ADVANCED PROCESS MODELLING FORUM 2014

Fuel cell system design and optimisation

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PSE Customer base
FC product users and (evaluations)

Americas

Air Products
BP Chemicals
Conoco Phillips
Dow Chemicals
DuPont
ExxonMobil
INEOS
Praxair

Bend Research
Energy Solutions
Johns Manville
LXEng
Procter & Gamble
SQM
Toyota Motor US

EMEA

BP Chemicals
BP Exploration
BASF
Bayer TS
Infineum
Linde Engineering
Repsol YPF
Sasol
Shell Global Solutions
Süd-Chemie
Sulzer
TOTAL

Atomic Weapons Establishment
Cadbury's
det Norske Veritas
FLS Automation
Friesland Foods
Nexia Solutions
Nestlé
PURAC
RWEnpower

(A large automotive company in Germany)

APAC

Idemitsu Petrochemicals
LG Chem
Mitsubishi Chemical
Samnam Petrochemical
SK Chemicals
SK Energy
SK Petrochemicals
Taiyo Nippon Sanso

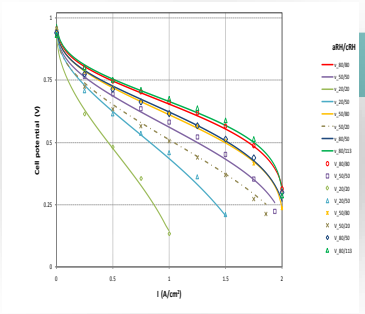
Samsung Electronics
KIER
Toshiba Fuel Cell Power

Toyota Motor Corp.
HONDA

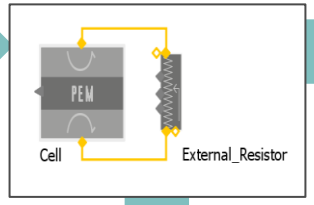
(DENSO)
(Hyundai Motor Company)

Life cycle of stack and system design

1 Data based validation of MEA model for stack design

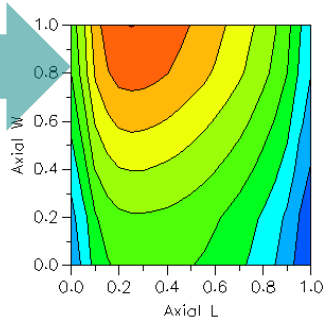


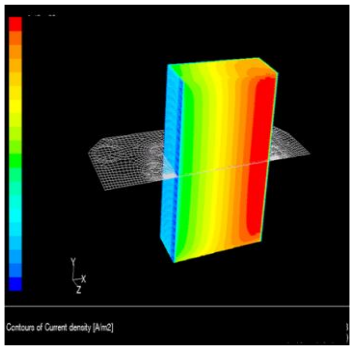
Single cell data processing with 1-D distributed model of fuel cell

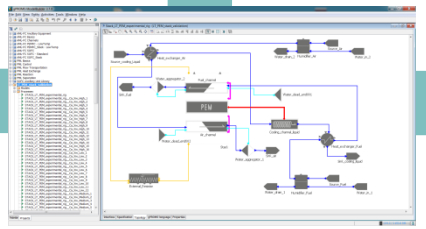


1. Stack model default parameters
2. Parameters refined by processing experimental data from single cell or stack

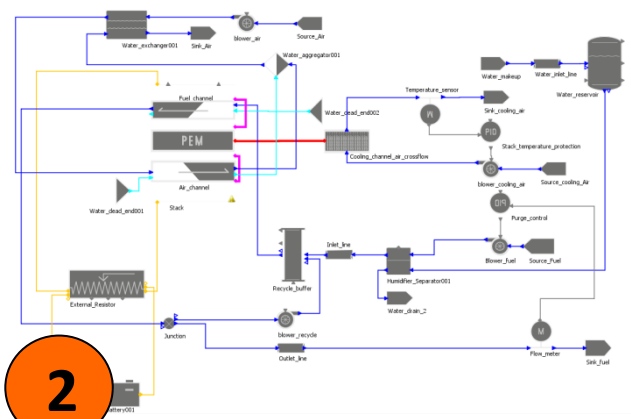
4 Detailed stack design (3-D stack model or link with CFD)







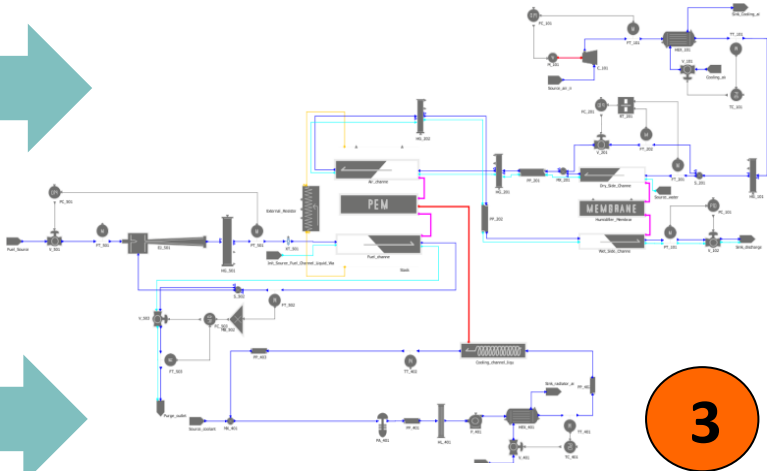
Vendor information for auxiliary equipment or validation by data processing



2

Stack performance in a simple system, water management, deactivation, design decisions (2-D stack model)

Auxiliary Units

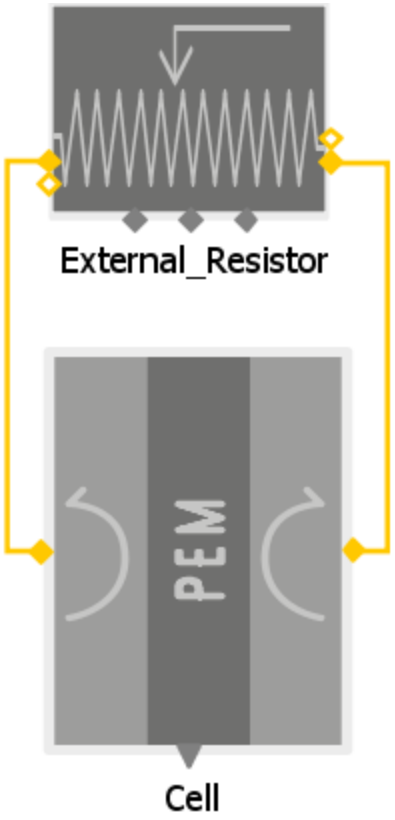


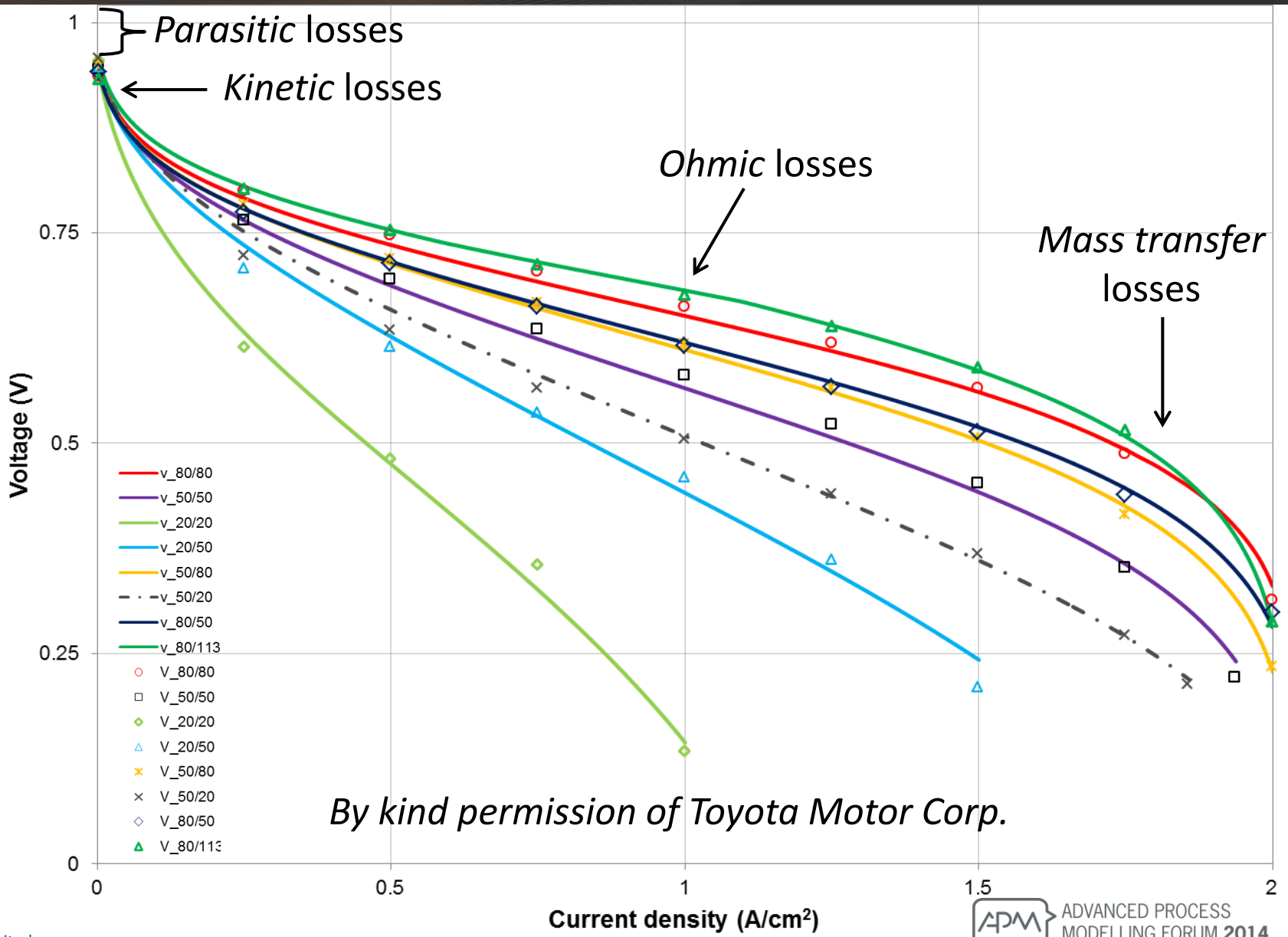
3

Design and optimisation of complete system for commercial applications (2-D stack model)

Making the most of experimental data

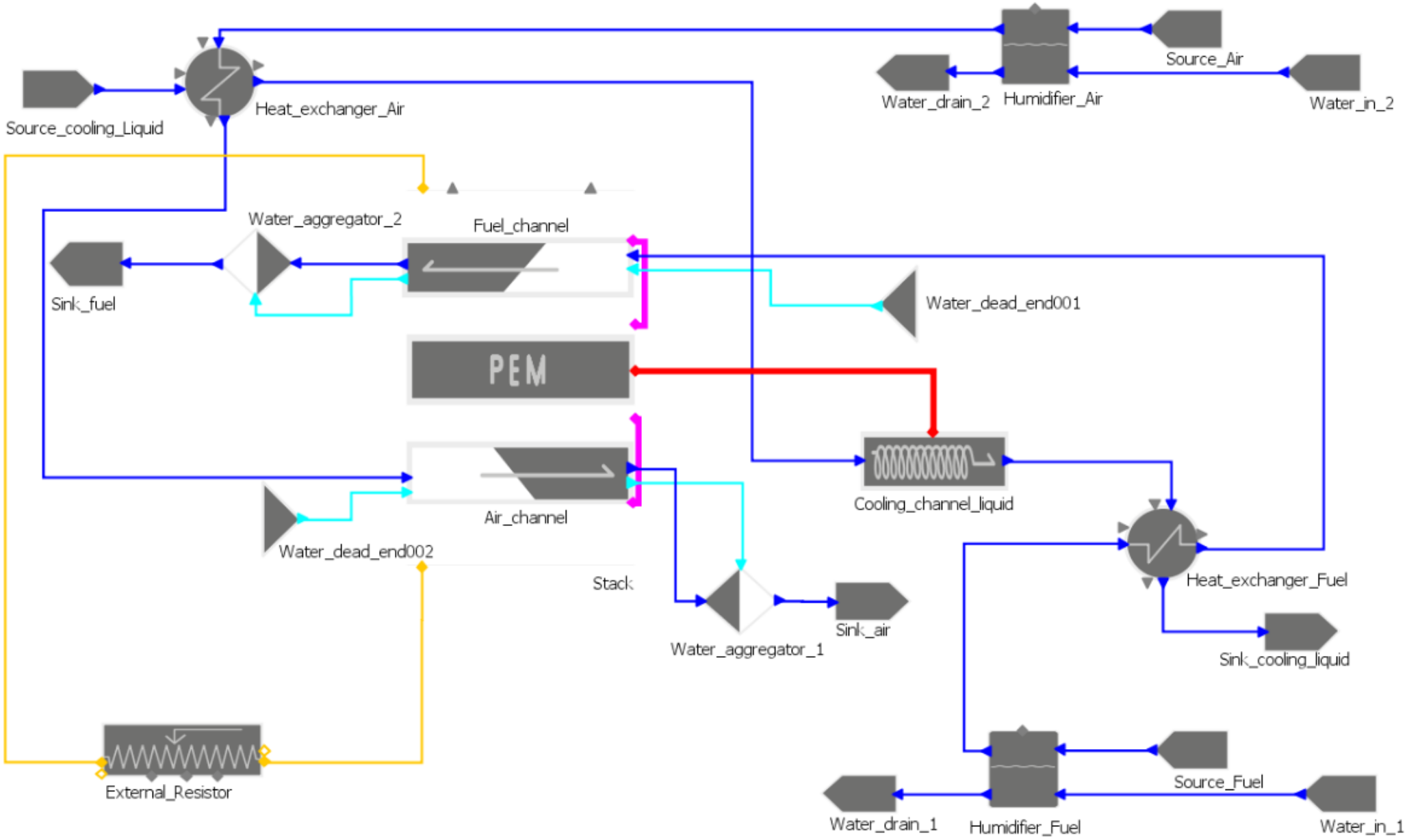
Single cell experiments





By kind permission of Toyota Motor Corp.

Setup for fuel cell stack experiments



From stand-alone stack information to fully integrated systems

Features of system model in fuel cell applications

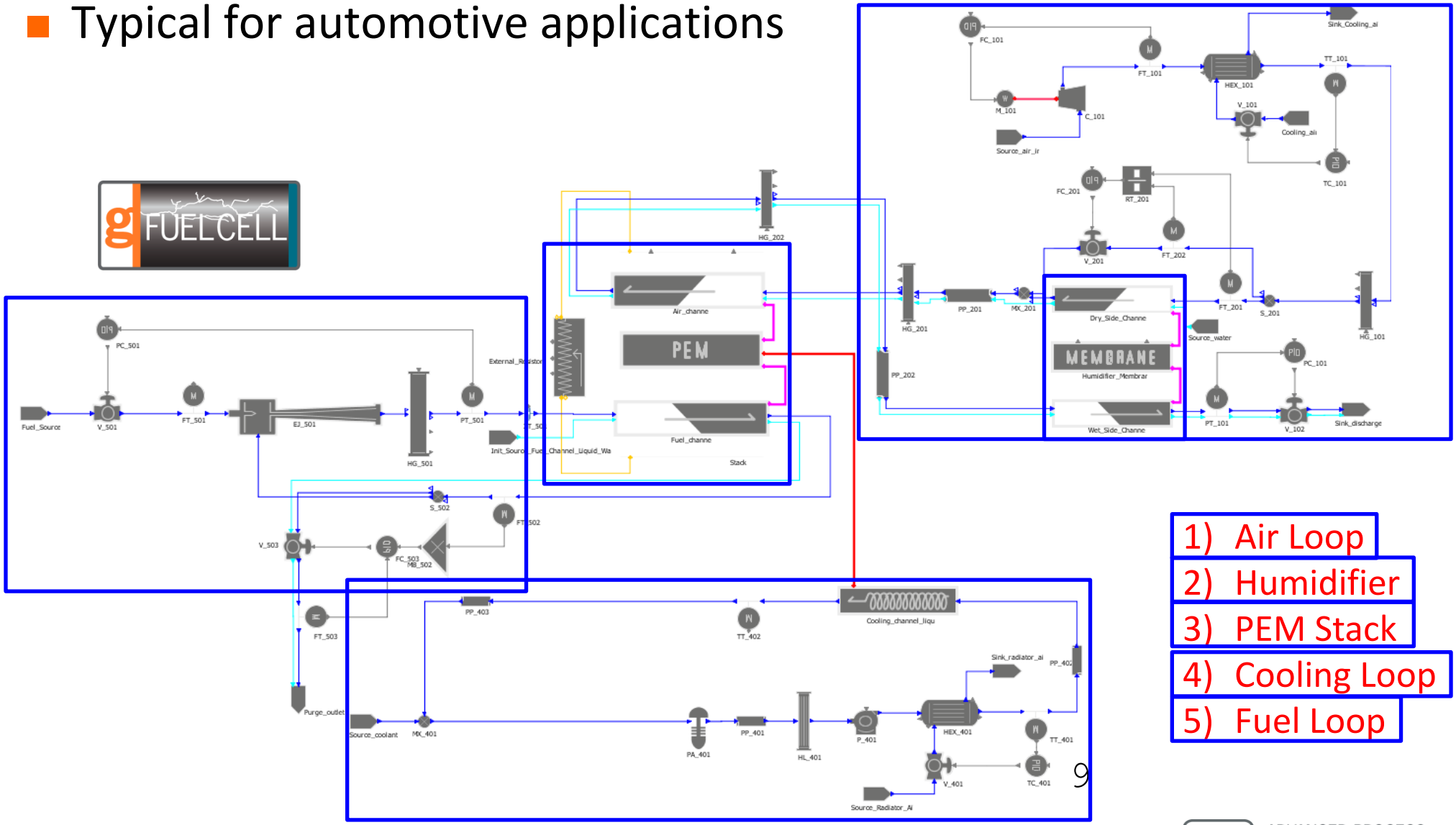
Successful commercialization of fuel cell technologies depends largely on how the fuel cell stack is integrated within the entire power plant system.

- Fully pressure driven models
- Include computation intensive, complex models

  (e.g. PEM stack, humidifier)
- Robust in simulating extremely dynamic operations
- Accommodate hierarchical control structures
- Predictive to high degree to reproduce the pilot plant information

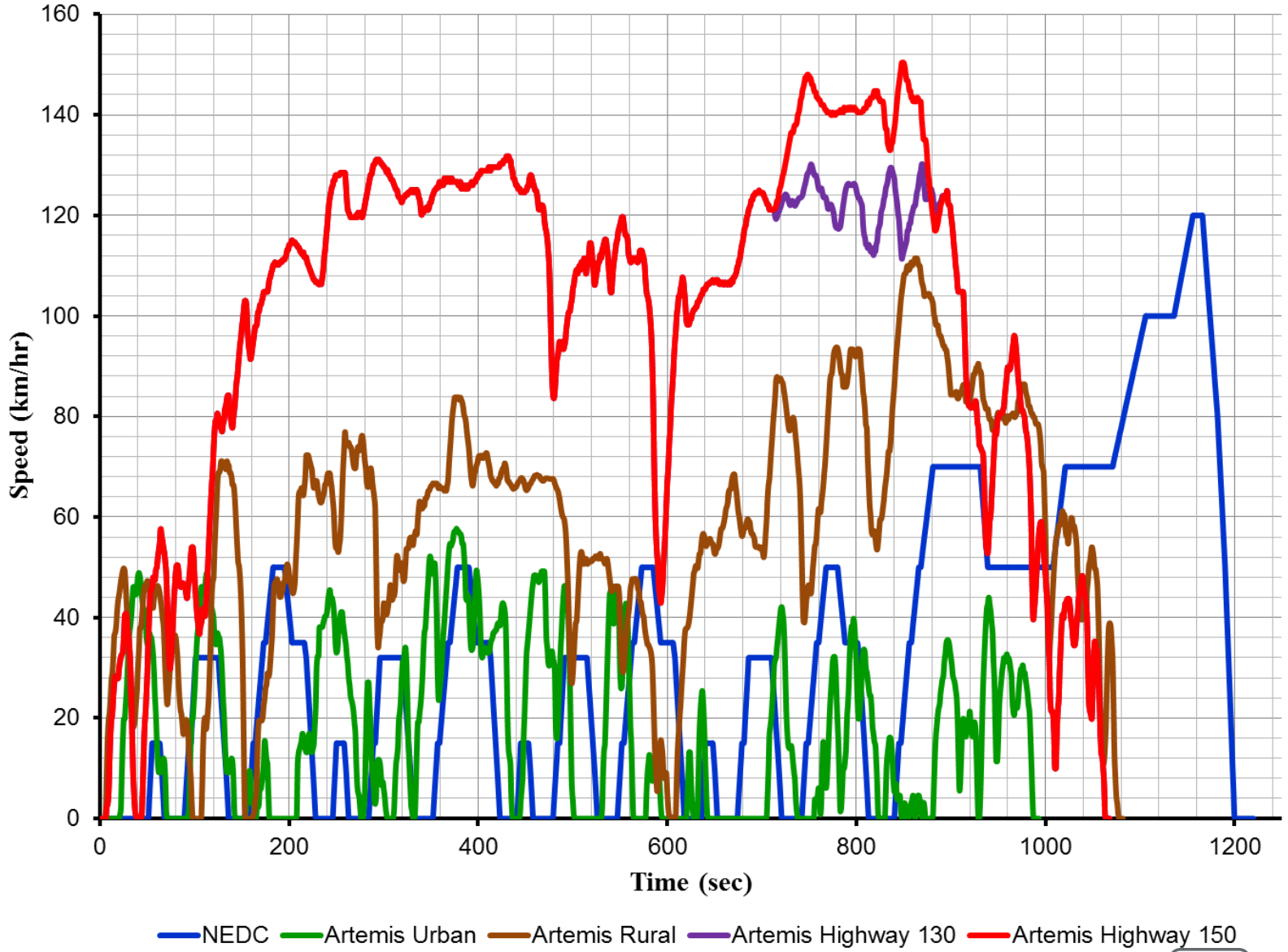
General Structure of a PEM FC System

- Typical for automotive applications

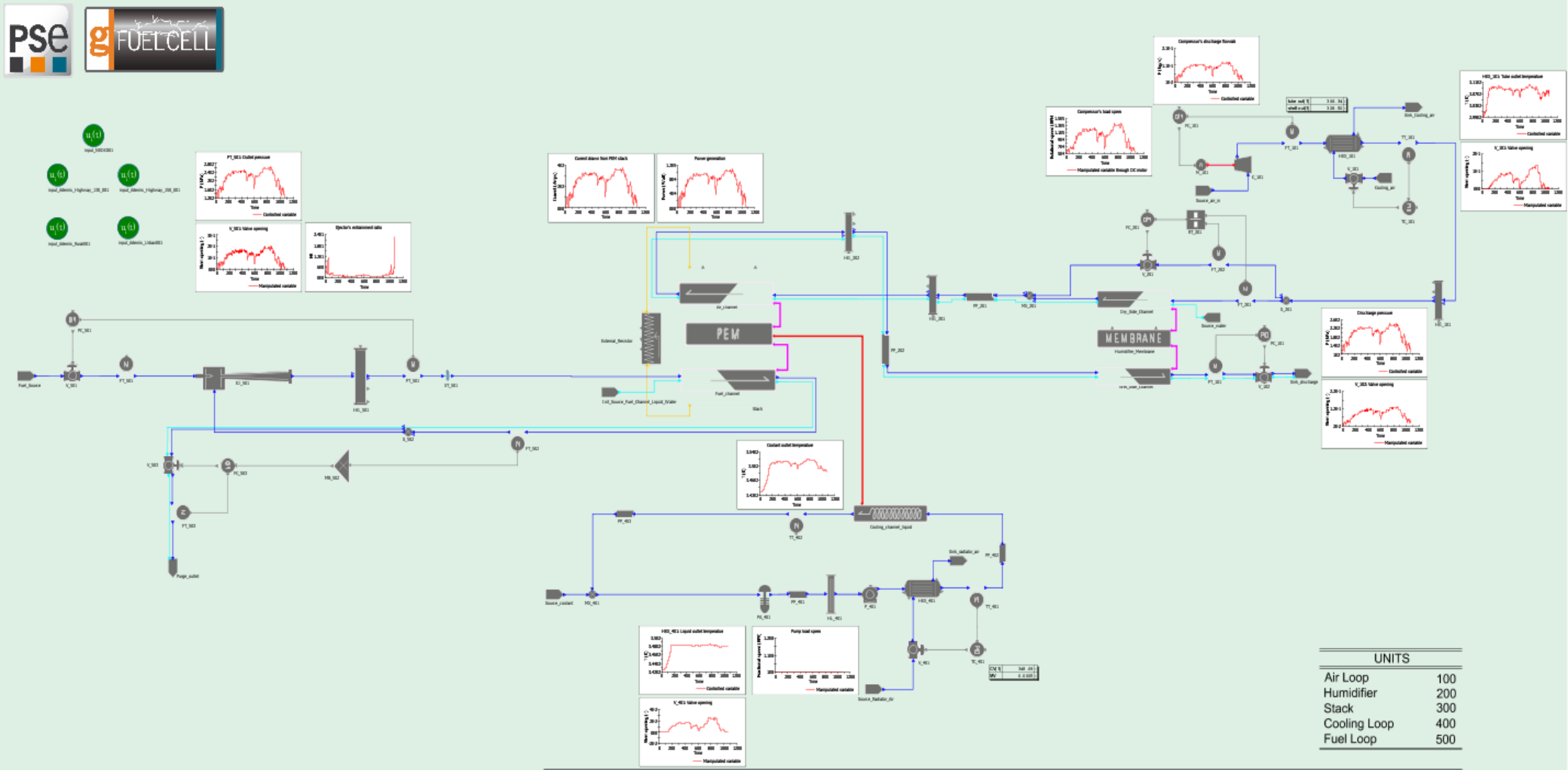


1) Air Loop
2) Humidifier
3) PEM Stack
4) Cooling Loop
5) Fuel Loop

Performance assessment based on industry standard driving cycles



High level output from simulation of Artemis Highway 150

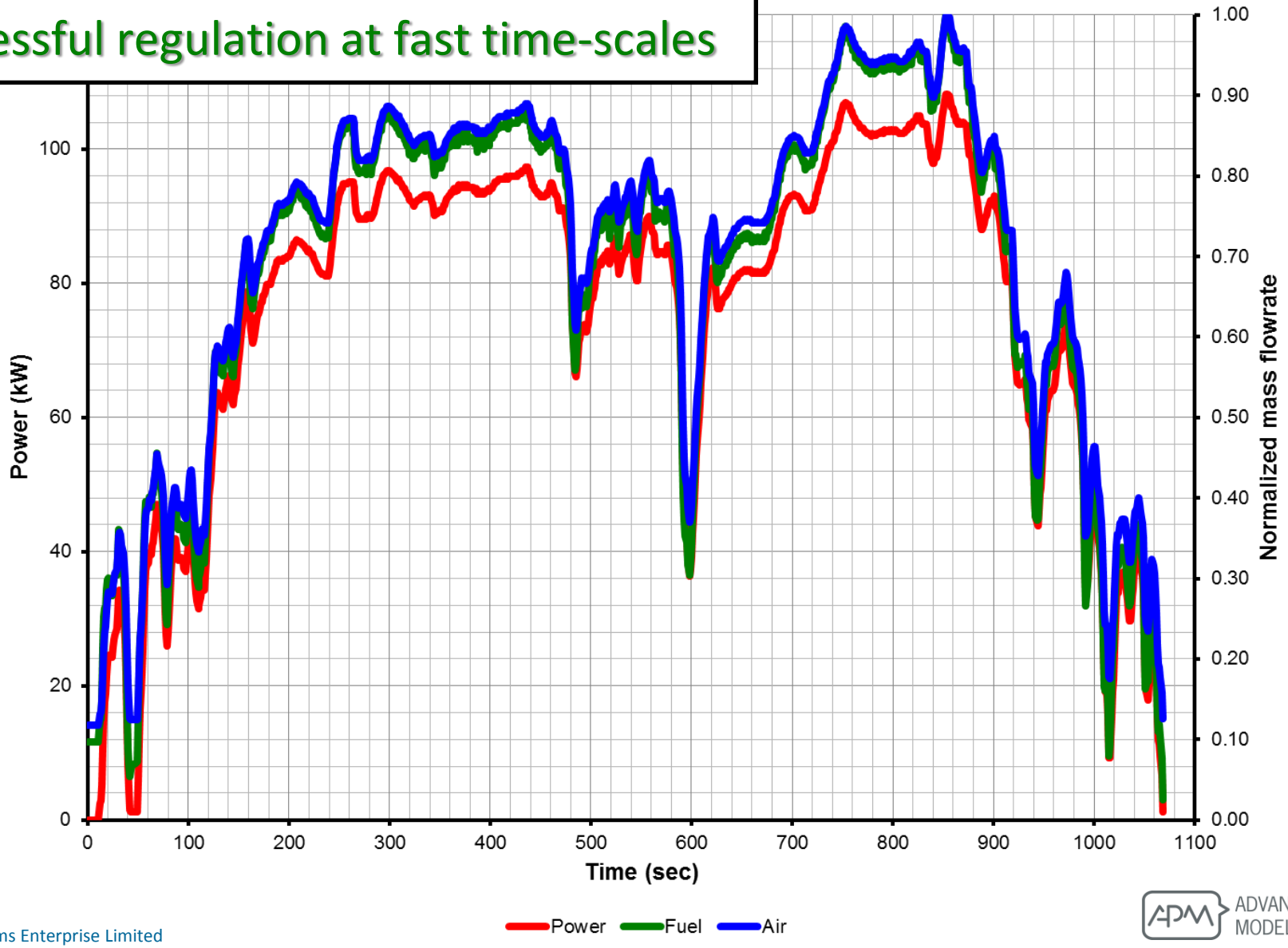


UNITS	
Air Loop	100
Humidifier	200
Stack	300
Cooling Loop	400
Fuel Loop	500

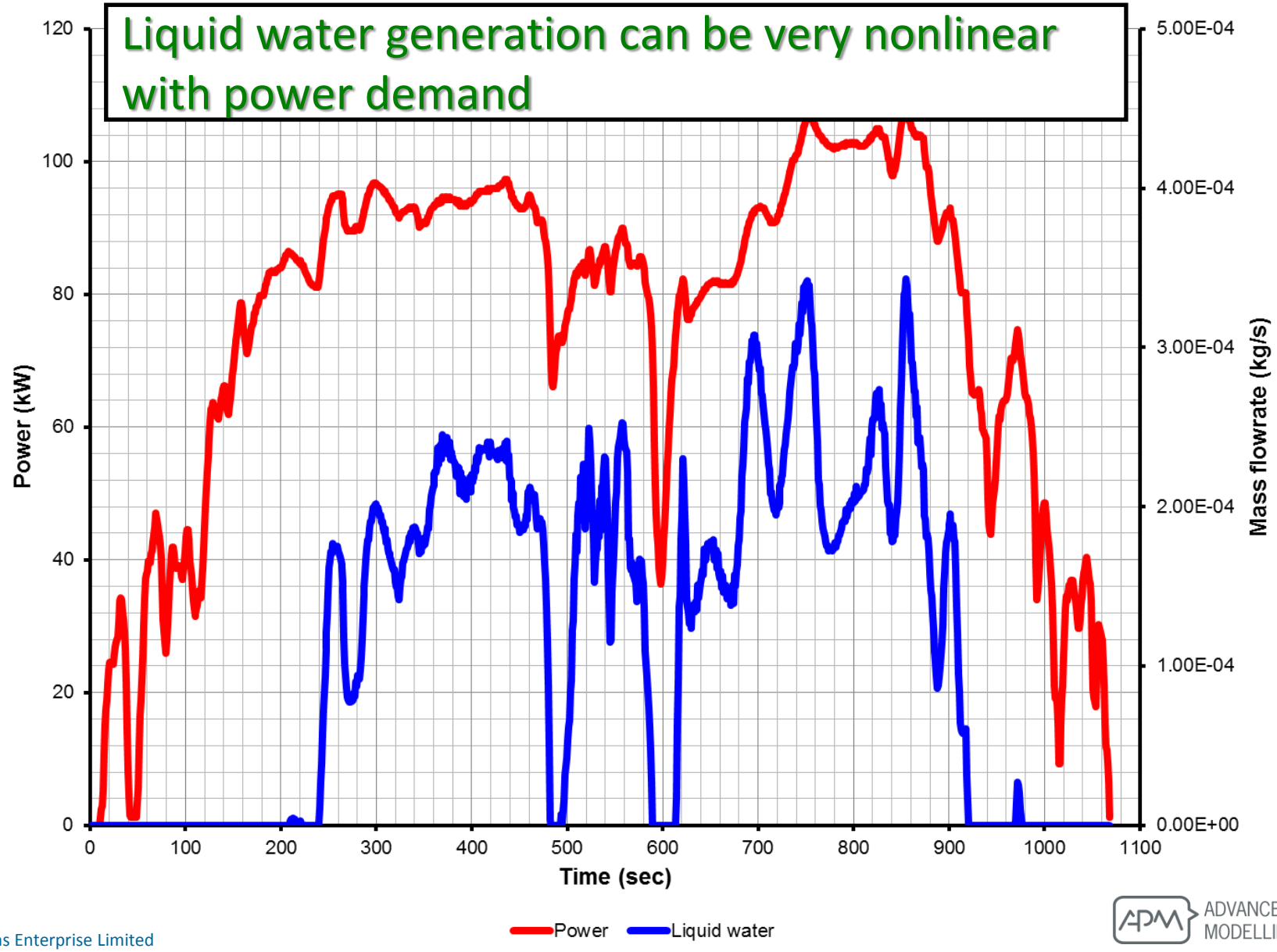
SYMBOLS									
C	Centrifugal compressor	HEX	Heat exchanger	NZ	Nozzle	PT	Pressure transmitter	XT	Composition transmitter
DF	Diffuser	HG	Header gas	P	Pump	RT	Ratio transmitter		
EJ	Ejector	HL	Header liquid	PA	Pressure anchor	S	Splitter		
FC	Flow controller	M	DC Motor	PC	Pressure controller	TT	Temperature transmitter		
FT	Flow transmitter	MX	Mixer	PP	Pipeline	V	Valve		

Basic Operations

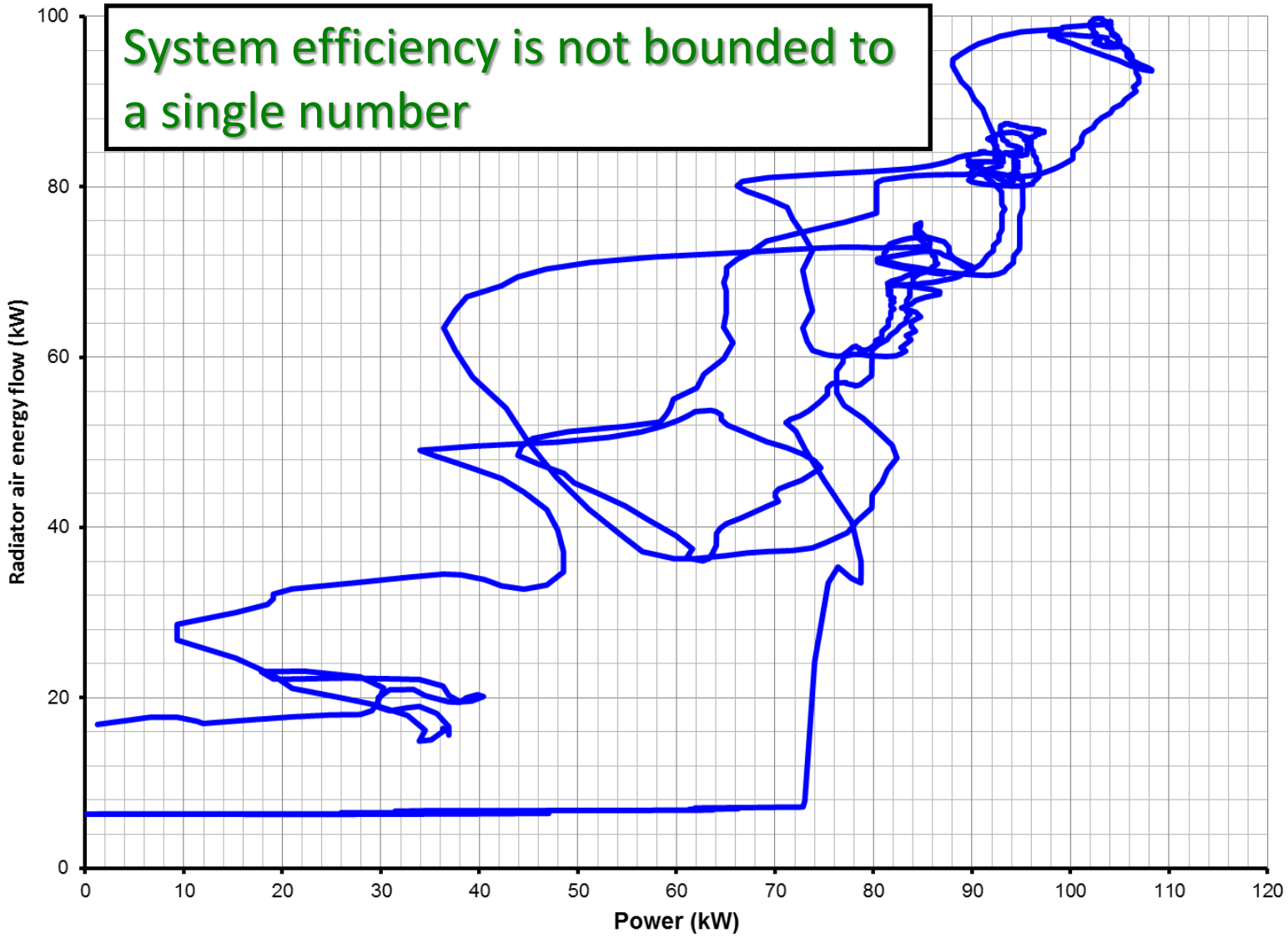
Successful regulation at fast time-scales



Nonlinear characteristics of the FC system

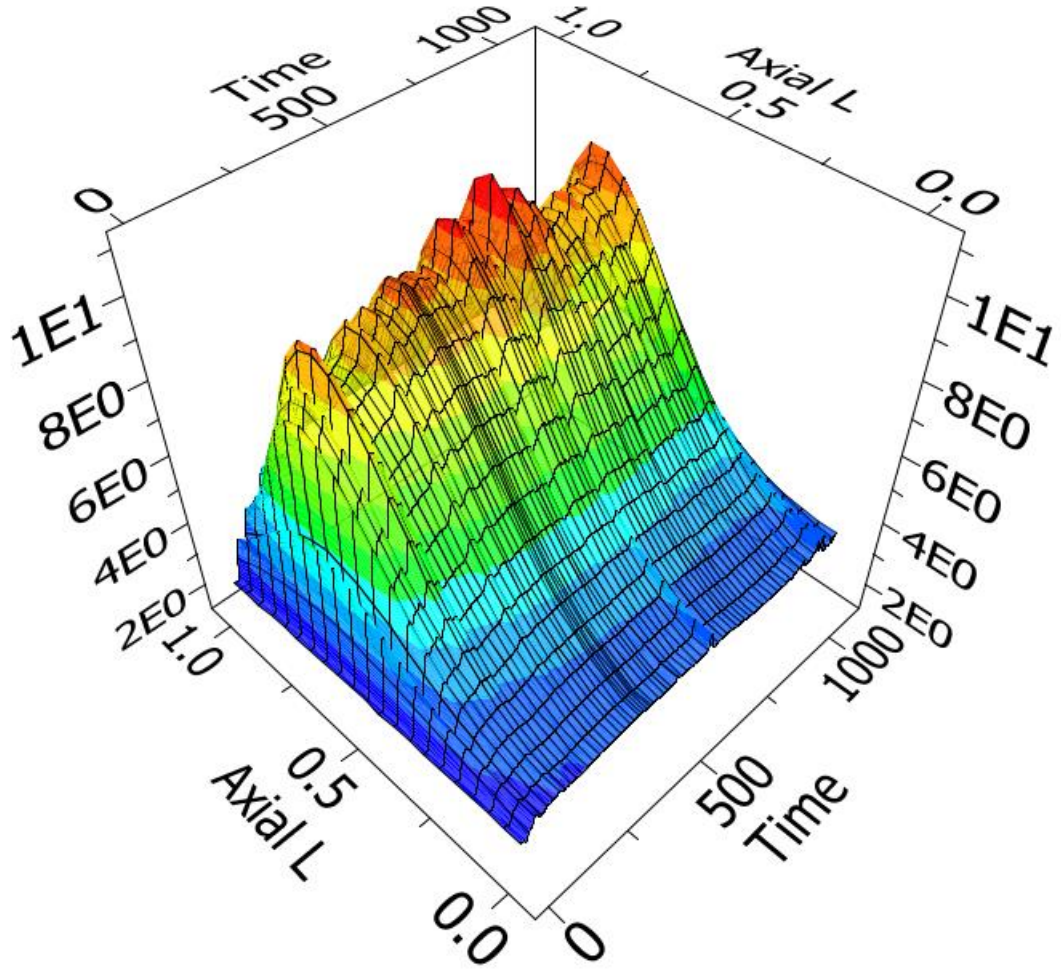


Cooling duty vs. Power demand



Model based diagnostics of stack in automotive applications

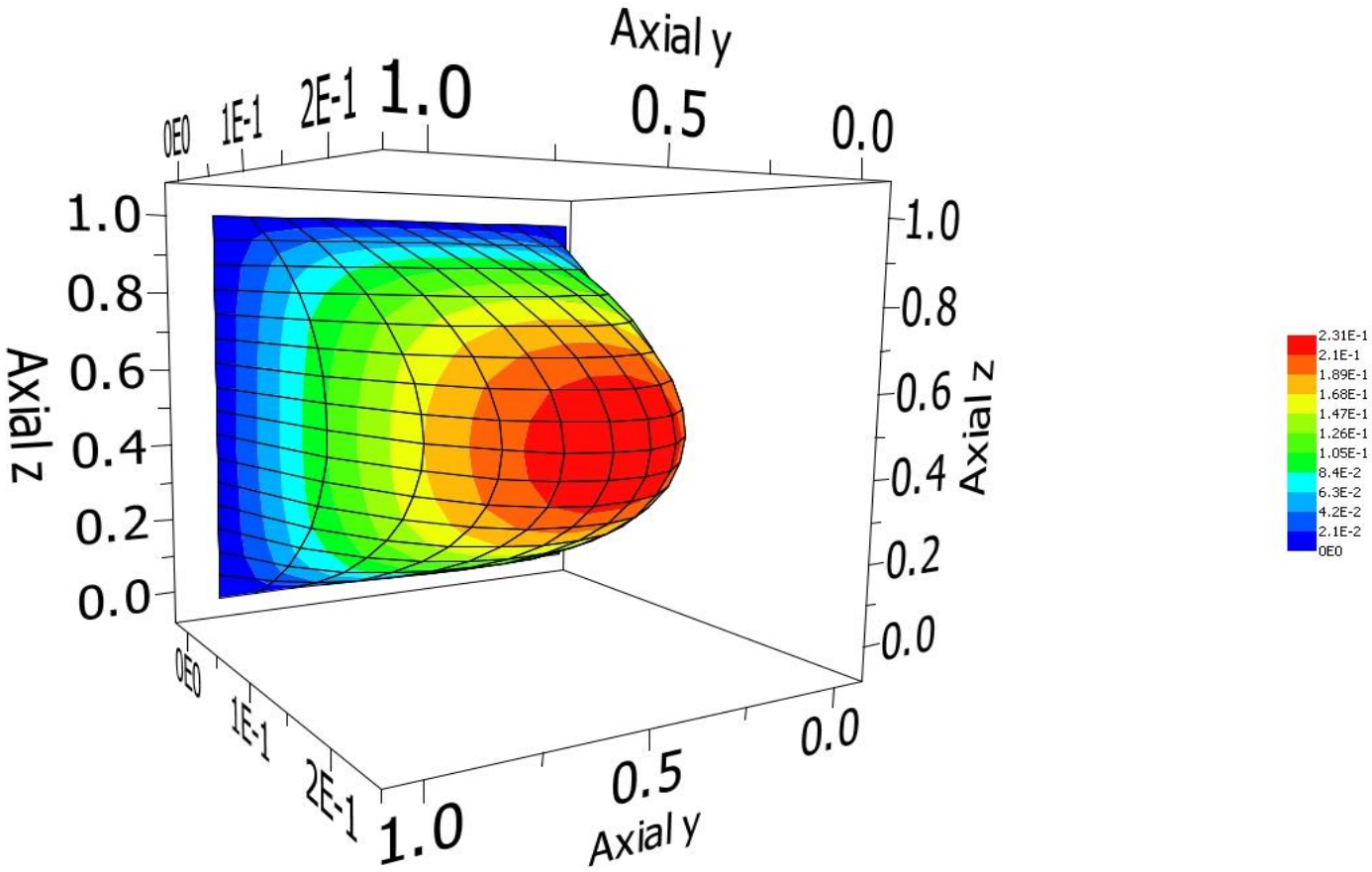
Detailed stack model allows monitoring the stack vitals in a driving cycle



gPROMS enters the realm of CFD resolution modelling

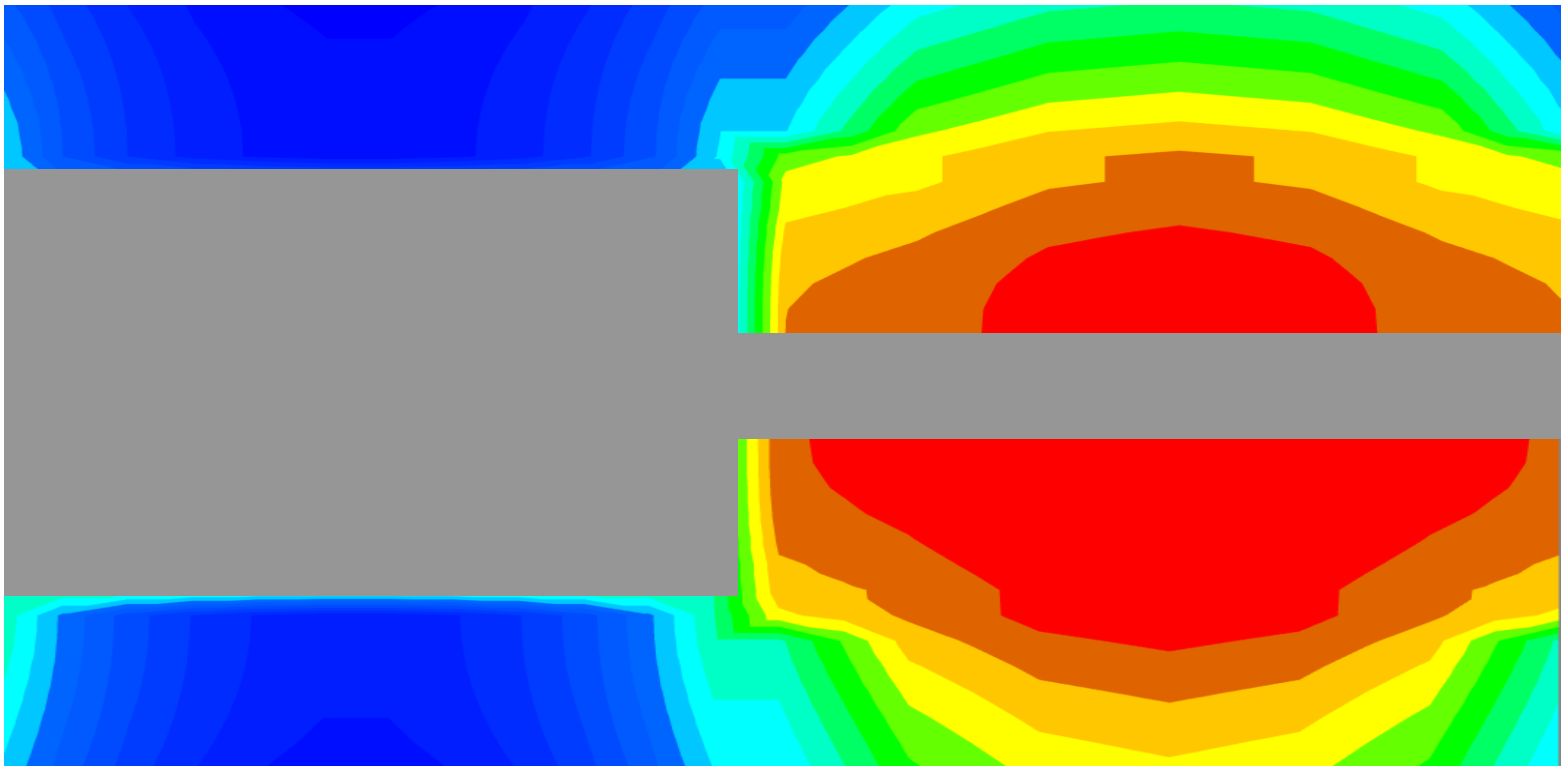
Navier-Stokes solution

Velocity Profile in Cooling Channel



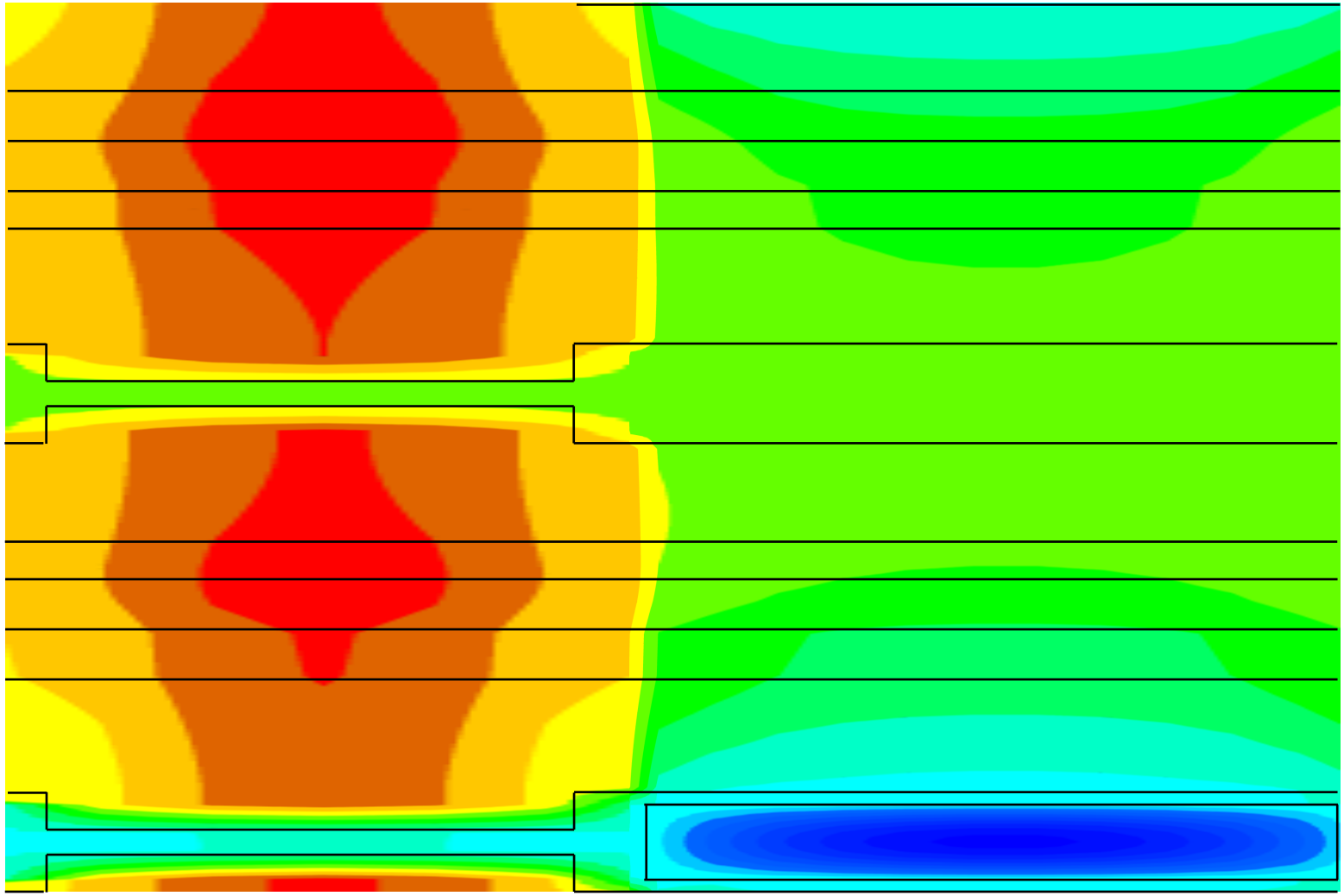
Reactant composition profiles

Hydrogen



Oxygen

Temperature profile – cooling every two cells



Lead-Acid Battery

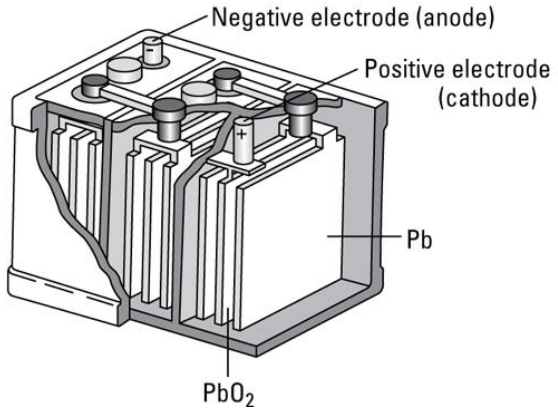
NEW MODELLING PROJECT- Automotive Batteries

- New Project: Model of a Lead-Acid Battery

MOTIVATION

- Start&Stop System of Cars

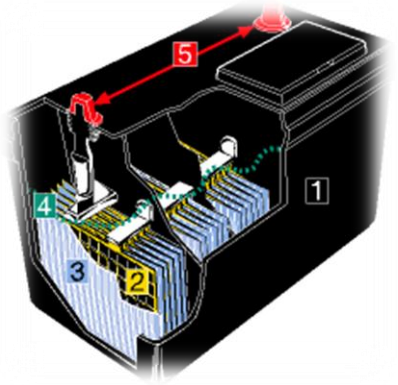
- More intense performance
- Reduced Battery Life

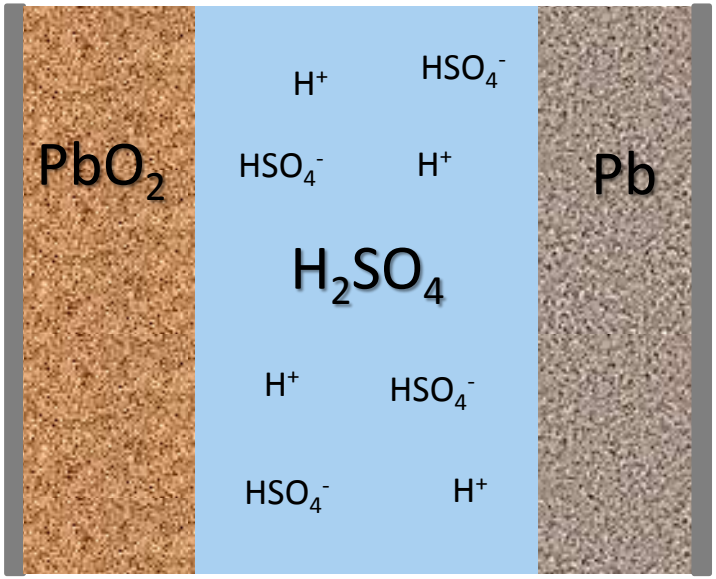


- Modelling:
  - Understand the batteries' operation
  - Advice on how to improve design

LEAD-ACID BATTERY

- MODEL:





CATHODE

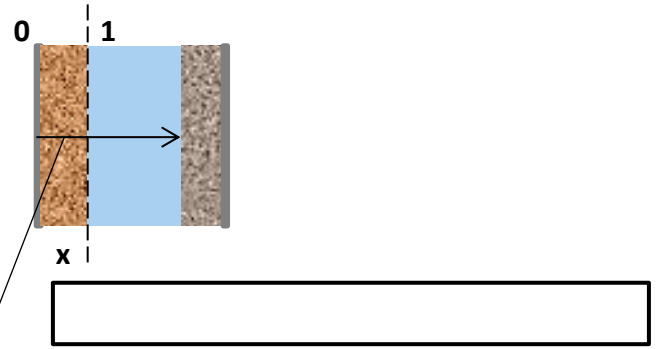
ANODE

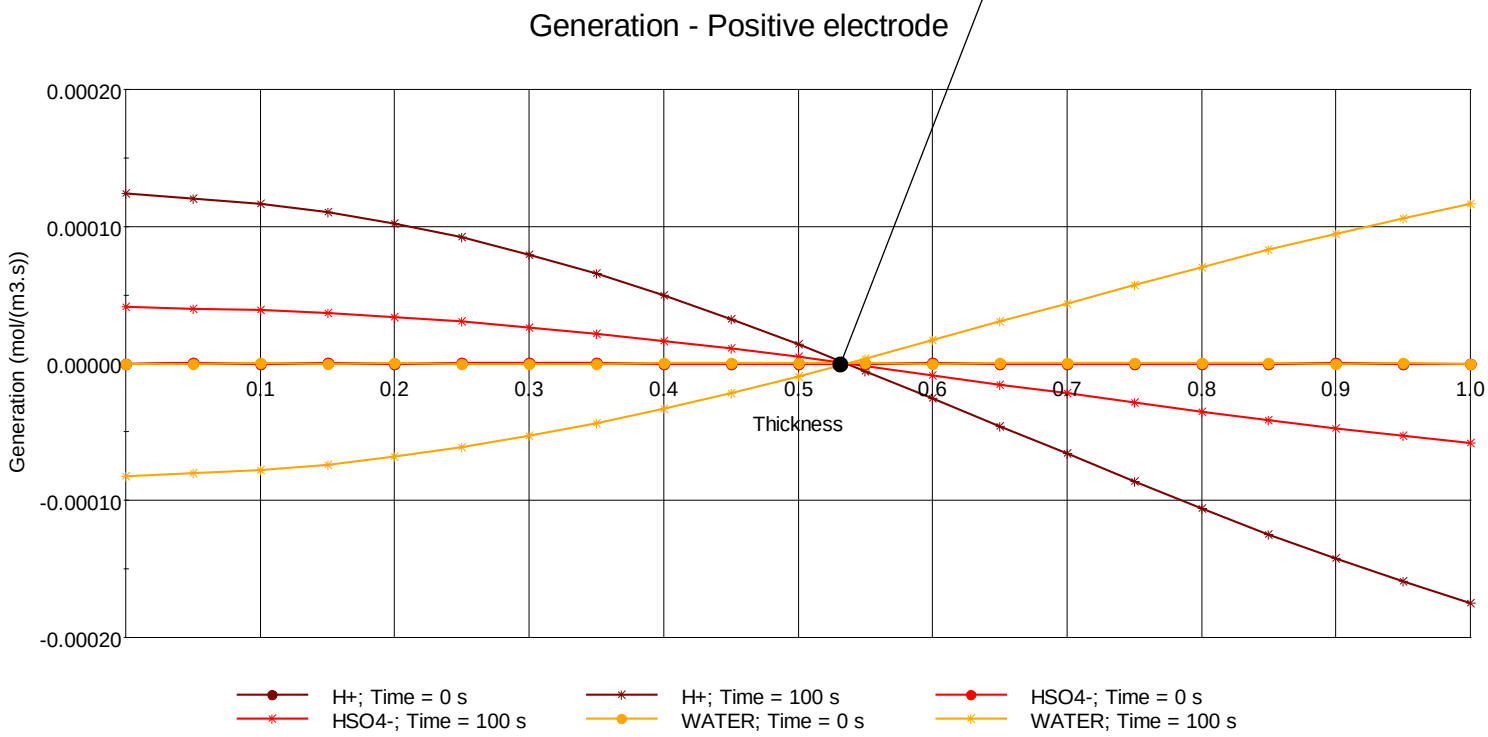
Electrochemistry and ionic mass transfer in 1D-Model

RESULTS – Electrochemistry at Open Cell state

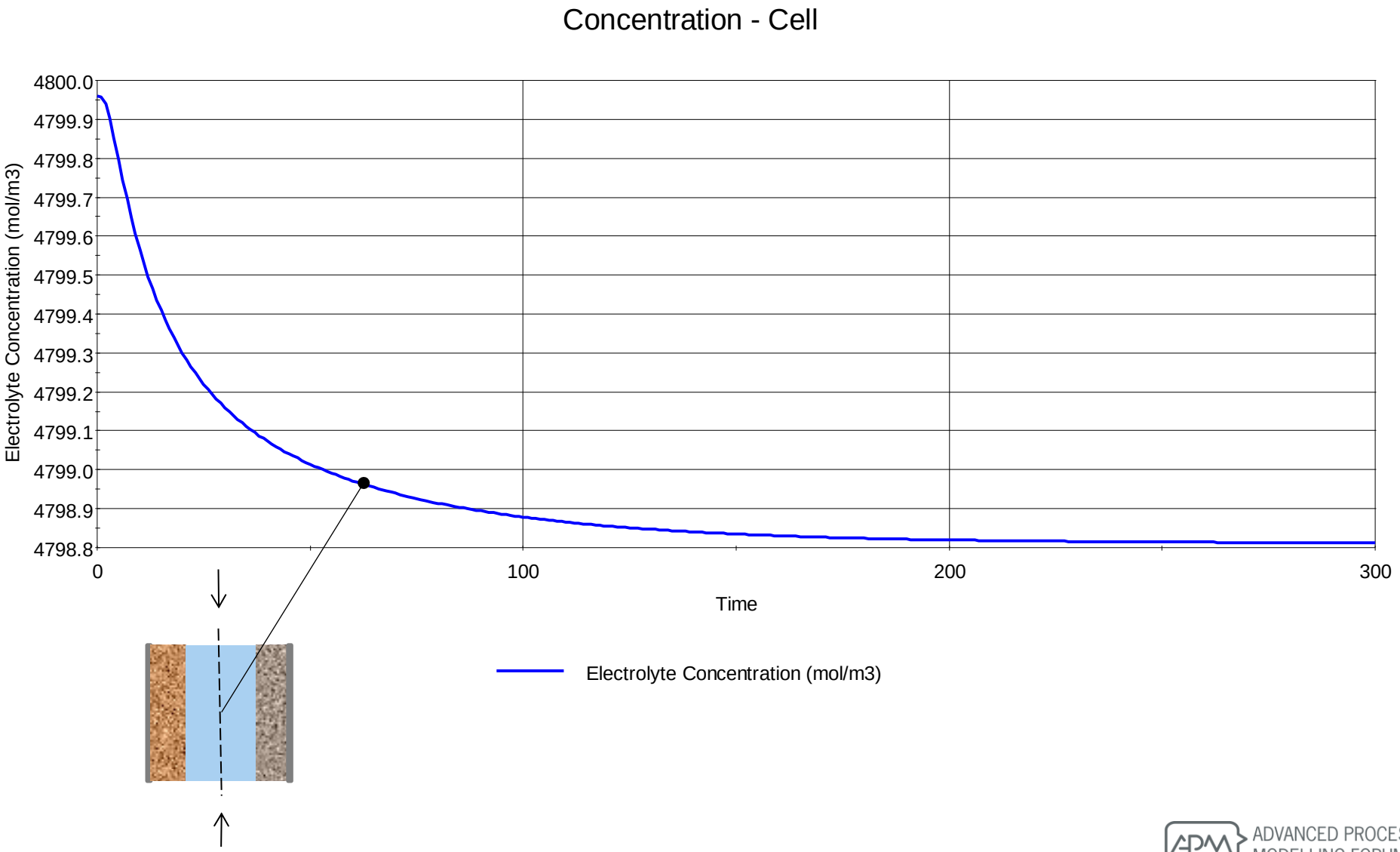
SPECIFICATIONS IN THE MODEL

- Same concentration through the cell
- Current = 0
- Electrodes' Charge: $Q_{Positive} = 3.15 \times 10^7\ C/m^3$;
  $Q_{Negative} = -3.15 \times 10^7\ C/m^3$



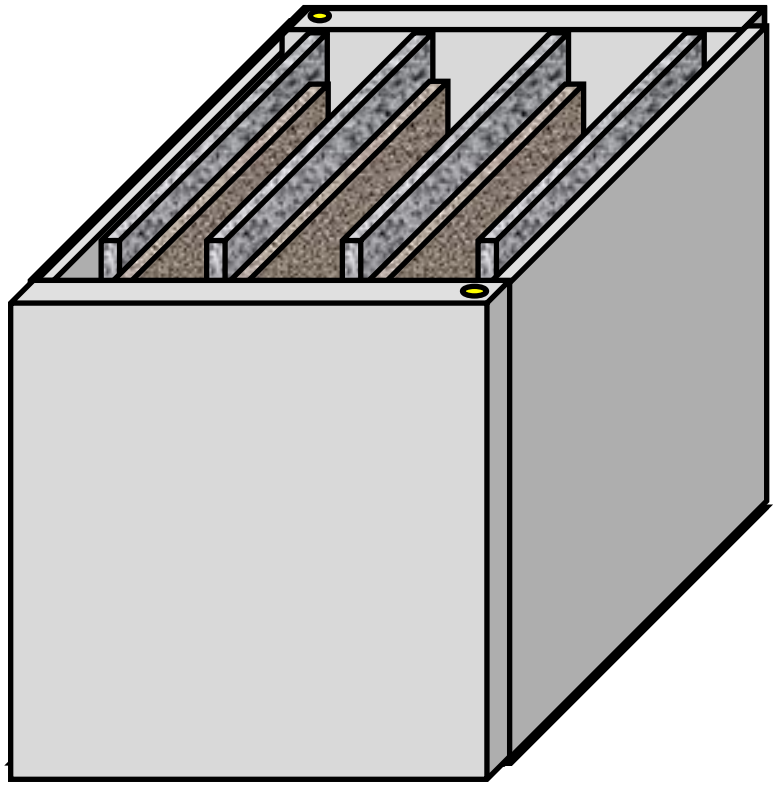


RESULTS – terminal concentration in bulk electrolyte

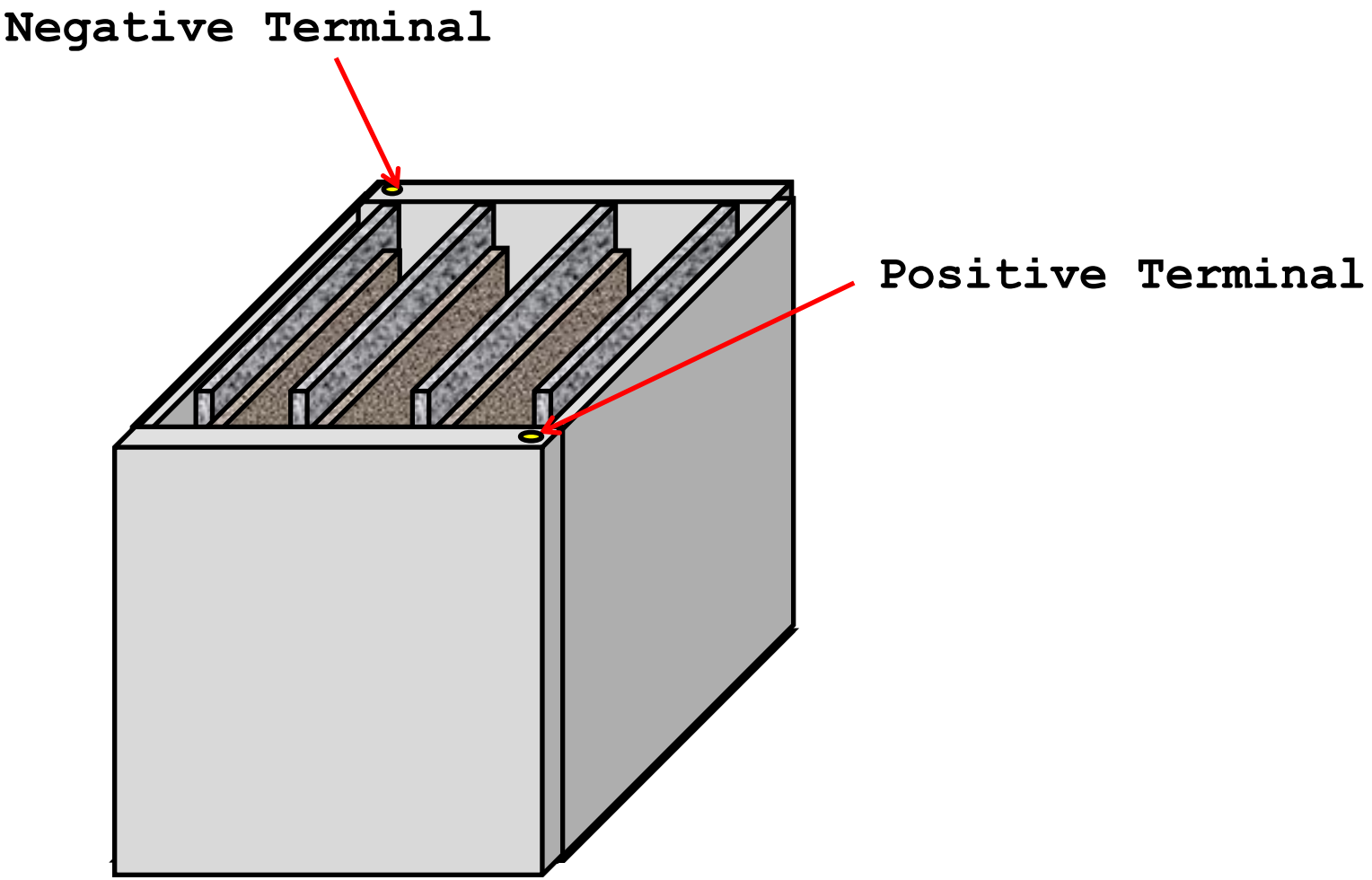


Ions composition and potential field in 2D-Model

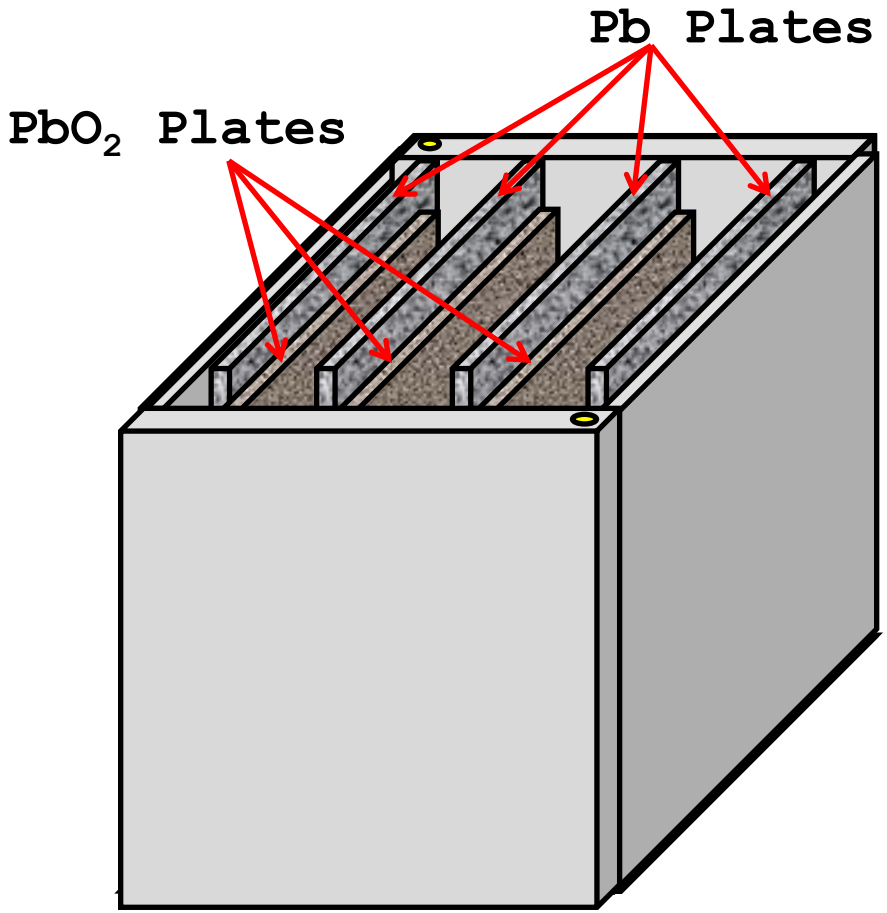
Lead-Acid Battery Arrangement



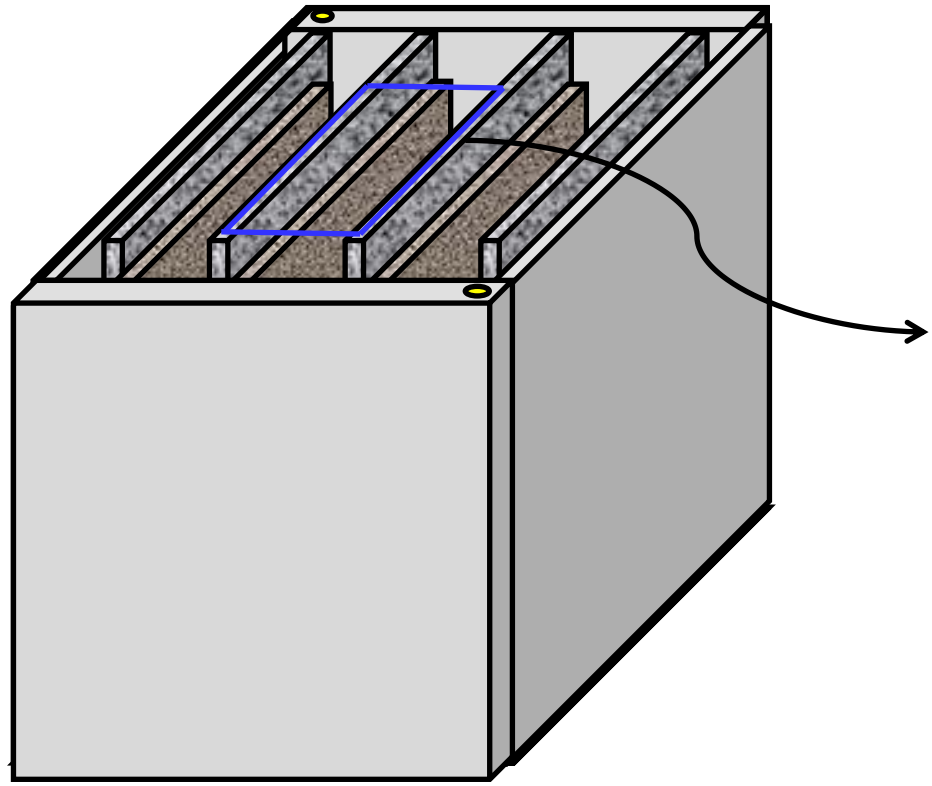
Lead-Acid Battery Arrangement

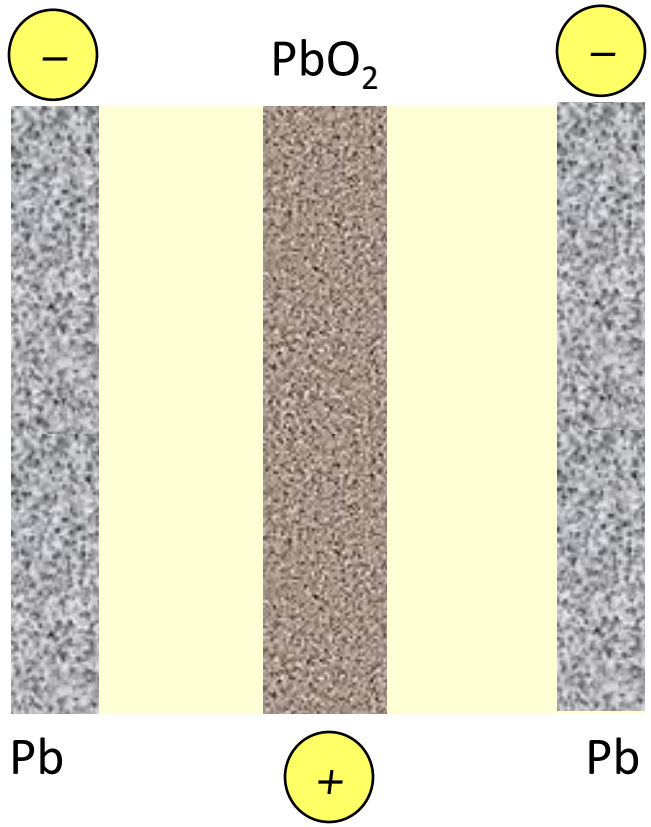


Lead-Acid Battery Arrangement



Lead-Acid Battery Arrangement





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MODELLING FORUM **2014**

Thank you