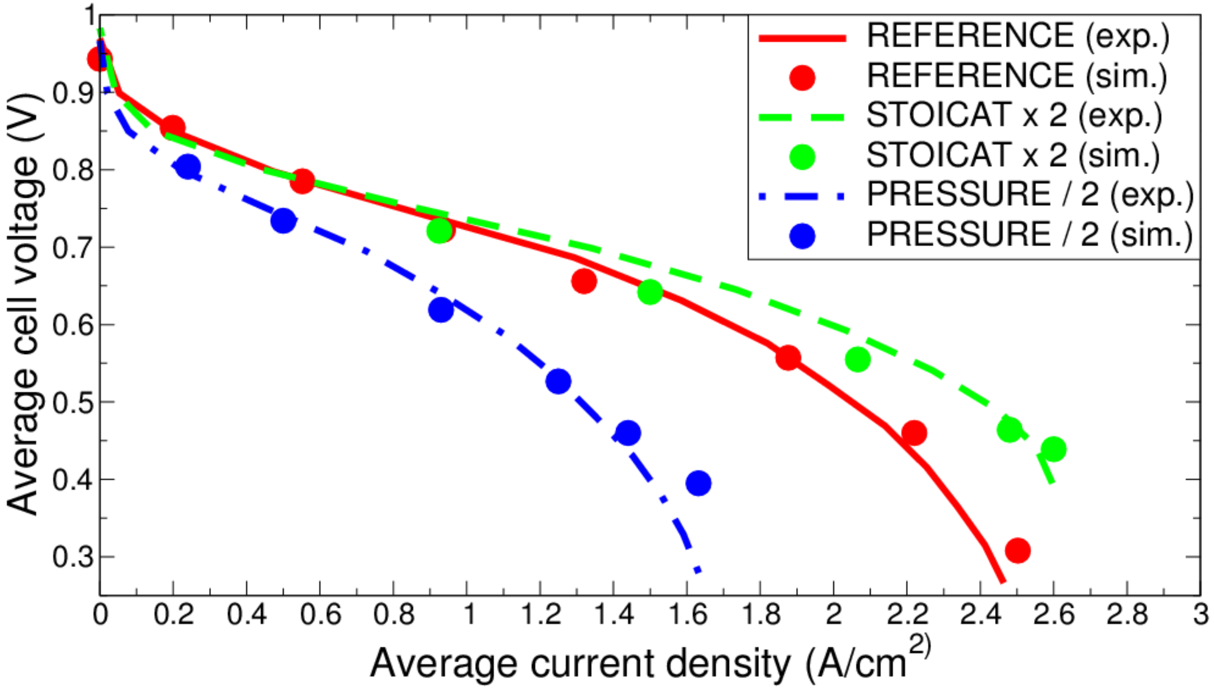


Exploded view of computational domains



Detailed Performance Analysis

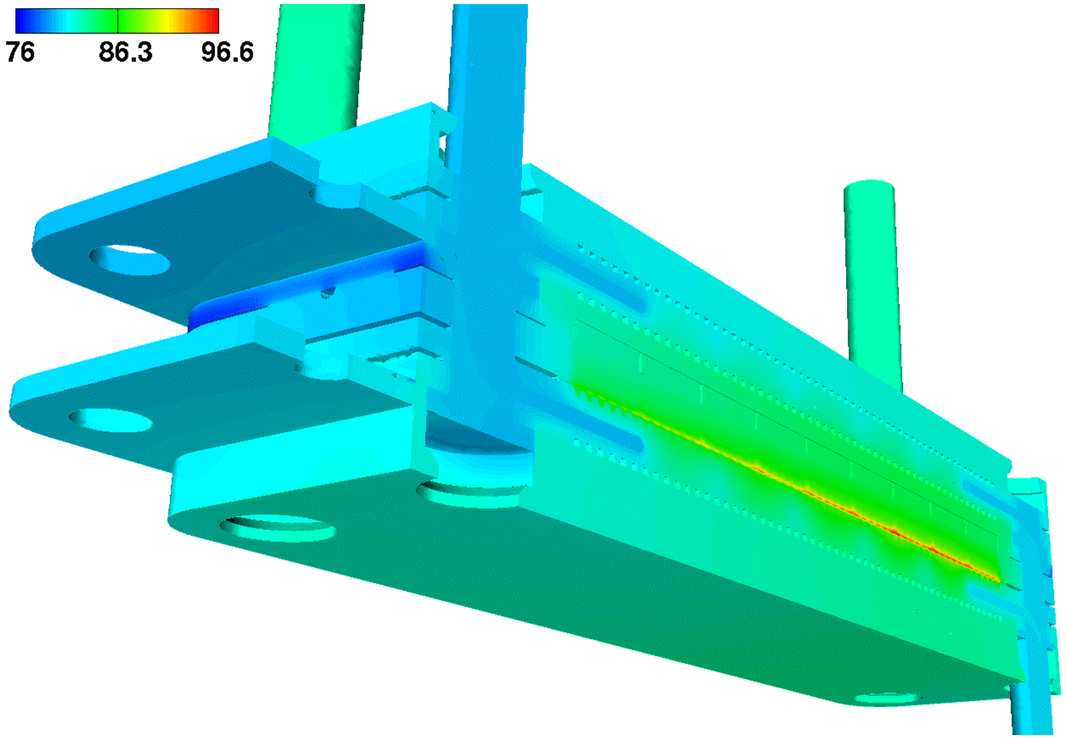
Polarization curves
for all variation cases

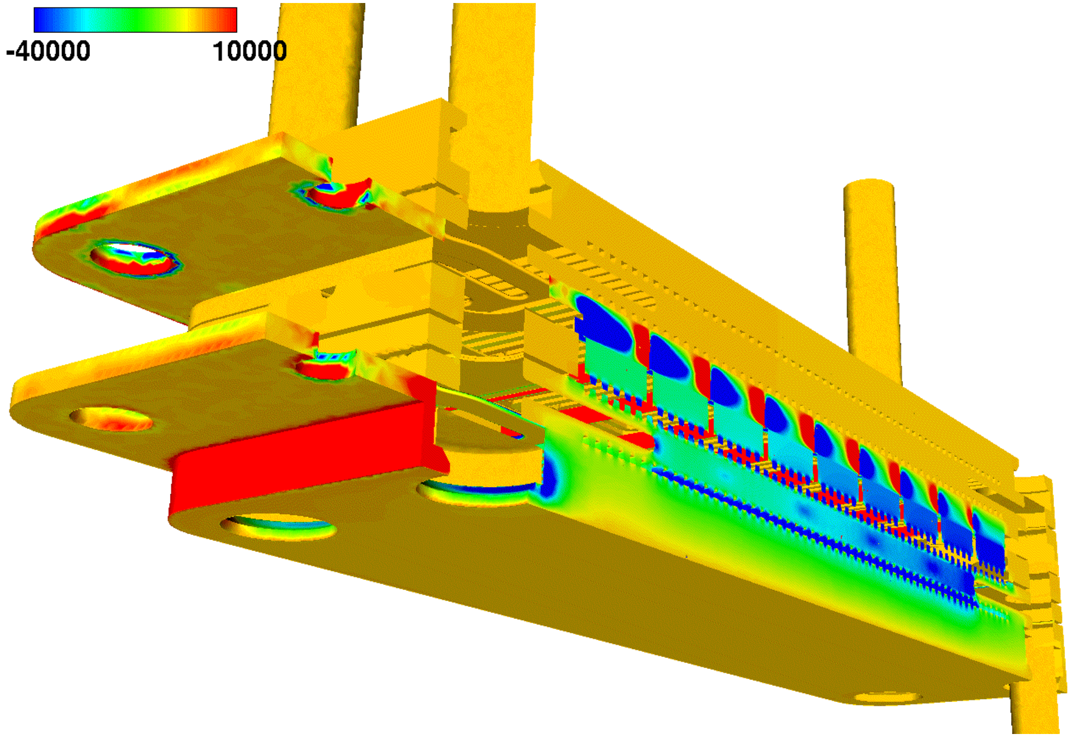


Variation case name	REFERENCE	STOICAT x 2	PRESSURE / 2
Inlet			
Stoichiometry cathode / anode (-)	1.5 / 1.3	**3** / 1.3	1.5 / 1.3
Relative humidity cathode / anode (-)	0.3 / 0.5	0.3 / 0.5	0.3 / 0.5
Temperature (°C)	80	80	80
Outlet			
Pressure cathode / anode (bar)	2.3 / 2.5	2.3 / 2.5	**1.15 / 1.25**

Detailed Performance Analysis

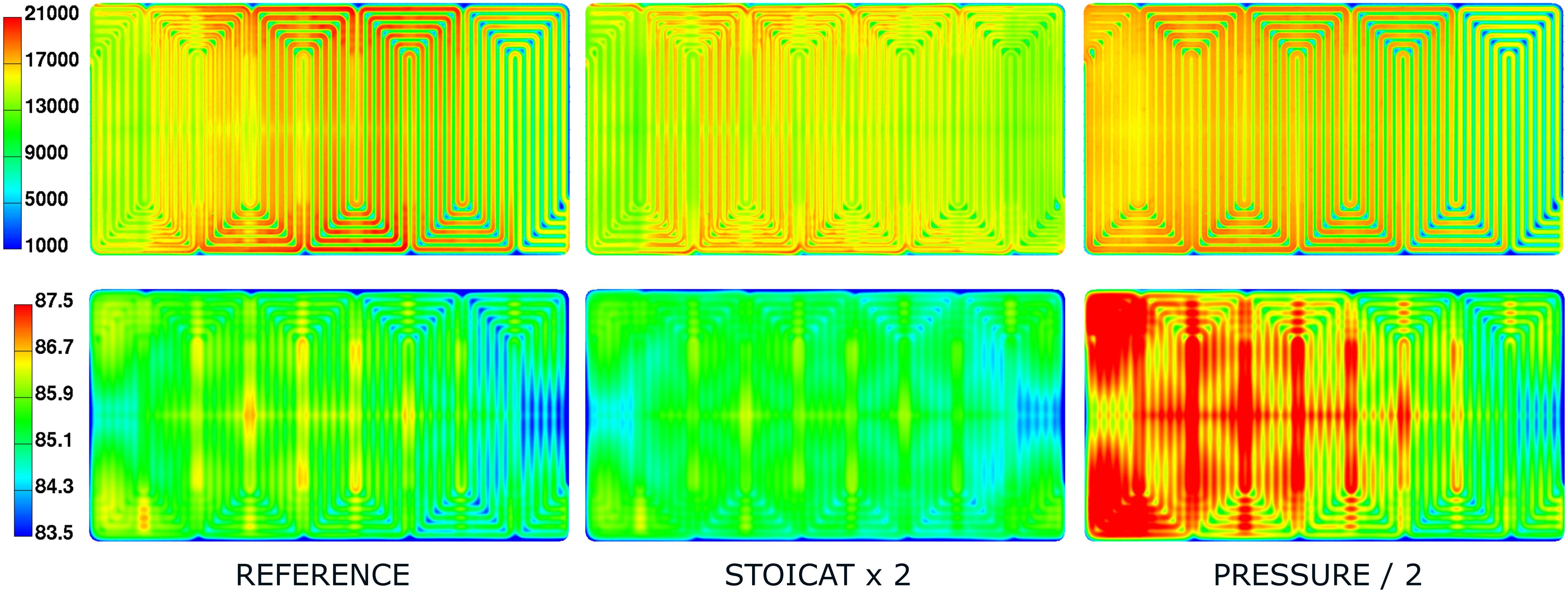
Temperature (°C) and current density (A/m²) for REFERENCE @ 2.5 A/cm²





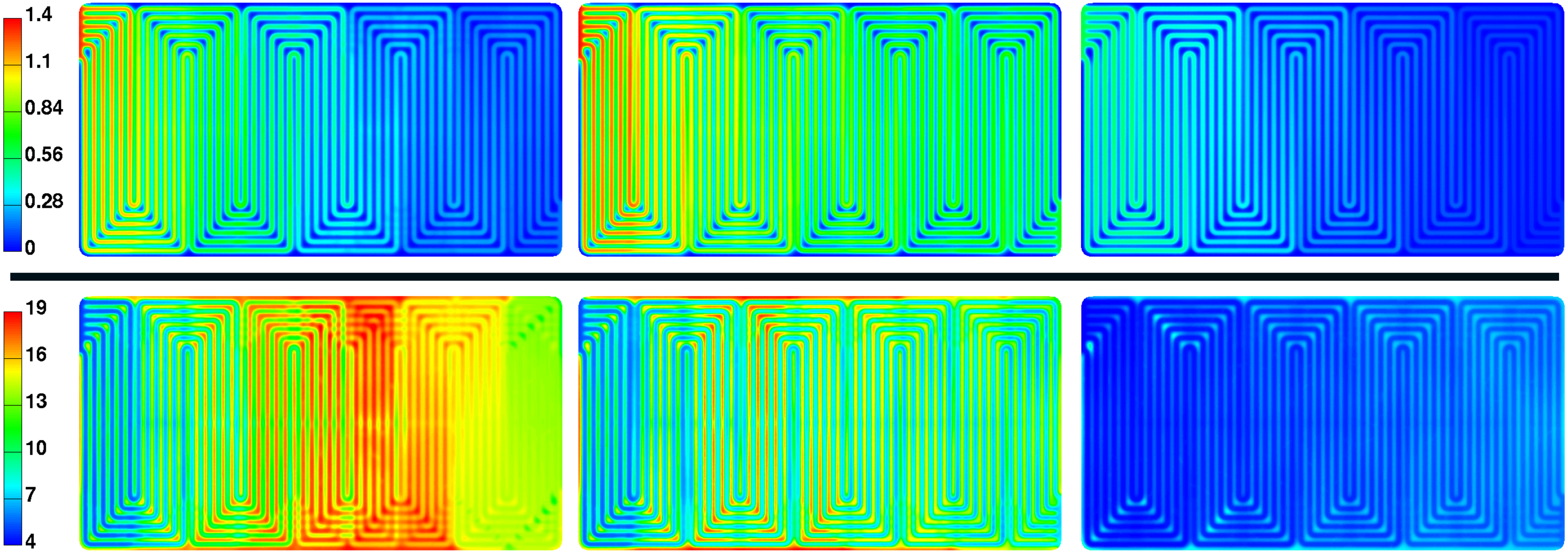
Detailed Performance Analysis

Current density (A/m^2) (top) and solid temperature (°C) (bottom) for 1.5 A/cm^2



Detailed Performance Analysis

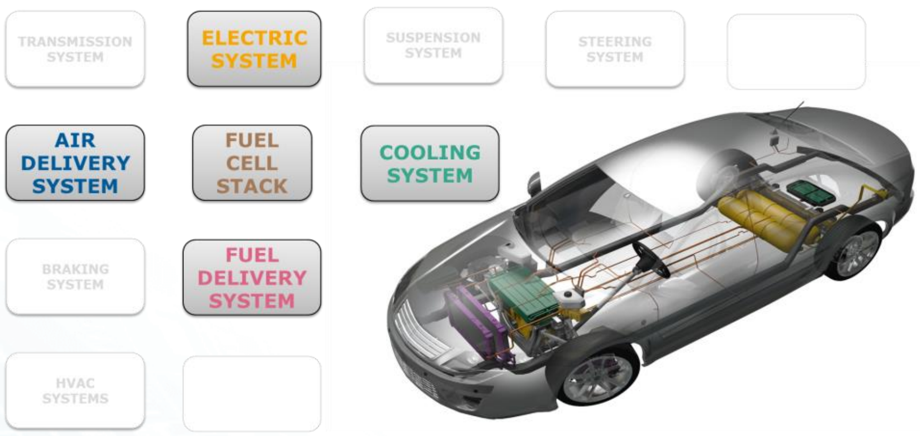
O_2 conc. at agglomerate surface (mol/m^3) (top) and water content (-) (bottom) for 1.5 A/cm^2

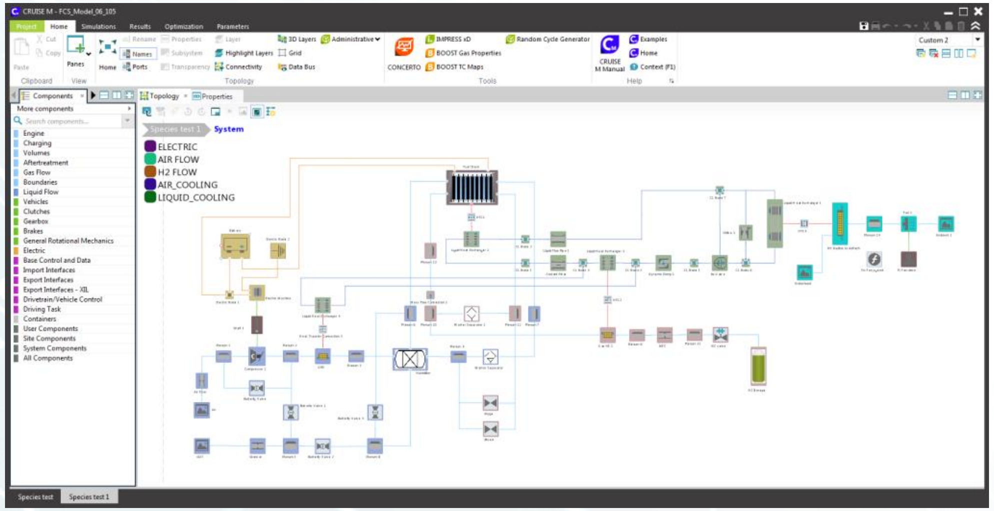


REFERENCE STOICAT x 2 PRESSURE / 2

System Layout

FC System Development

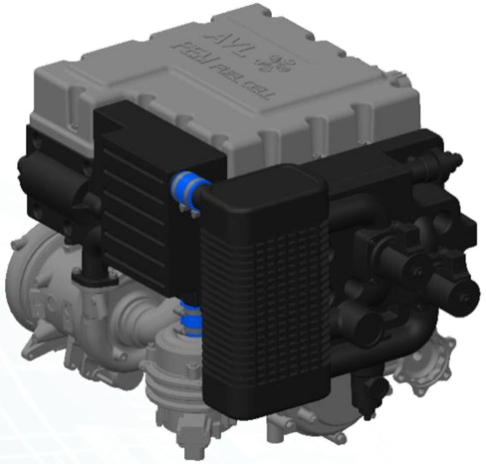


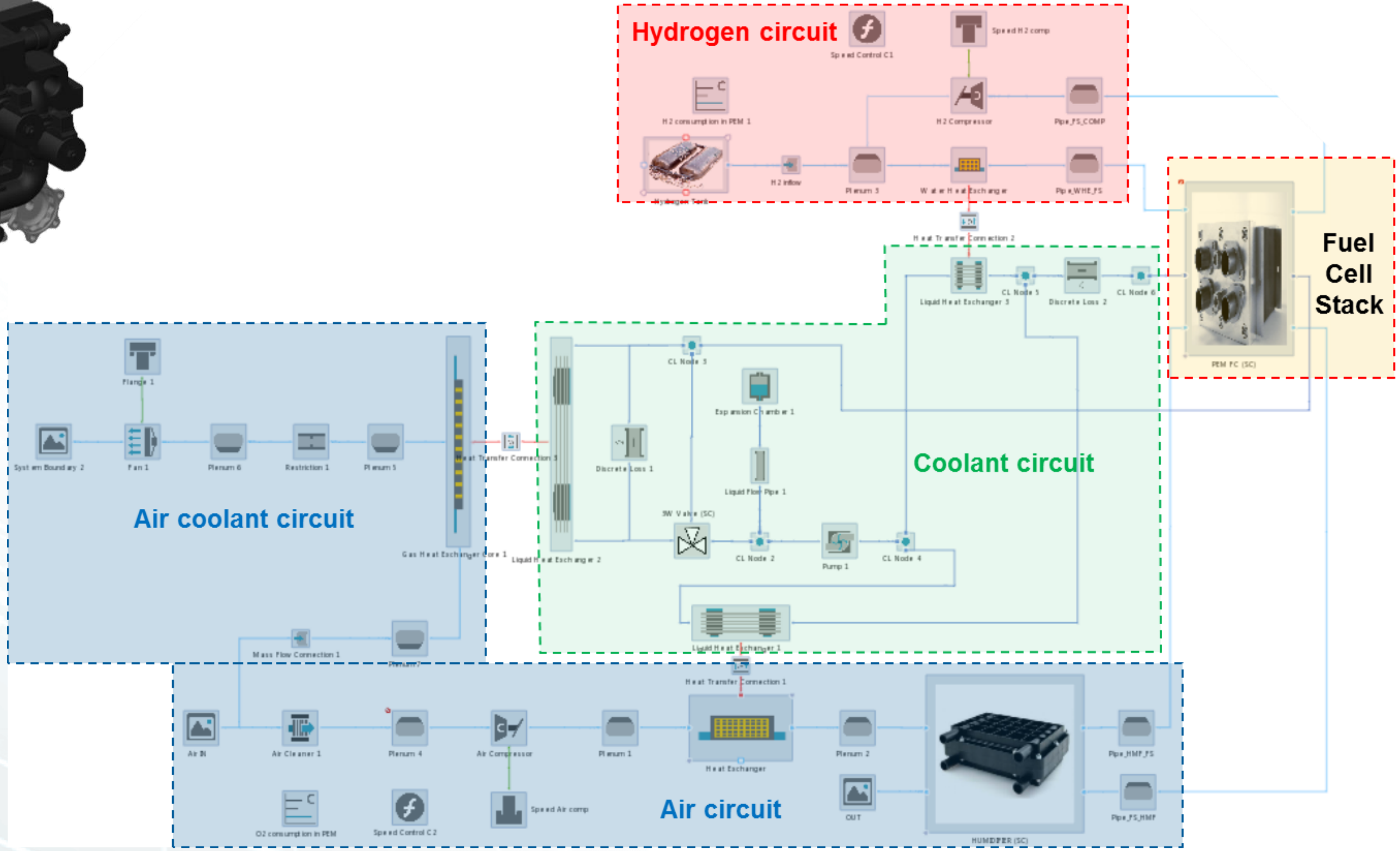


Application Scope

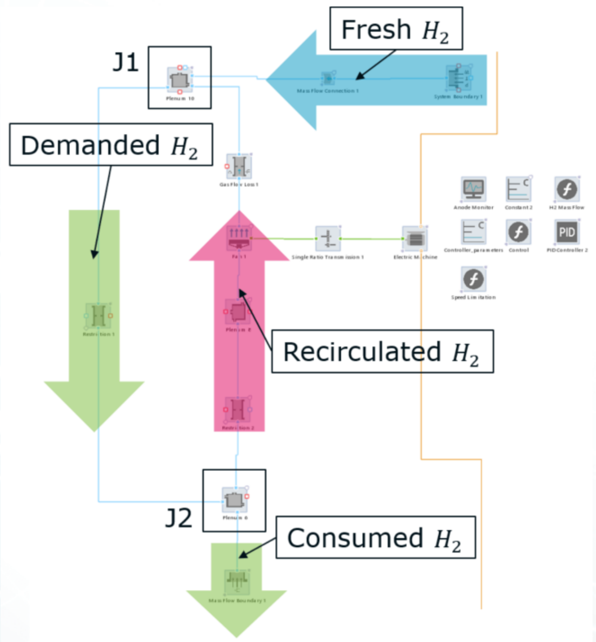
- Layout of **hydrogen and air supply and auxiliaries** (BoP - Balance of Plant)
- Layout of **cooling circuit**
- Development of **media supply control**
- Transient **response optimization**
- Real-time **control function development and testing**

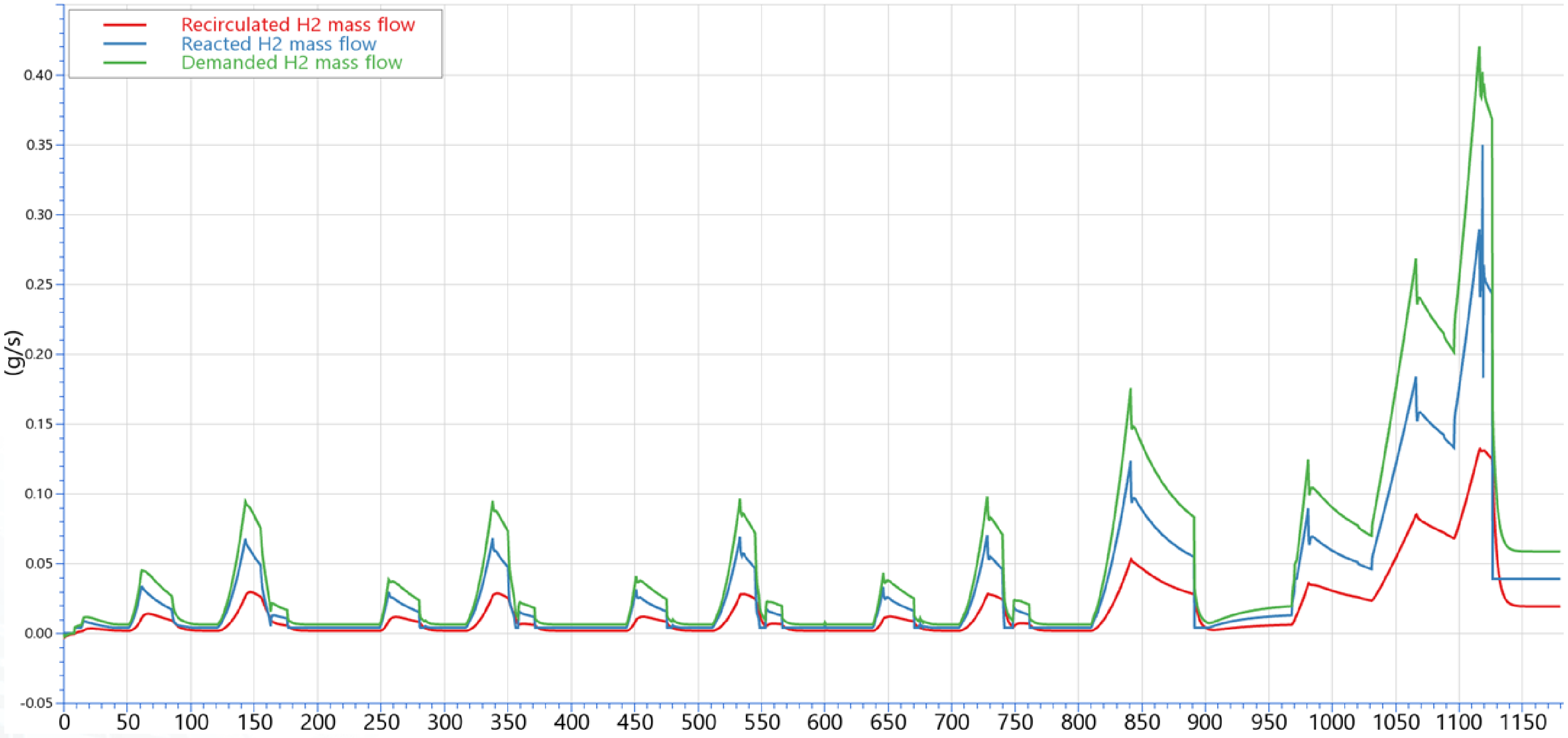
FC System Development / BoP Modelling





Detailed FC System Drive Cycle Results





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Detailed Thermal Network

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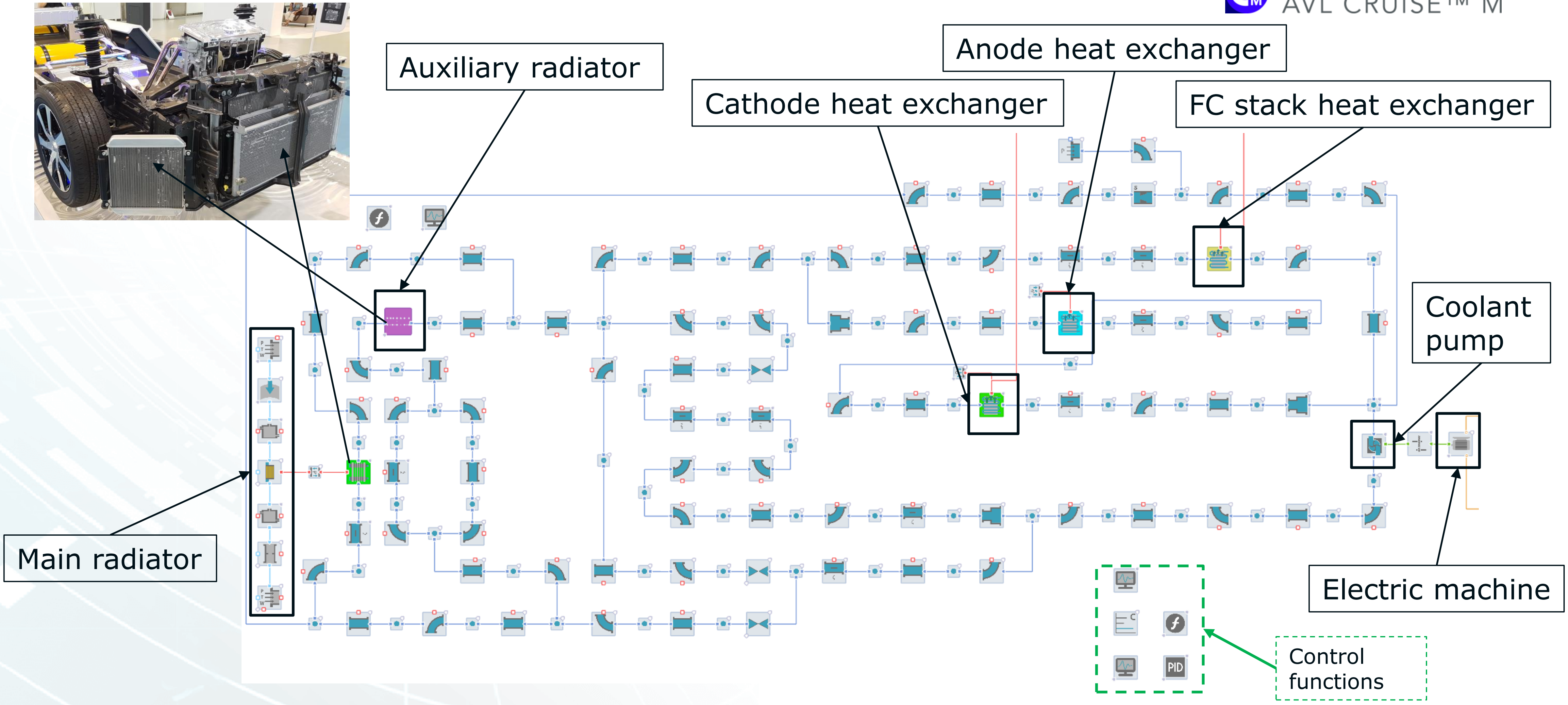
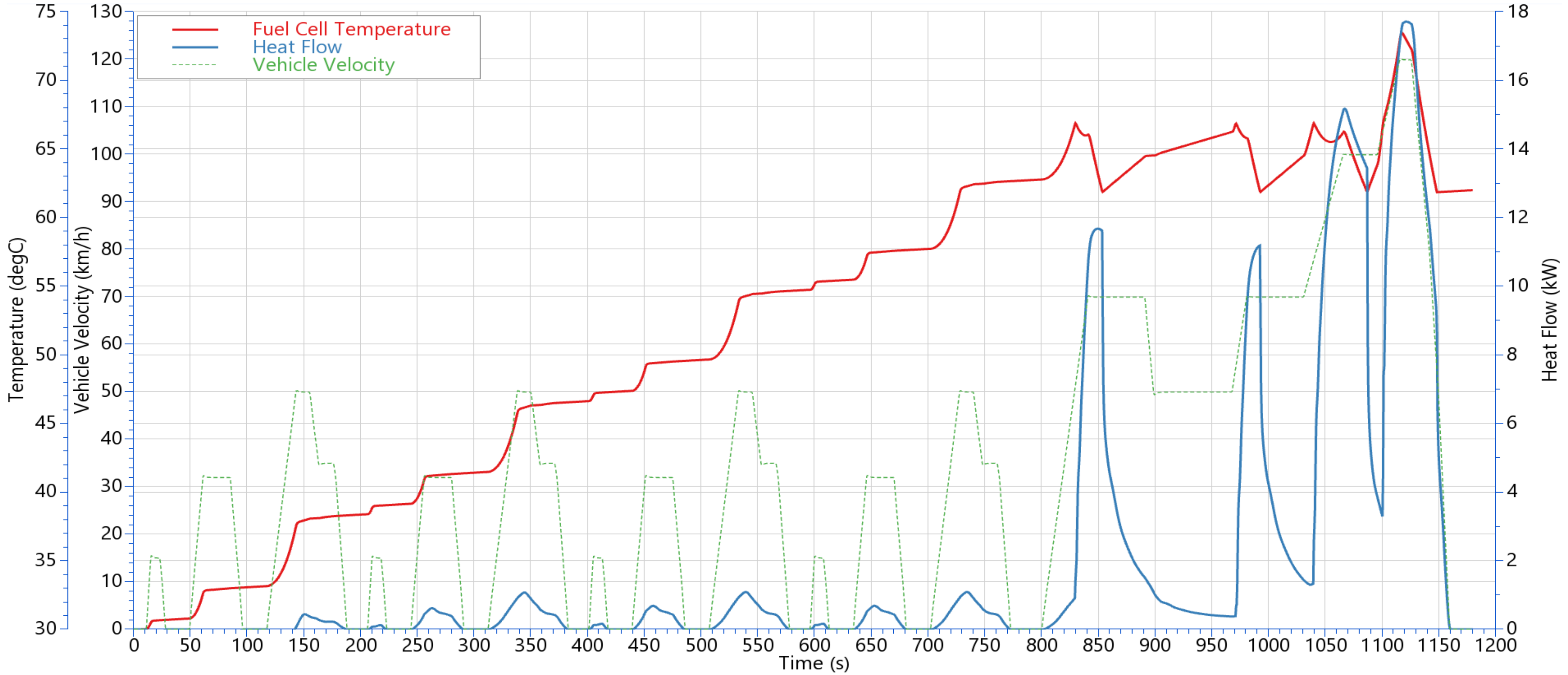


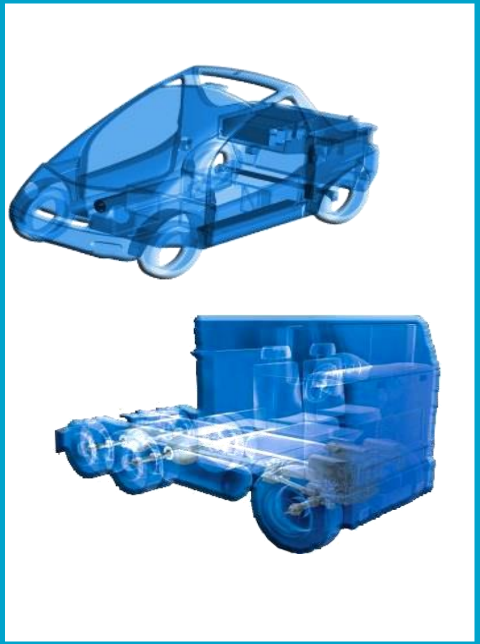
Detailed FC System Drive Cycle Results



SUMMARY

Scalable Modelling From Component To System

PT Concept Level



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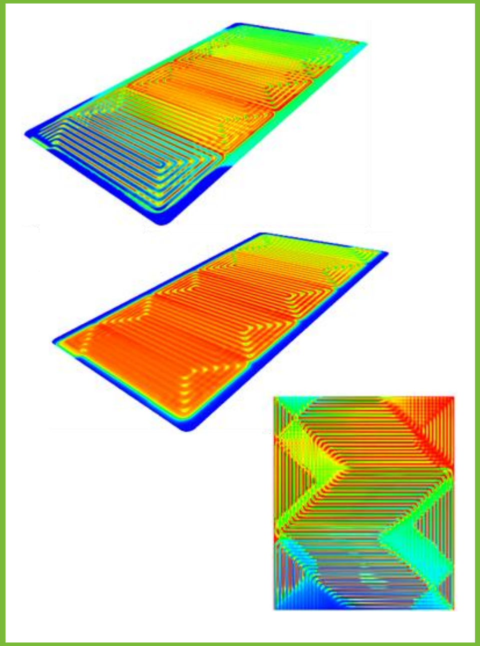
Detailed Cell Level



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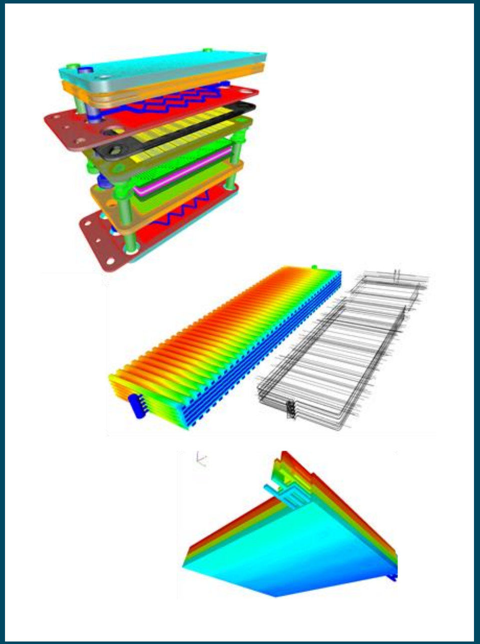
Detailed Stack Level



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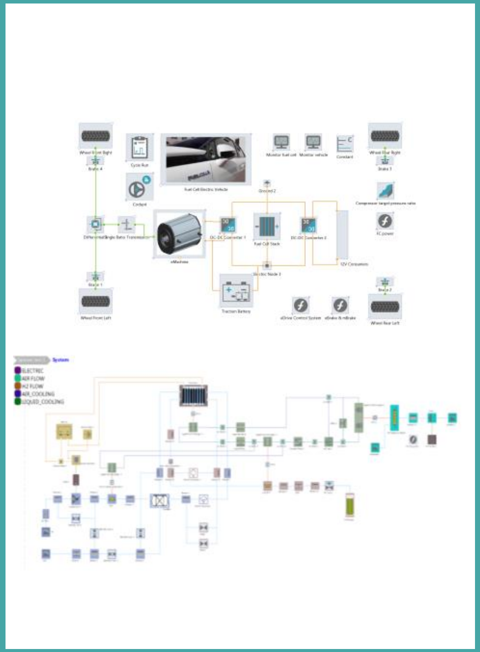
System Layout Level



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Thank You

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