COMPUTATIONAL MODELLING OF FUEL CELLS AND ELECTROLYZERS: AN OVERVIEW

International Workshop on Sustainable Energy, Power and Propulsion

19-21 January 2024

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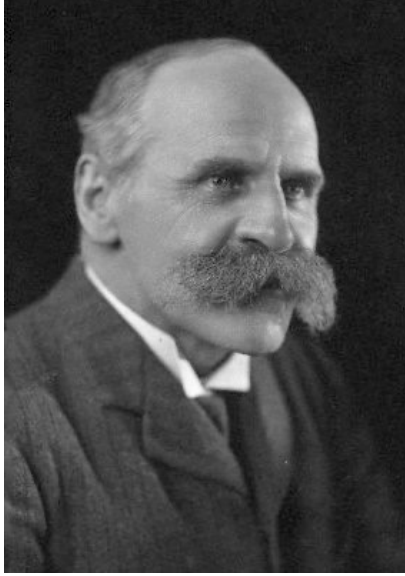
- About Forschungszentrum (Research Centre) Juelich
- Introduction to fuel cells/electrolyzers
- Different levels of modelling
  - Cell level
  - Stack level
  - Microscale
- Future work
- Summary and conclusions

PREAMBLE:

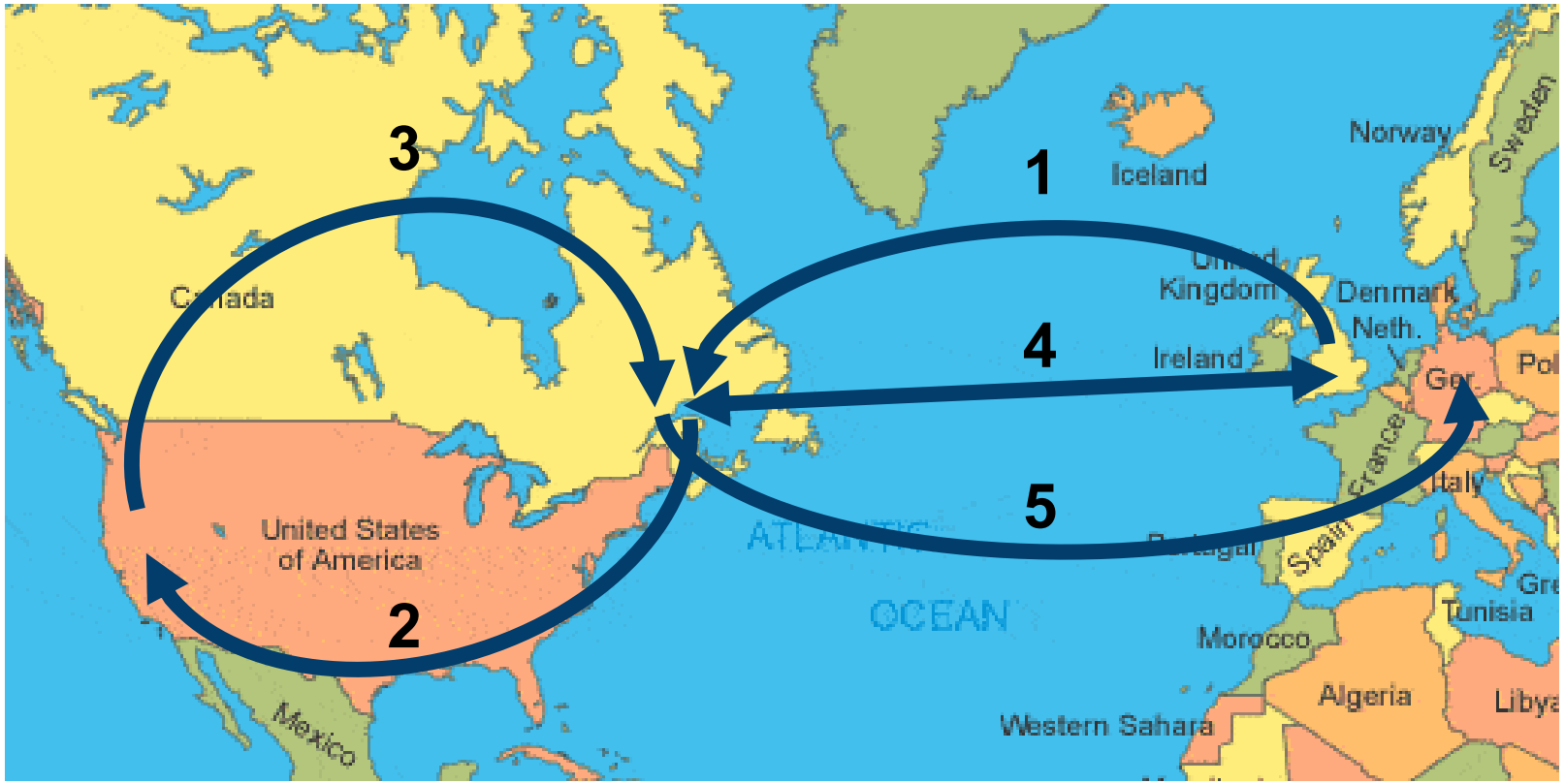


Personally, I think that four hundred years hence the power question in England may be solved somewhat as follows: The country will be covered with **rows of metallic windmills working electric motors** which in their turn supply current at a very high voltage to great electric mains. At suitable distances, there will be great power stations where during windy weather the **surplus power will be used for the electrolytic decomposition of water into oxygen and hydrogen**.

J.B.S. Haldane, 1923

AUTHOR:

- Originally from UK
- Educated in UK, US, Canada
- PhD Imperial College, Supervisor D.B. Spalding
- Background in CFD and heat transfer
- Employed at National Research Council Canada 1983-2013
- Juelich Research Centre (Germany) from 2013-23
- Started work on CFD modelling of fuel cells in 1999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Western Sahara
Mexico
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HELMHOLTZ

18 Centers – one Association

Helmholtz makes a key contribution to solving major challenges facing society, science, and the economy through top-level research at 18 Research Centers. We focus on six Research Fields: Energy, Earth and Environment, Health, Information, Matter, and Aeronautics, Space and Transport.

44,000
Employees

6
Research Fields

>11,000
Internal and external scientists from all over the world

>5.3
Billion euros total annual budget

FORSCHUNGSZENTRUM JÜLICH AT A GLANCE

1956

FOUNDED

on 12 December

Shareholders

90 % Federal Republic of Germany

10 % North Rhine-Westphalia

12

INSTITUTES

88

INSTITUTE SECTIONS

948*

million Euros of revenue in 2021

(43 % external funding)

7248*

PEOPLE AT WORK

934

VISITING SCIENTISTS

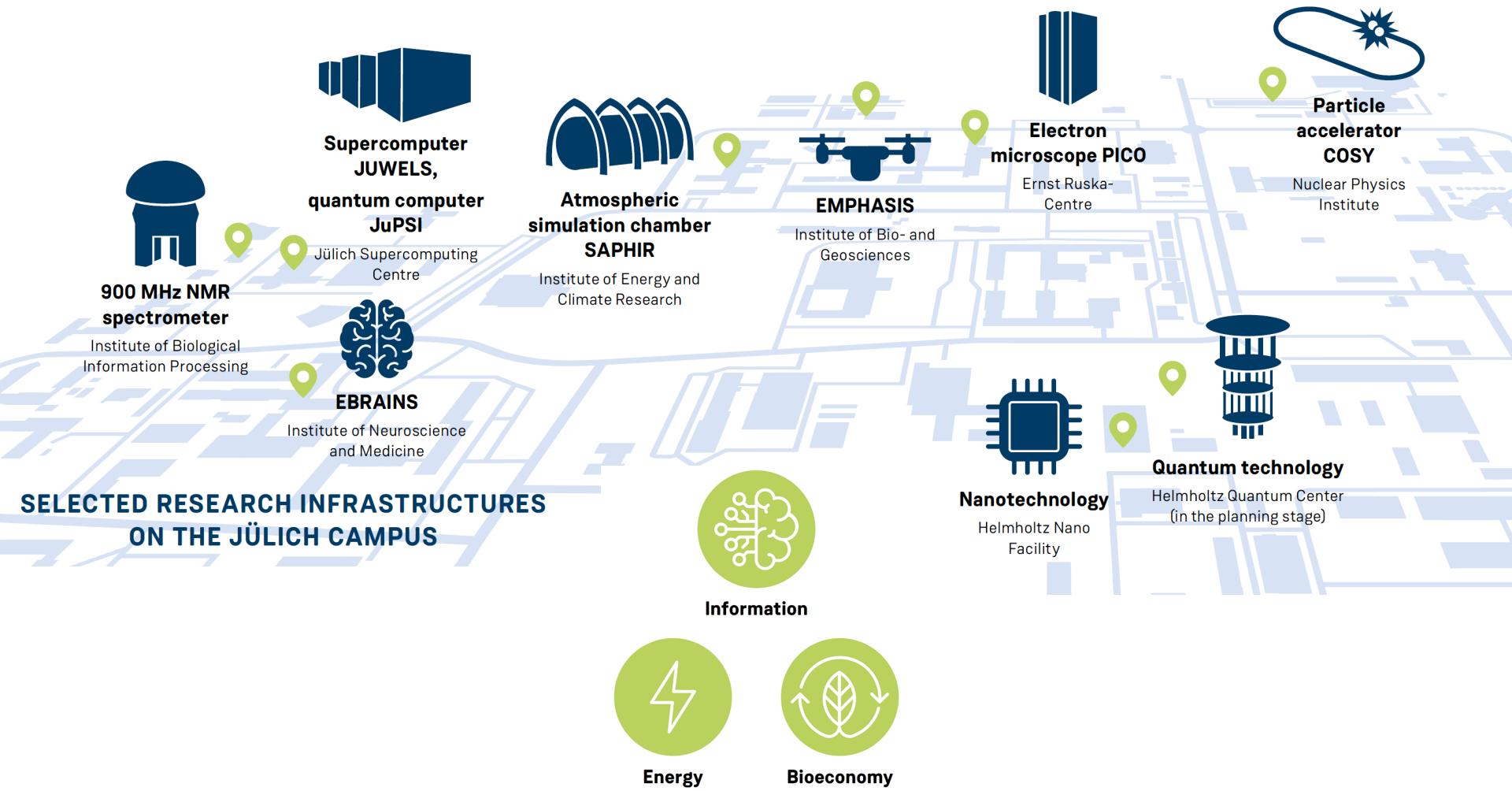
from **65** countries

Information

Energy

Bioeconomy

*As of 31.12.2022


Supercomputer JUWELS, quantum computer JuPSI
Jülich Supercomputing Centre
900 MHz NMR spectrometer
Institute of Biological Information Processing
EBRAINS
Institute of Neuroscience and Medicine
Atmospheric simulation chamber SAPHIR
Institute of Energy and Climate Research
EMPHASIS
Institute of Bio- and Geosciences
Electron microscope PICO
Ernst Ruska-Centre
Particle accelerator COSY
Nuclear Physics Institute
Nanotechnology
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Quantum technology
Helmholtz Quantum Center (in the planning stage)
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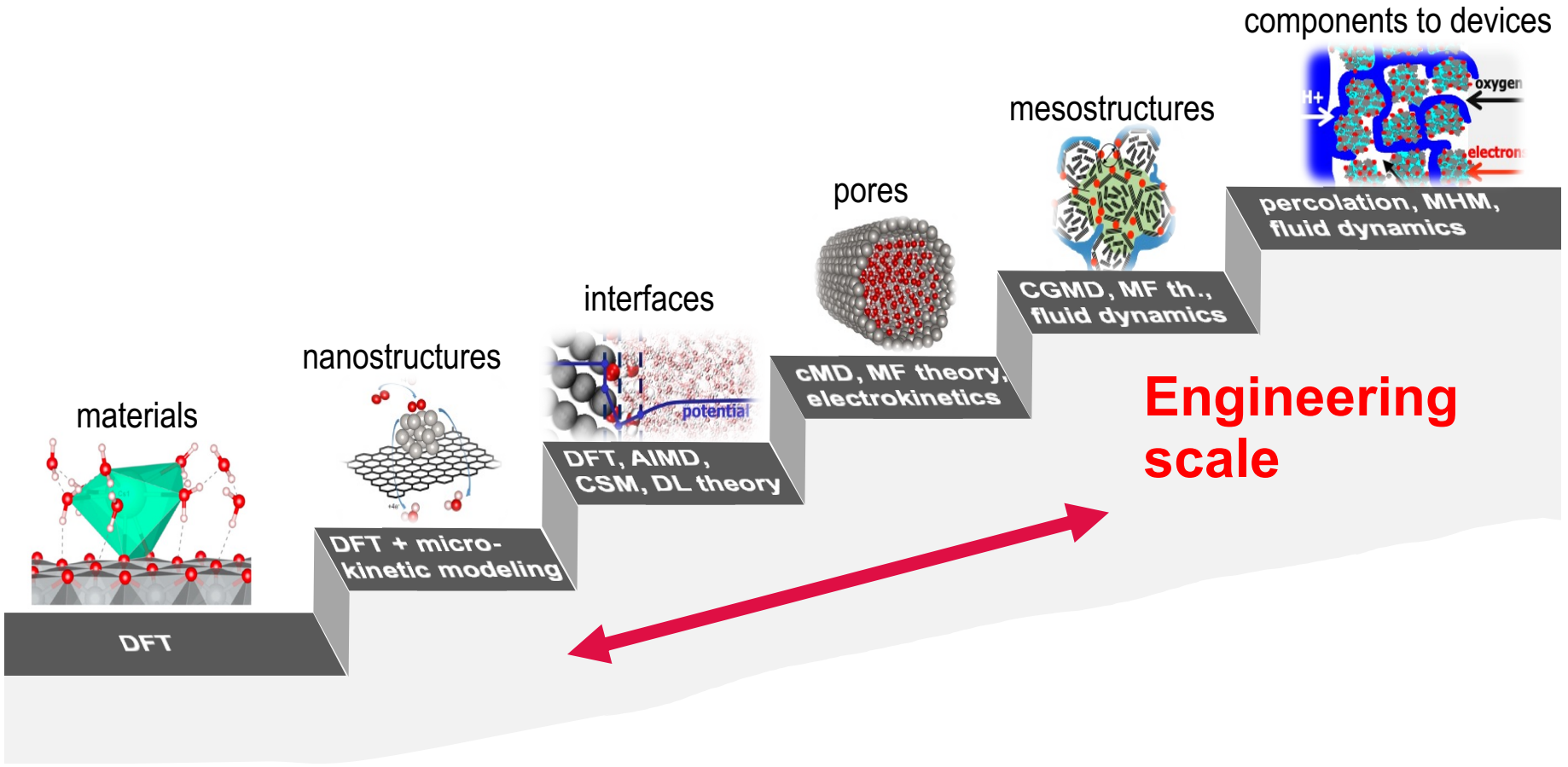
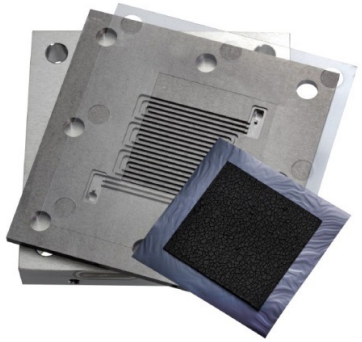
Information
Energy
Bioeconomy

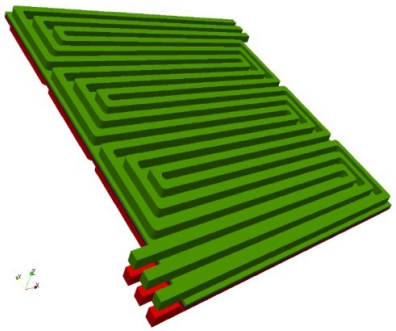
MODELLING IN IEK-13

Modelling spans all scales



ELECTROCHEMICAL CELL

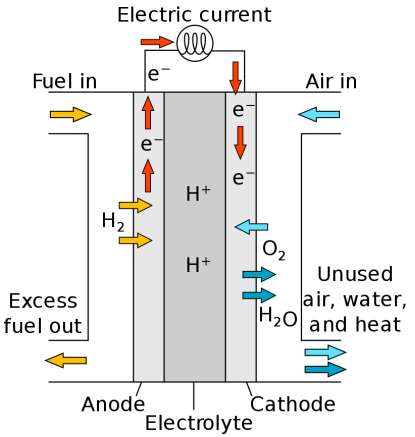




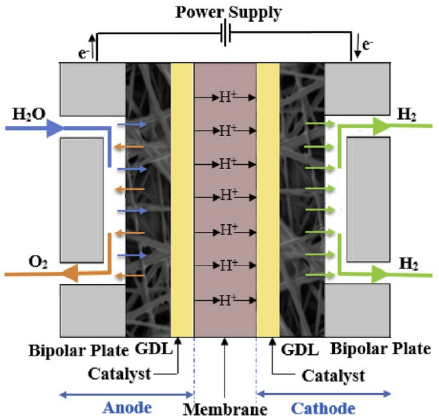
- **Fuel cell** converts chemical energy to electricity
- Uses hydrogen-rich fuel & oxygen reactants with water as product
- Environmentally friendly
- Commonly found types: **polymer electrolyte (PEFC)** used in **mobile applications** and **solid oxide (SOFC)** for **stationary power generation**
- Reaction rate/current density **strongly affected by** transport phenomena **& vice-versa**
- **Electrolyzer** is a fuel cell operating in reverse (converts electrical energy to chemical energy)

ELECTROCHEMICAL CELL

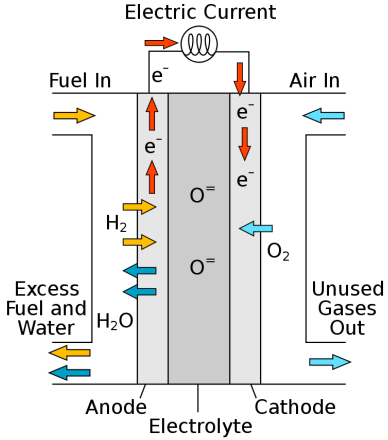
PEM fuel cell



PEM electrolyzer



SOFC (Solid oxide fuel cell)



… SOEC AEMWE

Anode:	$H_2 \rightarrow 2H^+ + 2e^-$	$H_2O \rightarrow O_2 + 4H^+ + 4e^-$	$H_2 + O^{2-} \rightarrow H_2O + 2e^-$
Cathode:	$2H^+ + 2e^- + ½O_2 \rightarrow H_2O$	$4H^+ + 4e^- \rightarrow 2H_2$	$O_2 + 4e^- \rightarrow 2O^{2-}$
Overall:	$H_2 + ½O_2 \rightarrow H_2O$	$H_2O \rightarrow H_2 + ½O_2$	$2H_2 + O_2 \rightarrow 2H_2O$

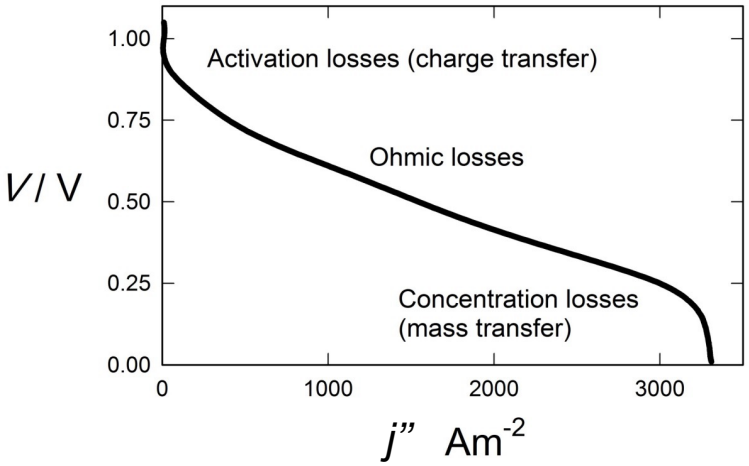
PEM: Proton-exchange membrane
SOFC: Solide oxide fuel cell
SOEC: Solide oxide electrolyzer cell
AEMWE: Anion exchange membrane water electrol

ELECTROCHEMICAL CELL

What is it? What does it do? How does it work?

- Actual electric potential differs from ideal due to losses:
  - Activation/kinetics
  - Ohmic resistance
  - Concentration/mass transfer

Polarisation diagram:
Voltage vs current density



- Actual potential,
  V = Ideal potential E – losses, η

$$E - \eta - V = j'' R_e$$

$$\eta = \sum_{a,c} \eta_e$$

CELL MODEL: BASIC EQUATIONS

Simplest formulation – Nernst minus losses

- Thermodynamic maximum potential

(May never be achieved even at zero current)

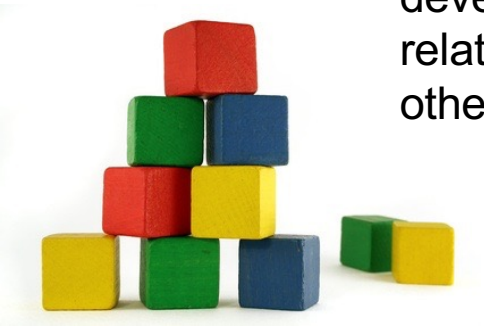
$$E = E^0 + \frac{RT}{zF} \ln K_P$$

- Expression for reaction rate (Butler-Volmer)

$$j'' = j_0'' \left[\exp\left(2\beta F \eta_e / RT\right) - \exp\left(-2\left(1-\beta\right) F \eta_e / RT\right) \right]$$

Both j_0 and K_P are functions of concentration

THE BASIC IDEA



Basic solver core library development: not related to fuel cells or other specific apps

App interface

Class library

App developer: Knowledge both of CFD & fuel cells

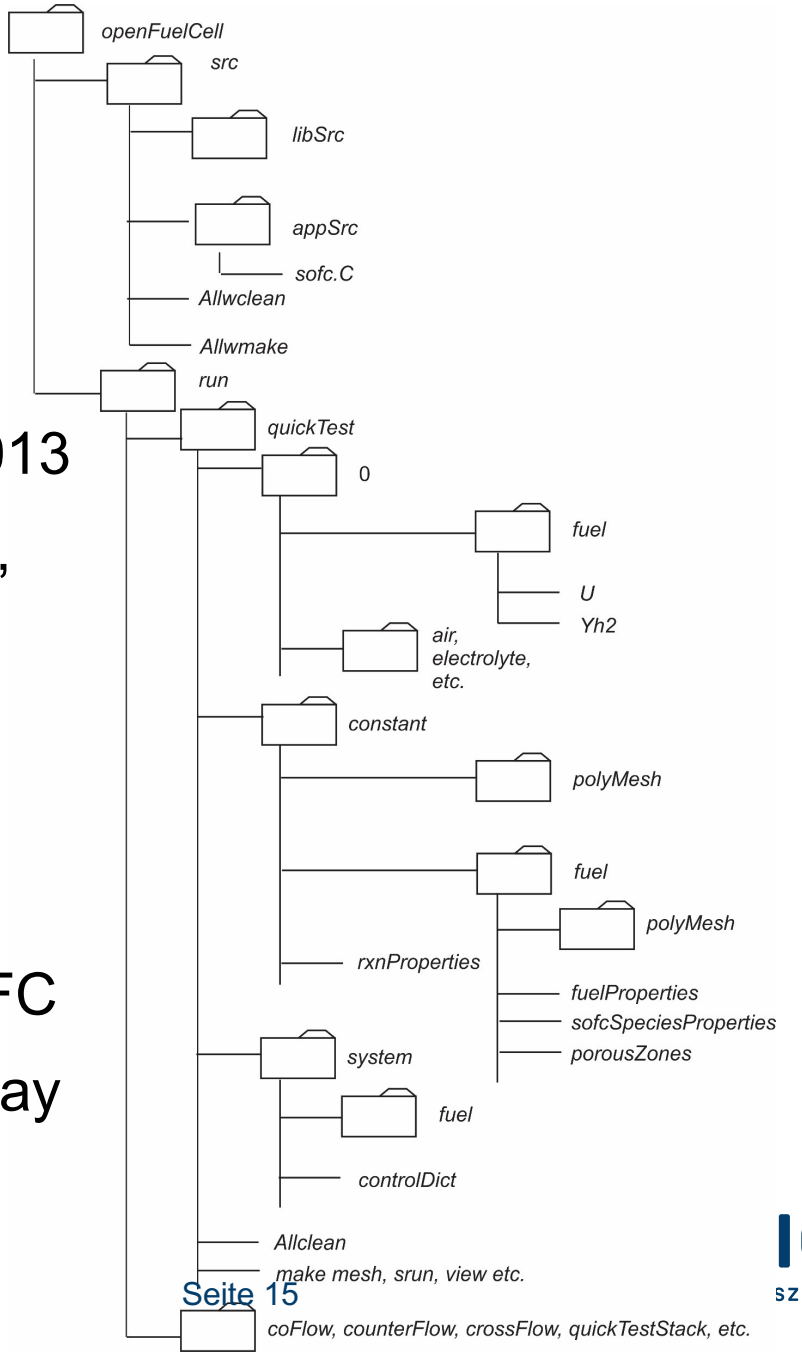
Application code

Fuel cell/electrolyser specialist, no interest in app internal details

openFuelCell

Version 1

- Developed using **OpenFOAM**
- **Git repo** posted **sourceForge** 2013
- Collaboration between FZJ, NRC, Queens U, Wikki
- Primarily SOFC (single-phase)
- Models (activation diffusion etc.) run-time selectable
- Later extended to stacks, HT-PEFC
- Minimal maintenance/support today



MODEL EQUATIONS

Part 1

GAS TRANSPORT

$$div(\rho \boldsymbol{u}) = 0$$

$$div(\rho \boldsymbol{u}\boldsymbol{u}) = -\text{grad}\, p + \text{div}(\mu\, \text{grad}\, \boldsymbol{u}) - \frac{\mu}{k_D}\boldsymbol{u}$$

$$div(\rho \boldsymbol{u} y_i) = \text{div}(\Gamma\, \text{grad}\, y_i)$$

'Branch' meshes

Mass fractions (partial pressures)

Mass & species sources

Electrochemistry

1. Nernst

$$E = E^0 + \frac{RT}{zF}\ln K_P$$

2. Kirchhoff-Ohm

$$E - \eta - V = j'' R_e \qquad \eta = \sum_{a,c} \eta_e$$

3. Butler-Volmer

$$j'' = j_0''\left[\exp(2\beta F\eta_e/RT) - \exp(-2(1-\beta)F\eta_e/RT)\right]$$

2-D surface mesh

Temperatures

Heat sources

Heat transfer

'Main' mesh

$$div(\rho c_p \boldsymbol{u} T) = \text{div}(\lambda\, \text{grad}\, T) + S$$

Open-source Computational Model of a Solid Oxide Fuel Cell. S.B. Beale, H.-W. Choi, J.G. Pharoah, H.K. Roth, H. Jasak, D.H. Jeon. Computer Physics Communications, 200, 15-26. 2016. https://doi.org/10.1016/j.cpc.2015.10.007

lCell web site

openFuelCell

Home | Documentation | Publications | Files | Git

The Project

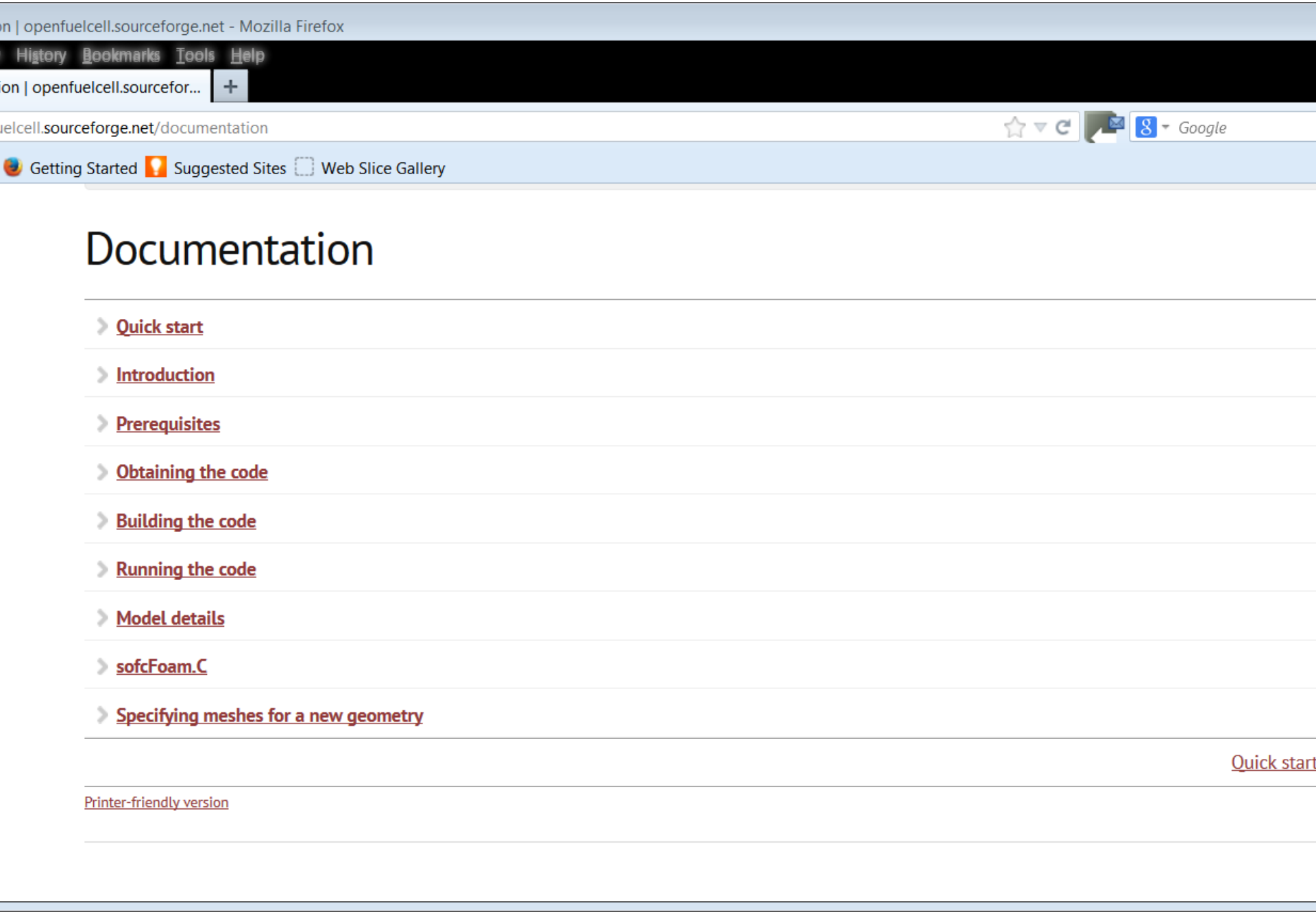
The openFuelCell project is a forum to develop open source computational fluid dynamics (CFD) software to model fuel cells. Fuel cells http://en.wikipedia.org/wiki/Fuel_cell are devices that convert hydrogen and oxygen to water and electricity, and are promising renewable energy conversion devices. Computational fluid dynamics tools are used to size and rate fuel cell systems. OpenFoam is an open source CFD toolbox, available for downloading at http://www.openfoam.com/, written in C++ and conforming to the object-oriented paradigm.

Members

The project is open to anybody who wishes to apply or produce open source fuel cell models. The founding members of the openFuelCell project are (in alphabetical order) Forschungszentrum Jülich, National Research Council Canada, Queen's University/Royal Military College Fuel Cell Research Centre, and Wikki Ltd.

Models

There are various types of fuel cells under development; at the present time the openFuelCell project is centred on solid oxide fuel cells (SOFCs). The first model to be released is a model of a single-cell SOFC operated in co-flow, counter-flow, or cross-flow with hydrogen and water on the fuel side, and dry air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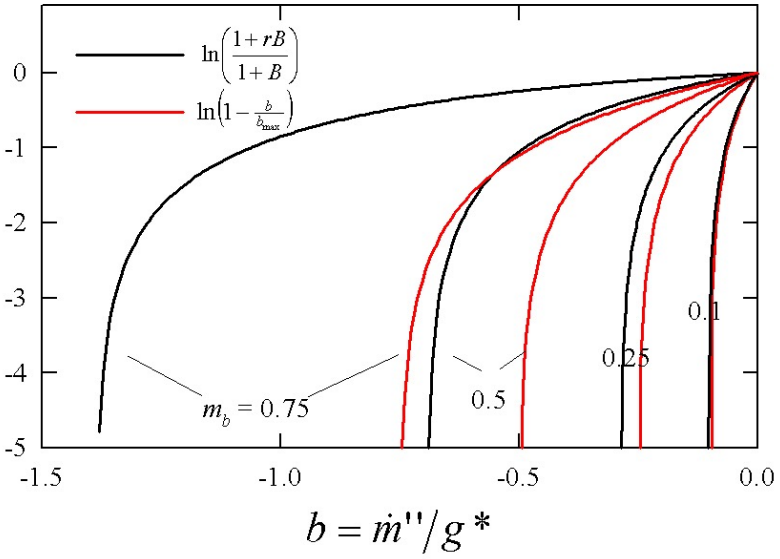
Introduction
Prerequisites
Obtaining the code
Building the code
Running the code
Model details
sofcFoam.C
Specifying meshes for a new geometry
Quick start
Printer-friendly version

MASS TRANSFER

$$\ln\left(\frac{y_w}{y_b}\right)$$



Mass fraction at electrode y_w

less (greater) than in channel, y_b

So-called 'concentration overpotential'

$$\eta = \frac{RT}{nF}\log_e\left(\frac{y_b}{y_w}\right)$$

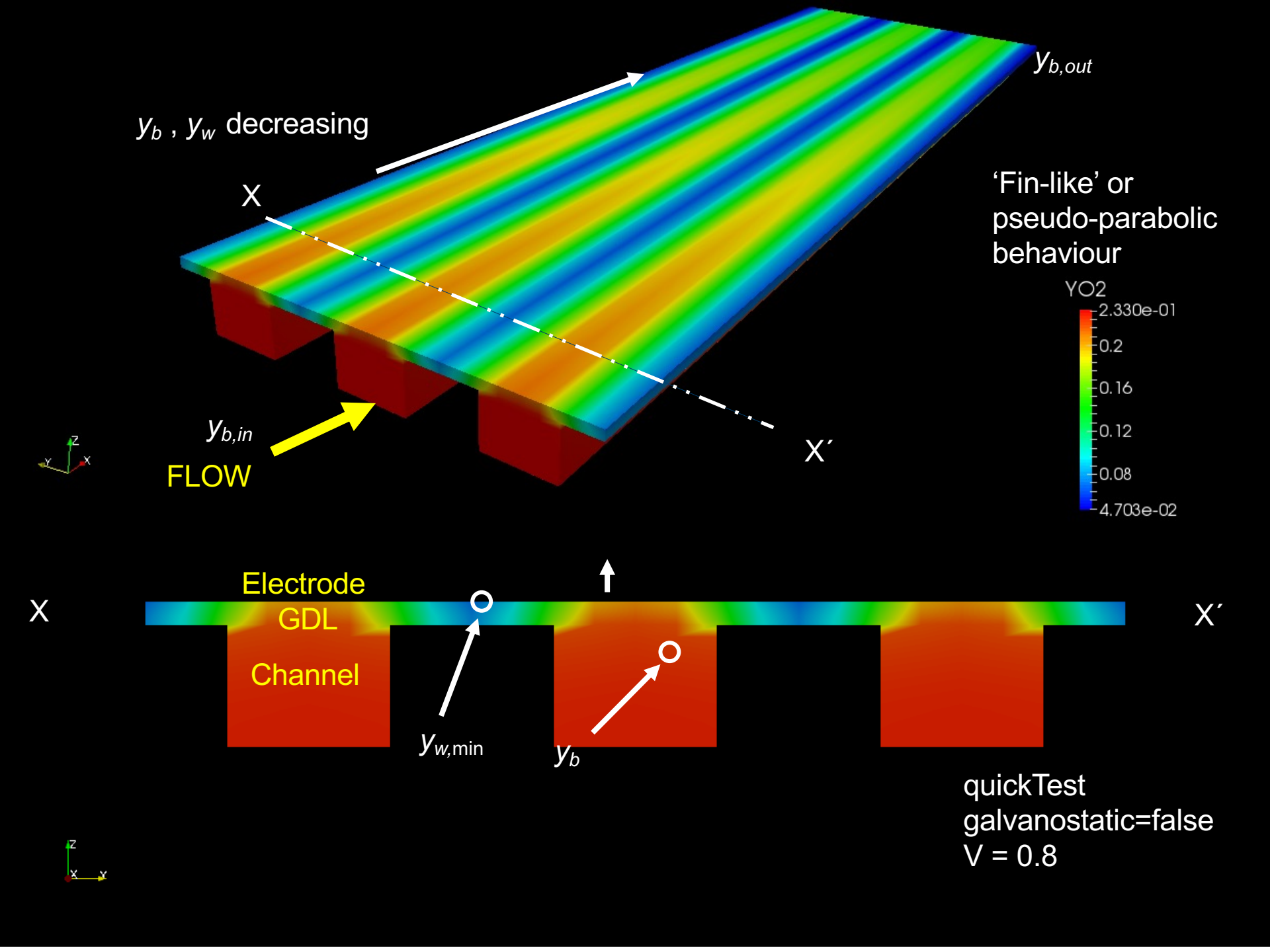
We write:

$$\frac{y_w}{y_b} = \frac{1+\frac{y_t}{y_b}B}{1+B}$$

B = **Spalding number** (mass transfer driving force)

If/when $y_w \rightarrow 0$ code stability important

Ideal code should work from open circuit to short circuit


$y_{b,out}$
y_b , y_w decreasing
X
X′
$y_{b,in}$
FLOW
'Fin-like' or pseudo-parabolic behaviour
YO2
2.330e-01
0.2
0.16
0.12
0.08
4.703e-02
Electrode
GDL
Channel
X
X′
$y_{w,min}$
y_b
quickTest
galvanostatic=false
V = 0.8

openFuelCell 2

Latest version

- Revised from version 1
- **Full two-potentials solved-for volumetrically**
- **Two-phase (L-G) or single-phase (G) at either/both electrode(s)**
- **Inter-phase L-G heat/mass transfer**
- **Water transport in MEA**
- Inherits **all** earlier SOFC work
- Documentation under development

openFuelCell2: A New Computational Tool for Fuel Cells, Electrolyzers, and Other Electrochemical Devices and Processes. S. Zhang, S. Hess, H. Marschall, U. Reimer, S.B. Beale, W. Lehnert. Computer Physics Communications. In press.

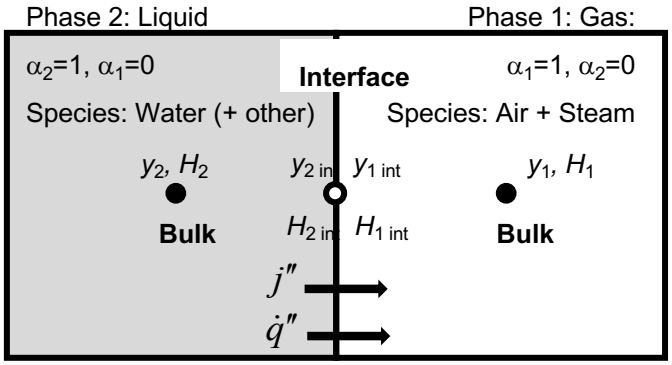
EVAPORATION/CONDENSATION

Mass transfer from heat transfer problem

α = volume fraction of phase (liquid/gas)

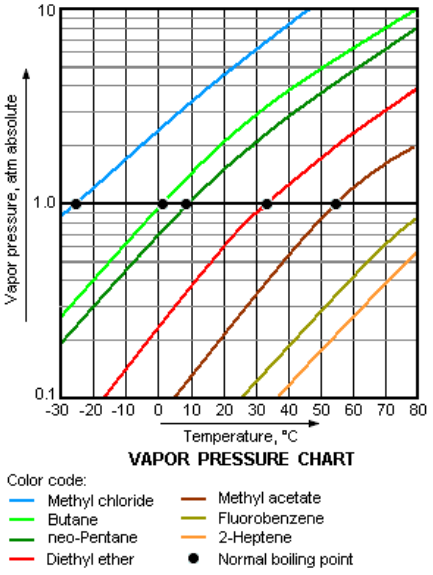
y = mass fraction of species in phase

$H = c_p T$ specific enthalpy



$$\ln\left(p_{\text{steam}}\right) = -\frac{H_{21}}{RT_{\text{int}}} + \ln\left(C\right)$$

$$\dot{m}''_{21} = \frac{h_1\left(T_{b,1} - T_{\text{int}}\right) + h_2\left(T_{b,2} - T_{\text{int}}\right)}{H_{21}}$$



EQUATIONS

Mixture transport

$$\frac{\partial \rho_\varphi s_\varphi}{\partial t} + \nabla \cdot \left(\rho_\varphi s_\varphi \mathbf{U}_\varphi \right) = R_\varphi$$

Liquid saturation

$$\frac{\partial \rho_\varphi s_\varphi \mathbf{U}_\varphi}{\partial t} + \rho_\varphi s_\varphi \mathbf{U}_\varphi \cdot \nabla \left(\mathbf{U}_\varphi \right) = -s_\varphi p_\varphi + \nabla \cdot \left(s_\varphi \mu_\varphi \nabla \mathbf{U}_\varphi \right) + \rho_\varphi s_\varphi \mathbf{g} + \mathbf{M}_\varphi + S_{\mathrm{Darcy},\varphi}$$

$$\frac{\partial \rho_\varphi s_\varphi Y_\mathrm{i}}{\partial t} + \nabla \cdot \left(\rho_\varphi s_\varphi \mathbf{U}_\varphi Y_\mathrm{i} \right) = \nabla \cdot \left(\rho_\varphi s_\varphi D_\mathrm{i}^{\mathrm{eff}} \nabla Y_\mathrm{i} \right) + R_\mathrm{i}$$

Interphase heat/mass transfer

$$\frac{\partial \rho_\varphi s_\varphi \left(h_\varphi + K \right)}{\partial t} + \nabla \cdot \left(\rho_\varphi s_\varphi \mathbf{U}_\varphi \left(h_\varphi + K \right) \right) = \nabla \cdot \left(\rho_\varphi s_\varphi \alpha^{\mathrm{eff}} \nabla h_\varphi \right) + Q_\varphi$$

Mass fractions (partial pressures)

Mass & species sources

Electrochemistry

$$\nabla \cdot \left(\sigma_\mathrm{P} \nabla \phi_\mathrm{P} \right) = J_\mathrm{P} \qquad \nabla \cdot \left(\sigma_\mathrm{E} \nabla \phi_\mathrm{E} \right) = J_\mathrm{E}$$

Full-field potentials

$$\sigma = \begin{cases} (0.514\lambda - 0.326) \exp\left(1268. \left(\frac{1}{303} - \frac{1}{T} \right) \right) & 1 \le \lambda \\ 0.1789\lambda \exp\left(1268. \left(\frac{1}{303} - \frac{1}{T} \right) \right) & \lambda < 1 \end{cases}$$

Water transport

$$\frac{\rho_\mathrm{m}}{\mathrm{EW}} \frac{\partial \lambda}{\partial t} + \nabla \cdot \left(\frac{\mathbf{i}}{F} n_d \right) = \frac{\rho_\mathrm{m}}{\mathrm{EW}} \nabla \cdot \left(D_\mathrm{m}^{\mathrm{eff}} \nabla \lambda \right) + R_\lambda$$

$$J_a = i_{a,0} s_g^\beta \prod_i \left(\frac{C_\mathrm{i}}{C_{\mathrm{ref,i}}} \right)^\gamma \left[\exp\left(\frac{\alpha_a z F \eta_a}{R_g T} \right) - \exp\left(-\frac{(1-\alpha_a) z F \eta_a}{R_g T} \right) \right]$$

$$J_c = i_{c,0} s_g^\beta \prod_i \left(\frac{C_\mathrm{i}}{C_{\mathrm{ref,i}}} \right)^\gamma \left[\exp\left(-\frac{\alpha_c z F \eta_c}{R_g T} \right) - \exp\left(\frac{(1-\alpha_c) z F \eta_c}{R_g T} \right) \right]$$

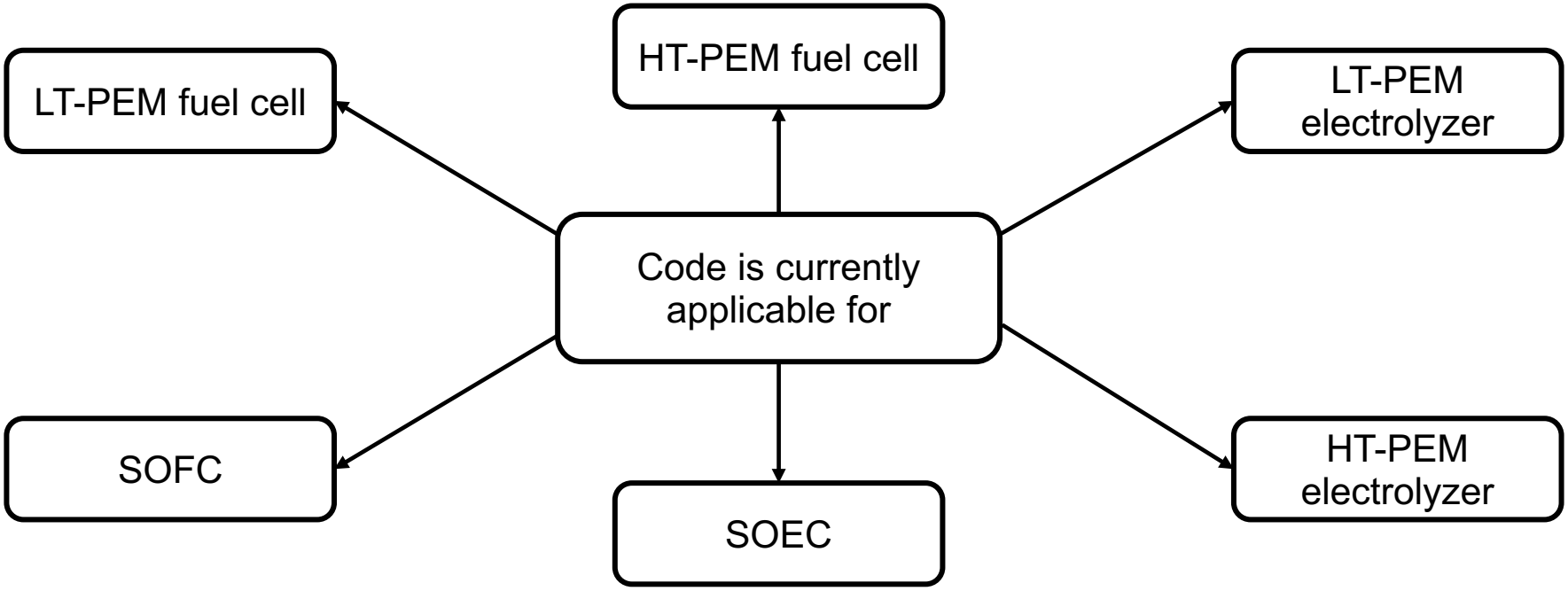
Temperatures

Heat sources

Heat transfer

$$\frac{\partial \rho C_p T}{\partial t} + \rho \mathbf{U} C_p \bullet \nabla T = \nabla \cdot \left(\kappa \nabla T \right) + Q$$

https://openfuelcell2.github.io/



openFuelCell https://github.com/openFuelCell2/openFuelCell2

openFuelCell2

openFuelCell2 is a computational fluid dynamics (CFD) toolbox for simulating electrochemical devices such as fuel cells and electrolysis. The solver is based on the open-source library, OpenFOAM®.

About the code

The source code was developed from a previous open-source repository called openFuelCell. It was also inspired by the standard solver **reactingTwoPhaseEulerFoam** in OpenFOAM®. The solver can consider coupled problems with multi-region and multi-physics issues, including single and two phase flows, multiple species components, charger transfer, and electrochemical reactions in different regions. More applications and solvers will be available in the future.

Running your own simulations

To install the openFuelCell2 libraries, please follow this installation guide.

Then, to test the tutorial cases, please see the tutorial guide.

Disclaimer

This offering is not approved or endorsed by OpenCFD Limited, producer and distributor of the OpenFOAM software via www.openfoam.com, and owner of the OPENFOAM® and OpenCFD® trade marks.

Acknowledgement

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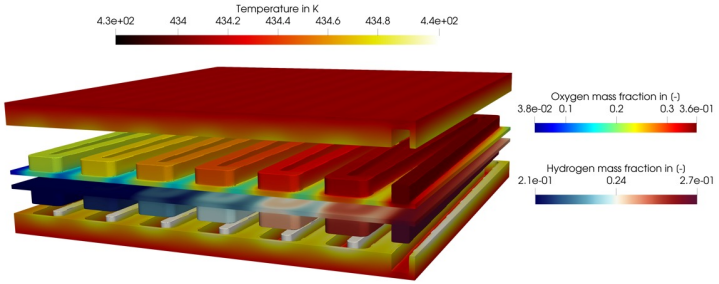
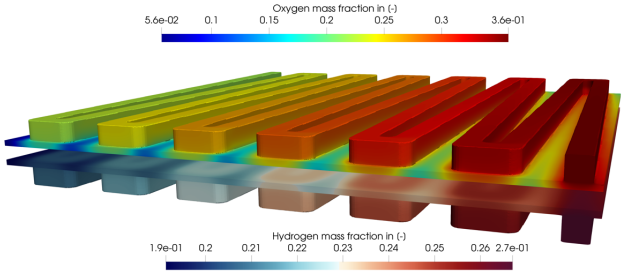
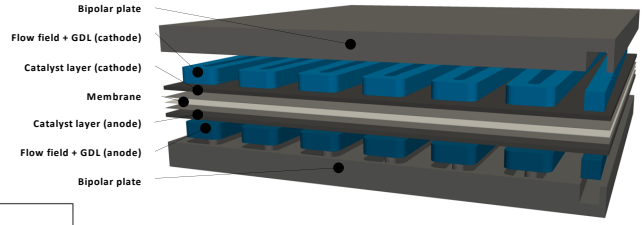
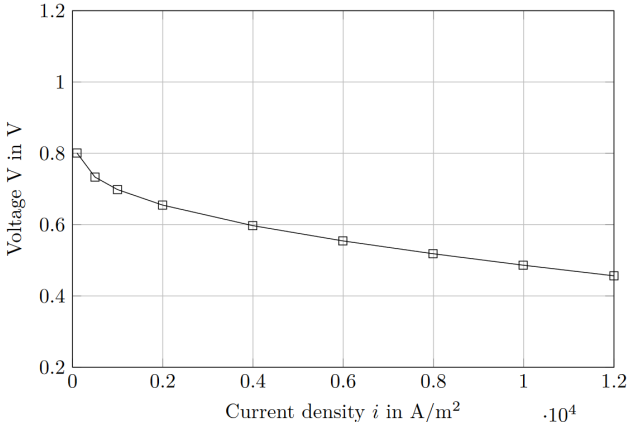
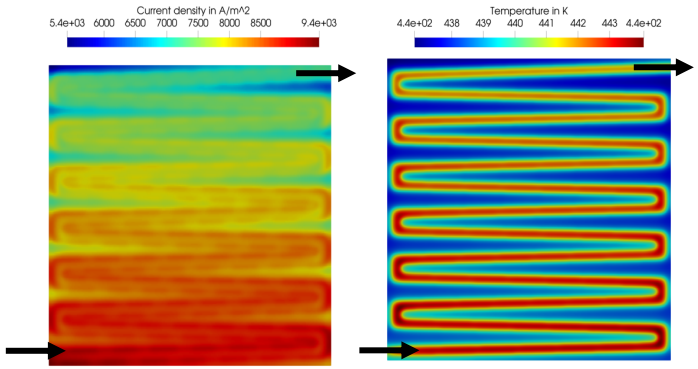
HIGH TEMPERATURE PEM FUEL CELL











openFuelCell2: A New Computational Tool for Fuel Cells, Electrolyzers, and Other Electrochemical Devices and Processes. S. Zhang, S. Hess, H. Marschall, U. Reimer, S.B. Beale, W. Lehnert. Computer Physics Communications. In press.

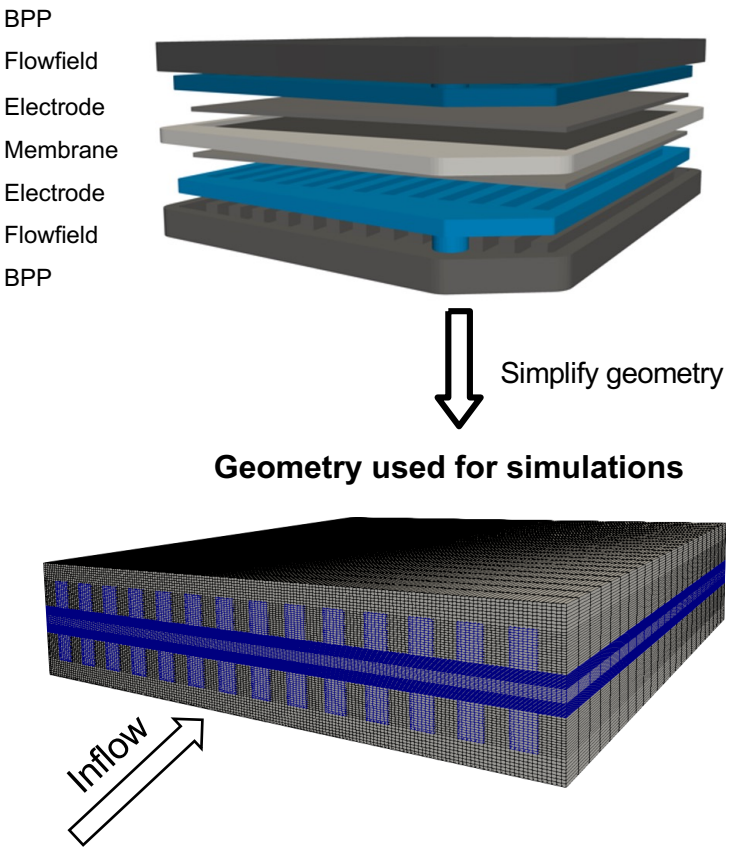
ALKALINE ELECTROLYZER CELL

Geometry – Experimental setup

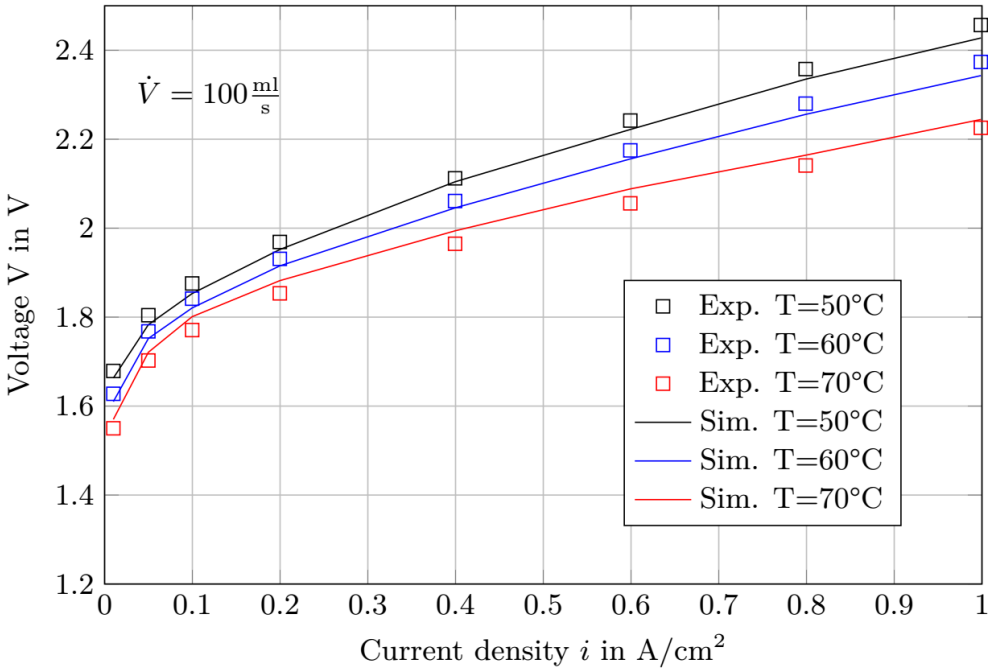
Part	Material	Dimensions (mm)
BPP	Nickel	1.5
Cathode	Nickel (porous)	0.5
Diaphragm	Zirfon PERL UTP 500	0.5
Anode	Nickel (porous)	0.5
Flow channel	Electrolyte/Gas	14 x 1.5
Rips	Nickel	1.5

Operating conditions:

- Volumetric flow rate: $\dot{V} = 100\mathrm{ml\,min^{-1}}$
- Temperature: $50°C \leq T \leq 70°C$
- Weight% KOH: $wt\%_{KOH} = 30$
- Pressure $p_{cat} = p_{an} = 1\mathrm{bar}$



ALKALINE ELECTROLYZER CELL



Note: Majority of the data were taken from literature $(i_0, \alpha_{cat}, \alpha_{an})$

→ **Not** specific for the used setup and electrodes

STACK MODEL

Distributed resistance analogy (macro-homogeneous model)

$$\frac{\partial(\rho_i \varepsilon_i \varphi_i)}{\partial t} + \mathrm{div}(\rho \varepsilon_i \vec{u}_i \varphi_i) = \varepsilon_i \sum_j \alpha_{ij} (\varphi_j - \varphi_i) + \mathrm{div}(\varepsilon_i \Gamma \,\mathrm{grad}\, \varphi_i) + \varepsilon_i \dot{S}'''$$

TRANSIENT + CONVECTION = INTER-PHASE + DIFFUSION + SOURCE

Continuity and momentum

$$\frac{\partial(\rho_i \varepsilon)}{\partial t} + \mathrm{div}(\rho_i \varepsilon_i \vec{u}_i) = \dot{m}'''$$

$$\dot{m}'' = \pm \sum MFi''$$

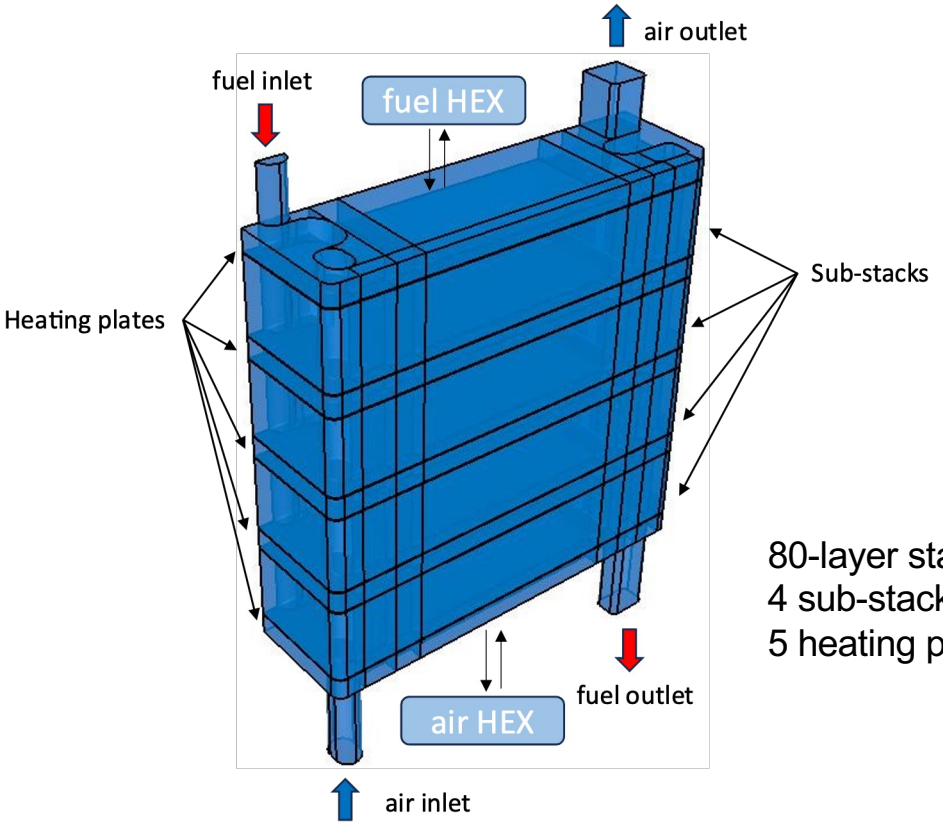
$$\frac{\partial(\rho_i \varepsilon \boldsymbol{u_i})}{\partial t} + \mathrm{div}(\rho_i \varepsilon_i \boldsymbol{u_i} \boldsymbol{u_i}) = -\,\mathrm{grad}\, p_i - F_i \varepsilon_i^2 \vec{u}_i + \mathrm{div}(\mu \,\mathrm{grad}\, \boldsymbol{u_i})$$

$$f^* = \frac{\tau_w}{\frac{1}{2}\rho u^2} = \frac{a}{\mathrm{Re}} \qquad F^* = \frac{2a}{\varepsilon} \frac{\mu}{D_h^2}$$

A Distributed Resistance Analogy for Solid Oxide Fuel Cells. S.B. Beale, S.V. Zhubrin. *Numerical Heat Transfer*, 47, 6, 573-591, June 2005.

STACK MODEL

Stack (Mark H2020)



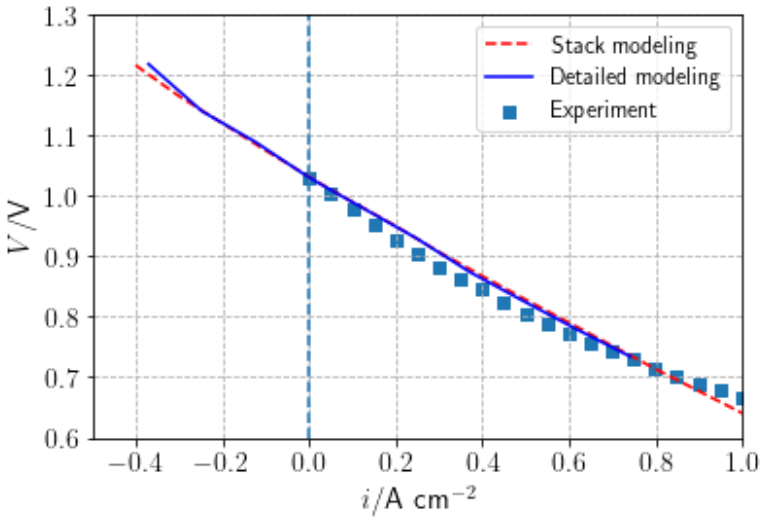
80-layer stack
4 sub-stacks
5 heating plates

Peters, Ro, et al. "Experimental Results of a 10/40 kW-Class Reversible Solid Oxide Cell Demonstration System at Forschungszentrum Jülich." Journal of The Electrochemical Society 170.4 (2023): 044509.

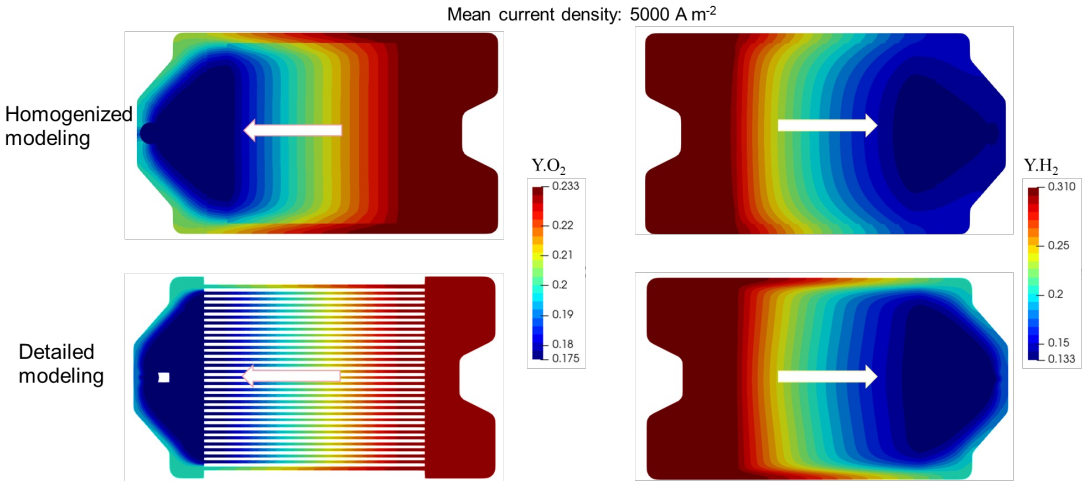
STACK MODEL

Repeating unit & short stack (Mark F-10)

I-V curves



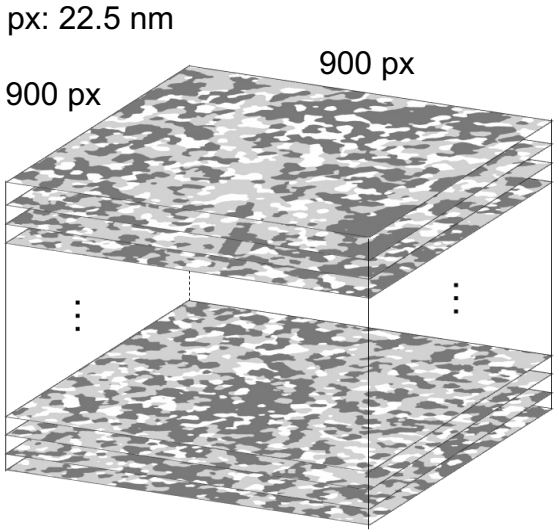
Species distributions



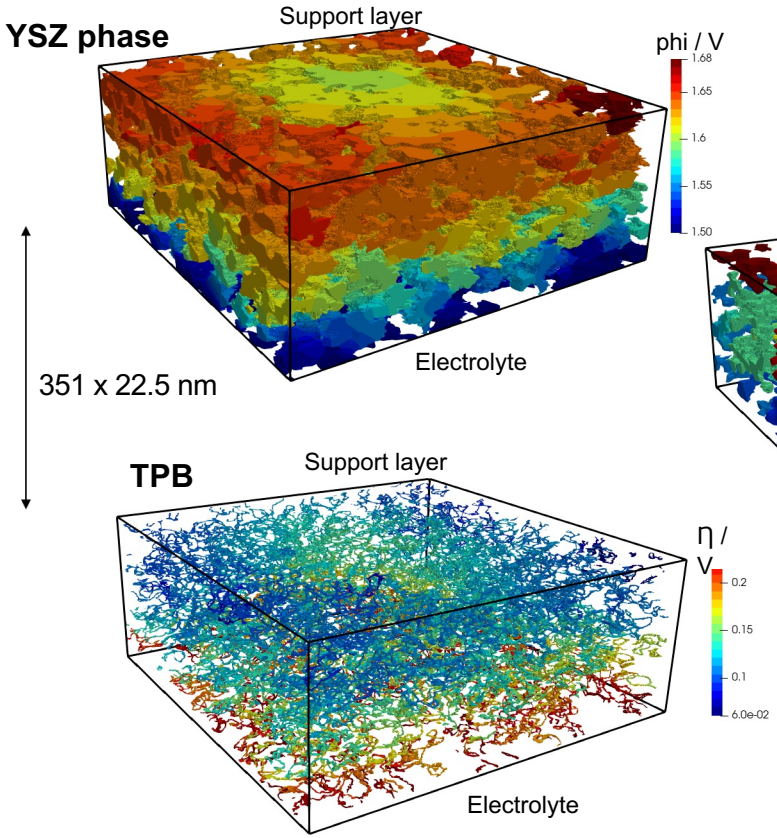
ModVal 2023, 2023 Duisburg, Germany.

MICROSCALE MODELS

Electrode: Reconstruction (351 images): 20.25 x 20.25 x 7.875 um^3, CFD mesh: 283.5 M



351 x 22.5 nm



Labeled FIB-SEM images

SOFC-XVIII ECS Meeting, 2023 Boston, USA.

Mean current density: ~0.6 A/cm^2

FUTURE WORK

- Degradation modelling
- AI/ML neural networks
- Bubble/drop dynamics
- Multi-scale models
- Combined electro-thermal-structural analysis
- Advanced kinetics
- Solvers
- Batteries

THE END

Thank you!

Preprint

Github