Permeation data analysis including a nonzero hydrogen concentration on the low pressure detector side

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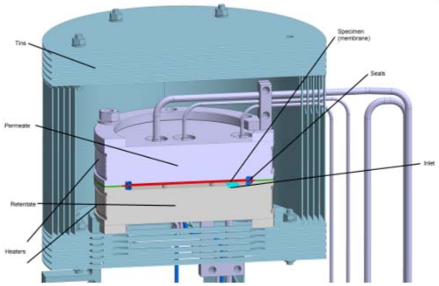
Karlsruhe , Computional Science and Mathematical Methods, 13th March, 2019

IKIT/INR/MET (Maschinenbau)



Determination of concentration dependent interstitial diffusion parameter regarding re-diffusion and small loading pressure: Situation of future fusion power plant 2 Pa tritium partial pressure (breeder unit) enriched to 1 Pa in purge gas system.

1.: Motivation
2.: Description of setup and simplification
3.: Status quo: FDM solver
4.: Status quo: Branch & Bond algorithm
5.: Desired Object: Gas release
6.: Other Projects

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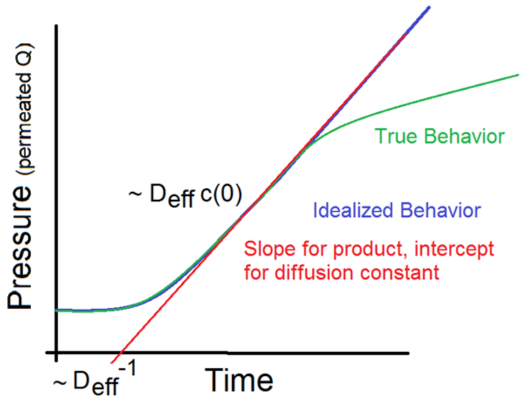
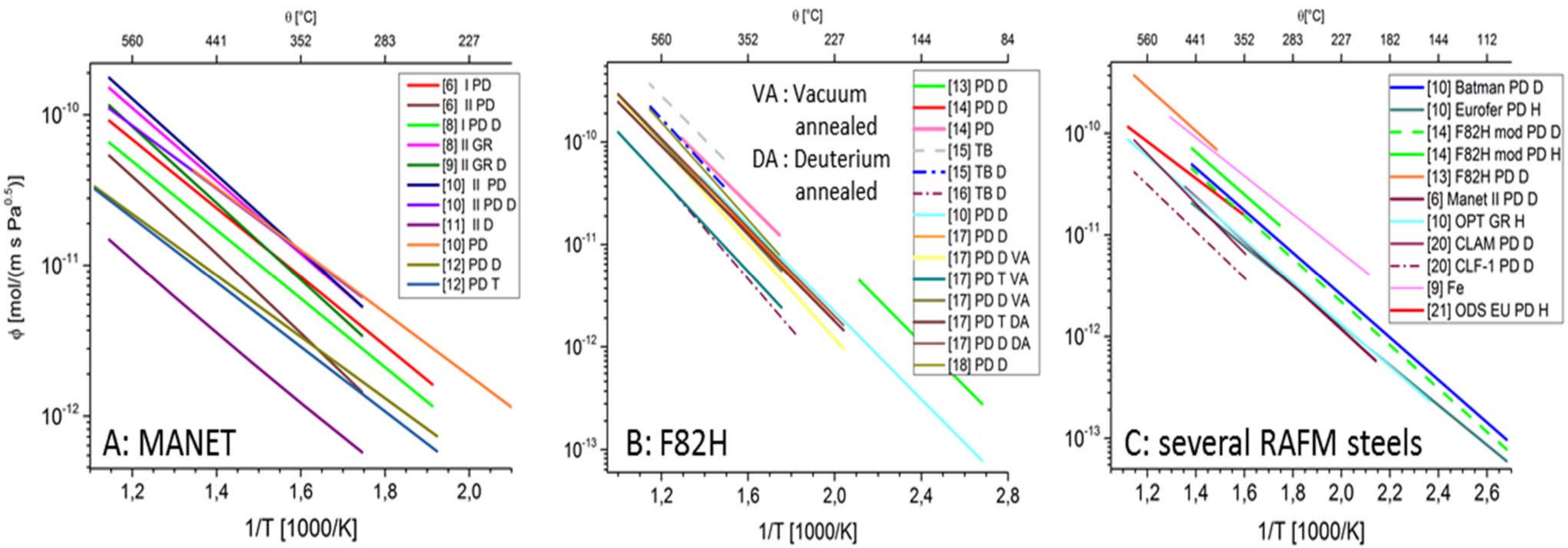
1.: Motivation



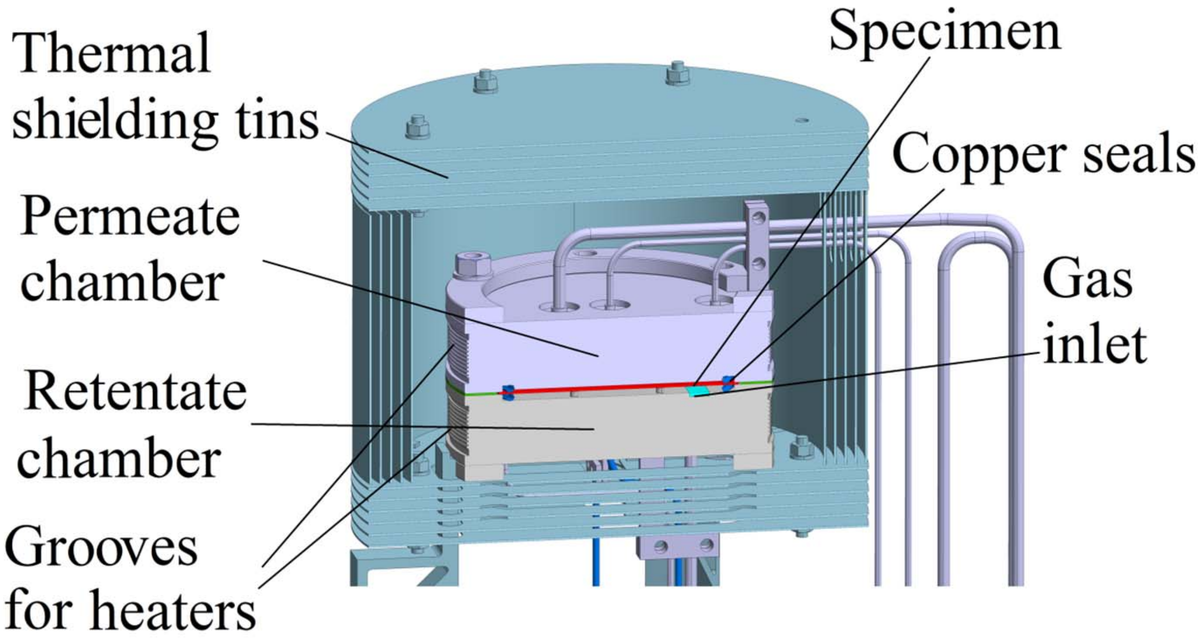
Time dependent non zero Q-concentration near measuring system (gauge or QMS) generates deviation from linear behavior.

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

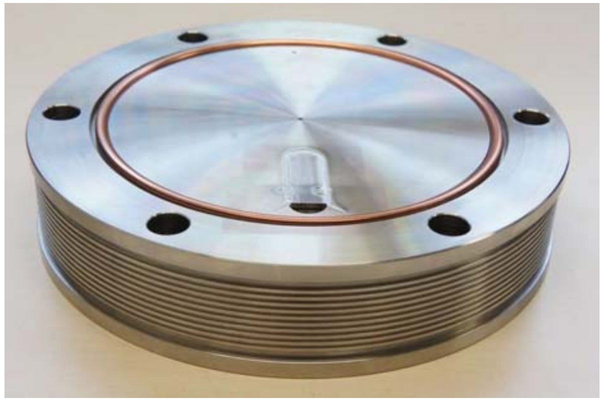
Daynes, Forcey transport equation solution



2.: Description of setup and simplification

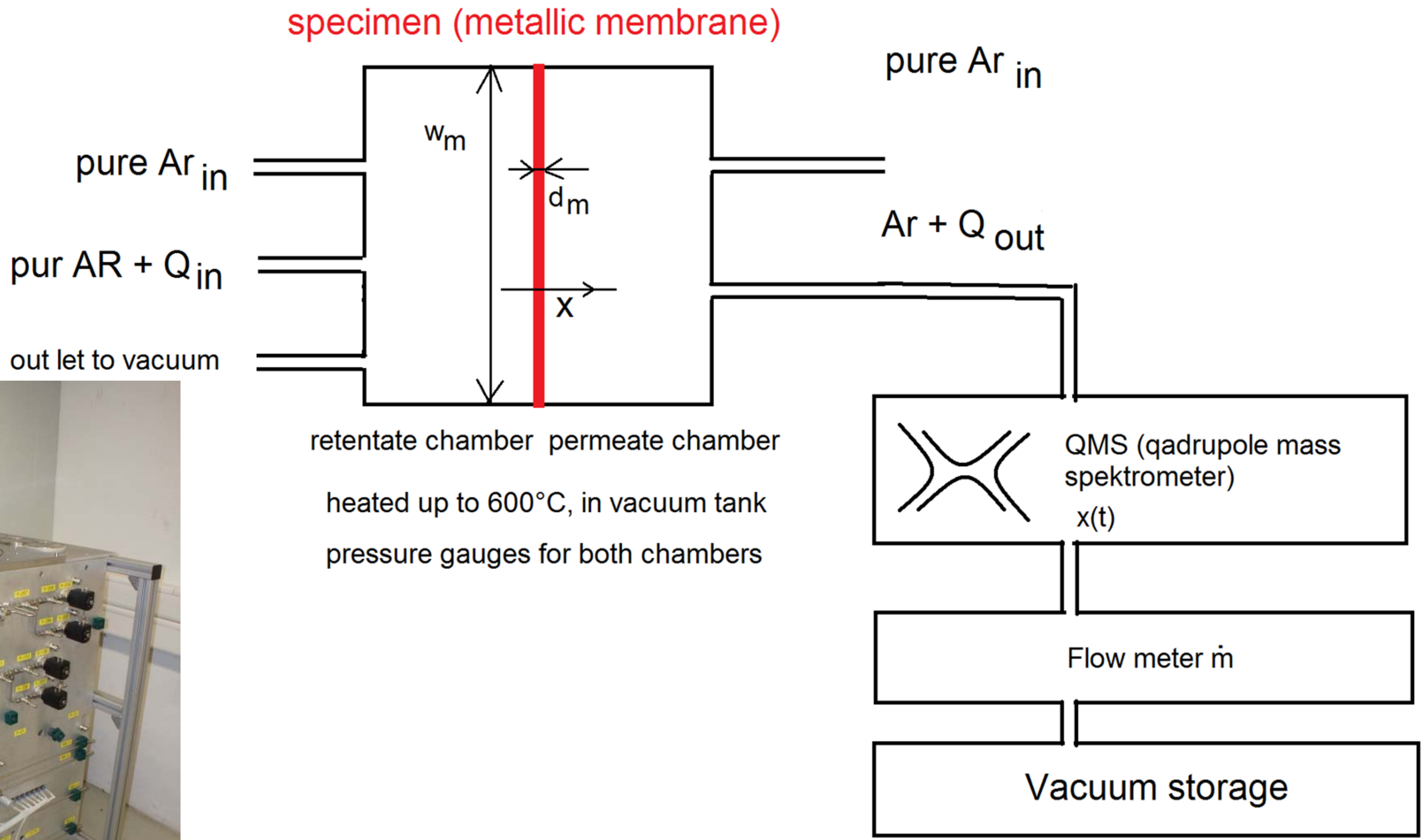


Therefore removing Q in permeate chamber.

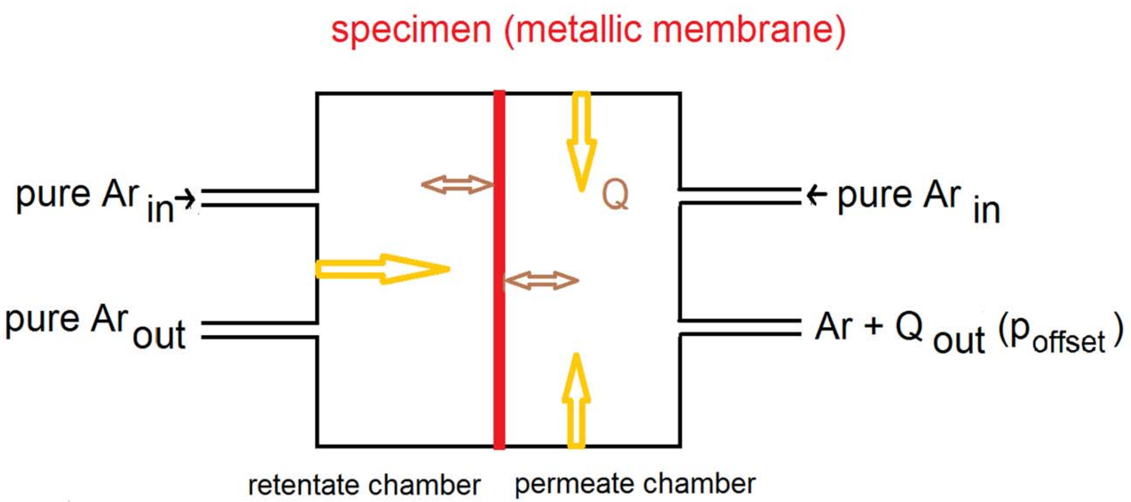


Permeate (secondary) chamber

Simplified Q-PETE experiment



3.: Status Quo FDM-solver: Before beginning of experiment: Purging with pure Ar:

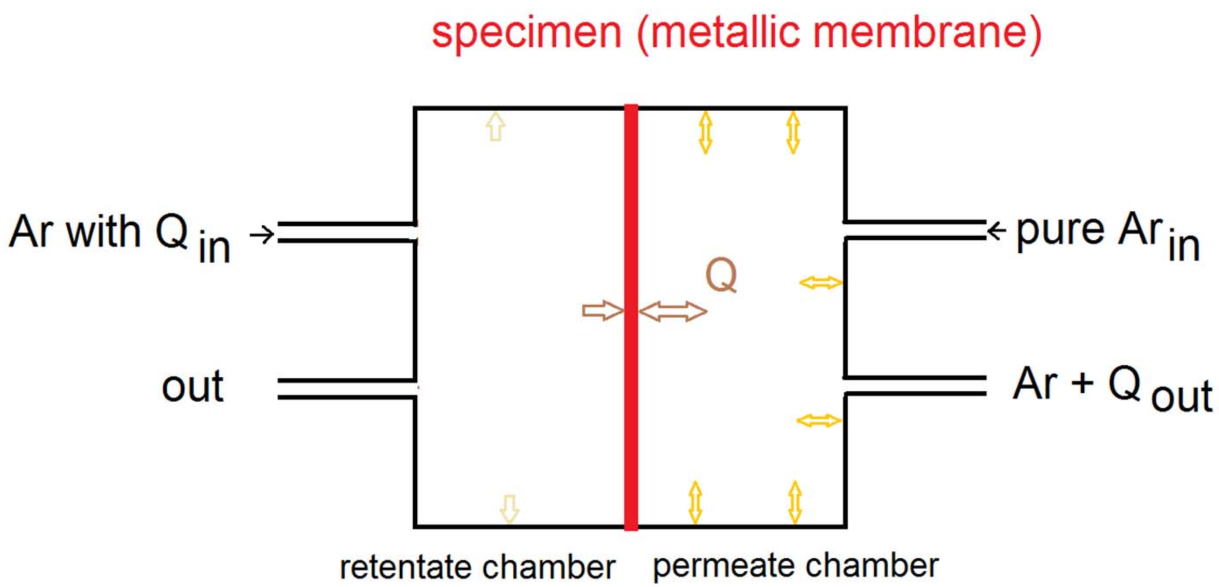


The stored Q is generating a constant assumed offset permeation. The membrane is in diffusive contact with the two volumes, equilibrium state given by k_S .

$$c(t,x) = k_s\sqrt{p_{offset}} = k_S\sqrt{\frac{j_{offset}\,p_{tot}}{\dot{m}_{Ar}}}, t < t_{start}, 0 \le x \le d_m$$

j_{offset} determined by QMS, specimen saturated with Q, no Q is additionally stored or emitted, p_{tot} absolute pressure in both volumes by pressure gauge, $\dot{m}_{Ar}$ by mass flow controller @RT

FDM solver: Boundary conditions after start of experiment:



$$c(x=0, t > t_{off}) \underbrace{=}_{FDM} c(1, t > t_{off}) = c(o)$$
$$= k_s \sqrt{p_{load}}$$

$$p_{offset} < p_{load}$$

$$j_{messure} = j_{offset} + \underbrace{j_{perm}}_{from\,membrane}$$

Partial Q-Pressure in retendate chamber, surface concentration linear increased in *1 s* after t_{off}

j_{offset} assumed constant, generated by thick structures thickness more than 20 mm (1.4404), emitting into vacuum also , membrane around 1.2 mm thickness.

FDM solver: Boundary condition of permeate (secondary) membrane side after start of experiment

$$j_{measure} = j_{offset} + -D_{eff}\frac{d_m^2\,\pi}{4}\frac{\partial c(x = w_m, t > t_{off})}{\partial x} \underbrace{=}_{FDM} j_{offset}$$

$$+ -D_{eff}\frac{d_m^2\,\pi}{4}\frac{c(x = w_m - 4\Delta x, t > t_{off}) - c(x = w_m - 2\Delta x, t > t_{off})}{2\,\Delta x}$$

$$(*)\quad c(n, t > t_{off}) = \underbrace{k_s\sqrt{j_{measure}\,\frac{p_{tot}}{\dot{m}_{Ar}\,\alpha}}}_{lit.=0,\; c(n,t>t_{off})=k_s\sqrt{\frac{R\,T_{abs}}{V_{gas}}\int_0^t j_{measure}dt}} \sim k_s\sqrt{\frac{D_{eff}\,(c(n-4,t)-c(n-2,t))}{2\,\Delta x}}$$

Δx = 12 µm (=d_m /n) from discretization of membrane in thickness direction normally n=100 elements, first element on retendate side, *n^{th}* element on permeate side. α=1 for homogeneous purge gas inlet, α=2 for point shaped inlet

Transient FDM-solver (any textbook):

$$\frac{\partial c}{\partial t} = D_{eff}\frac{\partial^2}{\partial x^2}$$

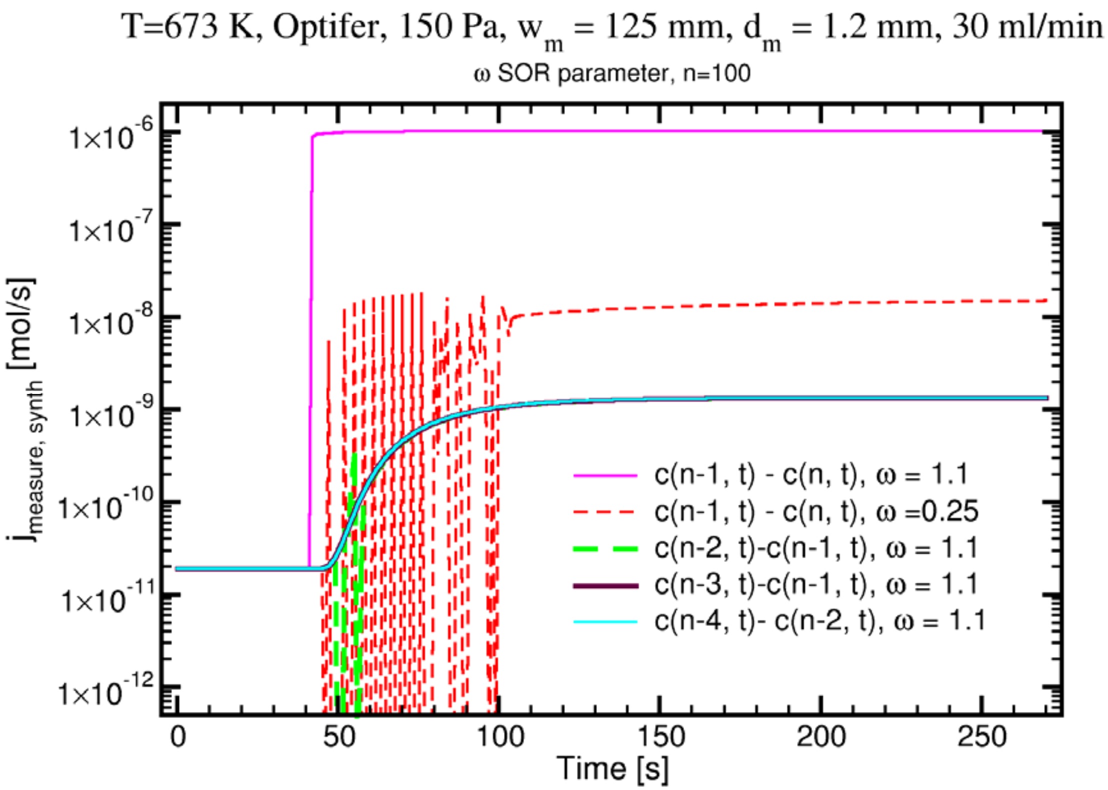
$$(**)\qquad c(i, t + \Delta t) = c(i,t) + \frac{D_{eff}\,\Delta t}{\Delta x^2}\left(c(i+1,t) - 2\,c(i,t) + c(i-1,t)\right)$$

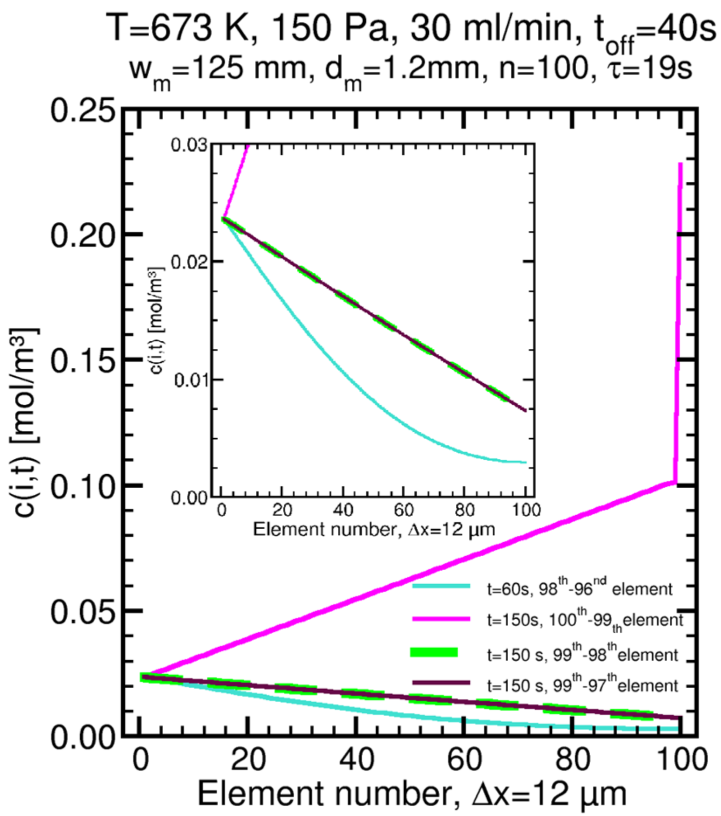
$$I = 2 \ldots .\, n-1, t > t_{off}$$

Used FDM-SOR-step (successive over relaxation)

$$c(i,t+\Delta t)_\omega = \underbrace{\omega}_{SOR}\ (c(i,t+\Delta t) - c(i,t)) + c(i,t)\,, \qquad 0 < \omega < 2$$

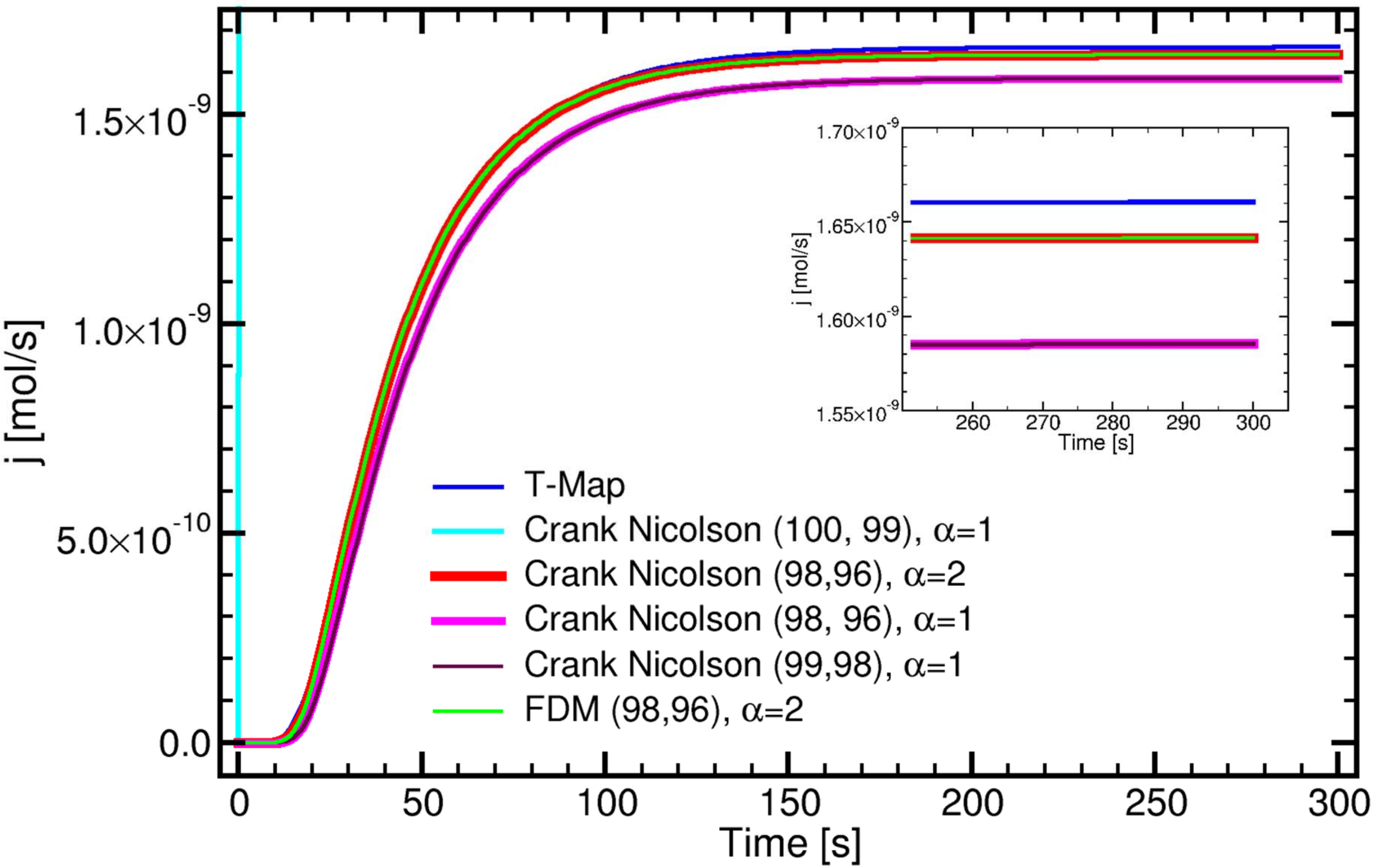
Optimized ω with Eigenwertanalysis of (*, **), only proposal: Change of (*) to Henrys law , translation of (**) into matrix, calculation with QR method for λ_{max}, now only $\omega=1.1$ carefully is used.





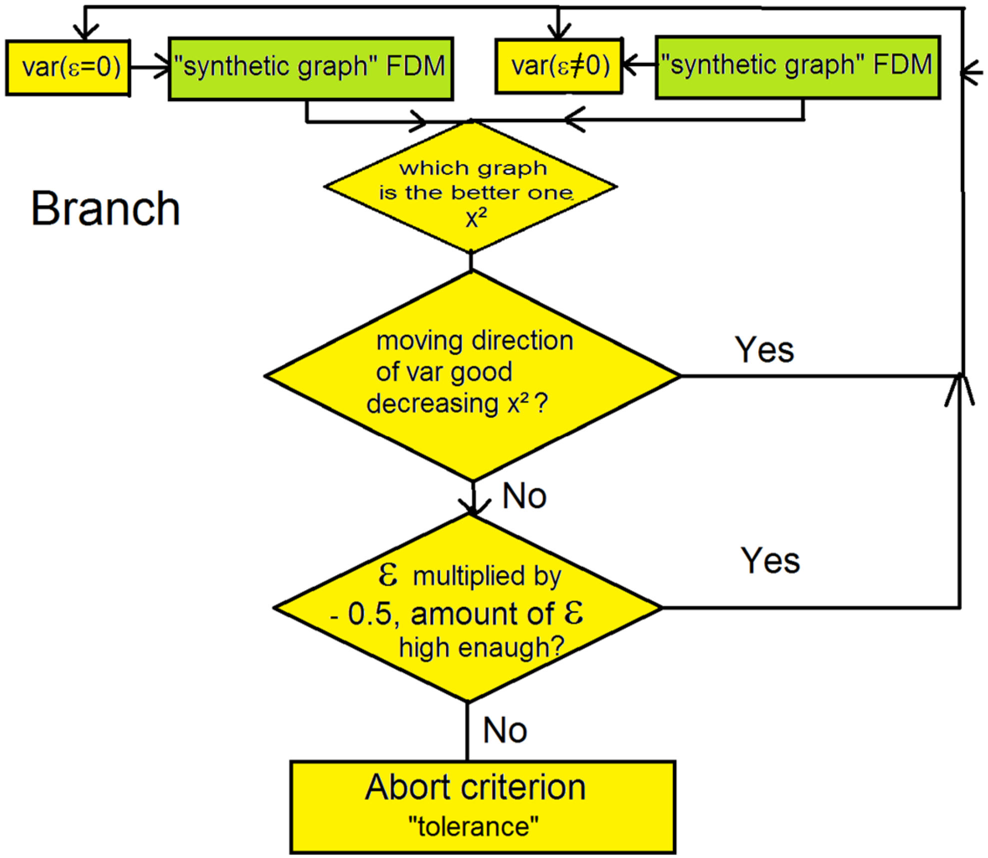
Comparison T-Map, Crank Nicolson and FDM

673 K, 2.5 $10^{-6} m^3/s$, 280 Pa, 1.4 10^5Pa, D_2, 100 elements



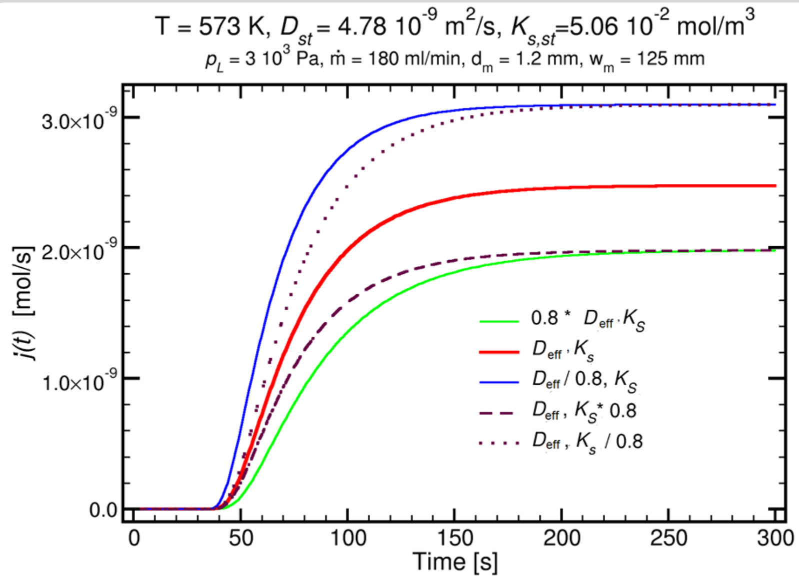
4.: Status quo: (Branch and Bound) B&B algorithm

Four desired variables: D_{eff}, c(0) (=c(1, t) res. $k_s\sqrt{p_{load}}$), t_{off} and j_{offset} serial treated within a super cycle. No explicit formulation possible, especially Daynes solution, comparison between measured permeation curve and “synthetic” graph from FDM module:

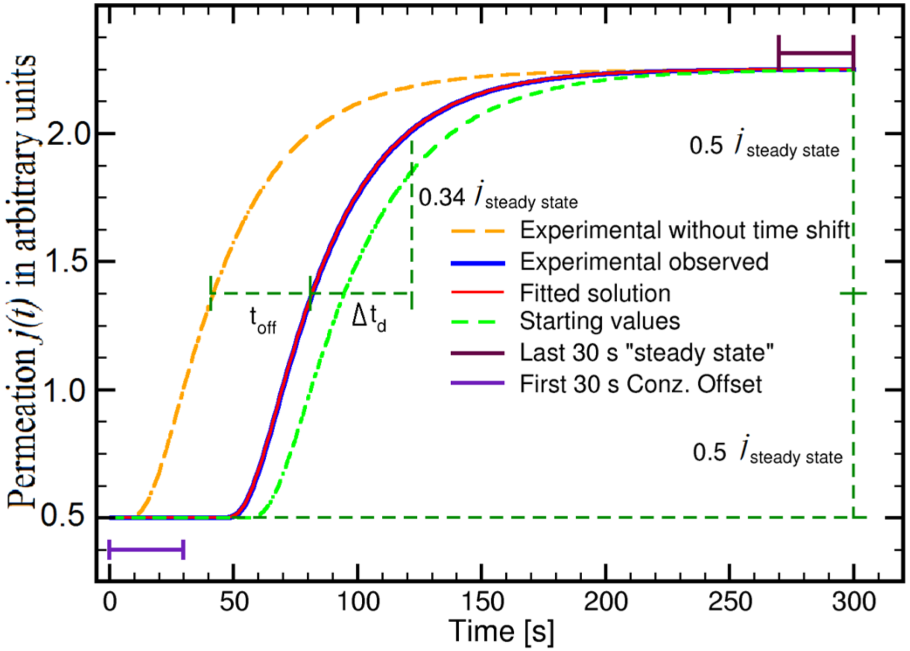


Initial values by analytical first order approximations

	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.	$D_{eff}, c(0); \ \ D_{eff}\ (1+\varepsilon), c(0)/(1+\varepsilon)$	$j_{stedy\ state} = const.$
5.	$j_{offset}; \ j_{offset}\ (1+\ \varepsilon)$	$j_{offset}\ > 0$



B&B: Determination of initial values:



$$j_{offset,initial} = \frac{1}{n_j} \sum_{i=1}^{n_j} j(i)_{measure}$$

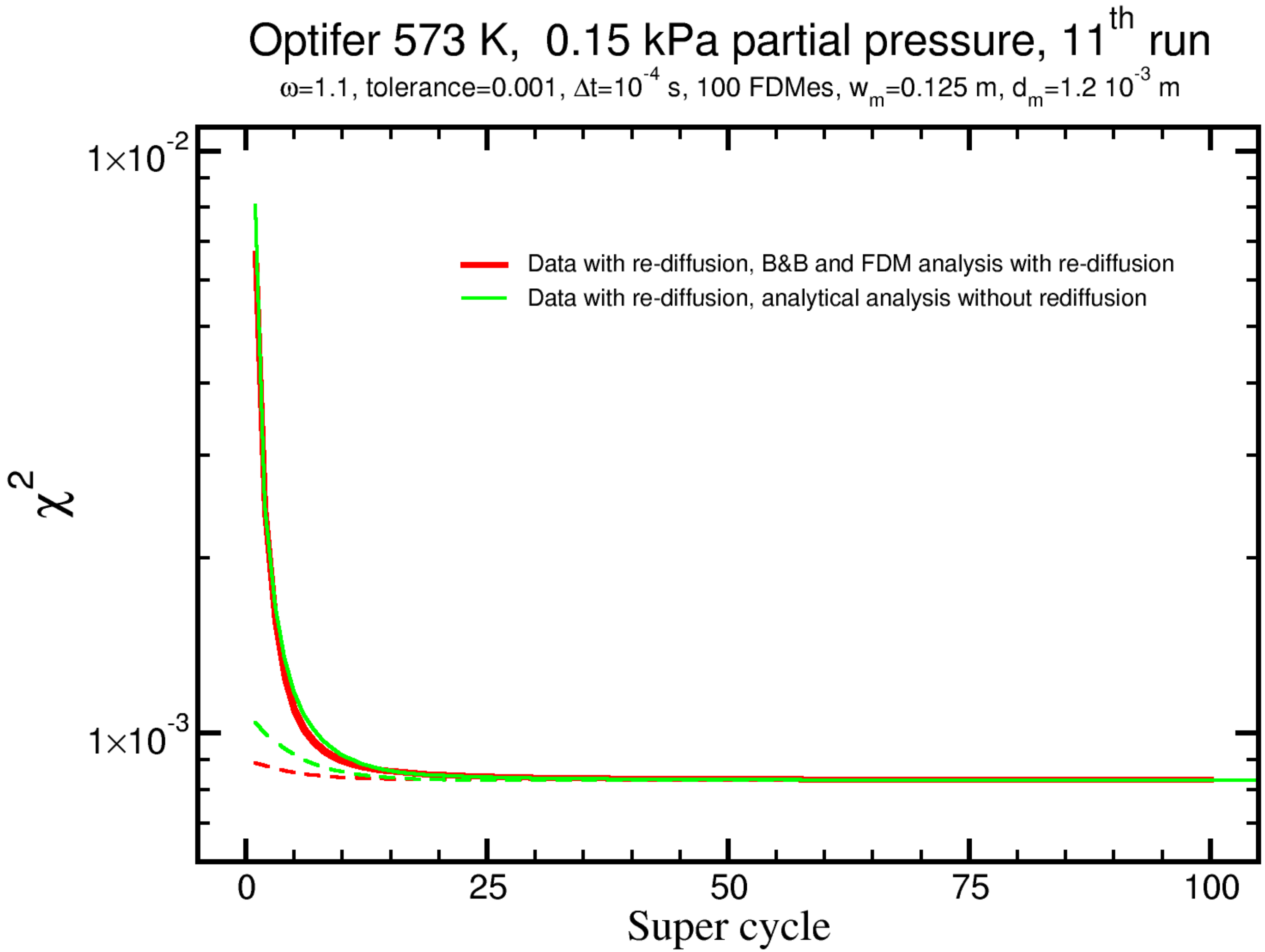
$$D_{eff,initial} = \frac{d_m^2}{\pi^2 \, \Delta t_d}$$

$$t_{off,initial} = t_{1/2} - 1.25 \, \Delta t_d$$

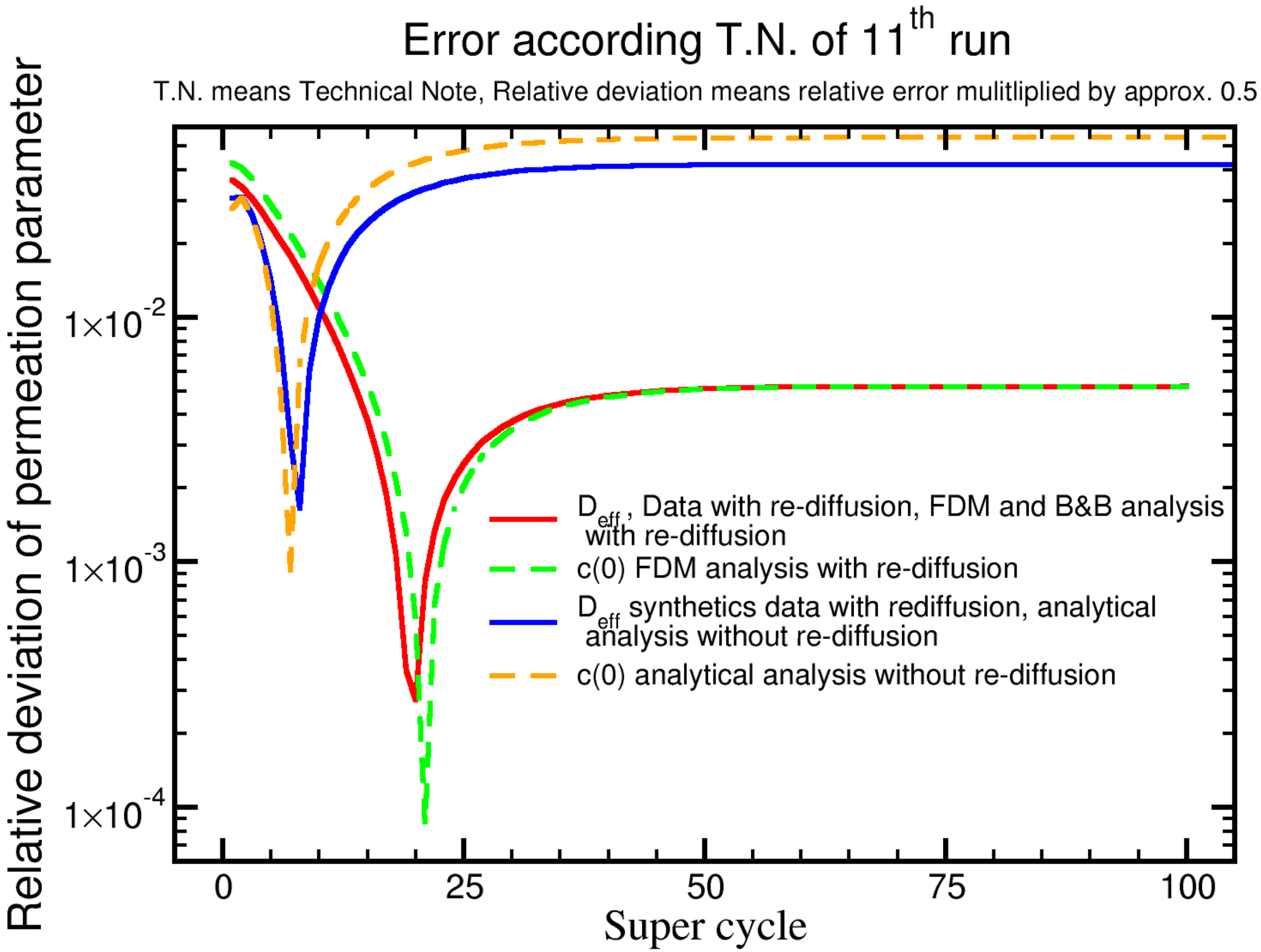
$$\Delta j = j_{steady\ state} - j_{offset,initial}$$

$$c(1, t \geq t_{off})_{initial} = \frac{\Delta j \;\; 4 \, d_m}{w_m^2 \, \pi \, D_{eff,initial} \sqrt{\dfrac{\Delta j \, p_{tot}}{\dot{m}_{therm} \, p_{load}}}}$$

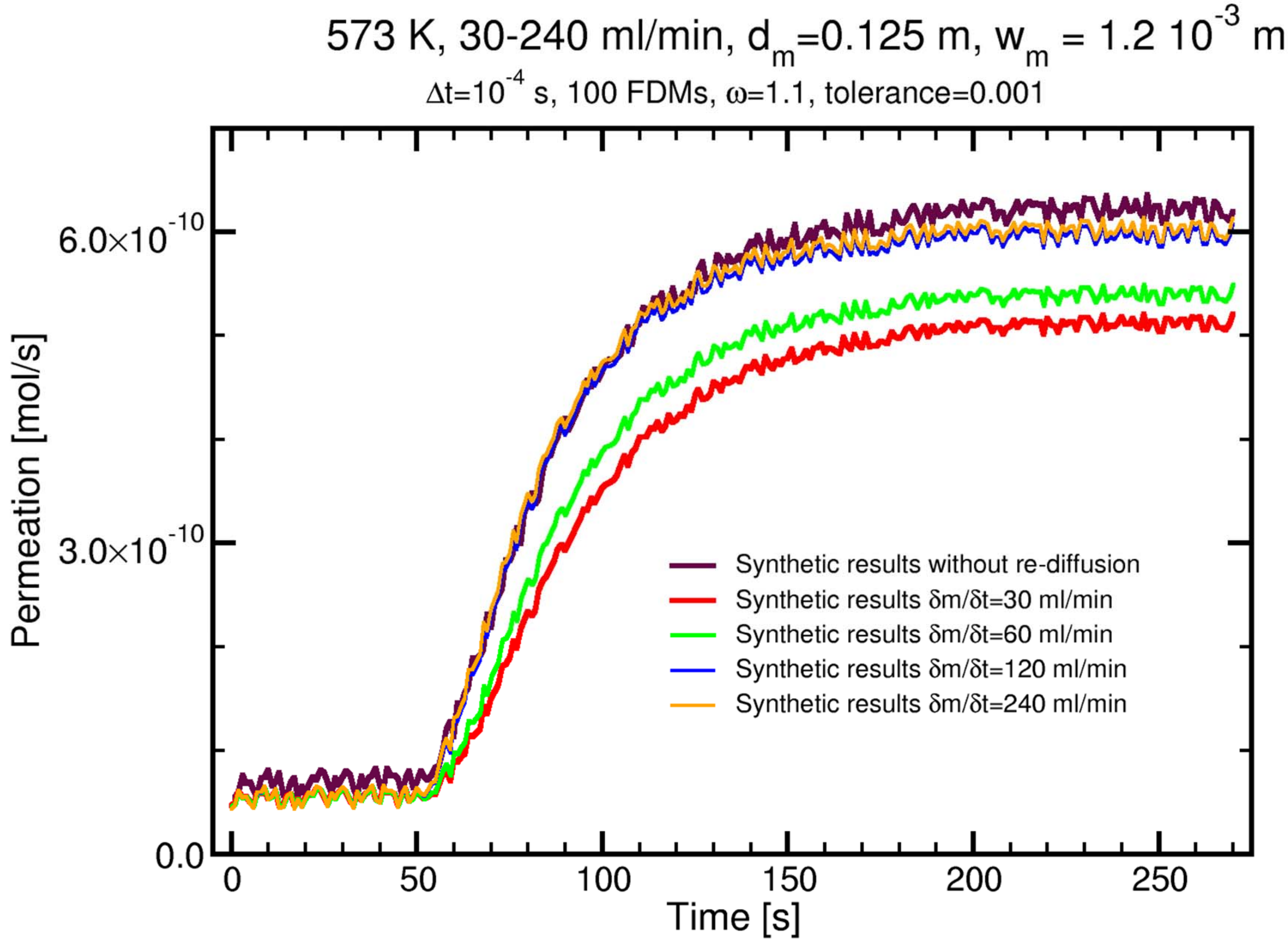
Example for χ^2



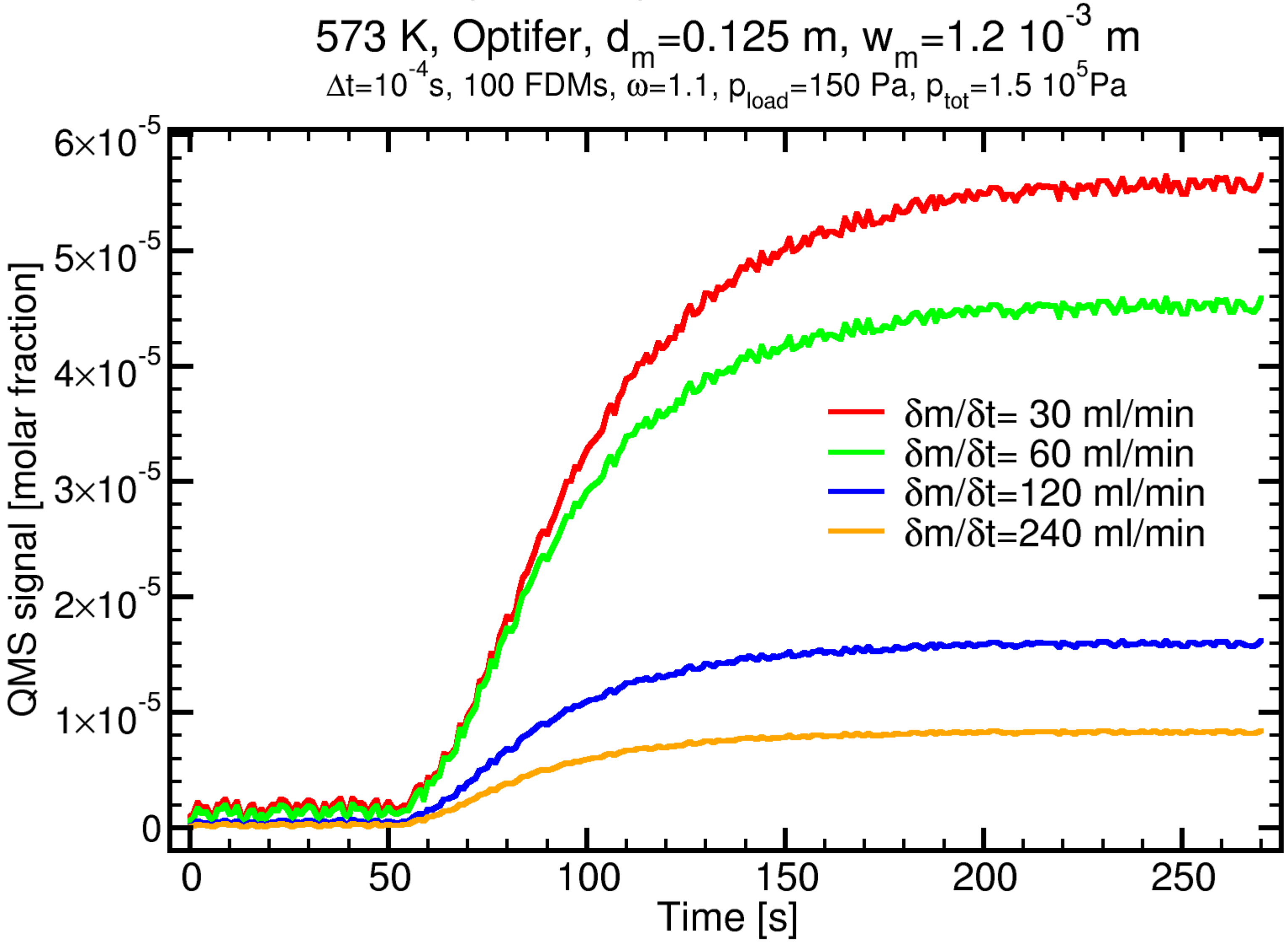
Example to former slide, comparison with analytical Daynes solution and FDM results



4. Expected advantage of Q-PETE setup: Influence on results by differing purge gas flux in permeate chamber:

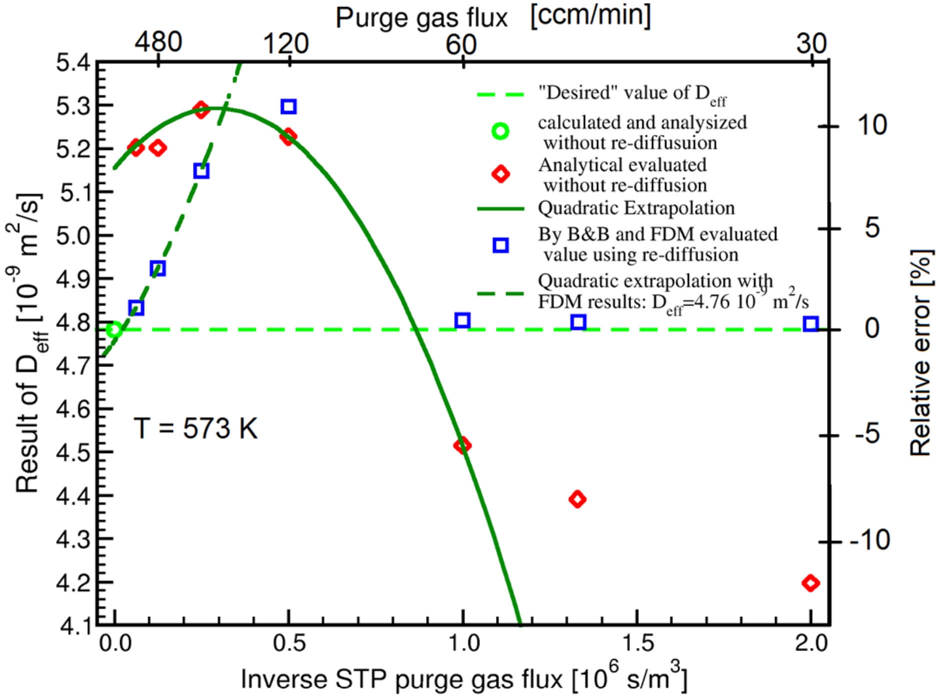


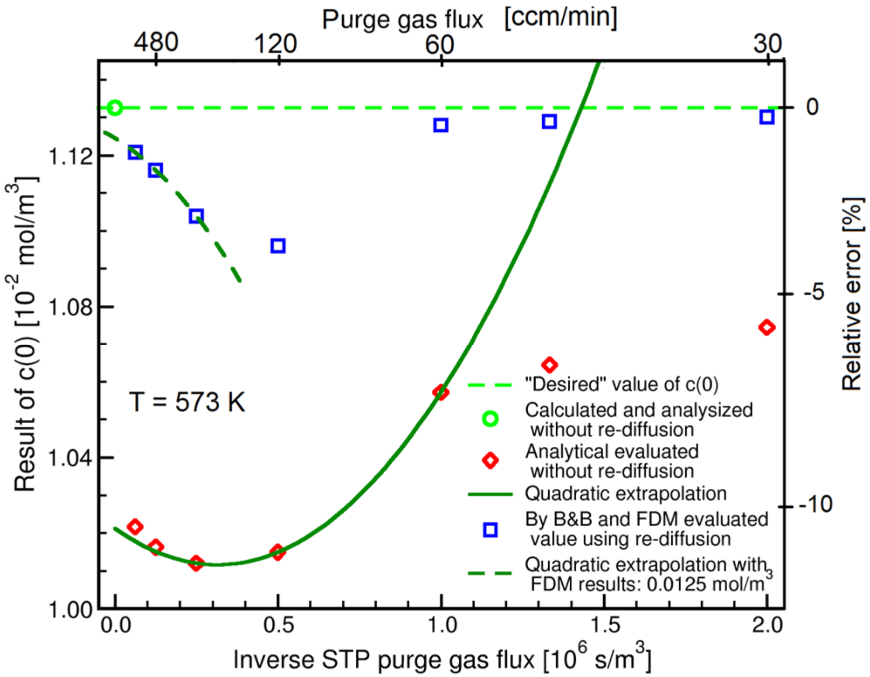
Expected advantage of Q-PETE setup: Influence on results by differing purge gas flux in permeate chamber aiming a differing Q-concentration there.



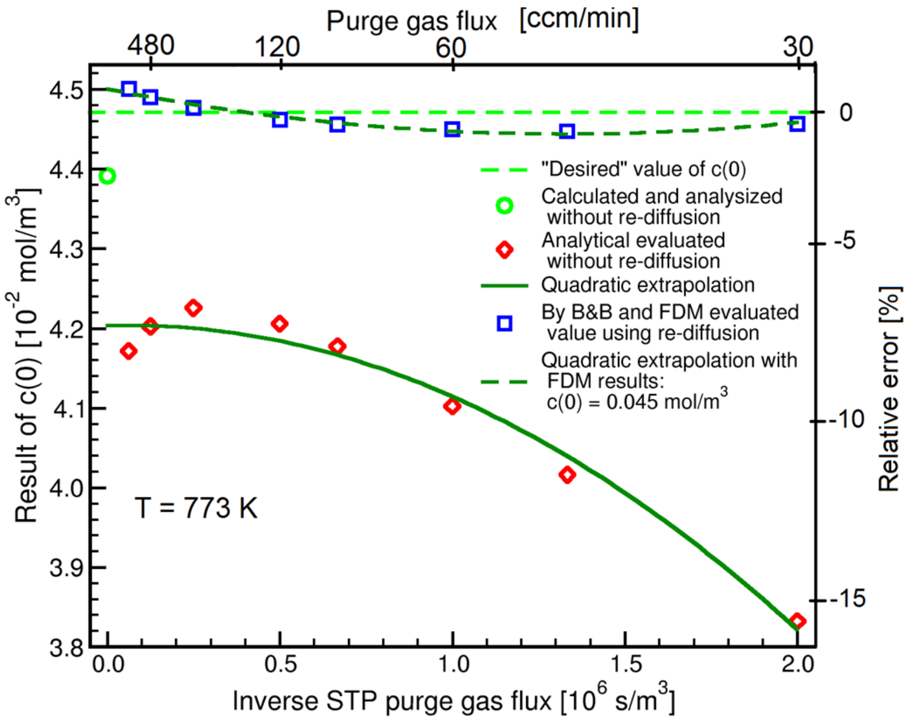
Re-recognition of diffusion constant and Sieverts´constant,

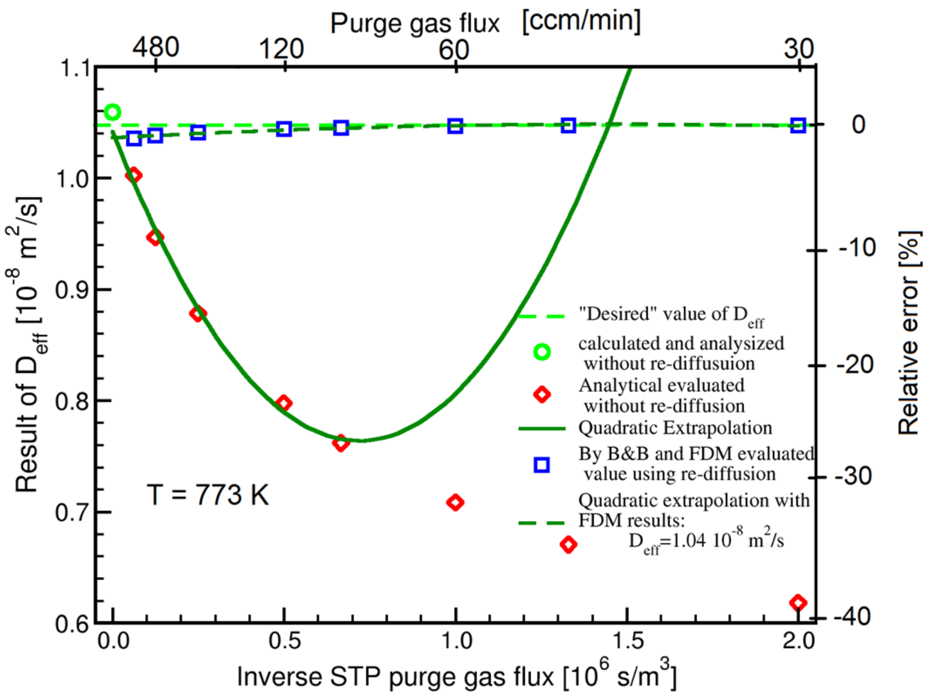
permeation constants of technical note as true regarded, time dependent synthetic permeation graph, analysis by FDM and B&B algorithm versus Daynes with B&B



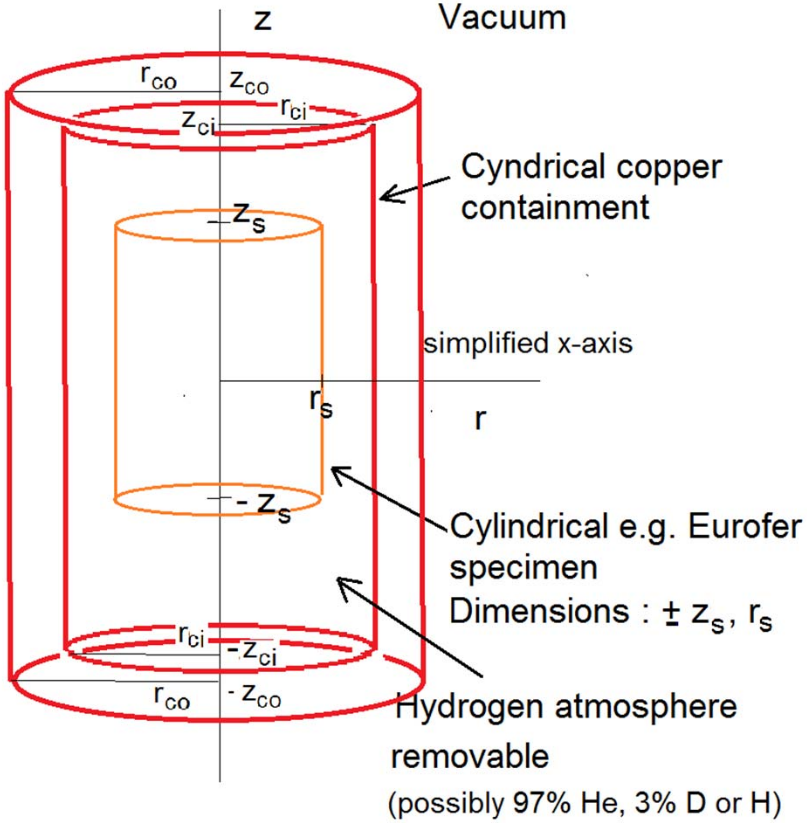


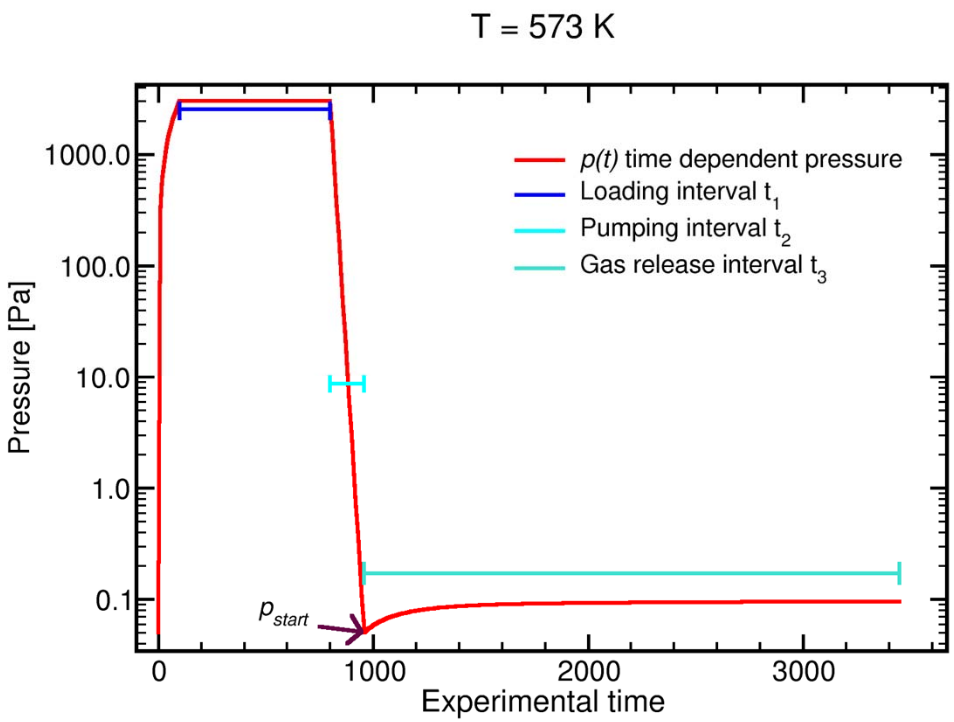
Re-recognition of diffusion and Sieverts´constant





5.: Desired object, gas release experiment





Equations simplified:

$$\frac{\partial c}{\partial t} = D_{sa}\Delta c \qquad \frac{\partial d}{\partial t} = D_{cu}\,\Delta d \qquad \Delta \underbrace{=}_{only\ r-dependence} \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}$$

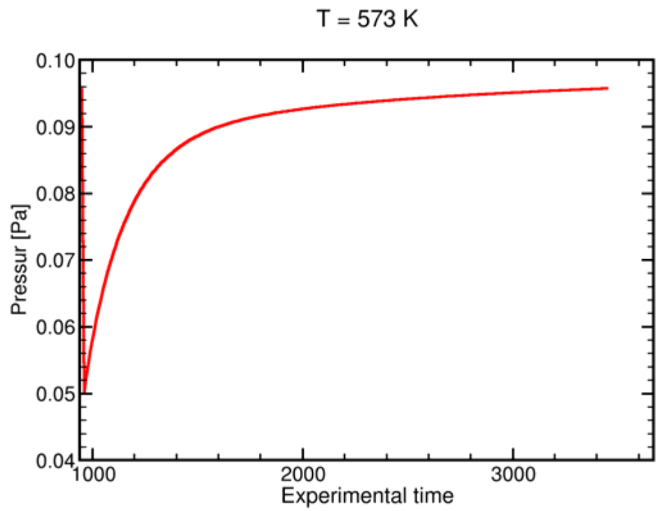
$$\frac{\partial m}{\partial t} = -A_{sa}\,D_{sa}\frac{\partial}{\partial r}\,c(r = r_{sa}, t) \;-A_{cu}\,D_{cu}\frac{\partial}{\partial r}\,d(r = r_{ci}, t)$$

$$p(t) = p_{start} + \underbrace{k_v}_{RT_{abs}/V_{gas}} \int_{t_1+t_2}^{t} \frac{\partial m}{\partial t}\,dt$$

$$c(r = r_s, \forall t) = k_{s,sa}\sqrt{p(t)} \qquad \frac{\partial}{\partial r}c(r = 0, \forall t) = 0$$

$$d(r = r_{ci}, \forall t) = k_{s,cu}\sqrt{p(t)}$$

$$d(r = r_{co},\ \forall t) = 0$$



Gas release Experiment, current status

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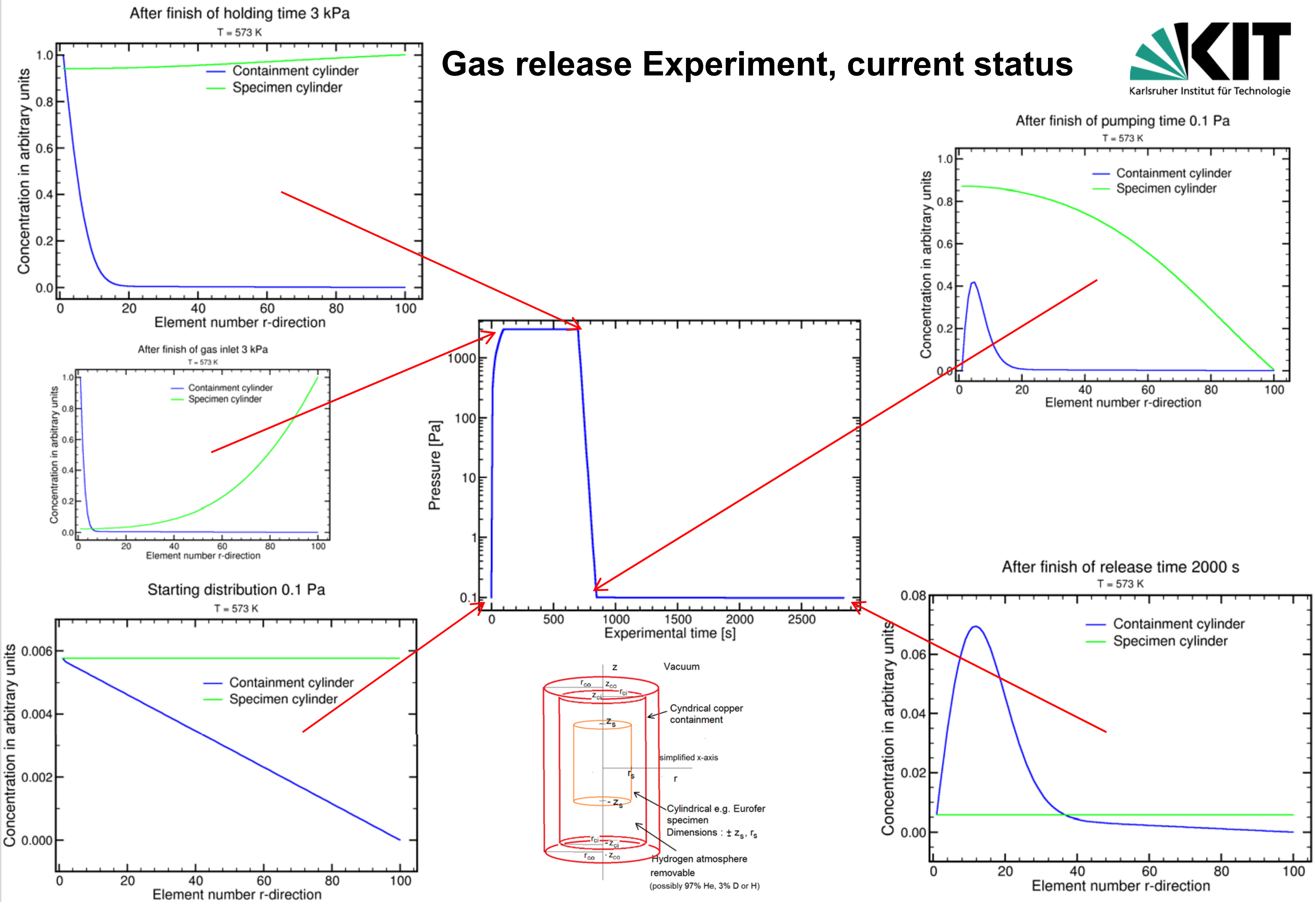
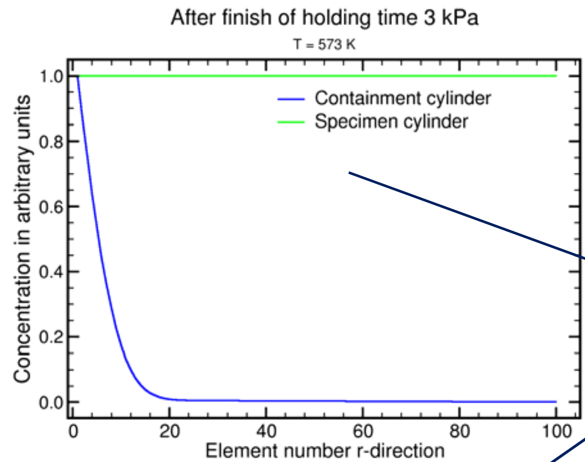
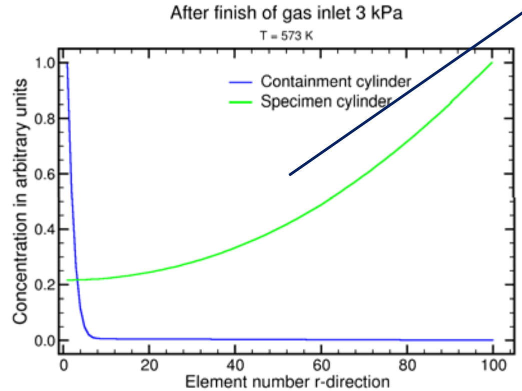
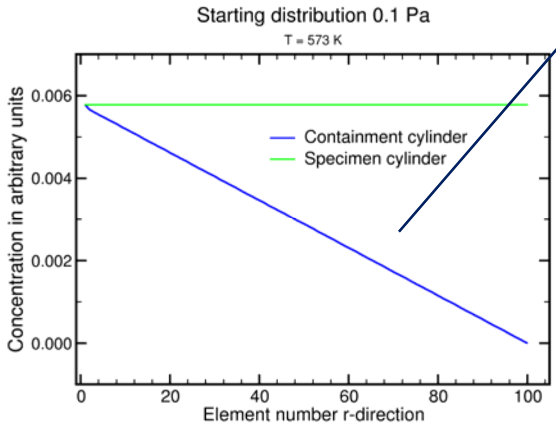


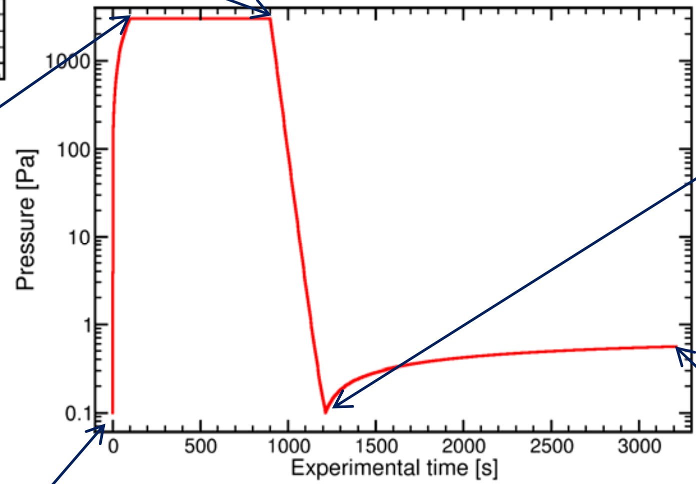
Gas release Experiment, current status

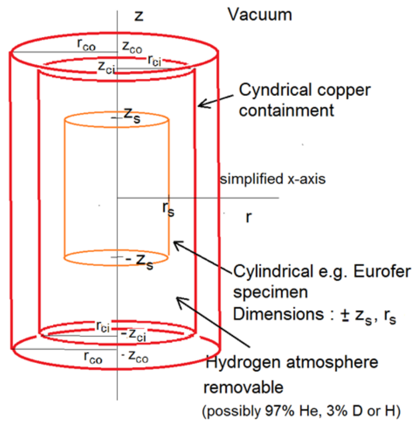
Extrapolation of inverse problem using 2D-Solver and additional cap surfaces 2400 h on bwUniCluster.

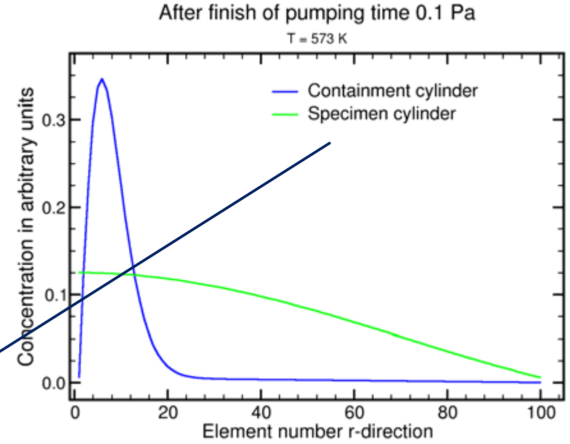


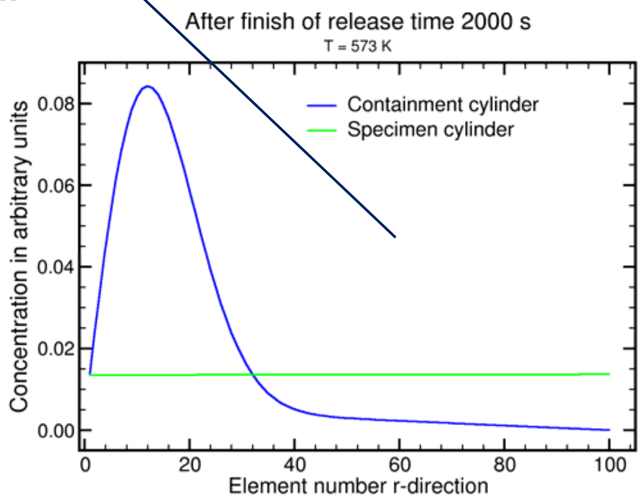








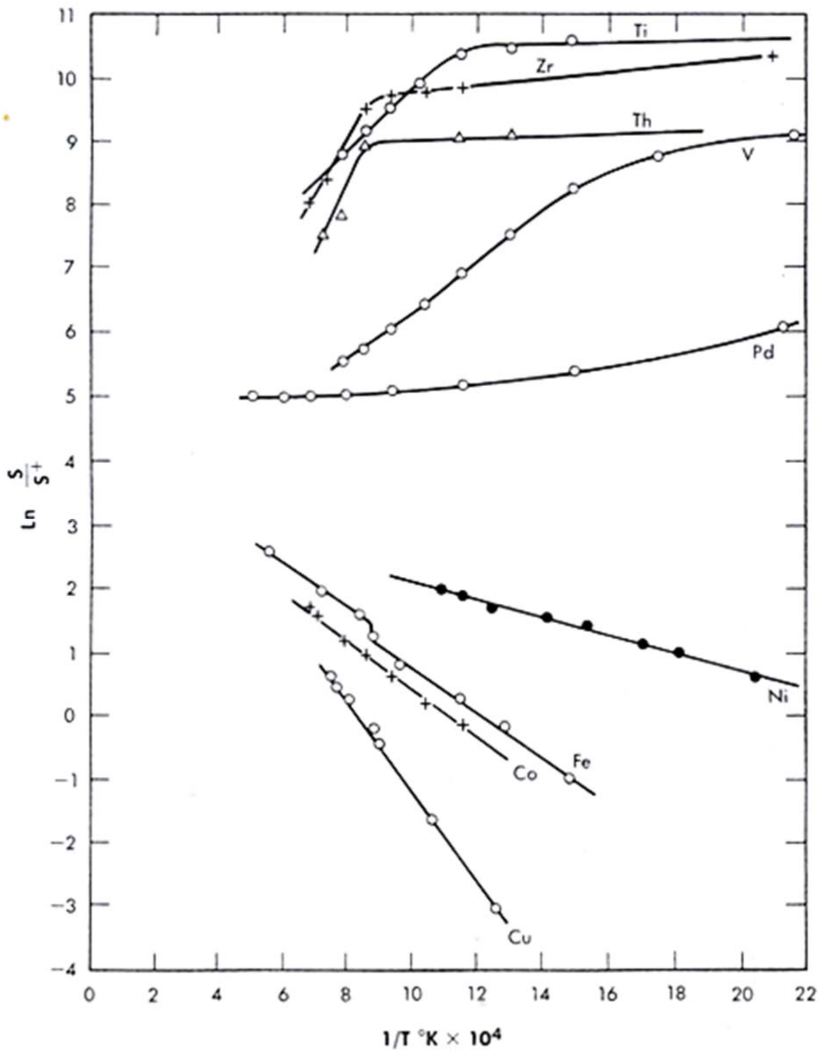


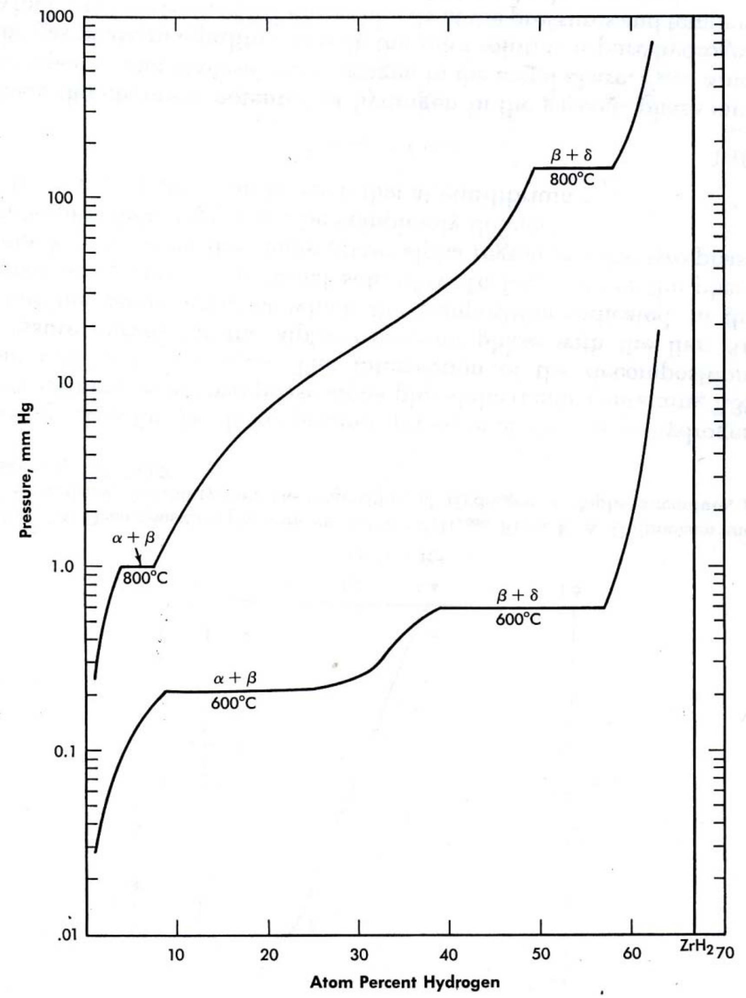


6.: Mögliche Anwendungsgebiete

Projekt	Problem-Typ	Analytische Lösung ohne Phasengleich-gewicht	Numerische Lösung mit Phasengleich-gewicht	Analytische Lösung mit Phasengleichgewicht
Q-PETE, (INR) Transport-parameter	kartesisch	Vorhanden, Inverses Problem (B&B)	Vorhanden, Inverses Problem (B&B)	Fehlt
Gas release (INR) Transport-parameter	zylinder	Teilweise vorhanden, Inverses Problem fehlt	In Arbeit, Inverses Problem fehlt (Open Foam)	In Vorbereitung
VSL (ITEP) Tritium Extraction	sphere	Vorhanden	Fehlt (Open Foam)	Fehlt
Tritium Extra-ction mit Superpermea-tion (ITEP) exothermes Material	kartesisch	Vorhanden für endothermes Material	Fehlt (Open Foam)	Fehlt
Wasserstoffspei-cher exothermes Material	zylinder	Fehlt	Fehlt (Open Foam)	Fehlt

Exothermic/endothermic metallic hydrides





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