Karlsruher Institut für Technologie

1. KIT-interner Workshop zur Wasserstoff- und Brennstoffzellen-Forschung

Contribution to Hydrogen research of INR

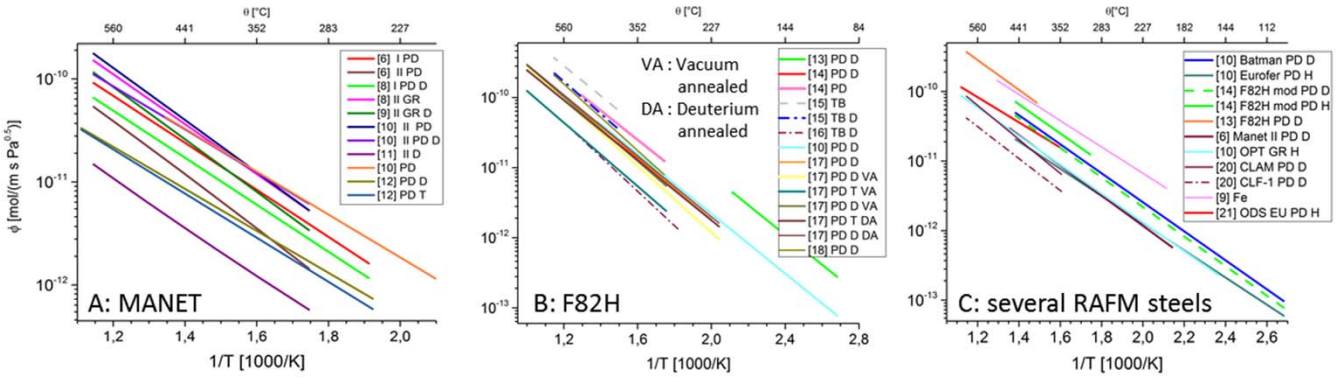
Karlsruhe, KIT

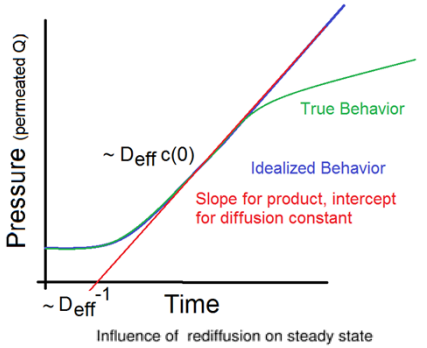
@ 2. März 2021 von 14 – 18 Uhr via Zoom,

Dr. Axel von der Weth, Dr. Daniela Piccioni Koch, Dr. Volker Pasler

1. KIT-interner Workshop zur Wasserstoff-und Brennstoffzellen-Forschung

Main issue: Experimental determination of diffusion constant and Sieverts´constant, currently for FUSION, endothermic RAFM steel

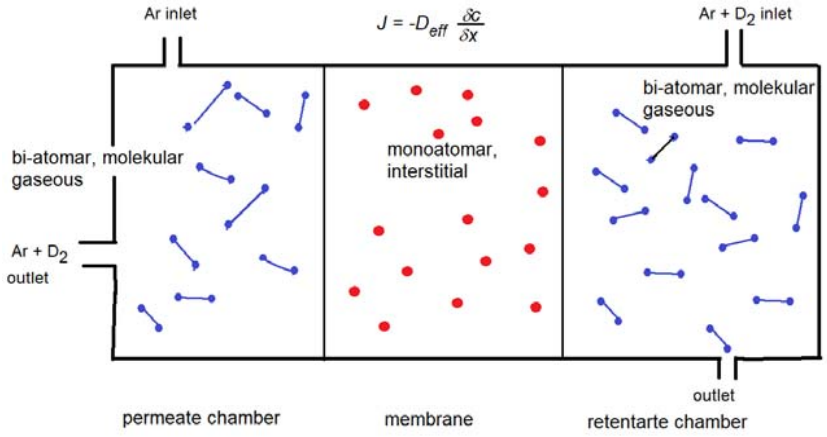


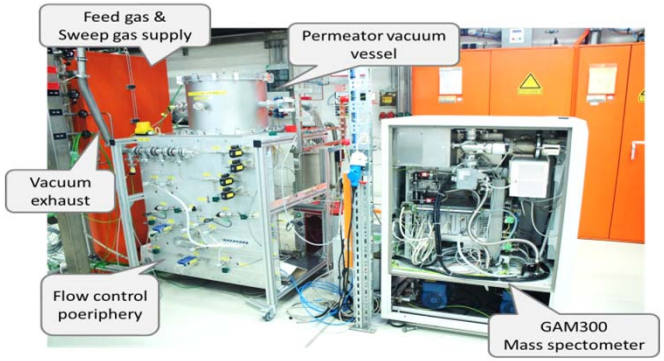


$$j(t)_{measure} = \underbrace{\frac{D_{eff}\,c(0)\,d_m^2}{w_m\,4\,\pi}}_{j_{steady\ state}} \left(1 + 2\sum_{k=1}^{\infty}(-1)^k e^{\frac{-k^2\pi^2 D_{eff}(t-t_{off})}{w_m^2}}\right)$$

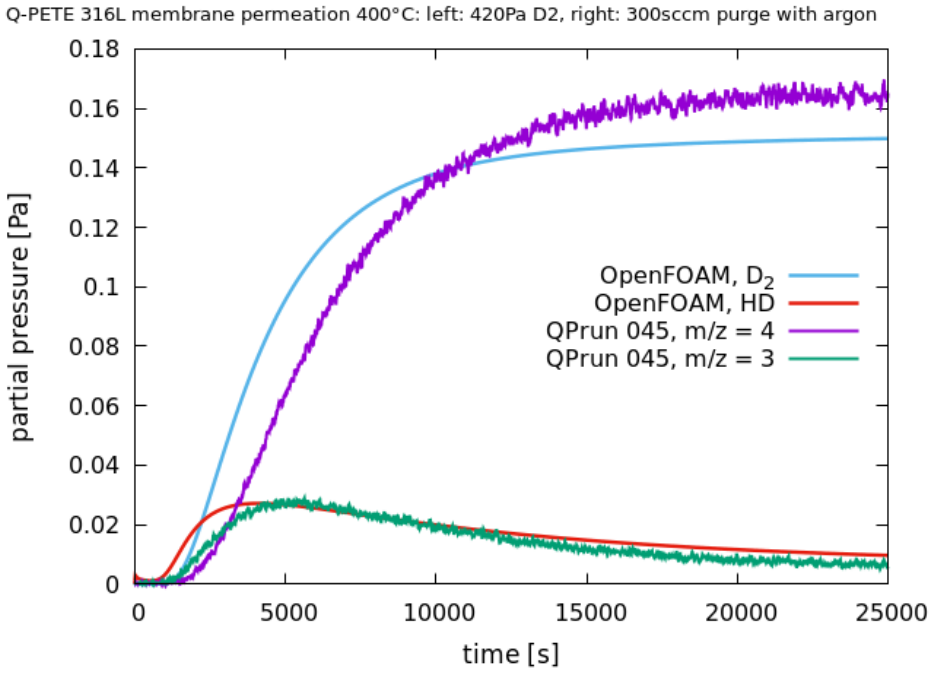
Daynes (1920)

Q-PETE (**H**ydrogen **Pe**rmeation **a**nd **T**ransport **E**xperiment



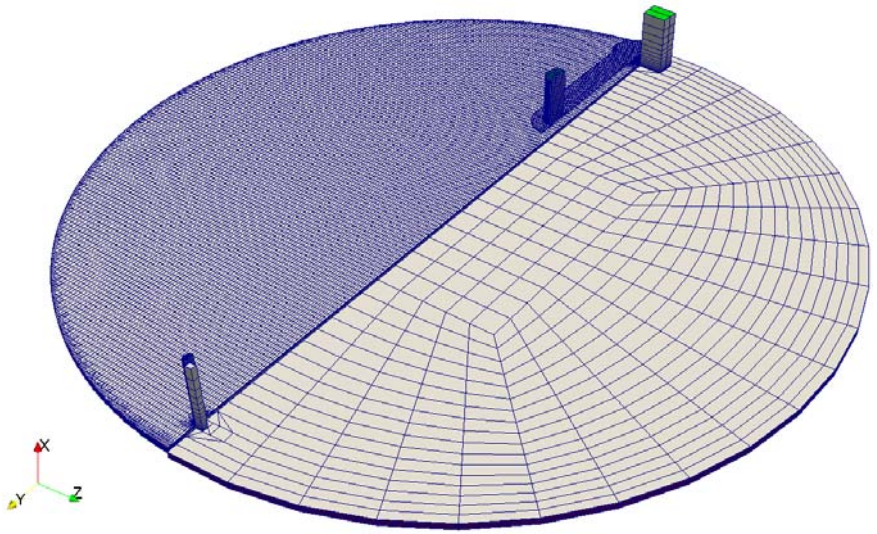


Open FOAM results of two isotops (H+D)



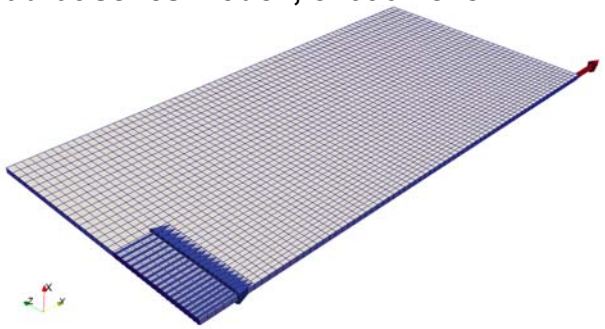
„Q-PETE“ in OpenFOAM: unterschiedlich komplexe Modellierungsansätze

“snappy hex mesh“ (CATIA), 406444 Zellen

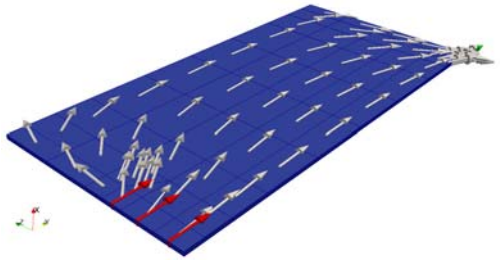


Halbkreismodell, 12180 Zellen

quadratisches Modell, 84096 Zellen



grobes optimiertes quadratisches Modell, 1674 Zellen

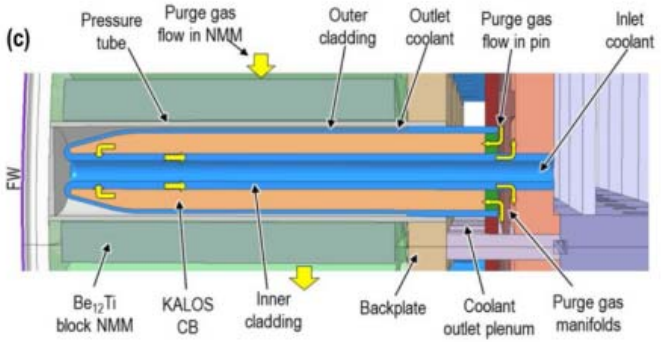


Simulation einer DEMO “Pin”- Bruteinheit mit OpenFOAM

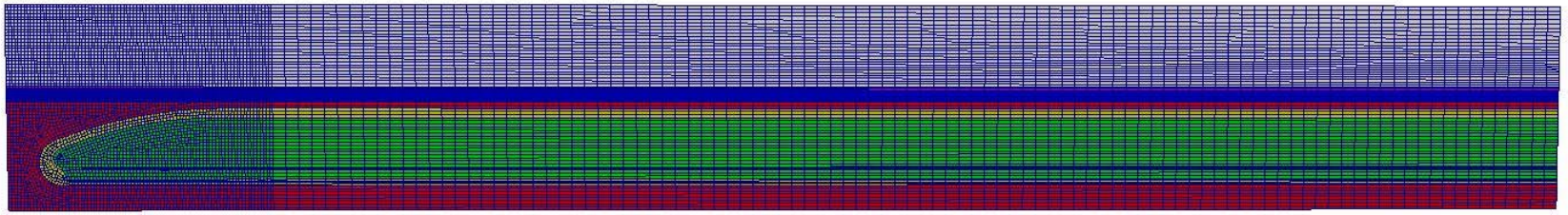
- Tritiumfreisetzung im Brutmaterial
- berechne Tritium in Spülgas, Kühlgas, Wänden.

Grundlage sind vorhandene Ergebnisse am INR

- 3D Modell mit thermohydraulischen Analysen
- 1D-Tritiumfreisetzung aus Neutronikrechnungen

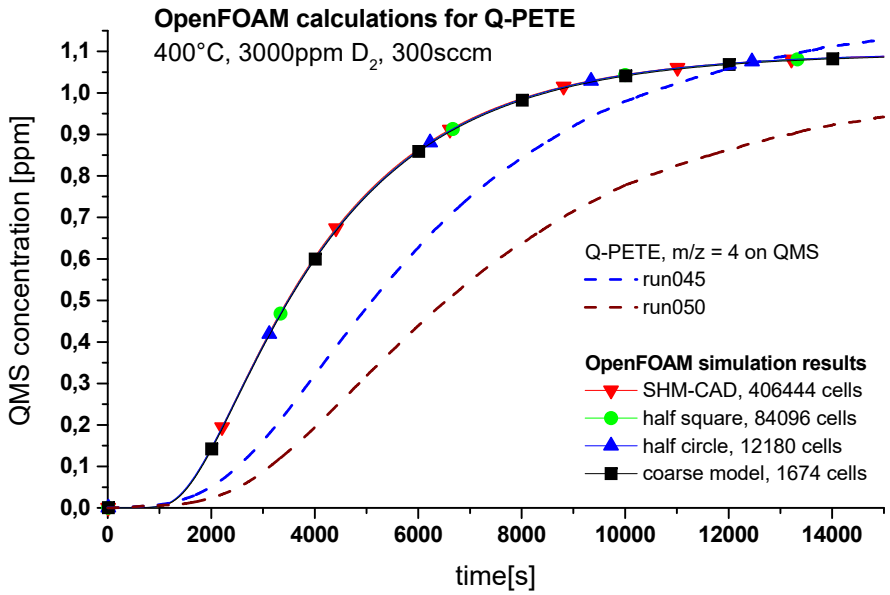


2D-Zylindersegment/Schnitt eines Pins (13167 Zellen)



OpenFOAM Ergebnisse für Q-PETE

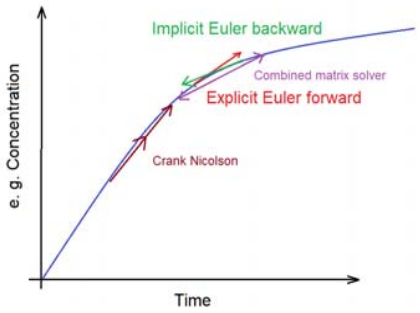
Möglichkeiten zur Vereinfachung des Mesh

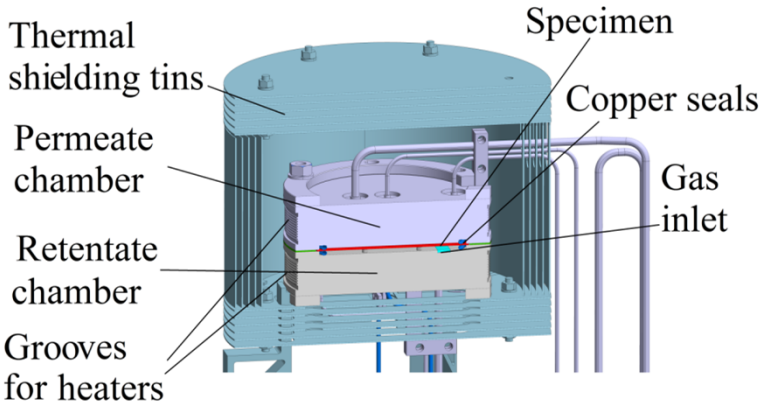


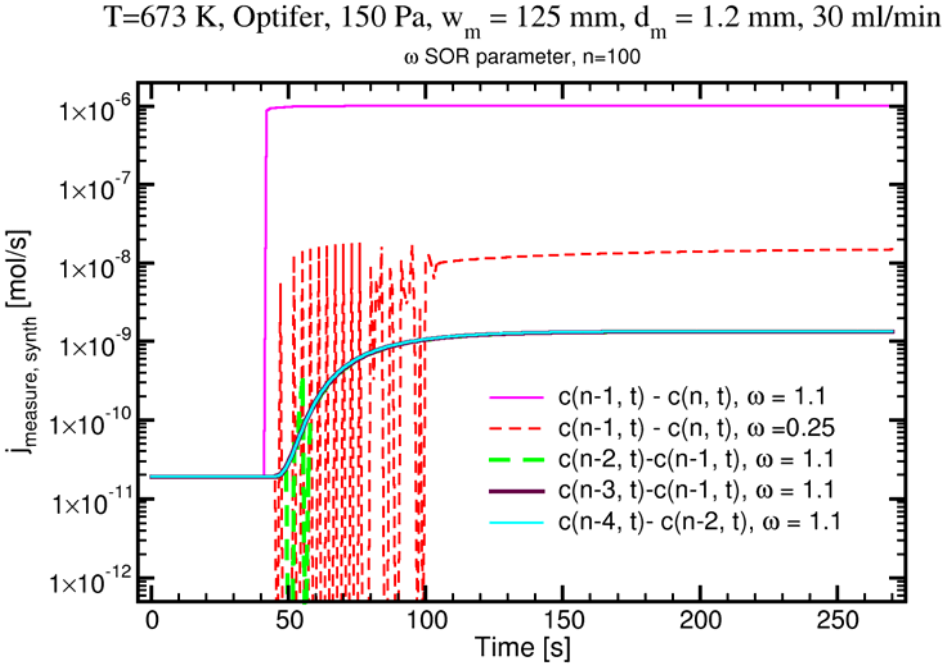
OpenFOAM Ergebnisse für Tritium-permeation ins Kühlmittel und Tritiumeintrag in die Stahlwände eines DEMO HCPB Pins

	1e-3Pa H_2 im Spülgas	300Pa H_2 im Spülgas
surface-limited (Oberflächengleichungen)	0.2% des erzeugten T 1.5 µg/pin	0.15% des erzeugten T 0.19 µg/pin
diffusion-limited (Sieverts Gesetz)	5% des erzeugten T 1.1 µg/pin	0.6% des erzeugten T 0.16 µg/pin

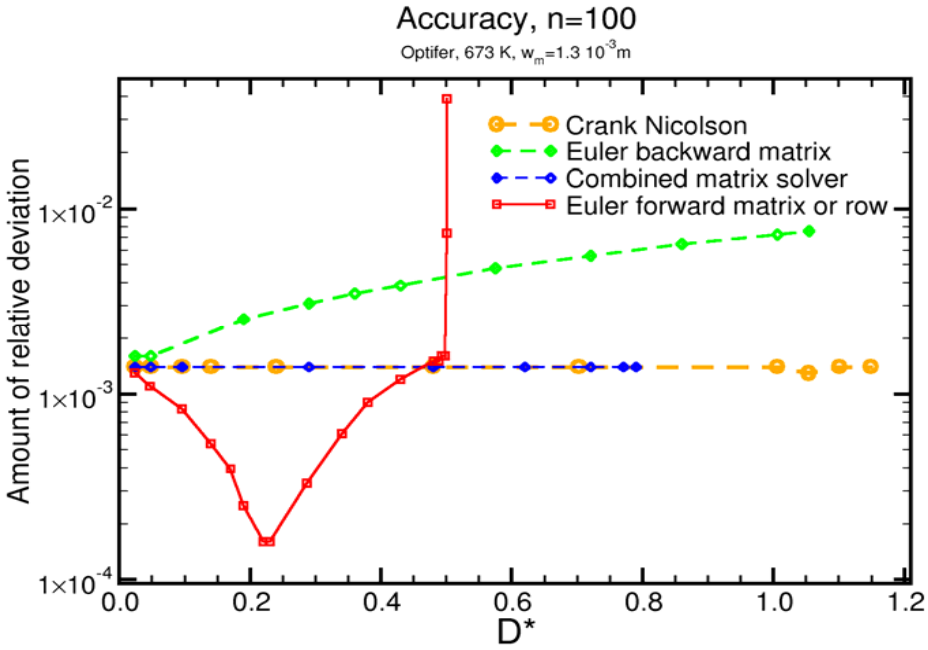
Application: Hydrogen paths in solid structures (embrittlement)

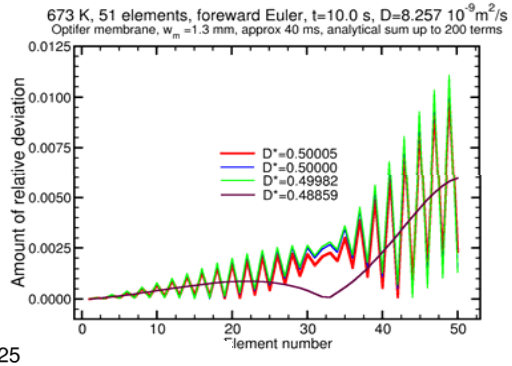

Implicit Euler backward
Combined matrix solver
Explicit Euler forward
Crank Nicolson
e. g. Concentration
Time


Thermal shielding tins
Permeate chamber
Retentate chamber
Grooves for heaters
Specimen
Copper seals
Gas inlet

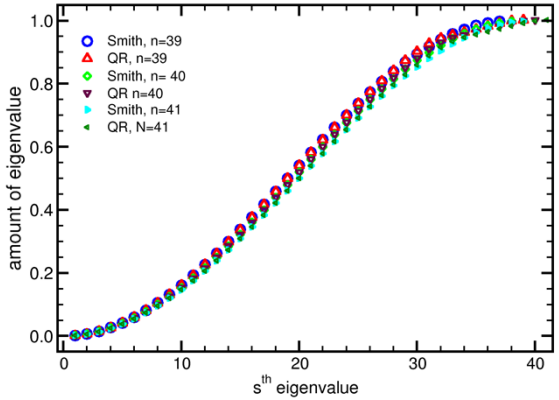

T=673 K, Optifer, 150 Pa, w_m = 125 mm, d_m = 1.2 mm, 30 ml/min
ω SOR parameter, n=100
j_measure, synth [mol/s]
1×10^-6
1×10^-7
1×10^-8
1×10^-9
1×10^-10
1×10^-11
1×10^-12
0
50
100
150
200
250
Time [s]
c(n-1, t) - c(n, t), ω = 1.1
c(n-1, t) - c(n, t), ω =0.25
c(n-2, t)-c(n-1, t), ω = 1.1
c(n-3, t)-c(n-1, t), ω = 1.1
c(n-4, t)- c(n-2, t), ω = 1.1

Solving algorithm: Rediffusion and optimal $D^*=(n-1)^2 D_{eff} dt/w_m^2 \leq 0.5$, former 17 hour @inrclu (fixed dt), optimised algorithm and use of $D^*=0.25$ (variable dt), now 40 -120 s @ UC2, n=100 elements



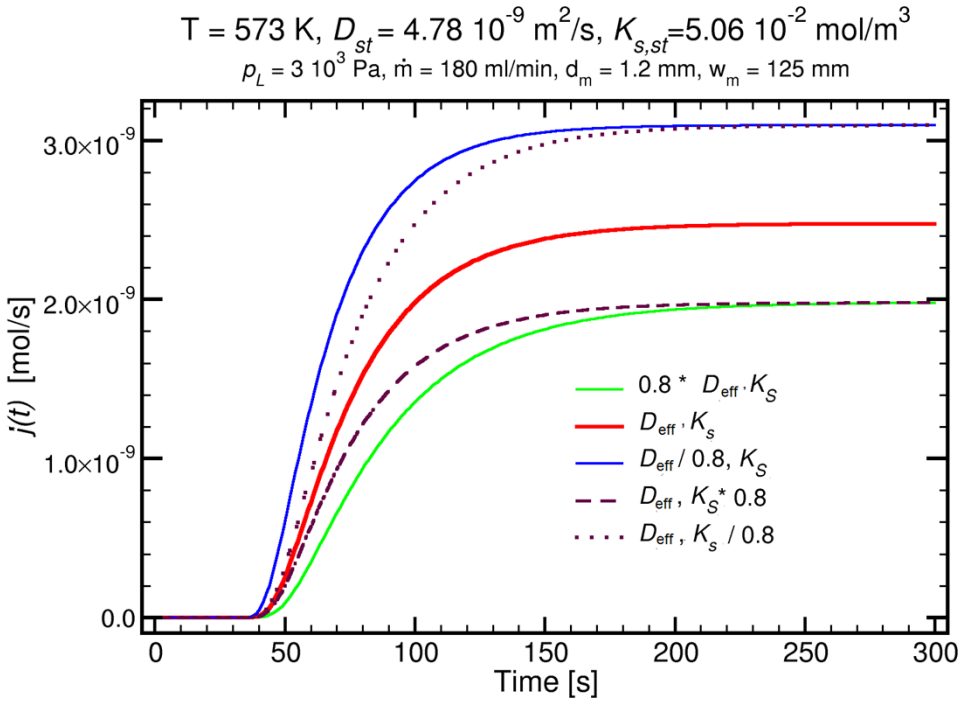


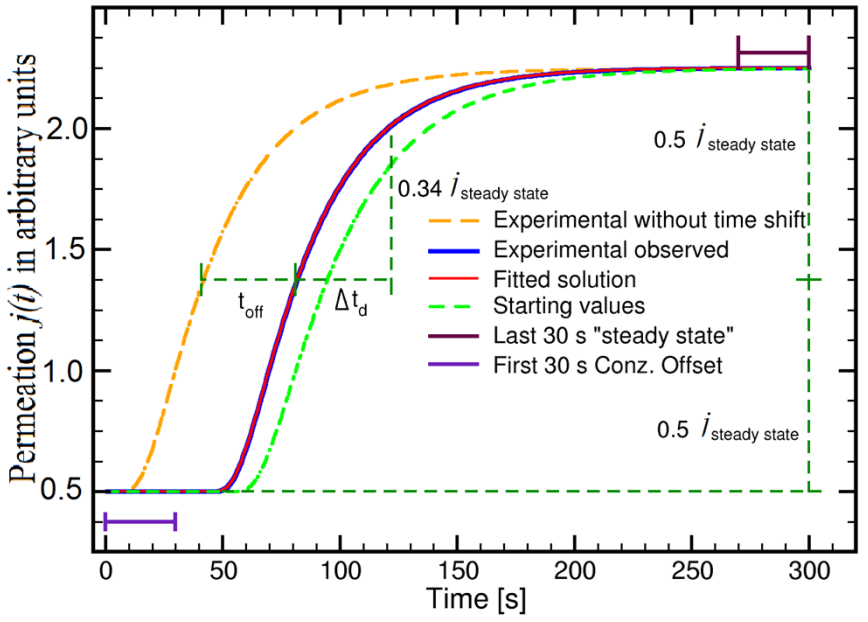
Euler forward, D*=0.25



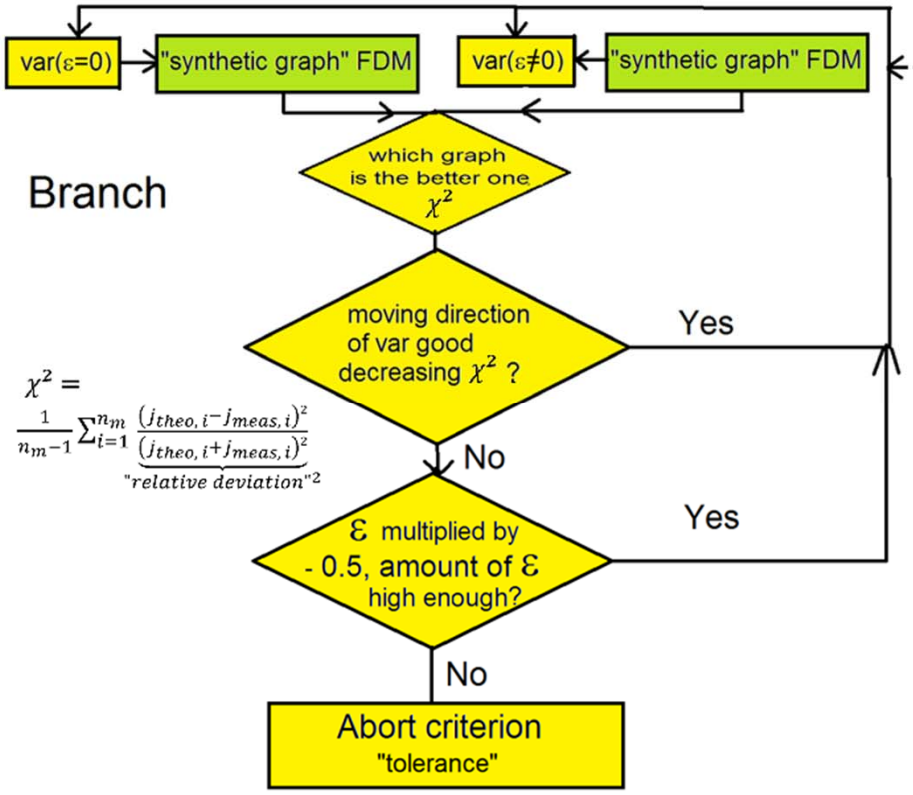
Co working in QR with Till Glage

B&B algorithm searching fitting solution depending on transport parameters



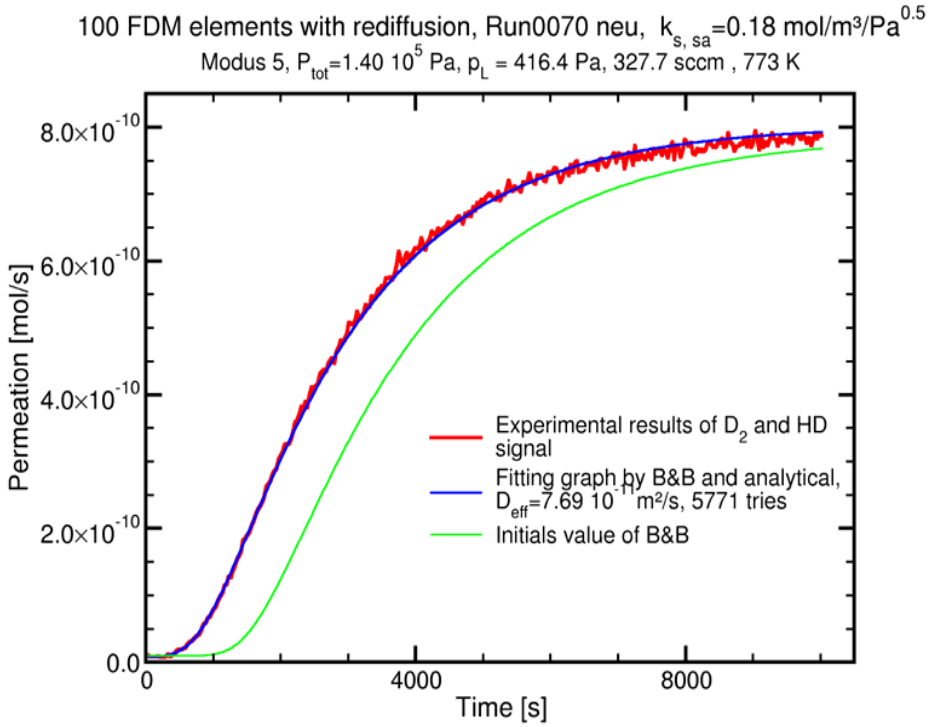


Solving inverse problem by B&B algorithm

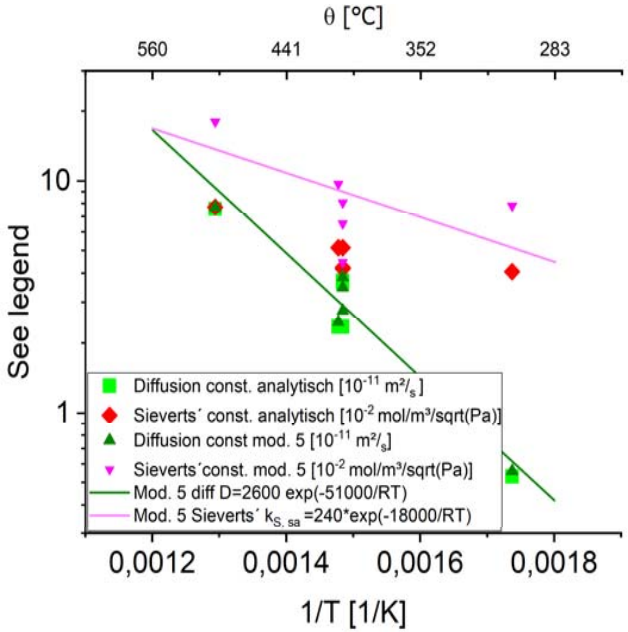


super cycle		bounds
1.	$t_{off};\ t_{off} + \epsilon$	
2.	$D_{eff}\ ;\ D_{eff}\ (1 + \varepsilon)$	$D_{eff} > 0$
3.	$c(0); c(0)(1 + \epsilon)$	$c(0) > 0$
4.	$D_{eff}, c(0);\ \ D_{eff}\ (1 + \varepsilon),$ $c(0)/(1 + \varepsilon)$	$j_{steady\ state} = const.$
5.	$j_{offset};\ j_{offset}\ (1 + \ \varepsilon)$	$j_{offset}\ > 0$

Q-PETE results

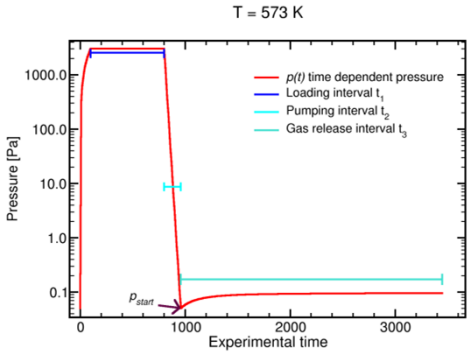


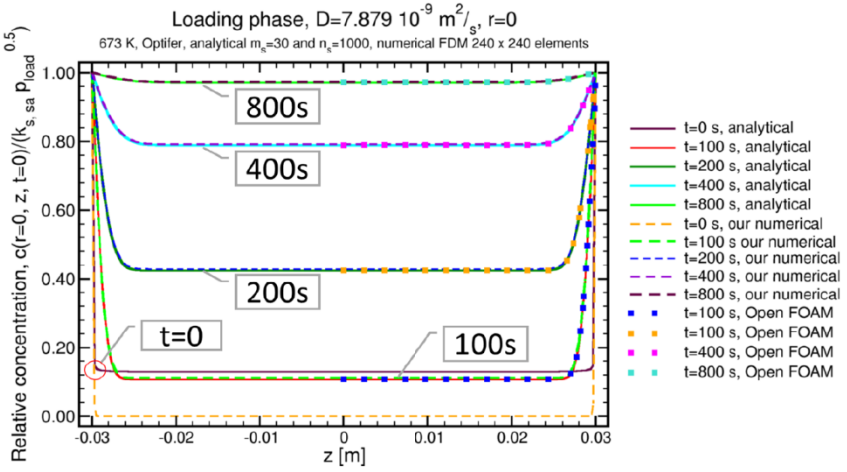
Possible Q-PETE application membrane of fuel cells



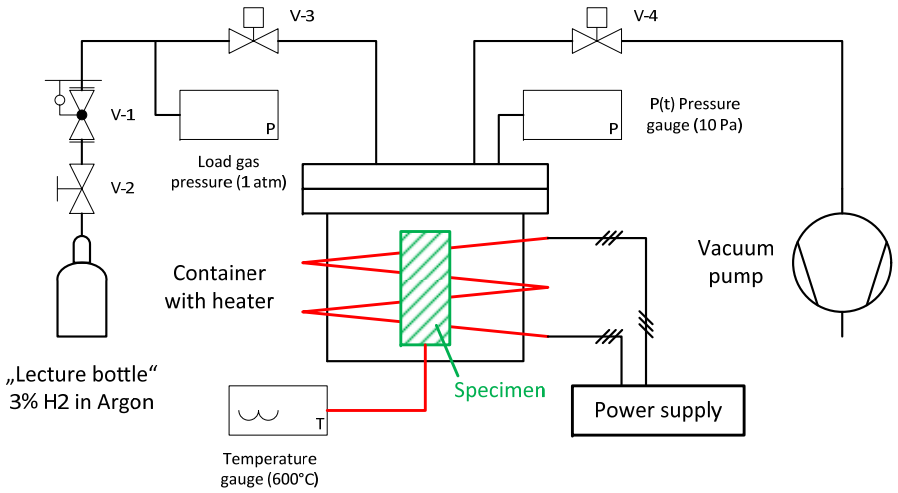
Endotherm, Grant et.al.: $E_{A,\ diff}$ = 52.4 kJ/mol, $E_{A,\ ks}$=16.5 kJ/mol (mod5)

Gas Releasase Experiment, status pre setup ready

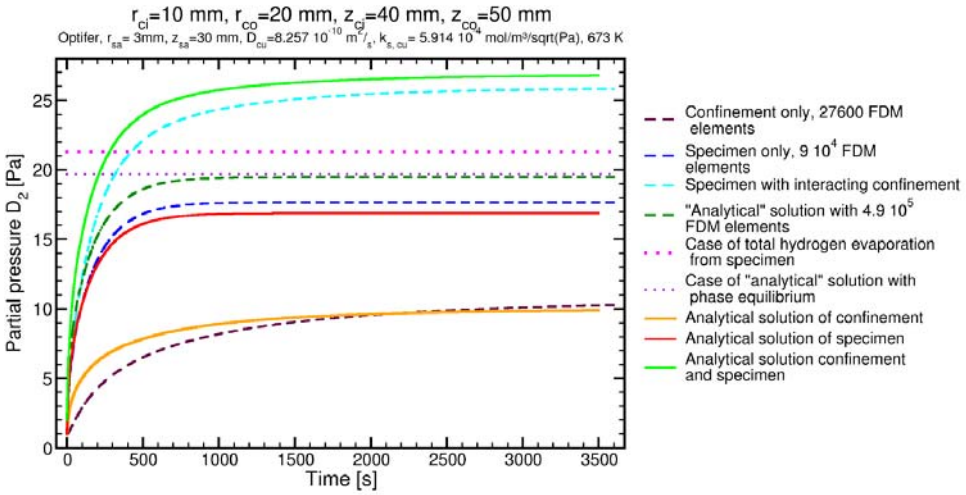




Analytical Solution: Co working with Marvin Schulz



First try with a CF tube with 19 mm diameter and 5 mm copper plating



Currently most interesting GRID experiment as storage description for “exothermal” hydrogen storage