Karlsruher Institut für Technologie

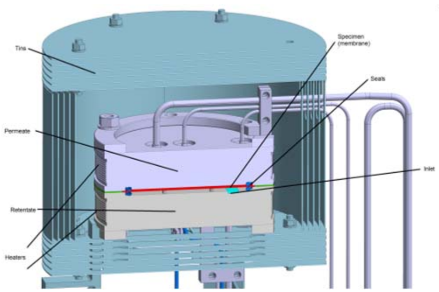
25-29 JUNE DSL2018
14th International Conference on Diffusion in Solids and Liquids
Amsterdam THE NETHERLANDS

Permeation data analysis including a nonzero hydrogen concentration on the low pressure detector side for a purged permeation experiment

Axel von der Weth*, Frederik Arbeiter, Dmitry Klimenko, Volker Pasler,
Georg Schlindwein

Amsterdam, DSL, 27th June 2018

IKIT/INR/MET (Maschinenbau)

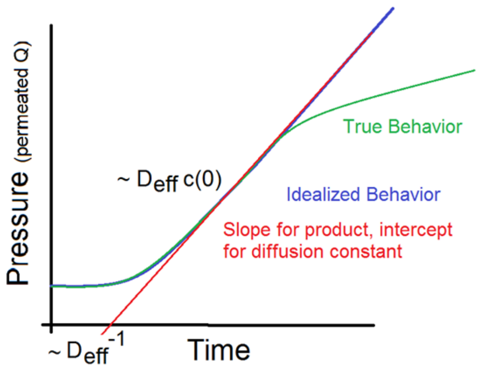


Determination of concentration dependent interstitial diffusion parameter regarding re-diffusion and small loading pressure: Situation of future fusion power plant 2 Pa tritium partial pressure (breeder unit) enriched to 1 Pa in purge gas system.

1.: Description of setup and simplification
2.: FDM solver
3.: Branch & Bond algorithm
4.: Results
5.: Conclusion

E-mail: axel.vonderWeth@kit.edu

1.: **Q-PETE** (hydrogen permeation transport experiment)

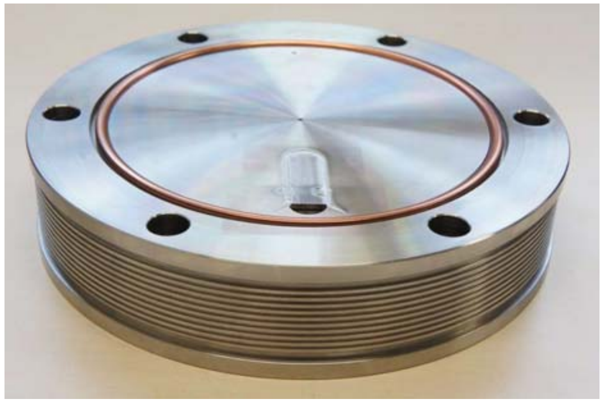


Time dependent non zero Q-concentration near measuring system (gauge or QMS) generates deviation from linear behavior.

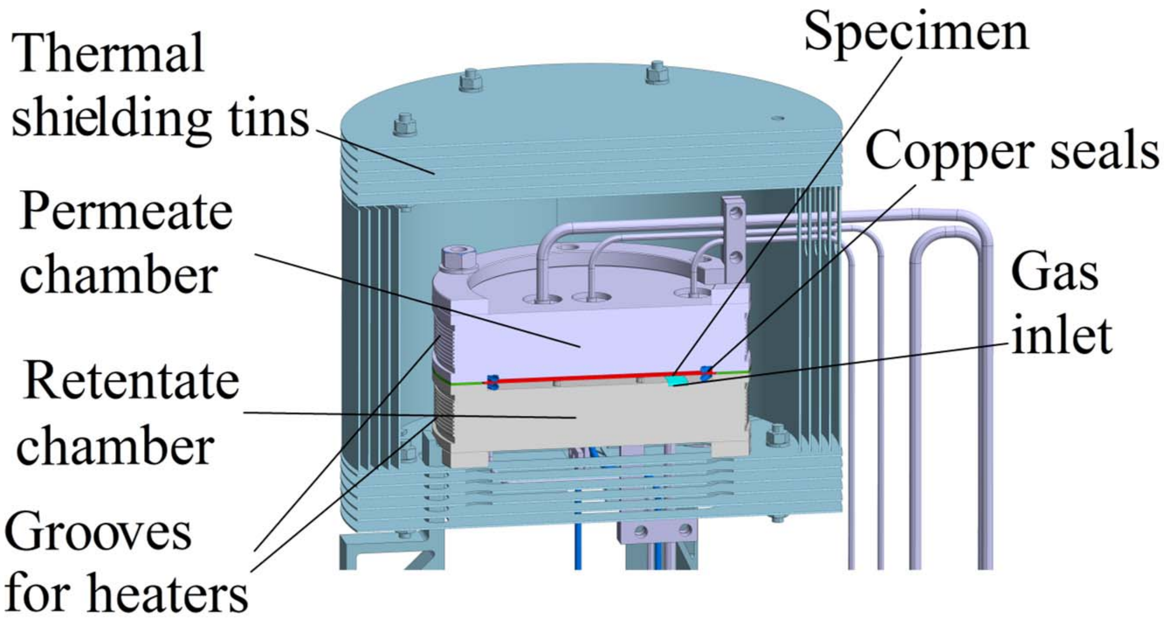
$$j(t)_{measure} = \underbrace{\frac{D_{eff}\, c(0)\, d_m^2}{w_m\, 4\,\pi}}_{j_{steady\ state}} \left(1 + 2\sum_{k=1}^{\infty}(-1)^k e^{\frac{-k^2\pi^2 D_{eff}(t-t_{off})}{w_m^2}}\right)$$

Daynes, Forcey transport equation solution

Therefor removing Q in permeate chamber.



Permeate (secondary) chamber



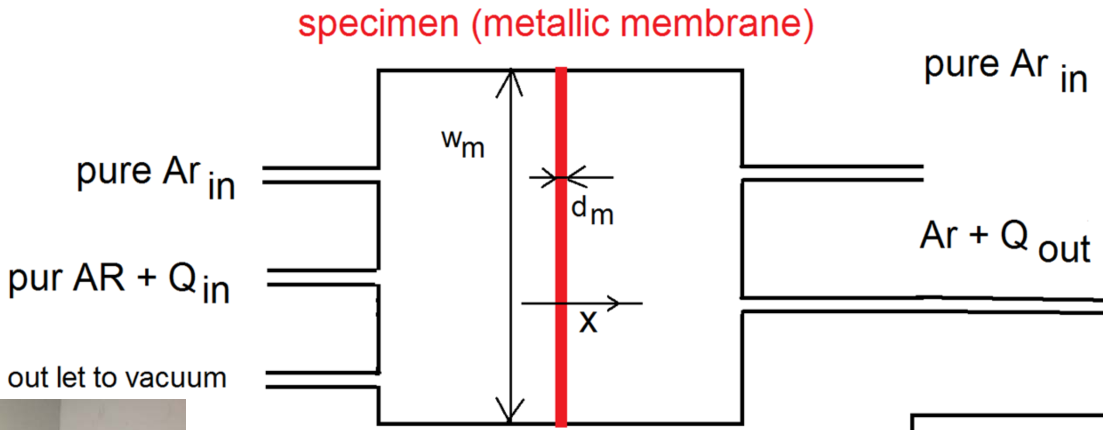
Simplified Q-PETE experiment

Ra	0.41 µm
Rz	2.89 µm
Rmax	3.99 µm
Rt	4.09 µm

Baffle surface

Ra	0.36 µm
Rz	2.21 µm
Rmax	2.38 µm
Rt	2.42 µm

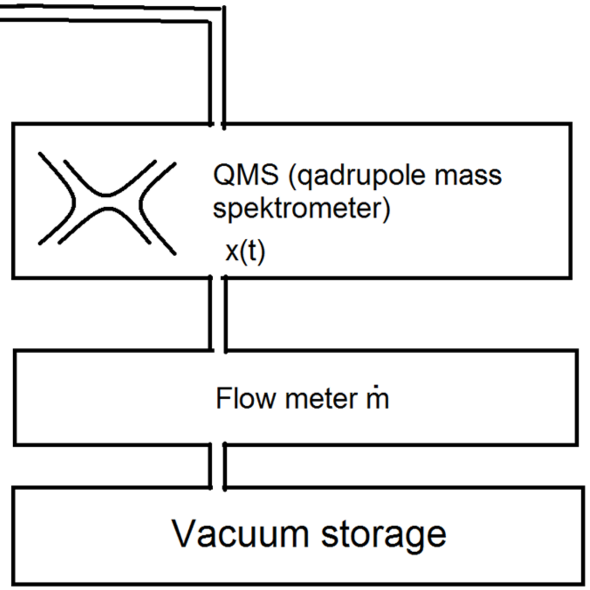
Sealing face

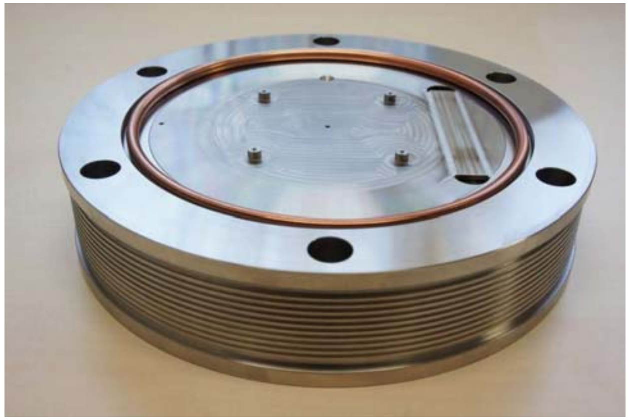


retentate chamber permeate chamber

heated up to 600°C, in vacuum tank

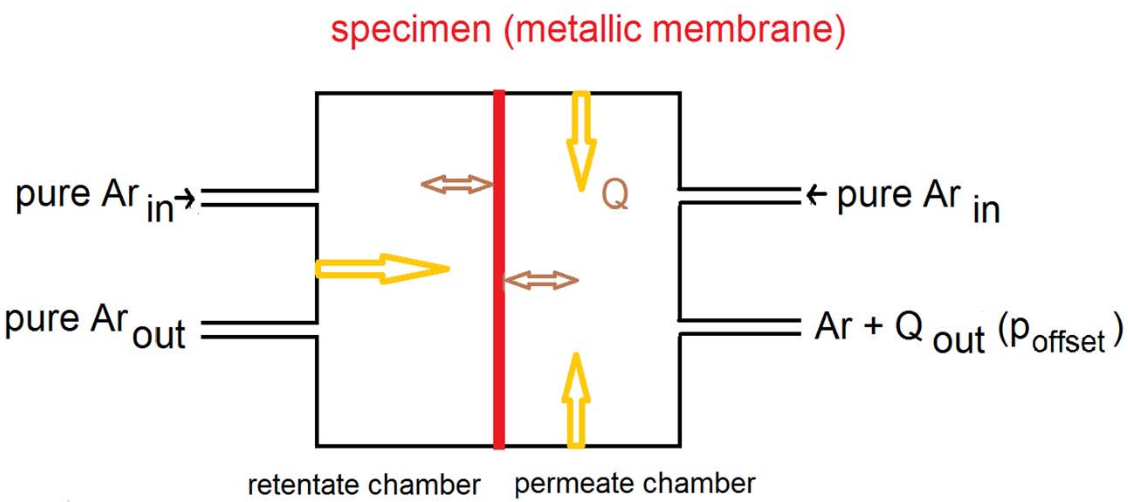
pressure gauges for both chambers





Retentate (primary) chamber

2.: (FDM) analysis: Before beginning of experiment: Purging with pure Ar:

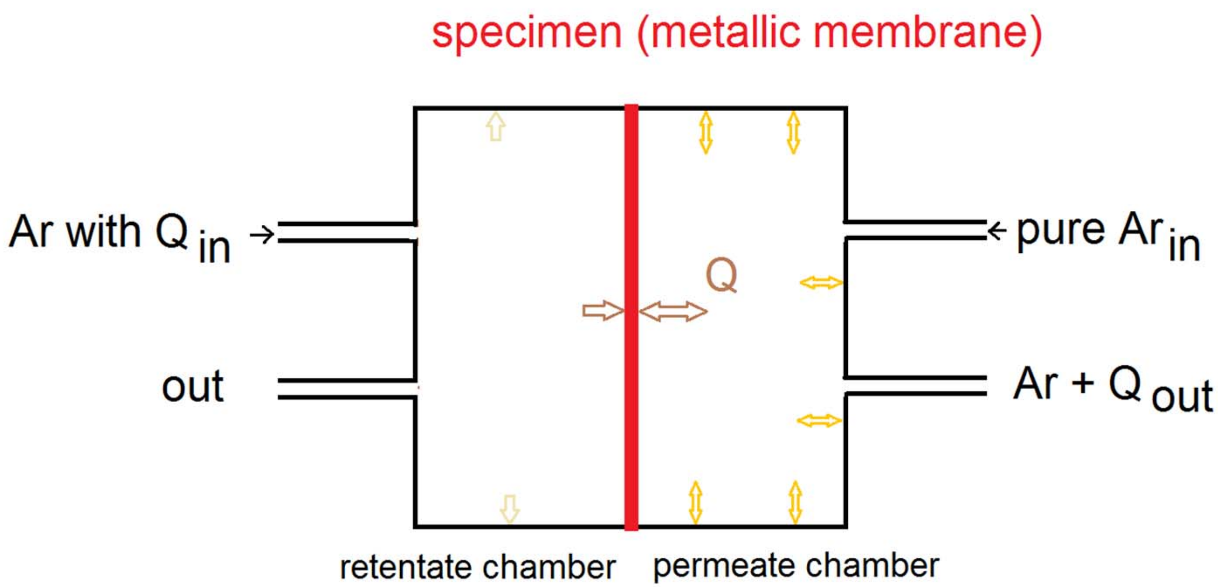


The stored Q is generating a constant assumed offset permeation. The membrane is in diffusive contact with the two volumes, equilibrium state given by K_S .

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

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:



$$c\left(x=0, t>\ t_{off}\right) \underbrace{=}_{FDM} \ c\left(1, t>t_{off}\right)=c(o)$$

$$= K_s \sqrt{p_{load}}$$

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

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

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

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

$$(*)\quad c(n, t > t_{off}) = K_s\,\sqrt{j_{measure}\,\frac{p_{tot}}{\dot{m}_{Ar}\,\alpha}}$$

$\Delta x = 12\ \mu m$ ($=d_m/n$) 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):

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

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

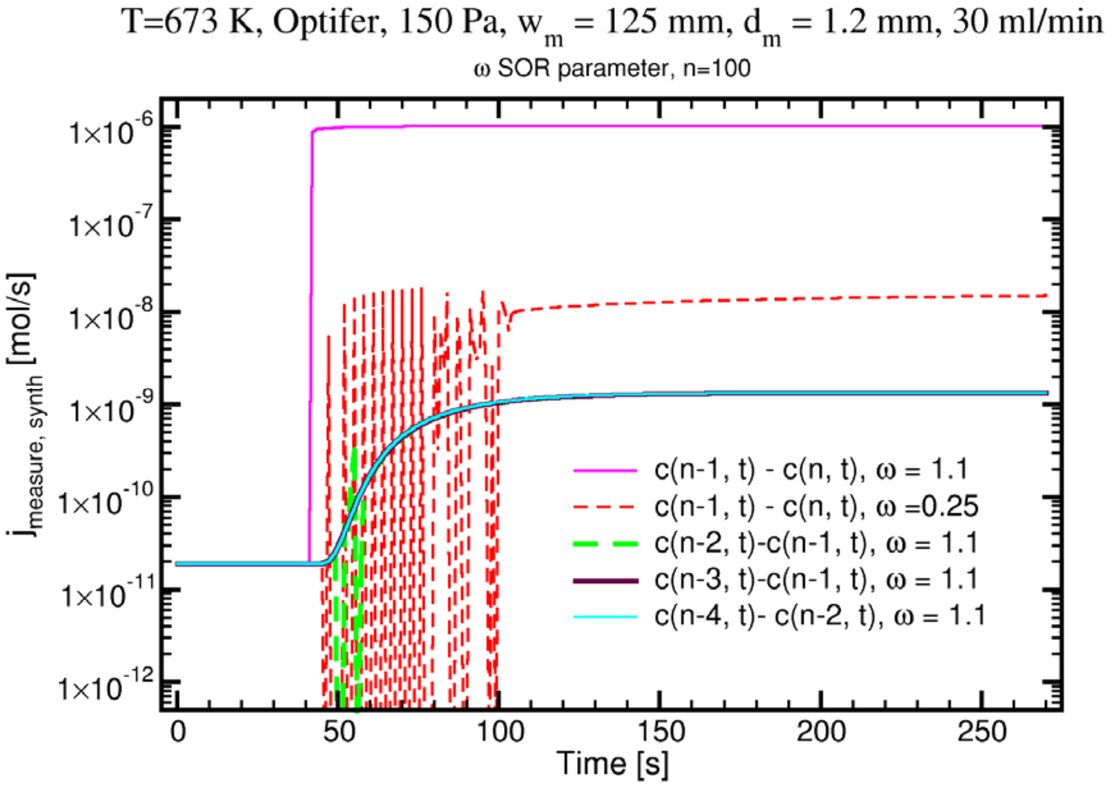
Pseudoadaptive time integration step (saving calculation steps and decrased step length in transient region) algorithm:

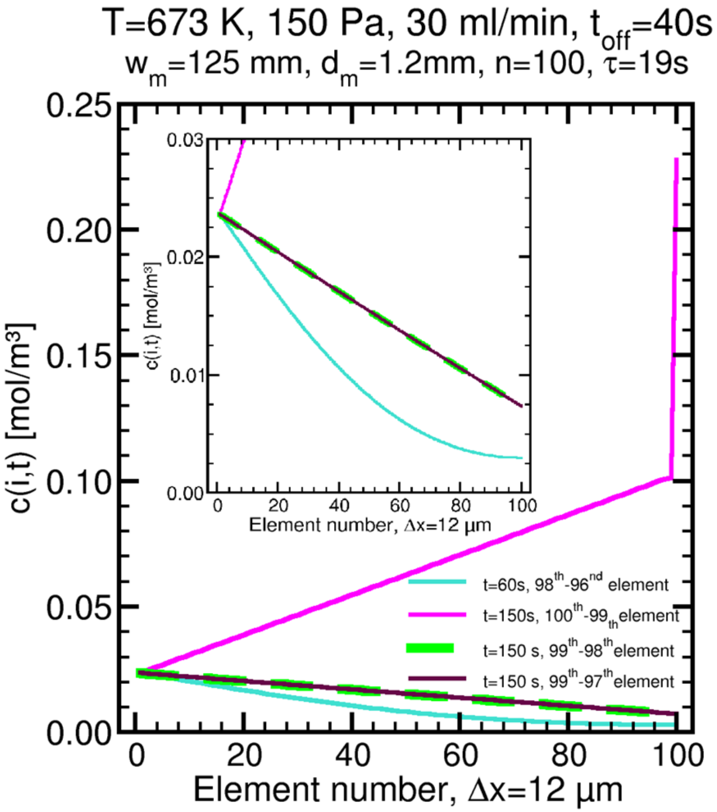
Δt is varied $2\,\Delta t_{soll}$ for $t<t_{off}$, $0.2 - 0.5\,\Delta t_{soll}$ for $t < t_{off} + \tau$, else $\Delta t = \Delta t_{soll}$ $\qquad \tau = \frac{w_m^2}{D_{eff}\,\pi^2}$

Used FDM-SOR-step (successive over relaxation)

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

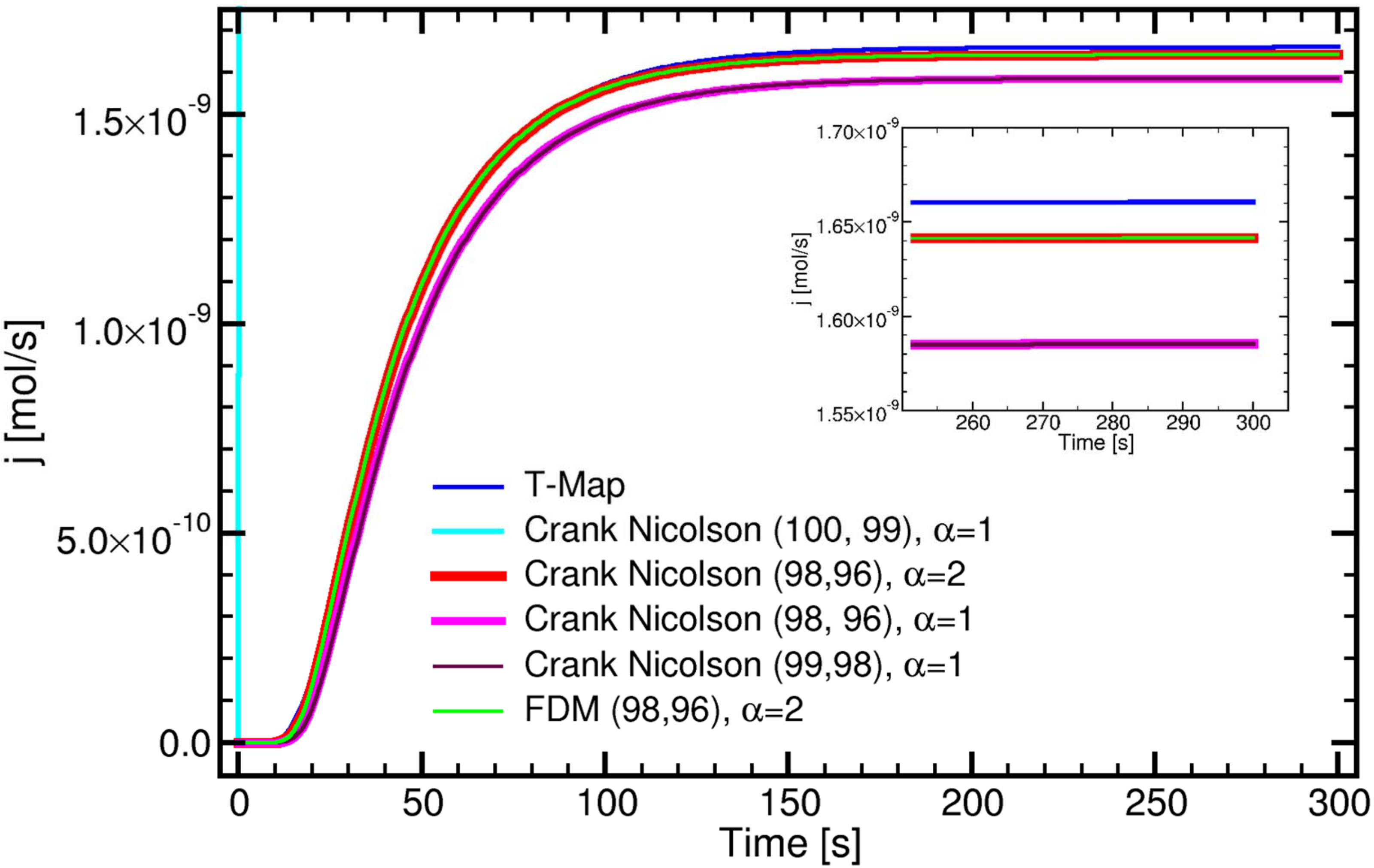
Optimized ω with Eigenwertanalysis of (*, **), only proposal: Translation of (*, **) into matrix, calculation with QR method for λ_{max}, now only $\omega=1.1$ carefully is used.





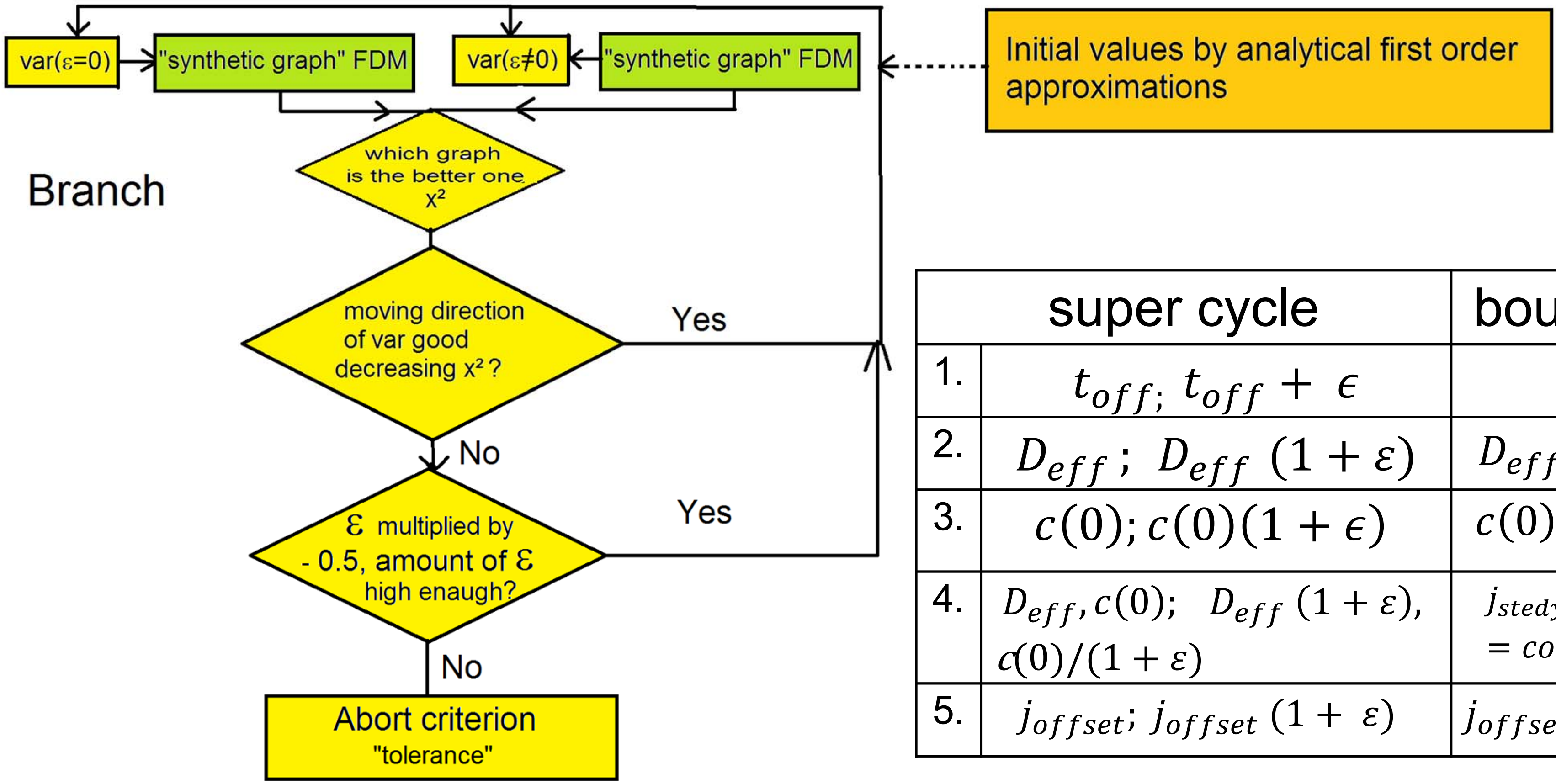
Comparison T-Map, Crank Nicolson and FDM

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

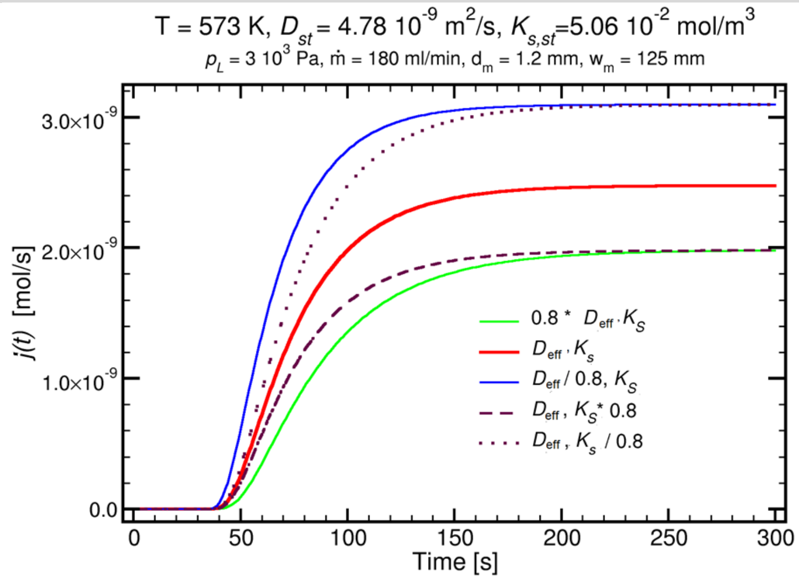


3.: (Branch and Bound) B&B algorithm

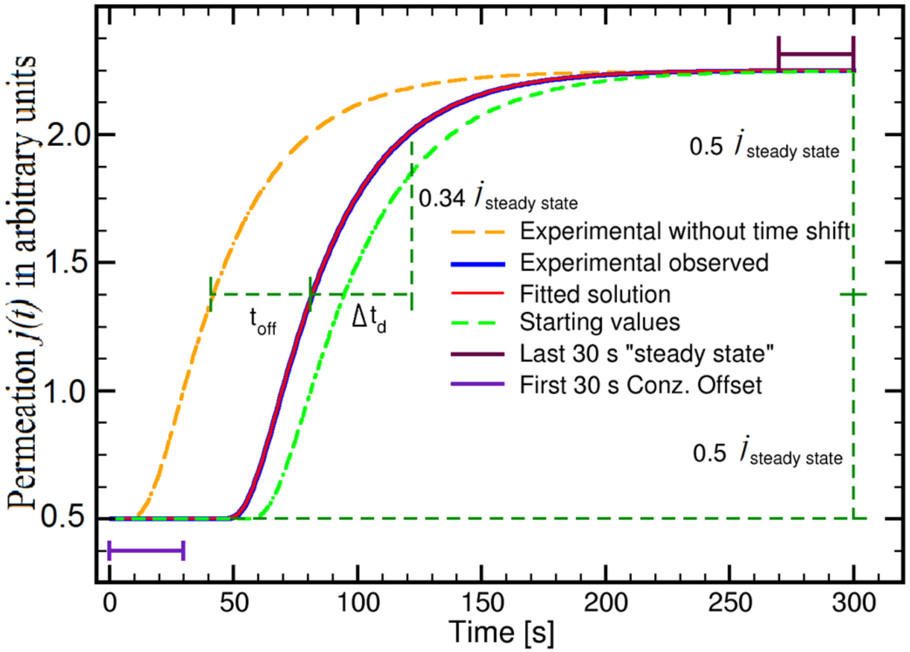
Four desired variables: D_{eff}, $c(0)$ (res. K_s), t_{off} and j_{offset} serial treated within a super cycle. No explicit formulation possible, especially Daynes solution, comparison between measured permeation curve and "synthetic" graph from FDM module:



	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:



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

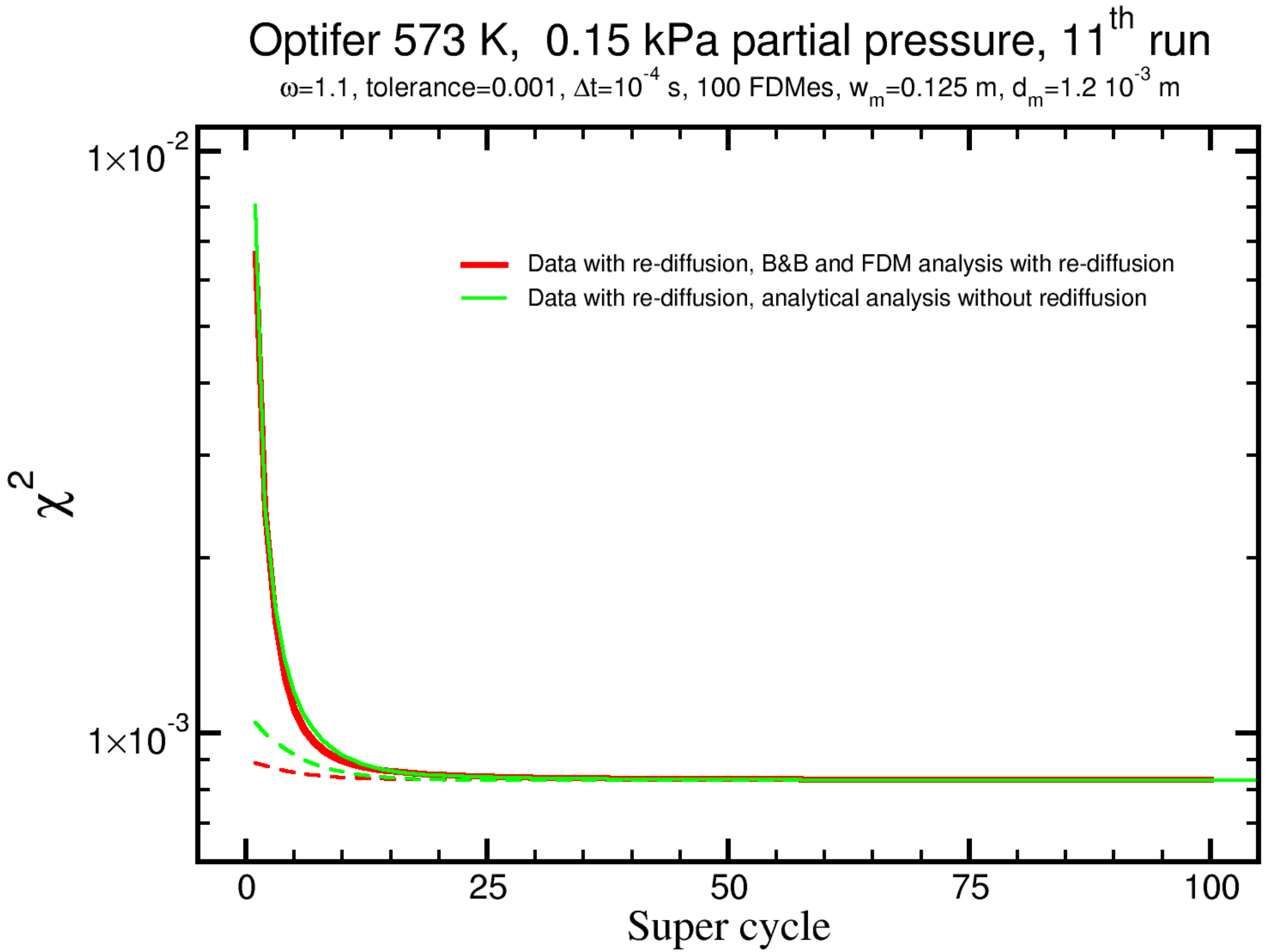
$$D_{eff,initial} = \frac{d_m^2}{\pi^2 \, \Delta t_d}$$

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

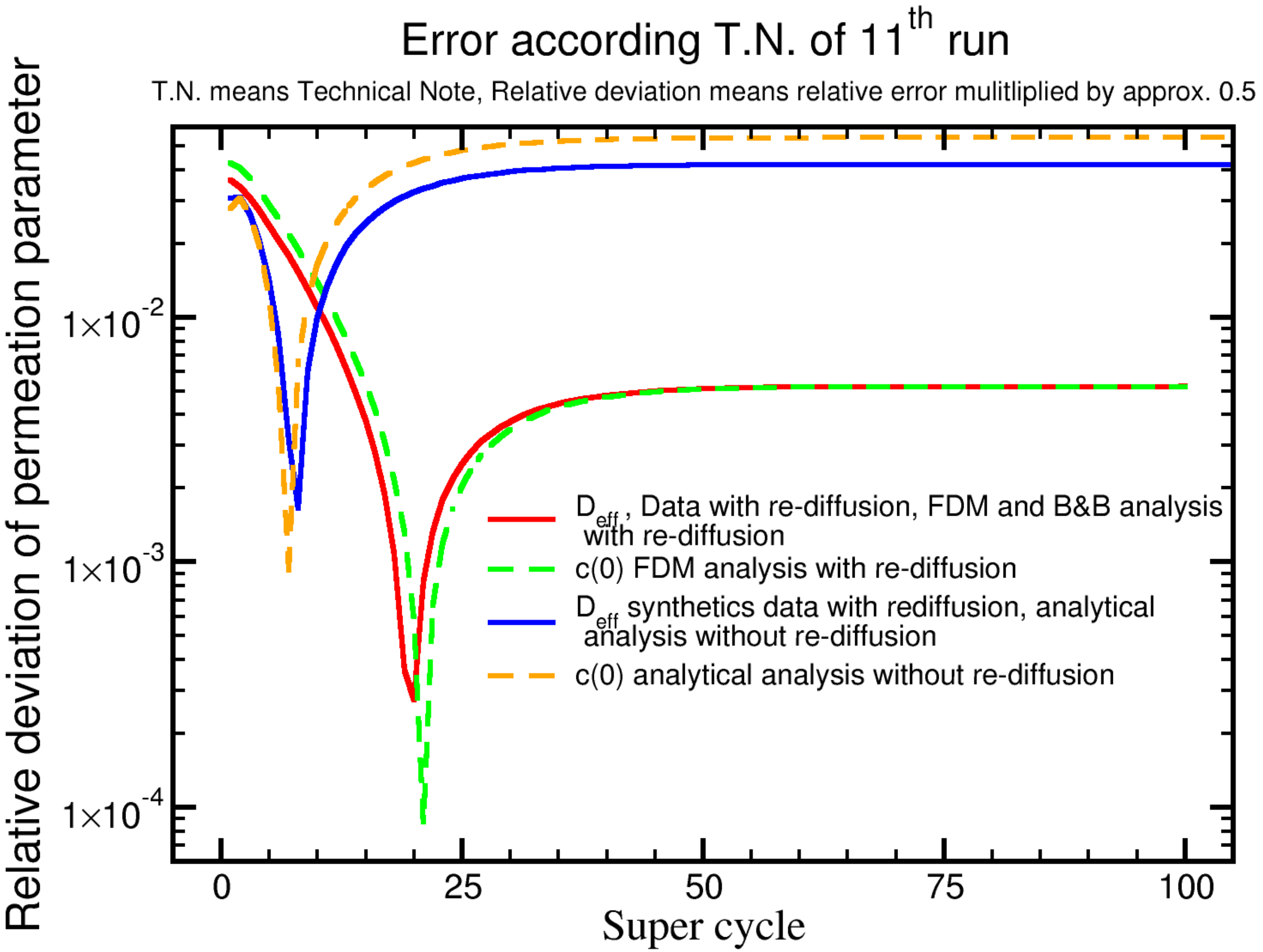
$$\Delta j = j_{steady\ state} - j_{offset,initial}$$

$$c(0)_{initial} = \frac{\Delta j \;\, 4 \, d_m}{w_m^2 \, \pi \, D_{eff,initial} \sqrt{\frac{\Delta j \; p_{tot}}{\dot{m}_{therm} \, p_{load}}}}$$

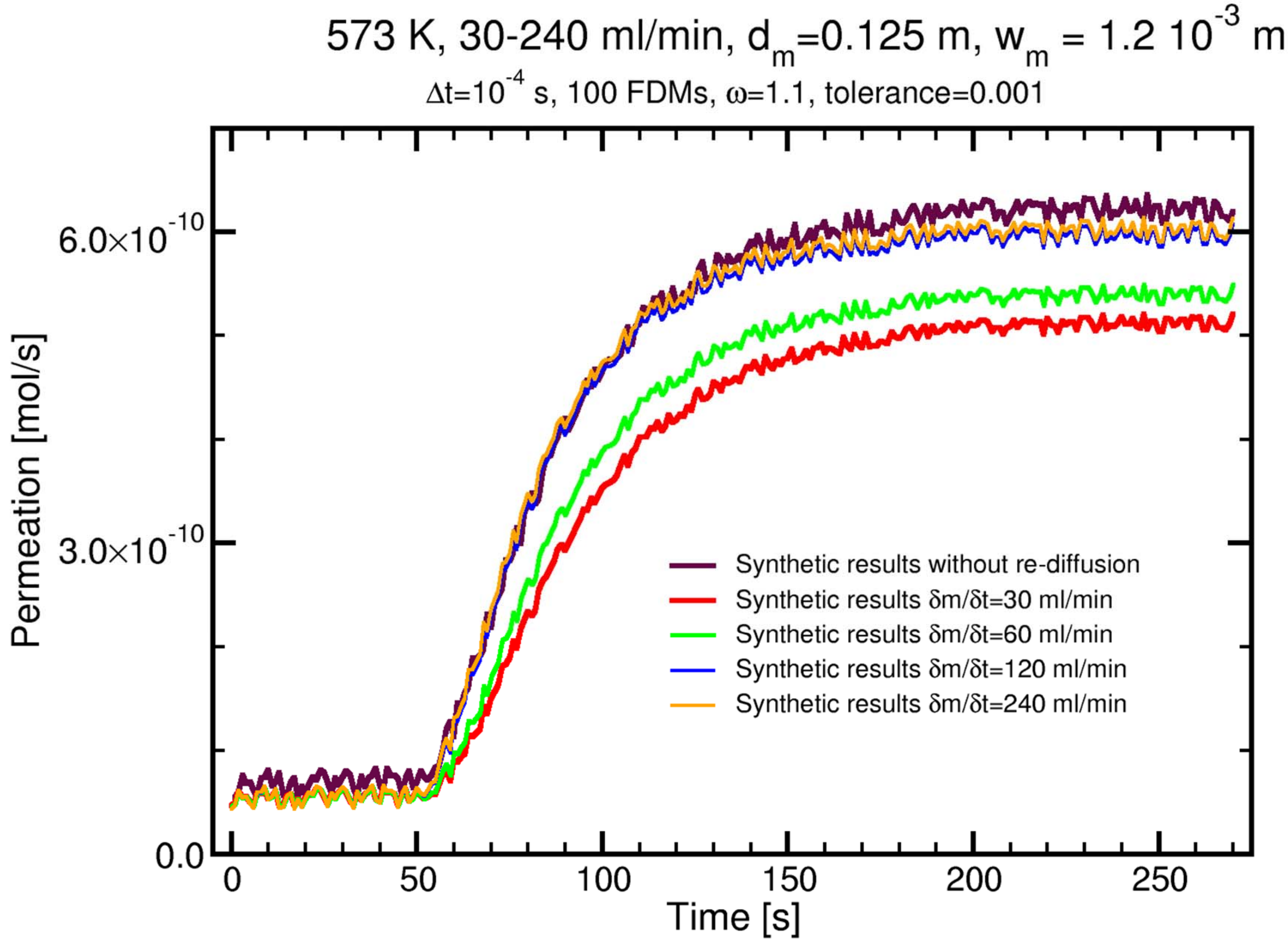
Example for χ^2



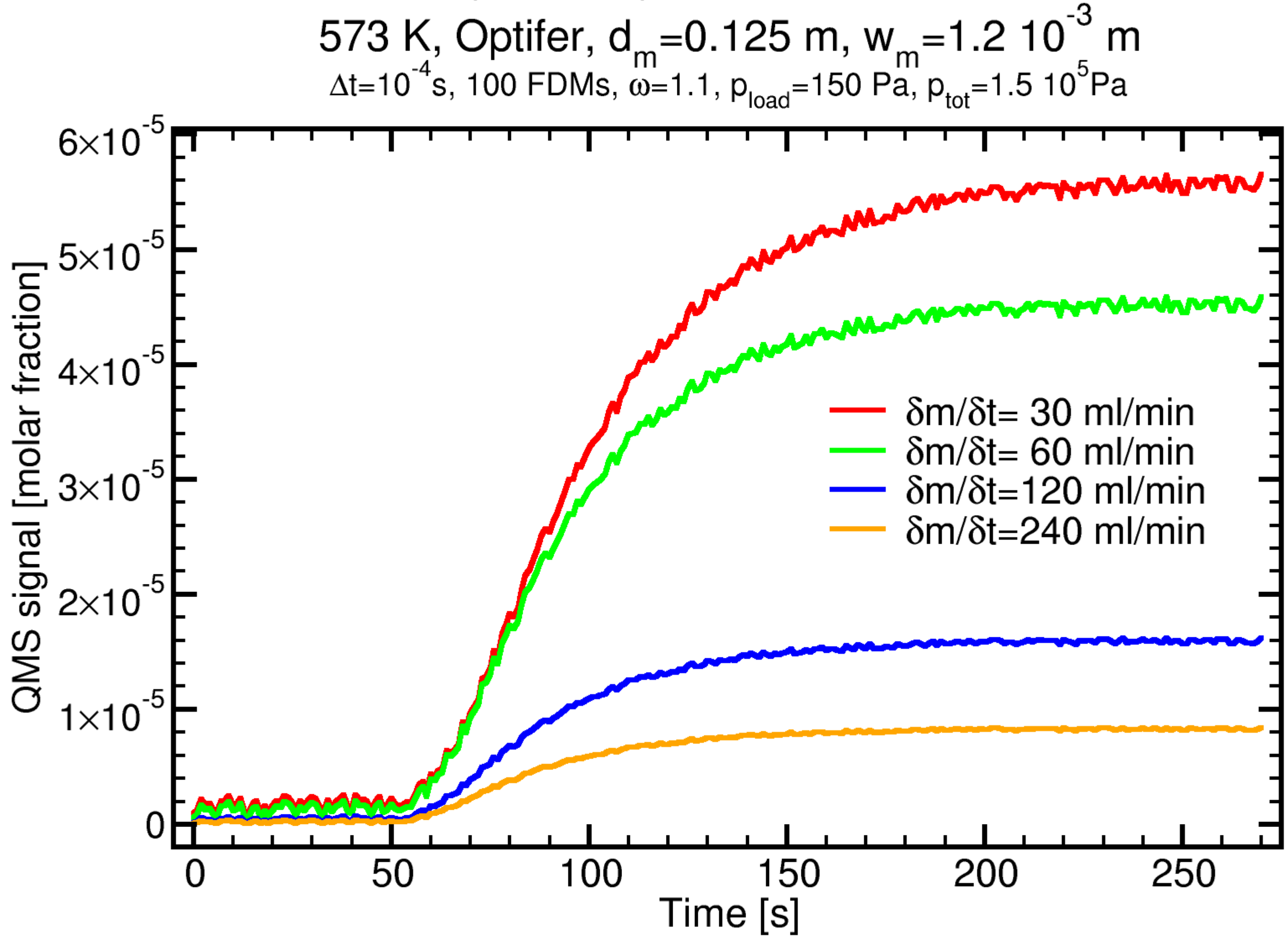
Example to former slide, comparison with analytical Daynes solution and FDM results



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

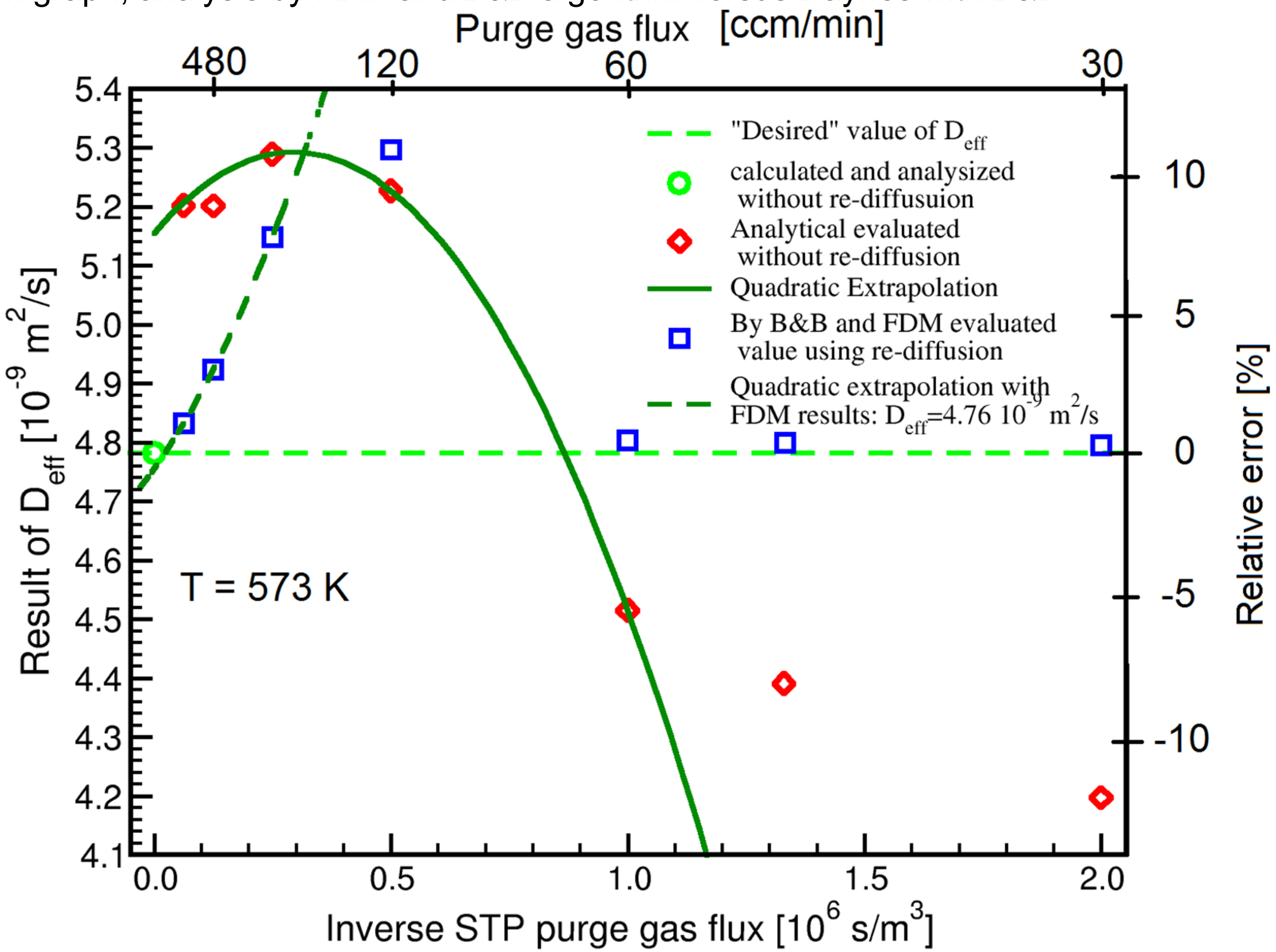


Expected advantage of Q-PETE setup: Influence on results by differing purge gas flux in permeate chamber aiming a differing Q-concentration there.

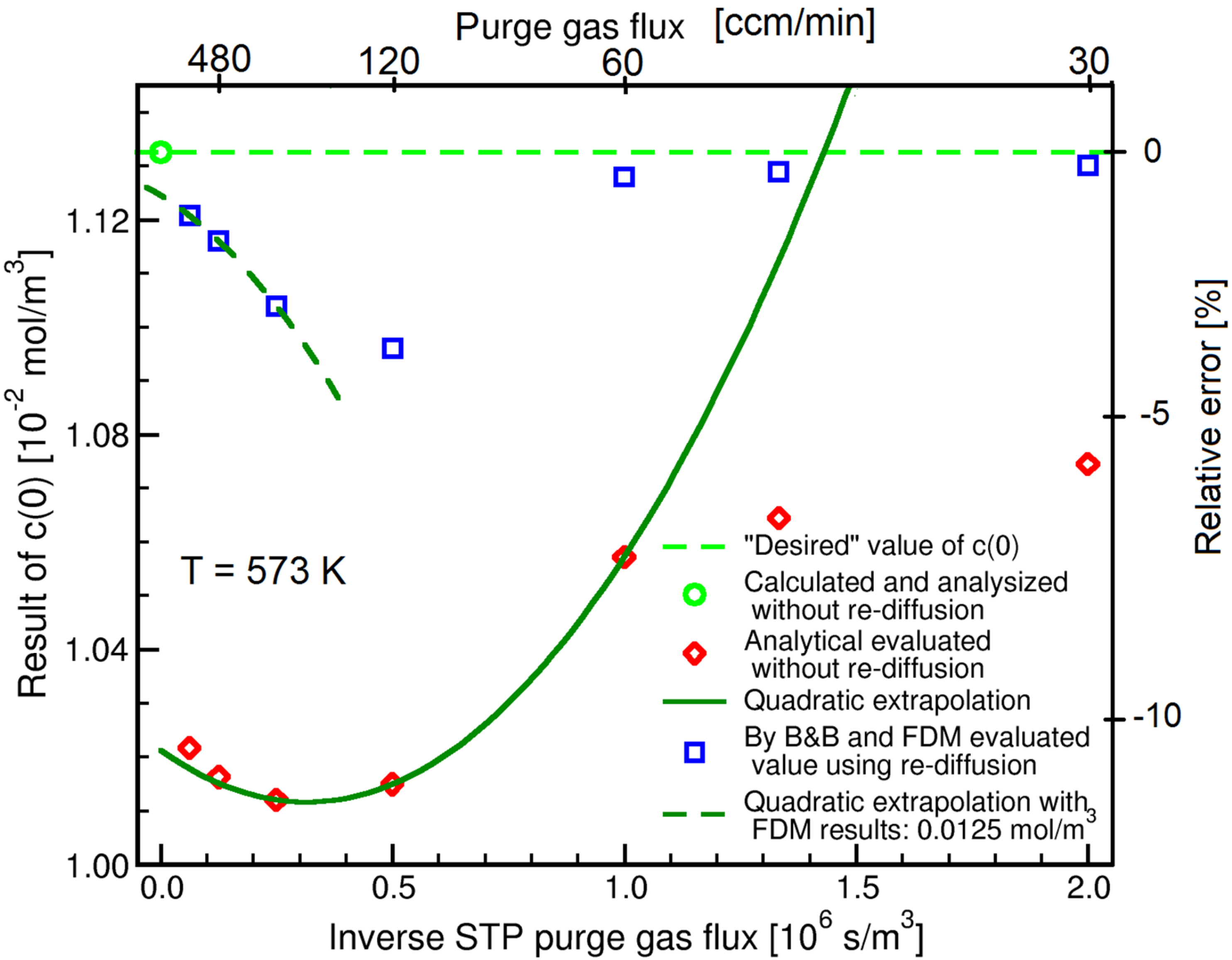


Re-recognition of diffusion constant and Sieverts´constant,

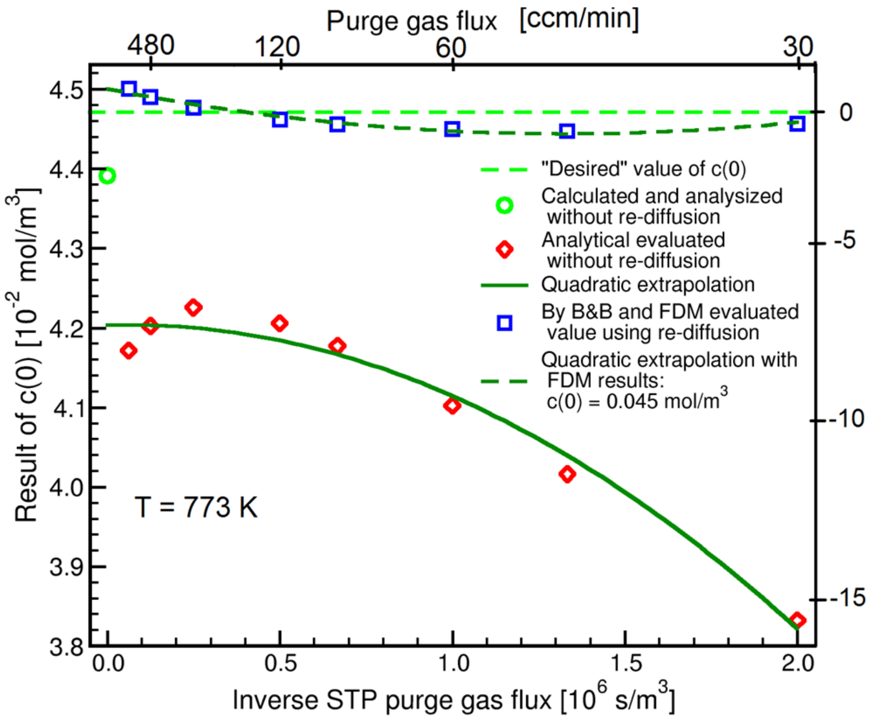
permeation constants of technical note as true regarded, time dependent synthetic permeation graph, analysis by FDM and B&B algorithm versus Daynes with B&B

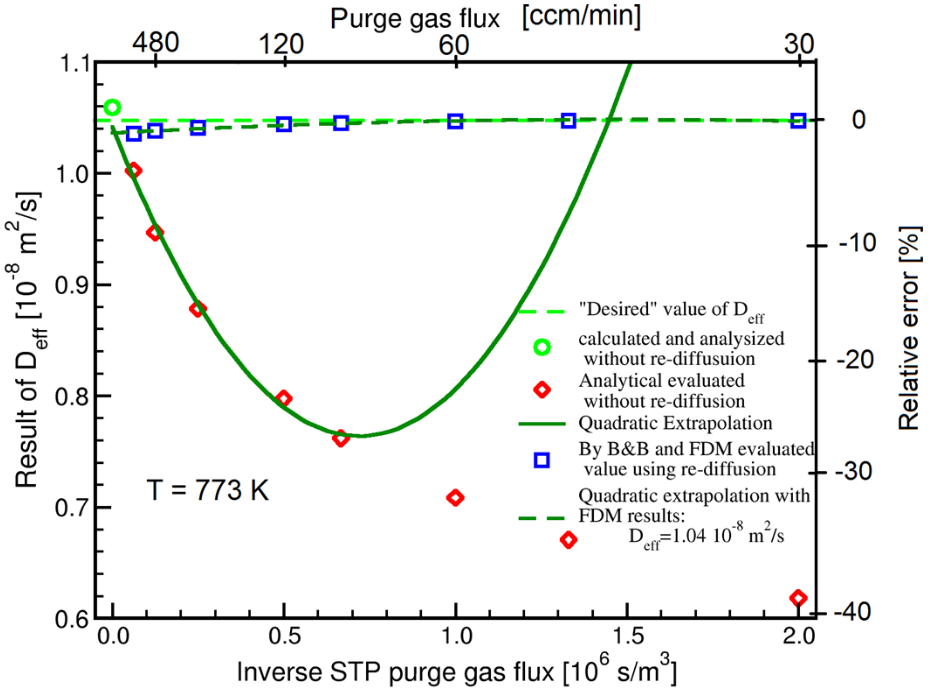


Re-recognition of diffusion and Sieverts´constant



Re-recognition of diffusion and Sieverts´constant





5.: Conclusion:

Karlsruher Institut für Technologie

- With the here published analysis the influence of re-diffusion by non vanishing Q-concentration in the permeate chamber containing the measuring application is described.
- The Q-PETE experiment will be able to control re-diffusion
- The here told FDM model can adjusted for experimental deviation (e.g. storage behavior of material) caused by numerical algorithm.
- Recognition error of B&B at the moment by 1%
- It can extended for other applications which use transport equation

Outlook: It is planed to start Q-PETE experiment using FDM & B&B algorithm. The future investigation of (semi-)analytical solution is desired

Thank You for Your attention !