SOFC-Life
(256885)

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Solid Oxide Fuel Cells – Integrating Degradation Effects into Lifetime Prediction Models

project data	
reference	FCH JU 256885
start date	01/01/2011
end date	31/12/2013
duration	36 months
total costs	5.700.000 €
FCH JU funding	2.400.000 €
	42 %

partners - research & university			
DTU-EC	Denmark	EPFL	Switzerland
VTT	Finnland	EMPA	Switzerland
CEA	France	ZHAW	Switzerland
FZ Jülich	Germany	Imperial College	United Kingdom
IHTE	Russia		

partners - industry			
TOFC	Denmark	HTCeramics	Switzerland
EDF	France	HEXIS	Switzerland

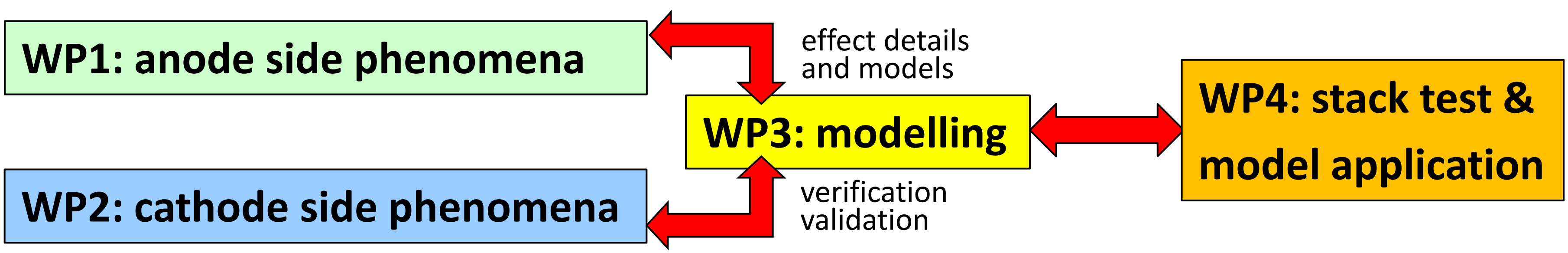
Project objectives & approach (1/3)

Objectives

- Understand the details of the major SOFC continuous degradation effects
- Develop models that predict single degradation phenomena
- Transfer the physical-chemical models to electrochemical models
- Re-assemble the single effect models to a full SRU life-time prediction model

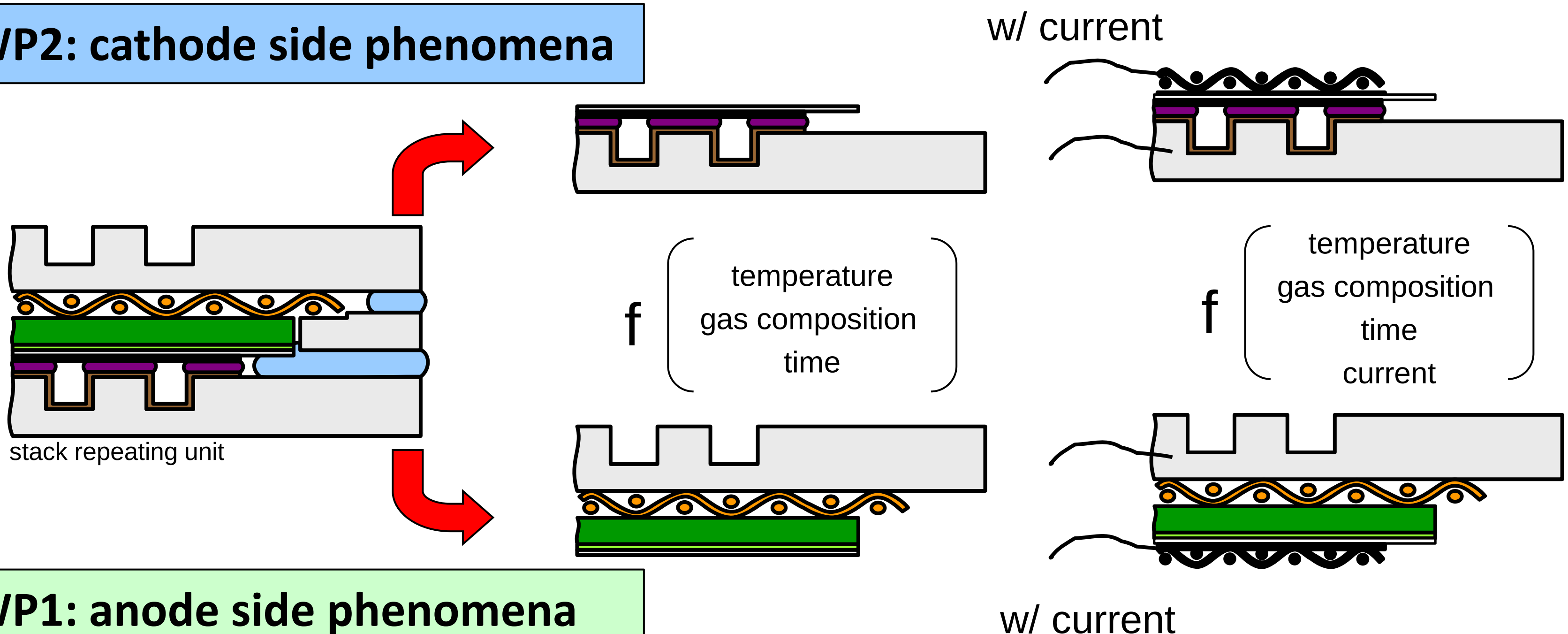
Approach

- dis-assemble the SOFC single repeating unit to model elements representing single degradation phenomena (anode and cathode compartment)



Approach

WP2: cathode side phenomena



WP1: anode side phenomena

result

changes in composition (phase) and morphology (*post-test*)

additional: changes in resistance (*in-situ*)

Main topics (degradation mechanism)

WP2: cathode side phenomena

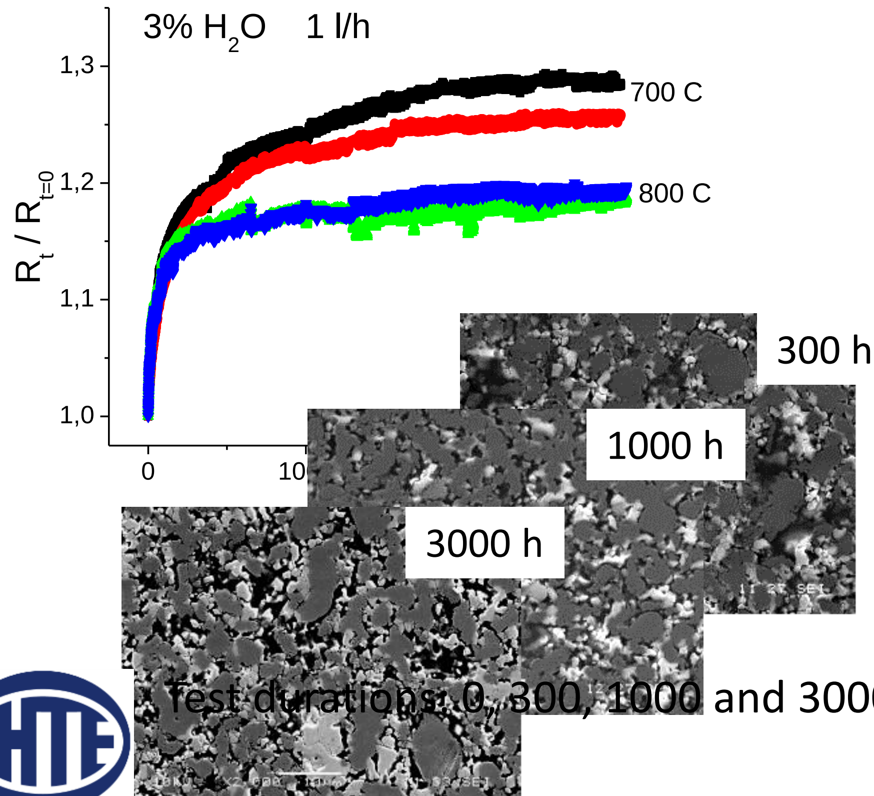
- the stability (chemical, kinetic and morphological) of state of the art cathode materials (impacting the cathode activity)
- processes at the cathode-interconnect interface (impacting electrical continuity and chemical composition of components, thus their electrochemical performance)

WP1: anode side phenomena

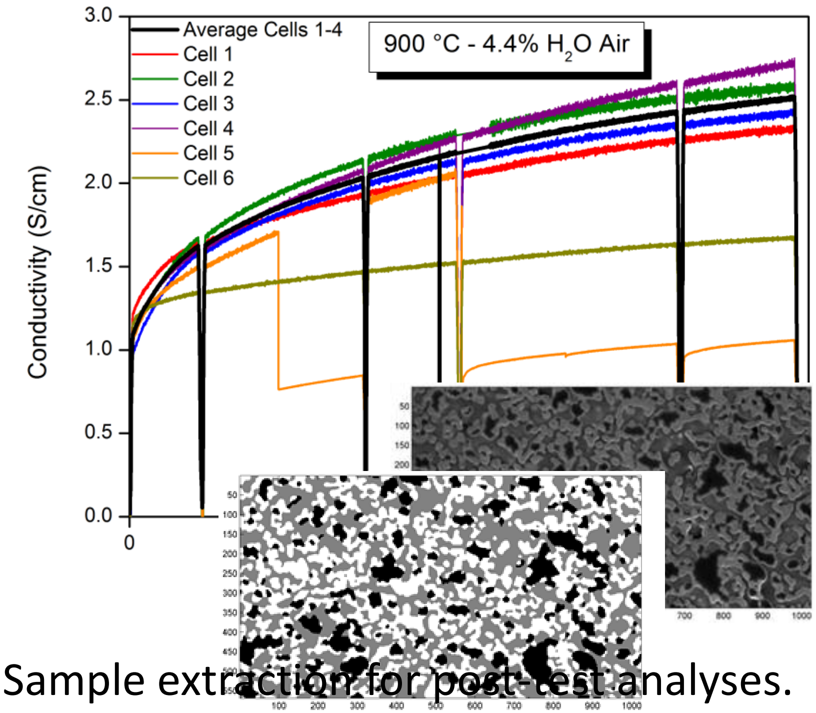
- morphological change in the anode cermet (impacting on anode activity and electrical continuity)
- nickel-steel corrosion (impacting on electrical continuity and conductivity)

Exposure tests of selected materials (combinations)

WP1: anode side phenomena



WP2: cathode side phenomena



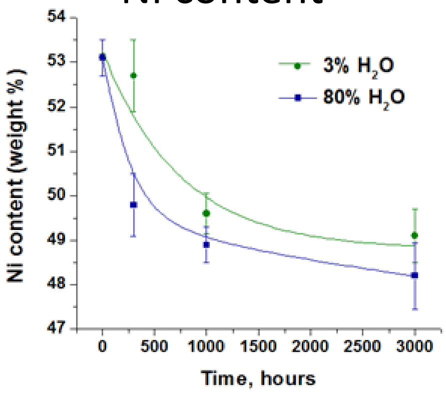
Test durations: 0, 300, 1000 and 3000 h. Sample extraction for post-test analyses.

SOFCLife

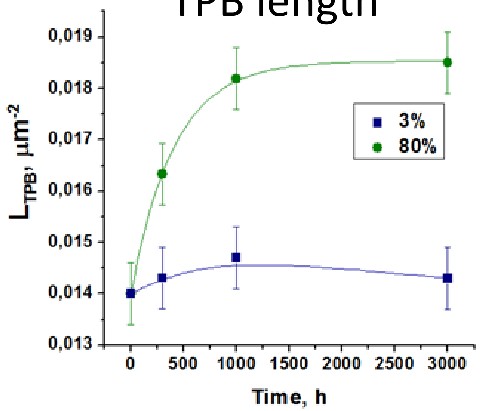
Post-test analysis

WP1: anode side phenomena

Ni content

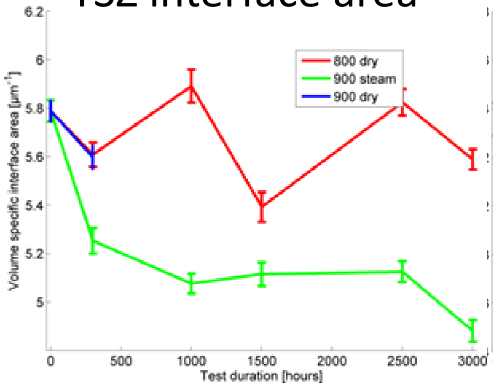


TPB length

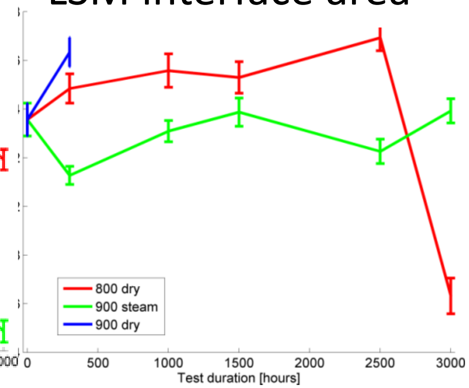


WP2: cathode side phenomena

YSZ interface area



LSM interface area



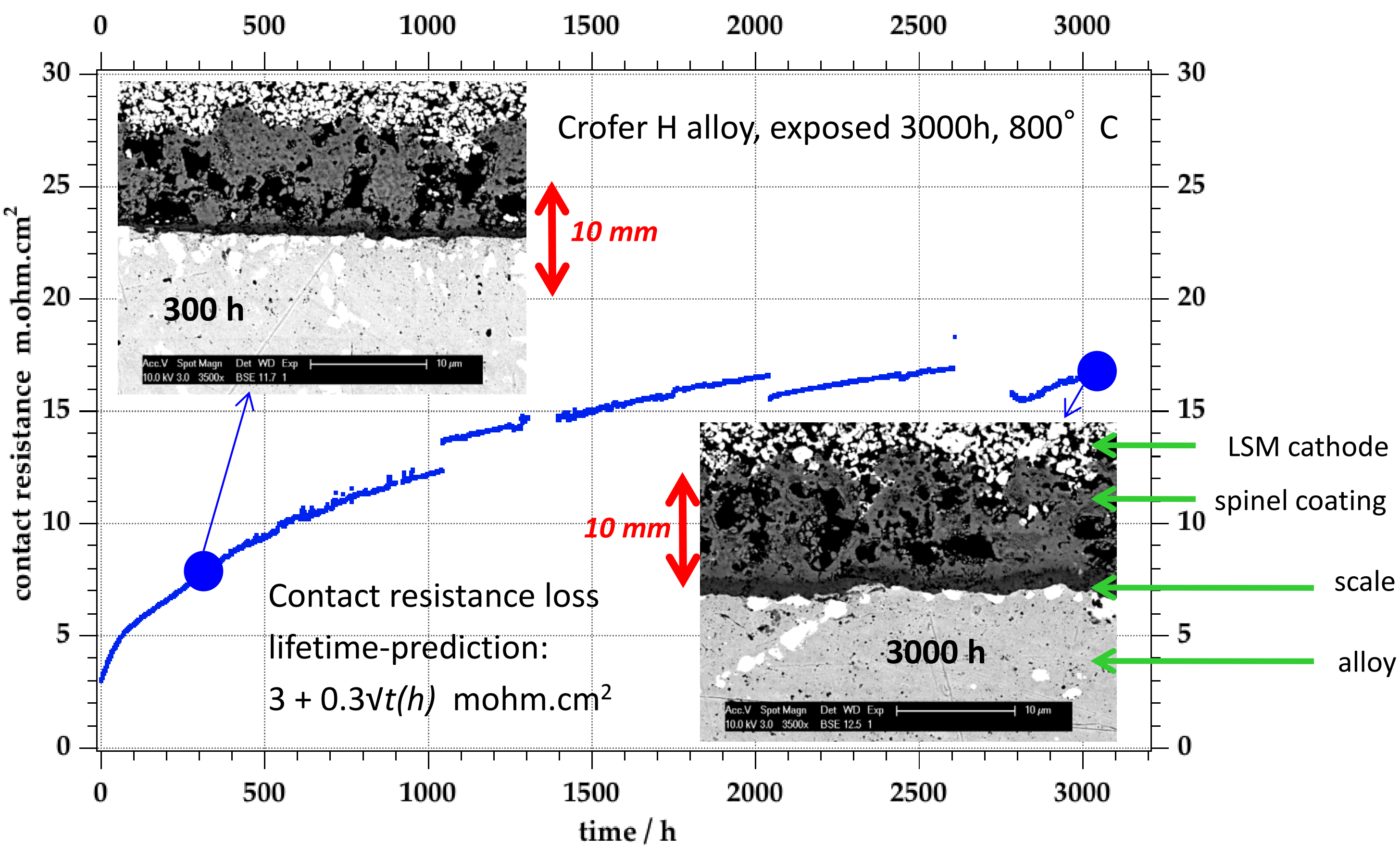
$$y = f(T, P_{H_2}, P_{H_2O}, \tau)$$

IHTE

DTU Energy Conversion
Department of Energy Conversion and Storage

WP2: cathode side phenomena

Cathode-Interconnect Interface



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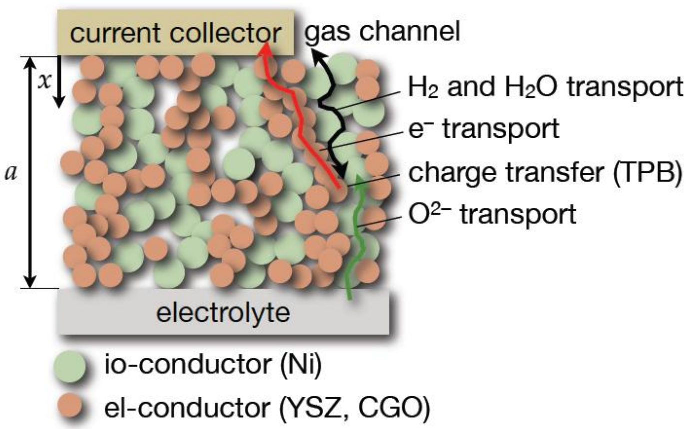
WP3: modeling and verification

anode side



Input from microstructure analysis

Ni	σ_{eff} ele	LSM
YSZ	σ_{eff} ion	YSZ

Active TPB length

Simulated processes

Charge-transport by Ohm's law

$$-\mathbf{div}(\sigma_{io}\nabla\phi_{io}) = p_{io}$$

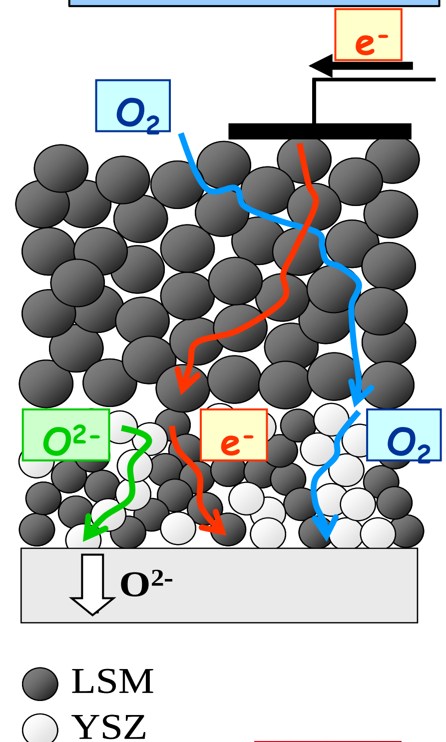
$$-\mathbf{div}(\sigma_{el}\nabla\phi_{el}) = -p_{io}$$

Charge-transfer by Butler-Volmer

$$p_{io} = A_{TPB}\, i_n = A_{TPB}\frac{i_0 F}{RT}\eta$$

$$\eta = U - U^{eq} = (\phi_{el} - \phi_{io}) - (\phi_{el}^{eq} - \phi_{io}^{eq})$$

cathode side



Output: prediction of electrode performance

$$\mathrm{ASR_{tot}} = \frac{U_{tot}}{i_{tot}} = \frac{\phi_{el}|_{x=0} - \phi_{io}|_{x=a}}{i_{tot}}$$

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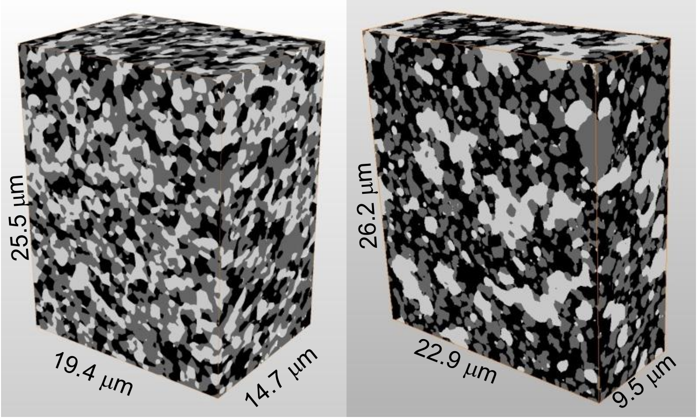
WP3: modeling and verification

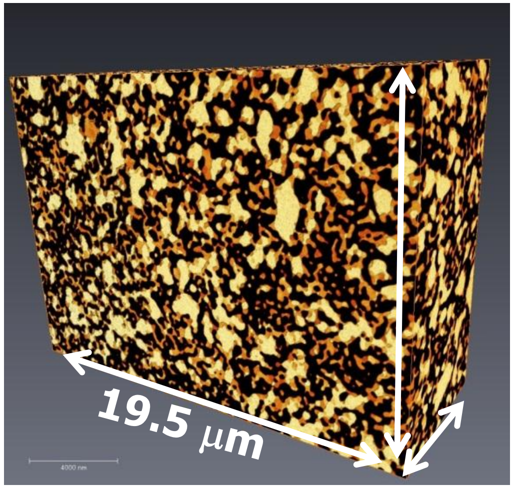
anode side

3D reconstruction by FIB/SEM tomography

cathode side



Microstructure quantification



Fresh Ni-8YSZ volume of
25.5 x 19.4 x 14.7 µm3

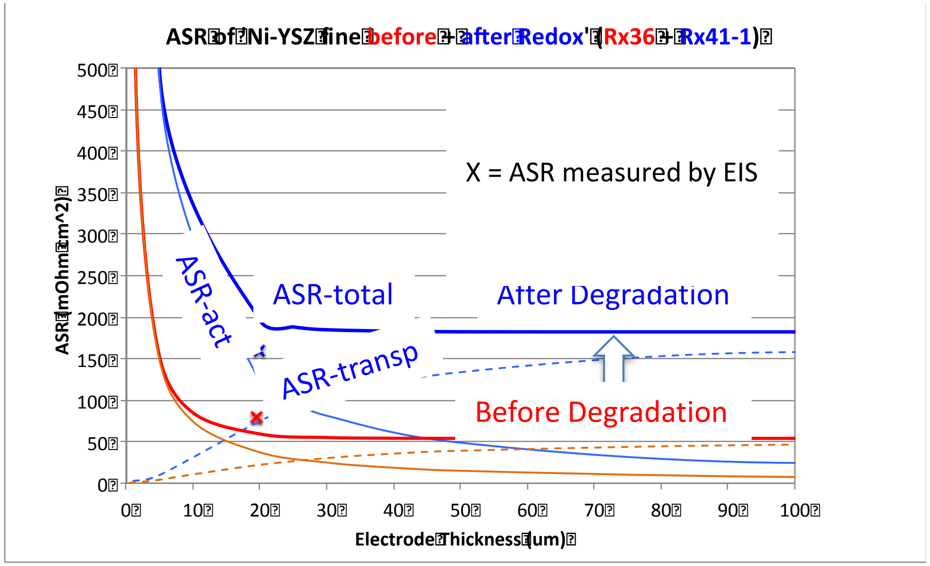
Fresh LSM-8YSZ volume of
19.5 x 14.8 x 7.6 µm3

WP3: modeling and verification

anode side

cathode side

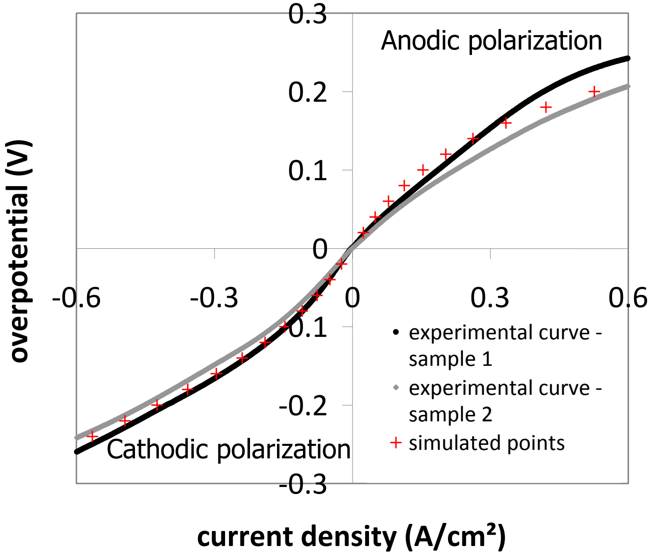
Prediction of ASR performance (before and after degradation)



The simulation provide total ASR and components of ASR related to charge transport and TPB-reactions.

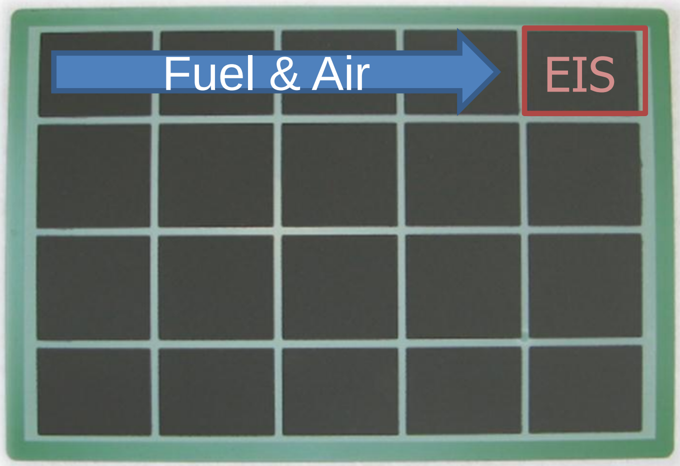
ASR_{total} predictions are in good agreement with EIS-measurements

Electrode modeling in anodic and cathodic polarization

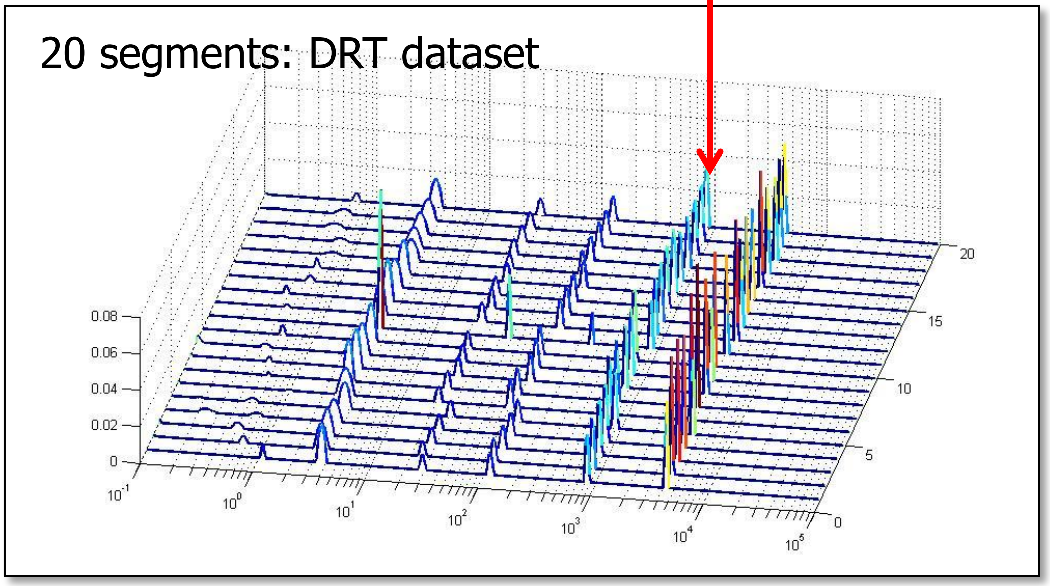


WP3: modeling and verification

- segmented 1-cell stack: 20 * 4 cm^2 electrode segments covering the whole flow field
- 1000 h tests (in H_2 and CH_4/H_2O) with periodical EIS allow to monitor ***local*** degradation processes



anode charge transfer

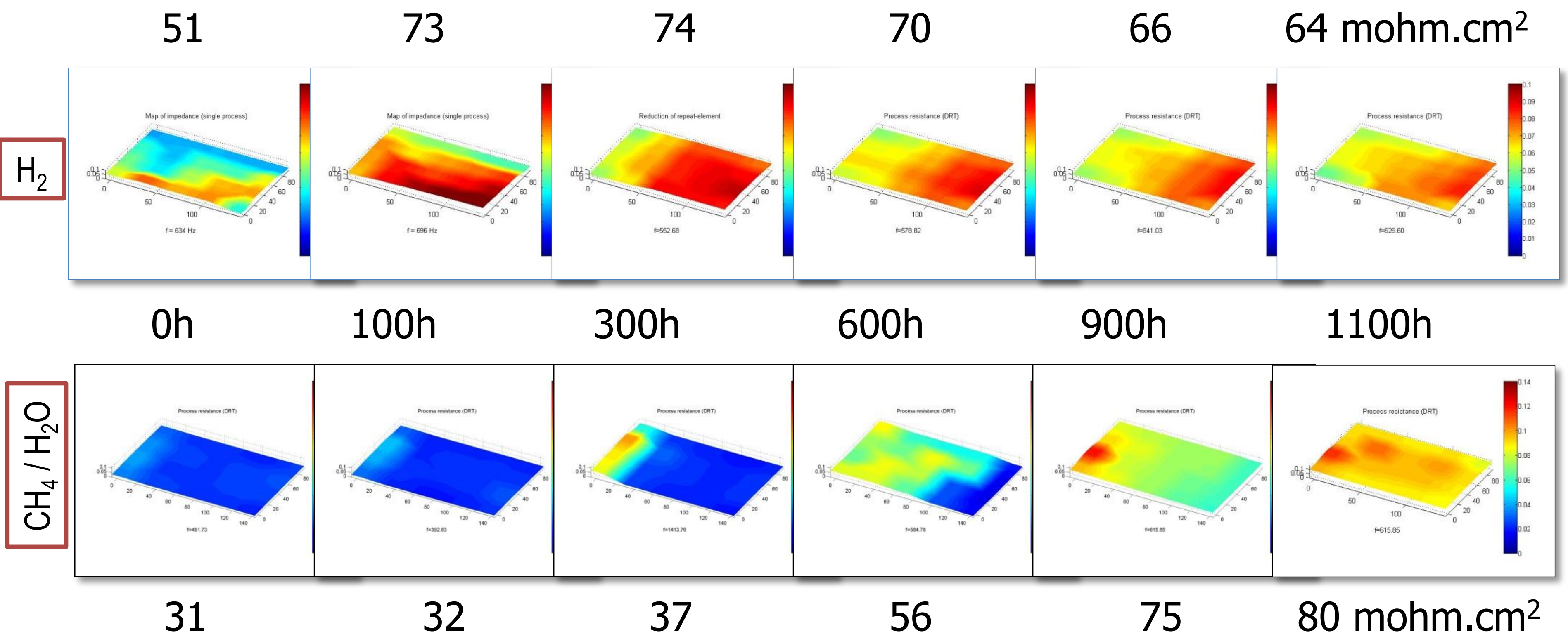


6 processes at well-defined frequencies identified on all 20 segments

Project achievements (8/9)

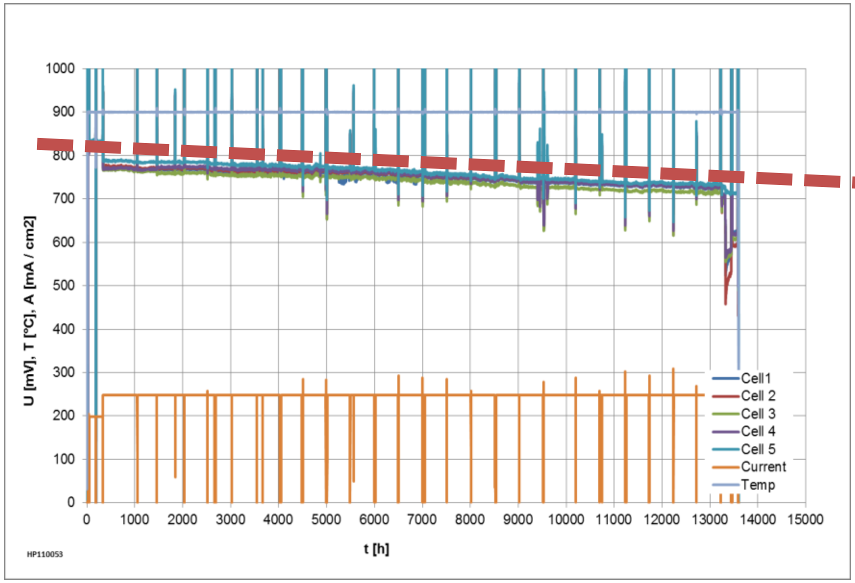
WP3: modeling and verification

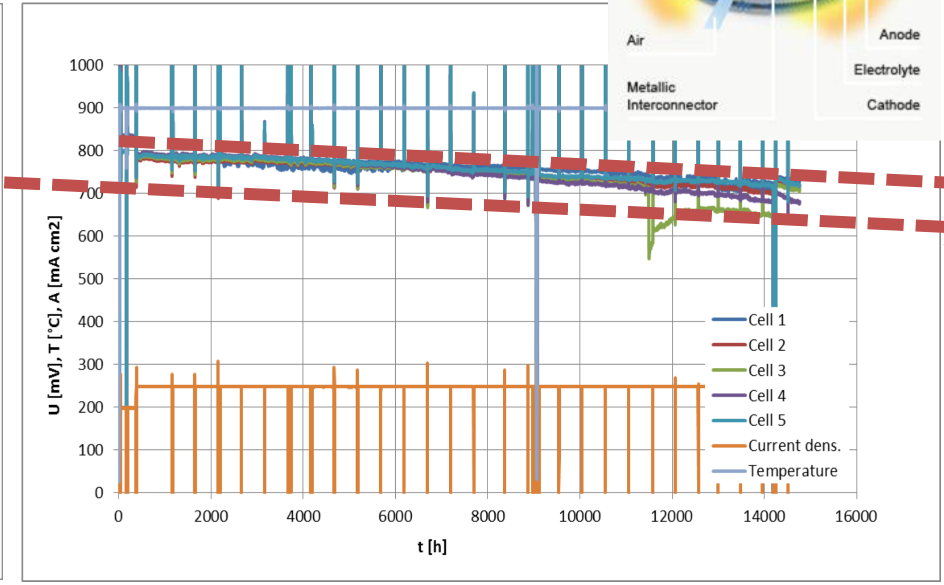
- example of local monitoring of anode charge transfer process, >1000 h, in H_2 and CH_4/H_2O fuel
- very different behavior (temporal and spatial) between the two cases

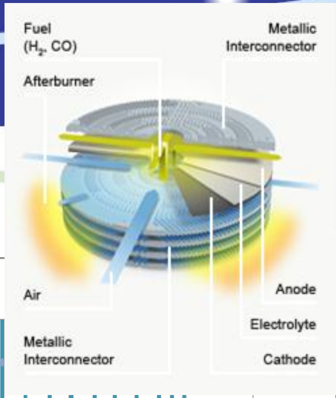


WP4: stack test & model application

for Hexis ECS-type SOFC







- Power density approx. 0.2 W/cm²; electrical efficiency approx. 37 % DC
- Degradation approx. 4 mV, i.e. 0.5 % / 1000 h over 13000 h
- Linear degradation, Fits well to the data measured on system level, as well as the model
- No progressive degradation but, lab incident destroyed one, harmed the other

Self Assessment Summary

Estimation of the probability that the project will achieve the objectives:

- Understand the details of the major SOFC continuous degradation effects

  From the four themes investigated only processes at the cathode-interconnect interface can be considered to be a major contribution to the overall degradation observed in SRUs and stacks.

➢ Objective is achieved.

- Develop models that predict single degradation phenomena

  Microstructural parameters as function of operating conditions and time for cathodes and anodes have been extracted for use in the respective sub-models. Due to a limited number of experiments on the stability of the LSCF cathode as function of time no sufficient data is available for the implementation of this cathode in the model.

➢ Objective will be partly achieved.

Self Assessment Summary

Estimation of the probability that the project will achieve the objectives:

- Transfer the physical-chemical models to electrochemical models

  Cellular automaton model developed to predict 3D microstructure evolution, and corresponding degradation of polarization resistance, of Ni/YSZ and Ni/CGO anodes and LSM/YSZ cathodes.

➢ Objective will be achieved for the anodes and cathodes mentioned.

- Re-assemble the single effect models to a full SRU life-time prediction model

➢ Objective will most likely be achieved.

Alignment to MAIP/AIP (1/1)

Relevance to call & AIP 2009

- Application area: Stationary power production and CHP
- Topic: SP1-JTI-FCH.3.1: Degradation and lifetime fundamentals

SOFC-Life addresses:
basic research activities directed to **degradation and lifetime fundamentals** of SOFC technology,
focusing on SOFC materials available and in industrial application today

(cf. MAIP section 3.4.3 page 15 - updated version adopted November 2011)

Relationship to Earlier and Other Current Projects

SOFC-Life

builds on experiences and data collected

in the projects Real-SOFC, SOFC600 and FlameSOFC,

follows protocols from FCTES^{QA} when appropriate,

and many others in which the partners have participated.

In turn protocols from SOFC-Life are being used in the project SCORED2.

Complementarity with Projects from Other Programs

Co-funding:

- VTT: (Finish) National Fuel Cell Technology Program (TEKES)
- IHTE: (National Russian Foundation for Fundamental Research)
- DTU-EC: Danish PSO-financed program (Top-up grant)

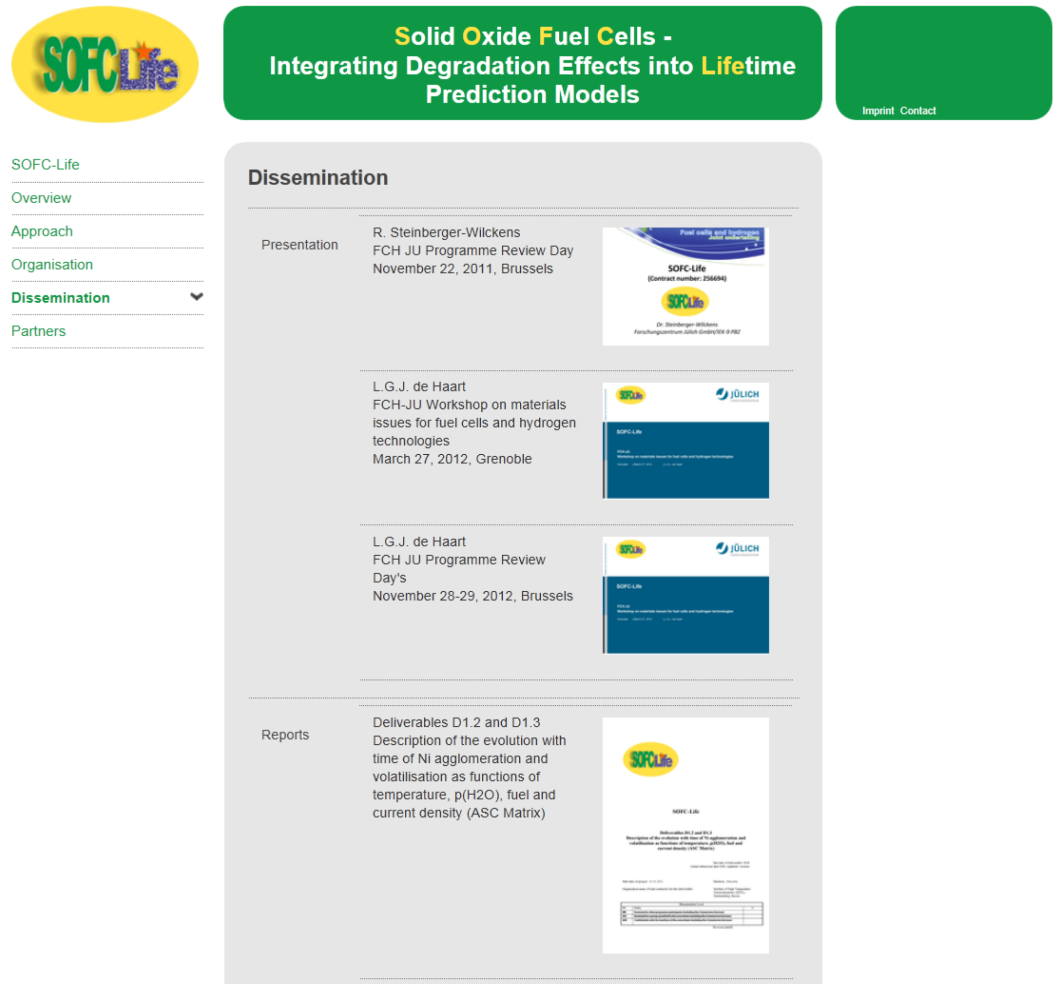
Participation in related / complementary projects:

- see above
- DTU-EC: SOFC Accelerated (Danish, EUDP); Towards Smart Grid Ready SOFC (Danish, ForskEl); METSAPP (EU)
- FZ Jülich: German project on SOFC Degradation to start June 2014

Cross-cutting, Dissemination & Exploitation Activities (1/1)

Cross-cutting & Dissemination Activities

- Publications,
  conferences presentations
- website www.sofc-life.eu



Cross-cutting & Dissemination Activities

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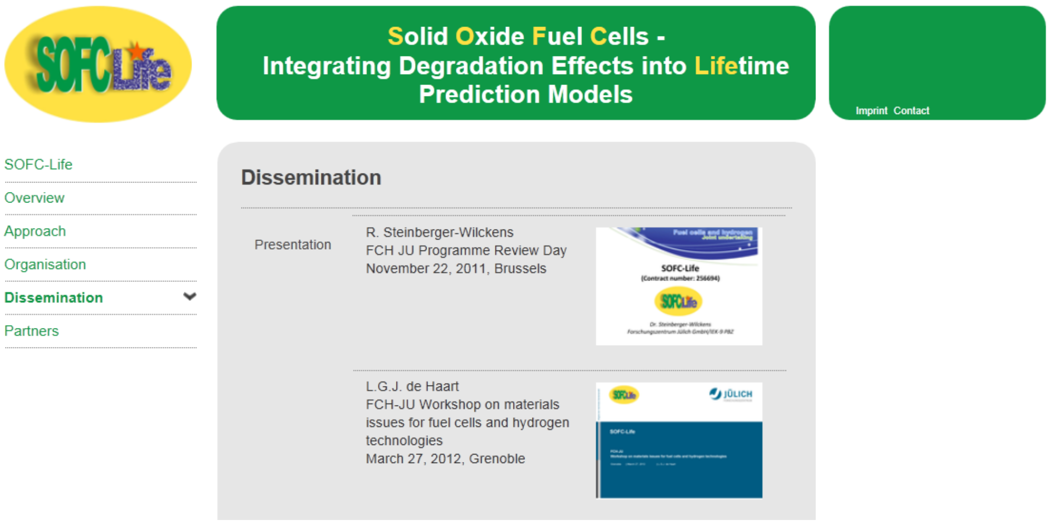

Exploitation & Post-Project Activities

- direct use of results by participating industries and SMEs

Further RTD activities

- Degradation models will require further refinement
  to make them applicable to a wider range of cell types and operating conditions.
- Basic understanding should be applied
  to develop soundly based accelerated tests.

Thank you for your attention

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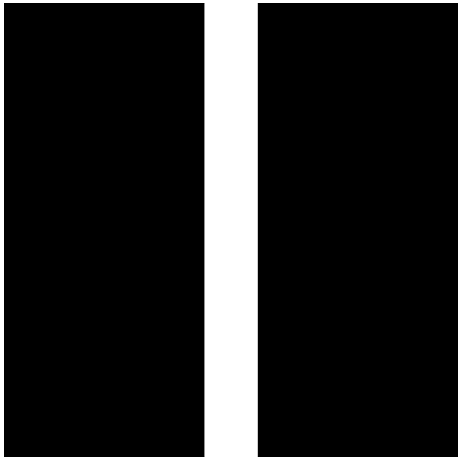
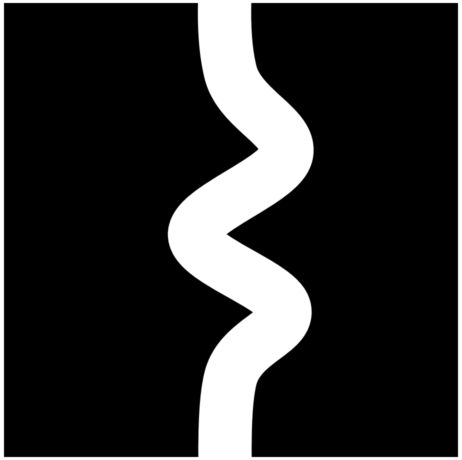
WP3: modeling and verification

Relationship between effective transport properties and microstructure

Porosity (ε)

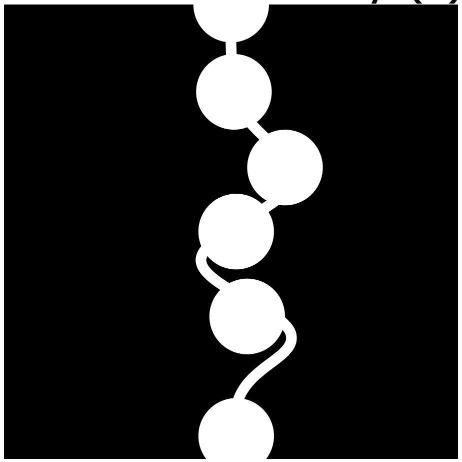


Porosity &
Tortuosity (τ)



Factor due to
extra pathway
lengths

Porosity &
Tortuosity &
Constrictivity (δ)



Factor due to
uneven path radii
(bottlenecks)

$$M = \frac{\varepsilon\delta}{\tau} \qquad \sigma_{eff} = M\sigma$$

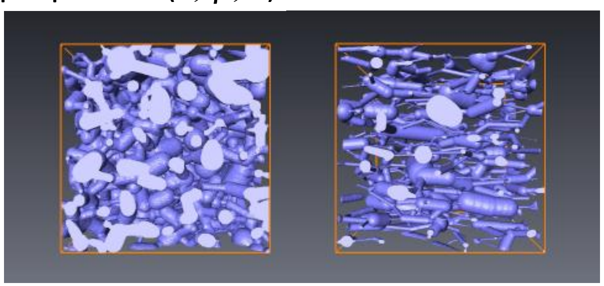
L. Holzer et. Al., Journal of Materials Science 48(7): 2934-2952, 2013

Back-up: (2/2)
Microstructure factor (M-factor)

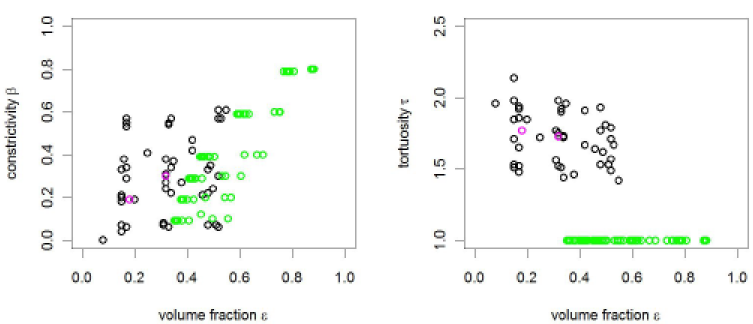
WP3: modeling and verification

Relationship between effective transport properties and microstructure investigated with virtual materials testing

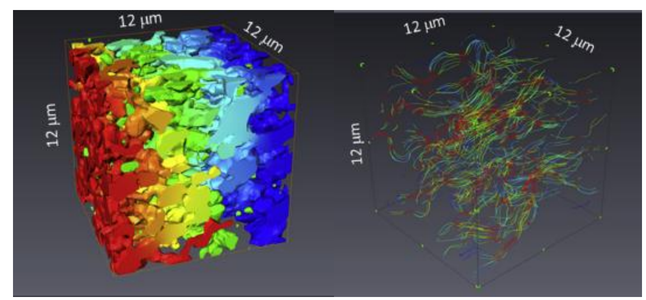
a) **More than 100 virtual microstructures** with specific properties (ε, β, τ) are created with **stochastic geometry**.



b) The virtual microstructures cover a **wide range of microstructure parameters** (ε, β, τ) :



c) **Finite Element Modeling** based on meshes from virtual microstructures is used to calculate the corresponding **effective conductivities σ_{eff}**



d) The database from virtual testing provides the relationship between microstructure parameters **(ε,τ,β)** and effective transport properties **(σ_{eff})**.

Using statistical error minimization leads to the following relationship:

$$\sigma_{\text{eff}} = \sigma_0 \boxed{2.03\,\varepsilon^{1.57}\,\beta^{0.72}/\tau^{2}}$$

'M-factor'

This expression can be used to describe effective electric and ionic conductivities as well as gas phase diffusivity