Multiphysics Simulation of an Anode-supported Micro-tubular Solid Oxide Fuel Cell (SOFC)

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Fraunhofer
IKTS

COMSOL
CONFERENCE
STUTTGART 2011
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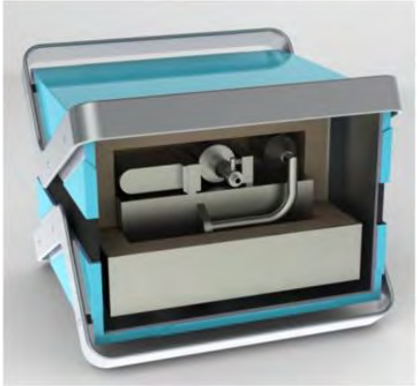
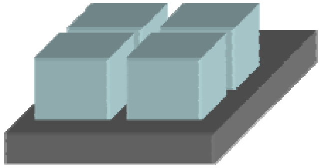
SOFC systems developed at IKTS

Different power rates

10 W	100 W	1 kW	10 kW	20 kW
				
ezelleron Power to go	eneramic by Fraunhofer	Vaillant		
Tubular SOFC	LPG SOFC	Natural gas SOFC	Biogas SOFC	Multiple CFY-Stacks

LPG Liquefied Petroleum Gas

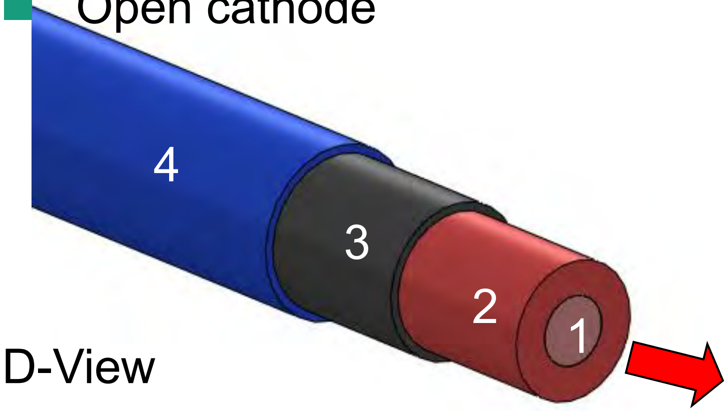
AGENDA

- Model setup
- Results
- Conclusion

Model of a tubular SOFC

Layout of a micro-tubular SOFC

- Specific advantages:
  - Fast thermal startup
  - High thermal stability
- Typical length in a range of some cm
- Anode Supported Cell (ASC)
- Open cathode



3D-View

Axisymmetric Sketch (scaled)

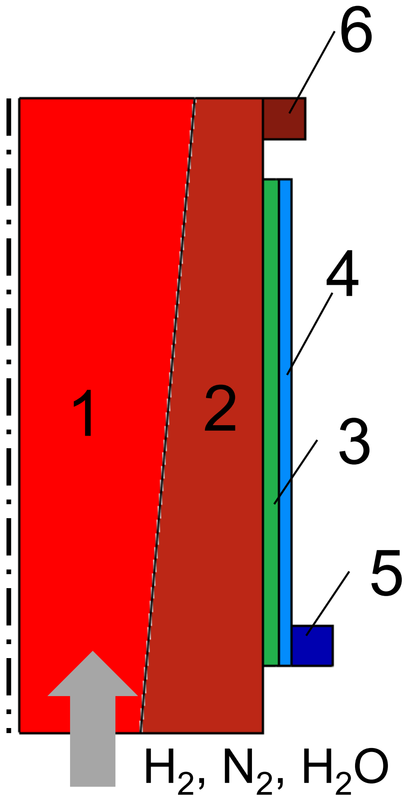
1 Anode channel

2 Porous anode

3 Electrolyte

4 Porous cathode

5/6 Current collectors



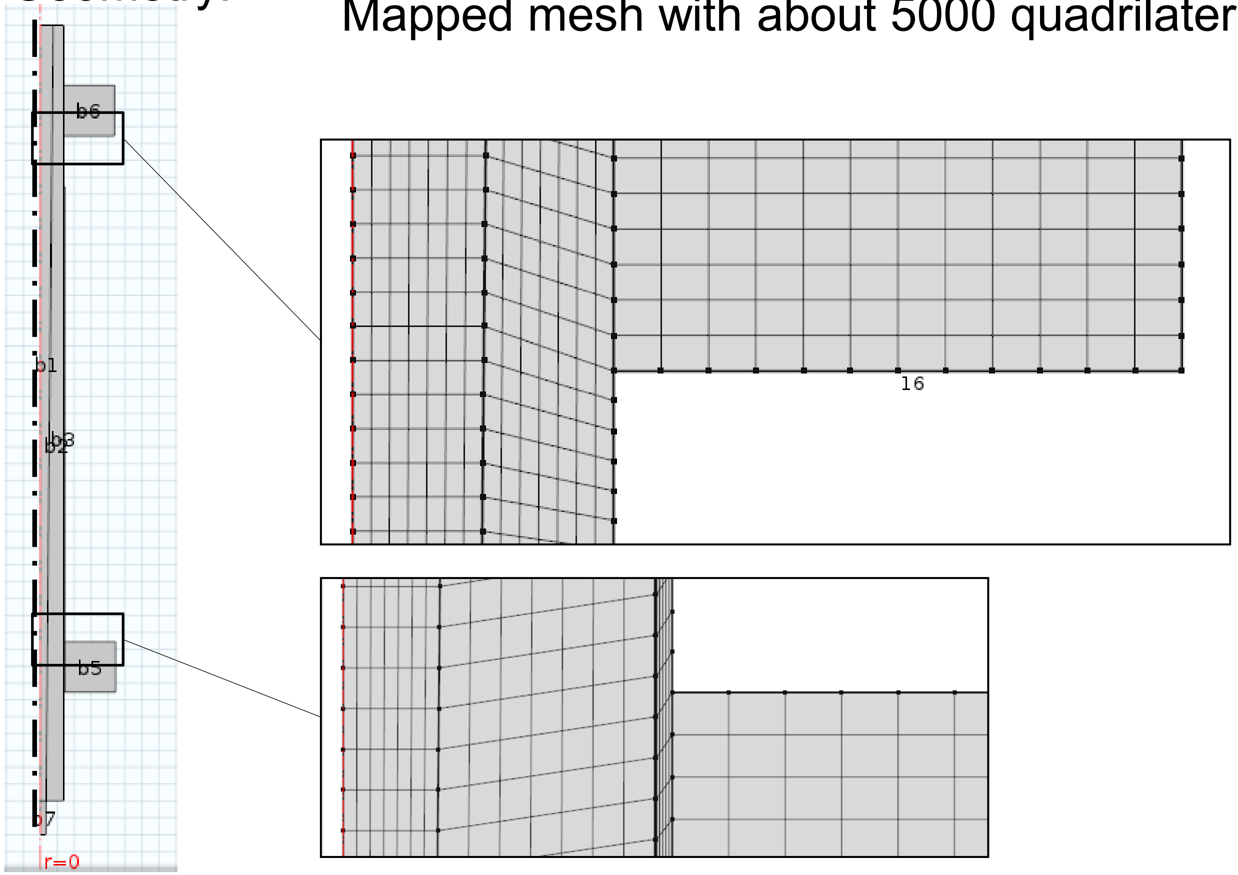
Model setup
Model development in COMSOL 4.2

- Axisymmetric model of microtubular SOFC
- Parameterized axisymmetric geometry of a single cell
- Multiphysics Simulation
  - Anode gas flow (Navier-Stokes equations, laminar)
  - Heat transfer(convection, conduction, radiation to the hotbox)
  - Diffusion (multicomponent Maxwell-Stefan diffusion)
  - Electrochemical submodel
    - Electric conduction
    - Reduced Butler-Volmer kinetics
  - Special treatment of porous zones (effective properties)
- In total seven physical modes

Model setup
Meshing

Geometry:

Mapped mesh with about 5000 quadrilateral elements



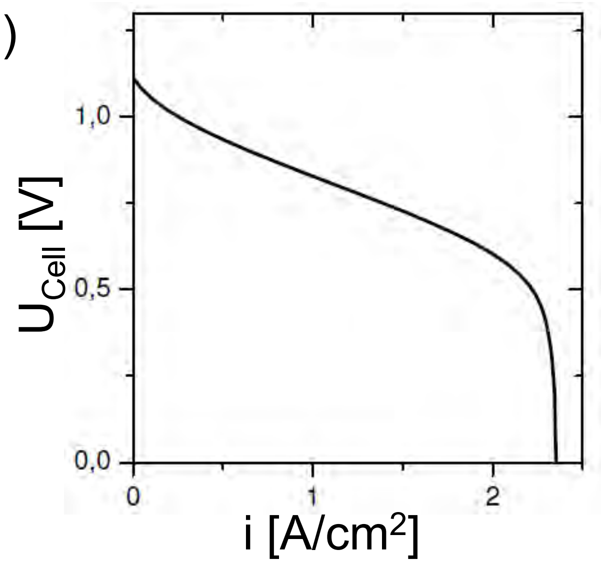
Model setup

Electrochemical submodel

- Aim: Description of characteristic polarization behaviour
- Conservation of charge (two electric currents modes)

$$\nabla \cdot \left(\vec{j}_{\mathrm{ele}} \right) + \nabla \cdot \left(\vec{j}_{\mathrm{ion}} \right) = 0$$

$$\nabla \cdot \left(-\sigma_{\mathrm{ele}} \nabla \phi_{\mathrm{ele}} \right) + \nabla \cdot \left(-\sigma_{\mathrm{ion}} \nabla \phi_{\mathrm{ion}} \right) = 0$$



- Faraday‘s law couples molar and current flow:

$$\vec{N}_i = \pm \frac{\vec{j}_{\mathrm{ele}}}{nF}$$

- Butler-Volmer equation at electrode/electrolyte interface:

$$\eta_{\mathrm{act}}^{a,c} = \left(\phi_{\mathrm{ele}}^{a,c} - \phi_{\mathrm{ion}}^{a,c} \right) - E_{\mathrm{rev}}^{a,c}$$

$$i_{BV} = \boxed{i_0} \left\{ \exp\left(\frac{\alpha_a F \eta_{\mathrm{act}}}{RT} \right) - \exp\left(-\frac{\alpha_c F \eta_{\mathrm{act}}}{RT} \right) \right\}$$

$$E_{\mathrm{Nernst}} = E_{\mathrm{rev}}^{c} - E_{\mathrm{rev}}^{a} = -\frac{\Delta G}{2F} + \frac{RT}{2F} \ln\left(\frac{x_{\mathrm{H_2}} x_{\mathrm{O_2}}^{0.5}}{x_{\mathrm{H_2O}}} \right)$$

$\vec{j}$	current density	α	symmetry factor	R	universal gas constant
σ	electric conductivity	F	Faraday constant	ΔG	Gibbs free energy
ϕ	potential	η_{act}	activation overpotential	x_i	molar fraction
i_0	exchange current density	T	temperature	$\vec{N}$	molar flux

Model setup
Mass transport submodel

- Inside the anode channel, multicomponent diffusion for ternary mixture is used:

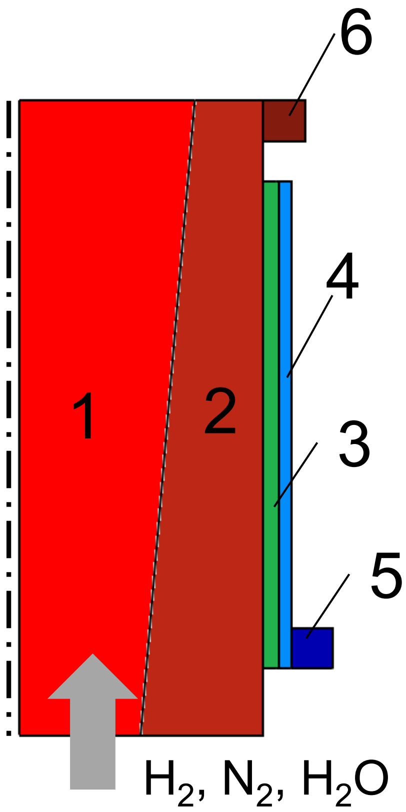
$$\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{X_i X_j}{\mathcal{D}_{ij}} \left(\frac{\vec{J}_j}{\rho_j} - \frac{\vec{J}_i}{\rho_i} \right) = \nabla X_i$$

- Inside the porous electrodes, Knudsen diffusion is dominant:

$$D_K^{\text{eff}} = \frac{\varepsilon}{\tau} \cdot \frac{1}{3} d_p \sqrt{\frac{8RT}{\pi M_i}}$$

$$D_K^{\text{eff}} = \boxed{a_{\text{Knudsen}}} \sqrt{\frac{T}{M_i}}$$

Fit parameter



1 Anode channel
2 Porous anode
3 Electrolyte
4 Porous cathode
5/6 Current collectors

T Temperature
p Pressure
D_{ij} Binary diffusion coeff.
$\vec{J}_i$ Diffusion flux
d_p Pore diameter
R Gas constant
ε Porosity
τ Tortuosity
x_i molar fraction
ρ density

Model setup

Heat sources in SOFCs

- Reversible losses:

$$q''_{rev,a/c} = T\cdot\Delta S_{a/c}\frac{i_{a/c}}{2F}$$

- Irreversible losses:
  - Ohmic heating

$$q''' = \sigma\cdot\nabla^2\phi$$

  - Overpotential losses

$$q''_{irrev,a/c} = \eta_{act,a/c}\cdot i_{a/c}$$

- Heat fluxes at outer surface:

$$q'' = q''_{\mathrm{convection}} + q''_{\mathrm{radiation}} = \frac{\mathrm{Nu}\cdot k}{D_h}\left(T - T_{amb}\right) + \sigma_0\cdot\varepsilon_{\mathrm{rad}}\left(T^4 - T^4_{amb}\right)$$

T	Temperature
ΔS	Molar entropy change
$i_{a/c}$	Current density at a/c-ele interface
F	Faraday constant
σ	Electric conductivity
ϕ	Electric potential
η_{act}	Activation overpotential
k	Thermal conductivity
D_h	Hydraulic diameter
$\varepsilon_{\mathrm{rad}}$	Radiative emissivity
σ_0	Boltzmann constant
T_{amb}	Ambient temperature (furnace)

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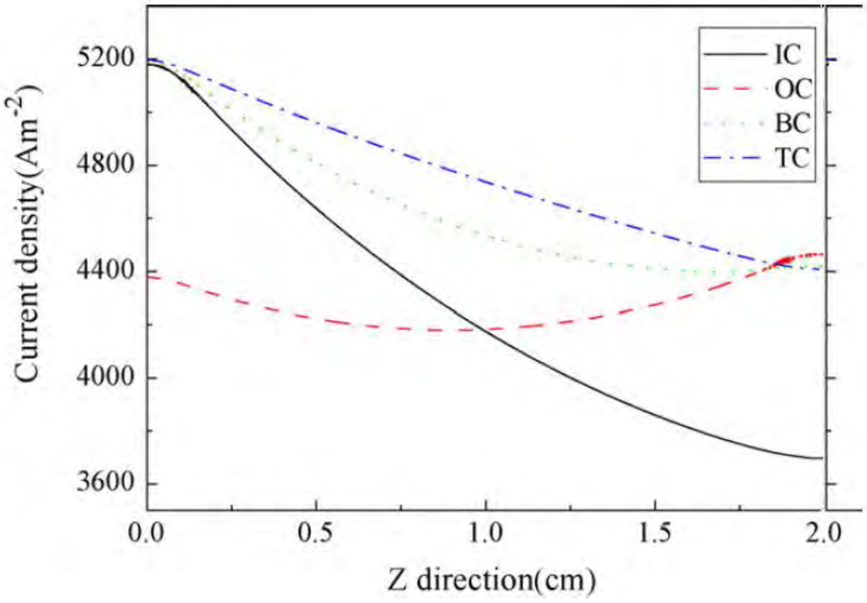
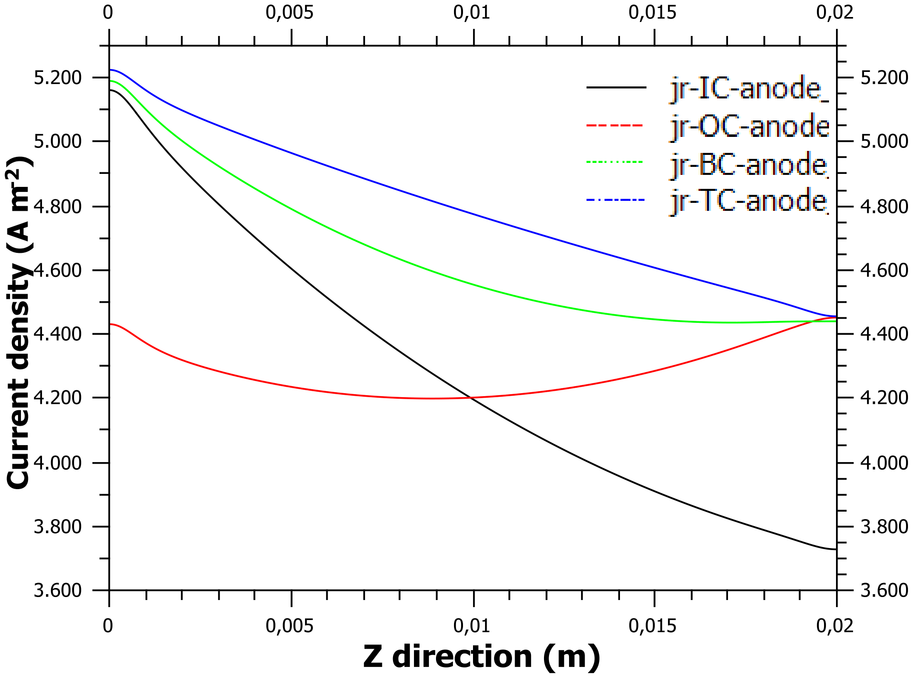
Validation

Comparison to published data

Cui 2007 Model



Own Model



Geometry:

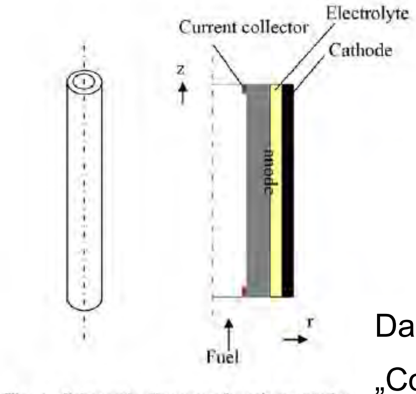


Fig. 1. Schematic diagram of a micro-tubular

Plot of current density at anode/electrolyte interface

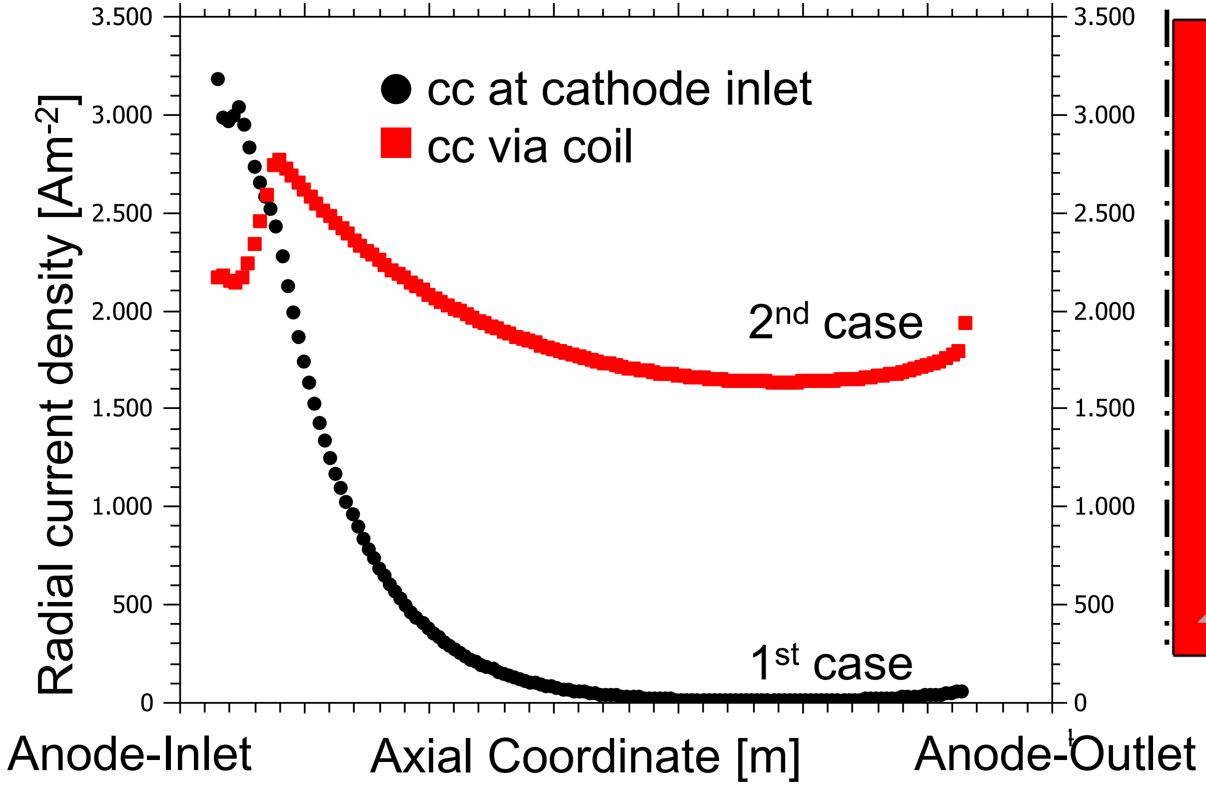
IC	anode inlet current collector
OC	anode outlet current collector
BC	both current collector
TC	total anode current collector

Daan Cui et al., 2007, Journal of Power Sources 174 (2007) 246–254
„Comparison of different current collecting modes of anode supported micro-tubular SOFC through mathematical modeling“

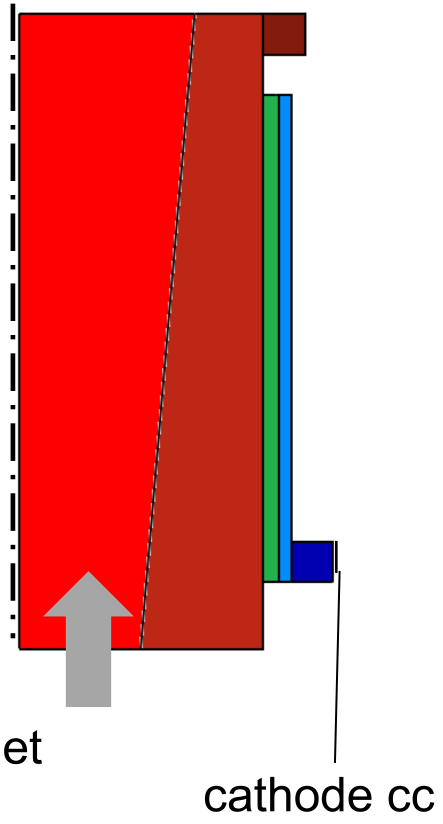
Distribution of current density

Influence of cathodic current collection (cc)

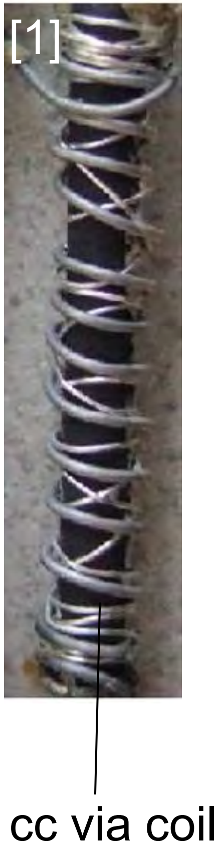
current density at anode/electrolyte interface



1st case:



2nd case:



U_{Load}=0.9 [V]

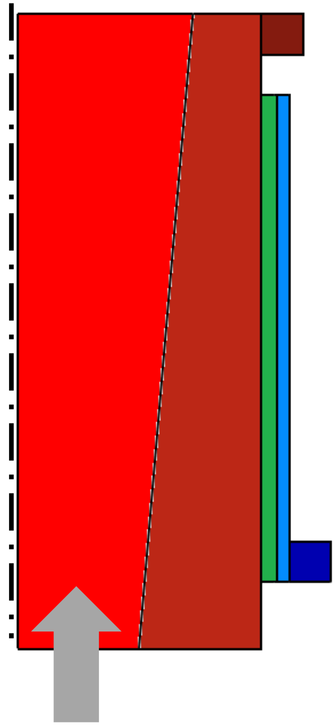
[1] V. Lawlor,G. Buchinger,C.Hochenauer, S. Cordinor, S. Griesser,A. Olabi, D. Meissner, The Second European Fuel Cell Technology and Applications Conference,Rome, Italy, 2007.

Model of a tubular SOFC
Some results

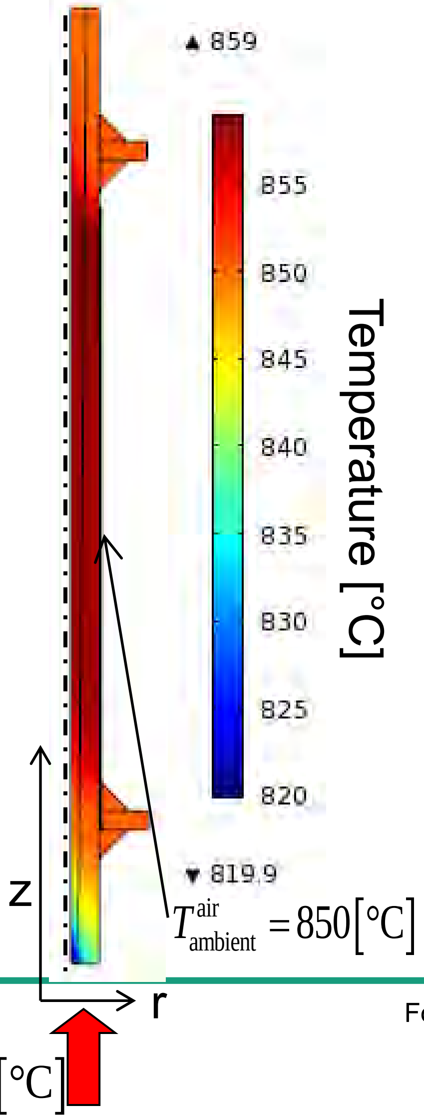
molar fractions:
$H_2:H_2O:N_2=0.35:0.03:0.62$

$U_{load}=0.7[V]$

Geometry:



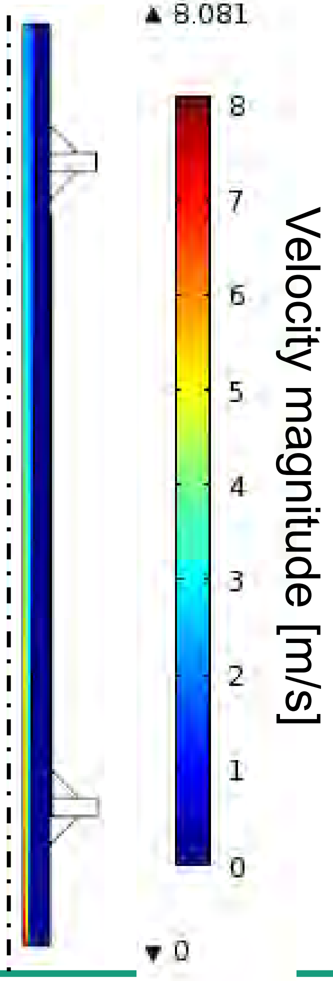
Temperature



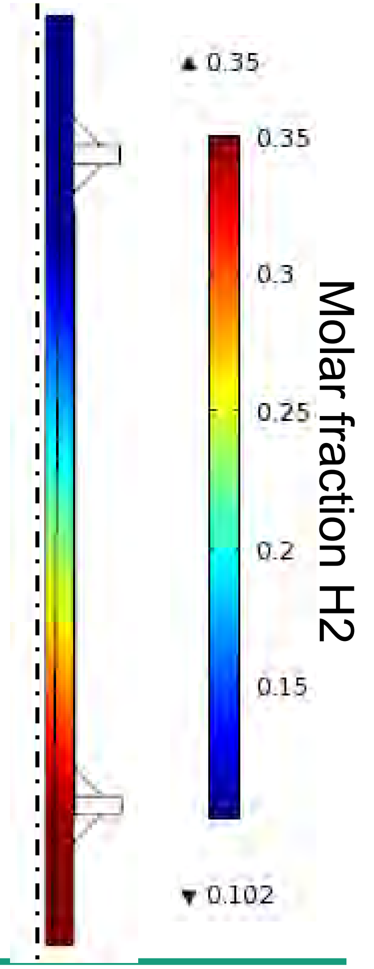
$T_{ambient}^{air}=850[°C]$

$T_{in}^{fuel}=820[°C]$

Velocity



Molar fraction H_2



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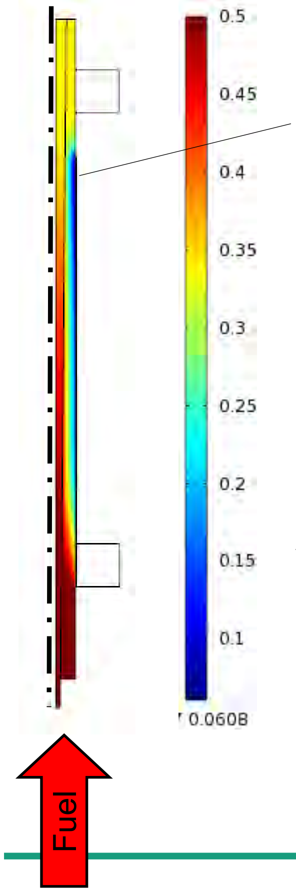
Model of a tubular SOFC

Some results

Hydrogen mole fraction



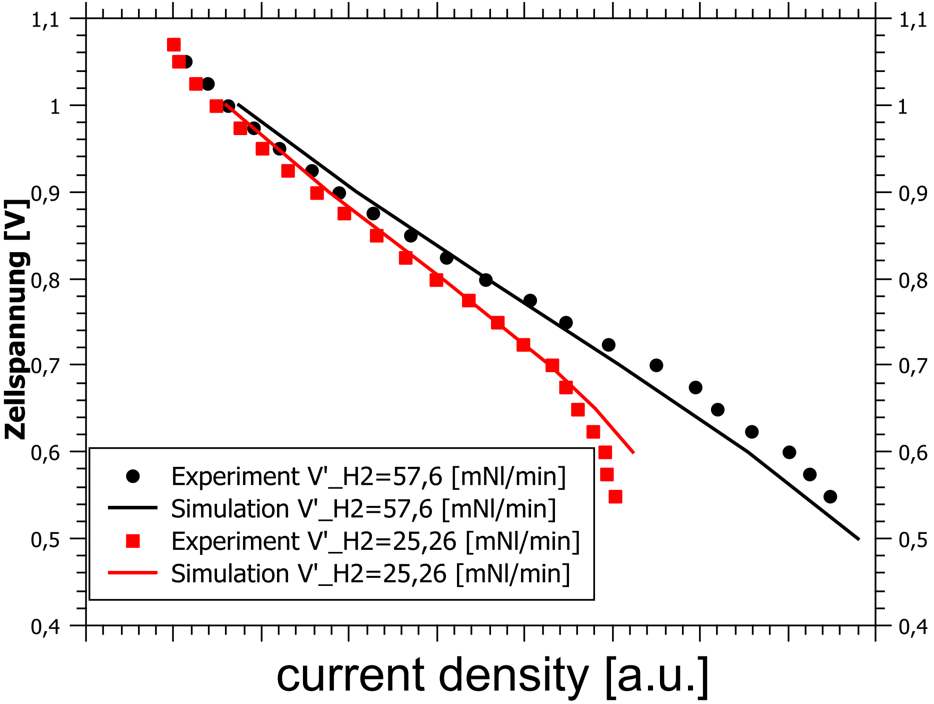
Hydrogen starvation

$x_{H2,in}=0.5$, $x_{H2O,in}=0.03$

T=800 [°C]

$U_{Zelle}=0.7$ [V]

Cell potential vs. current density



AGENDA

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Conclusion

- Multiphysics simualtions help to understand internal phenomena
- Comparison of different current collection modes
- Influence of mass transport shown

- In progress:
  - Transient simulations
  - Variation of geometric parameters

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