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Thoughts of an Isovoluminetric Thermal Desorption Experiment

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INR, CN KIT, 3th June, 2019

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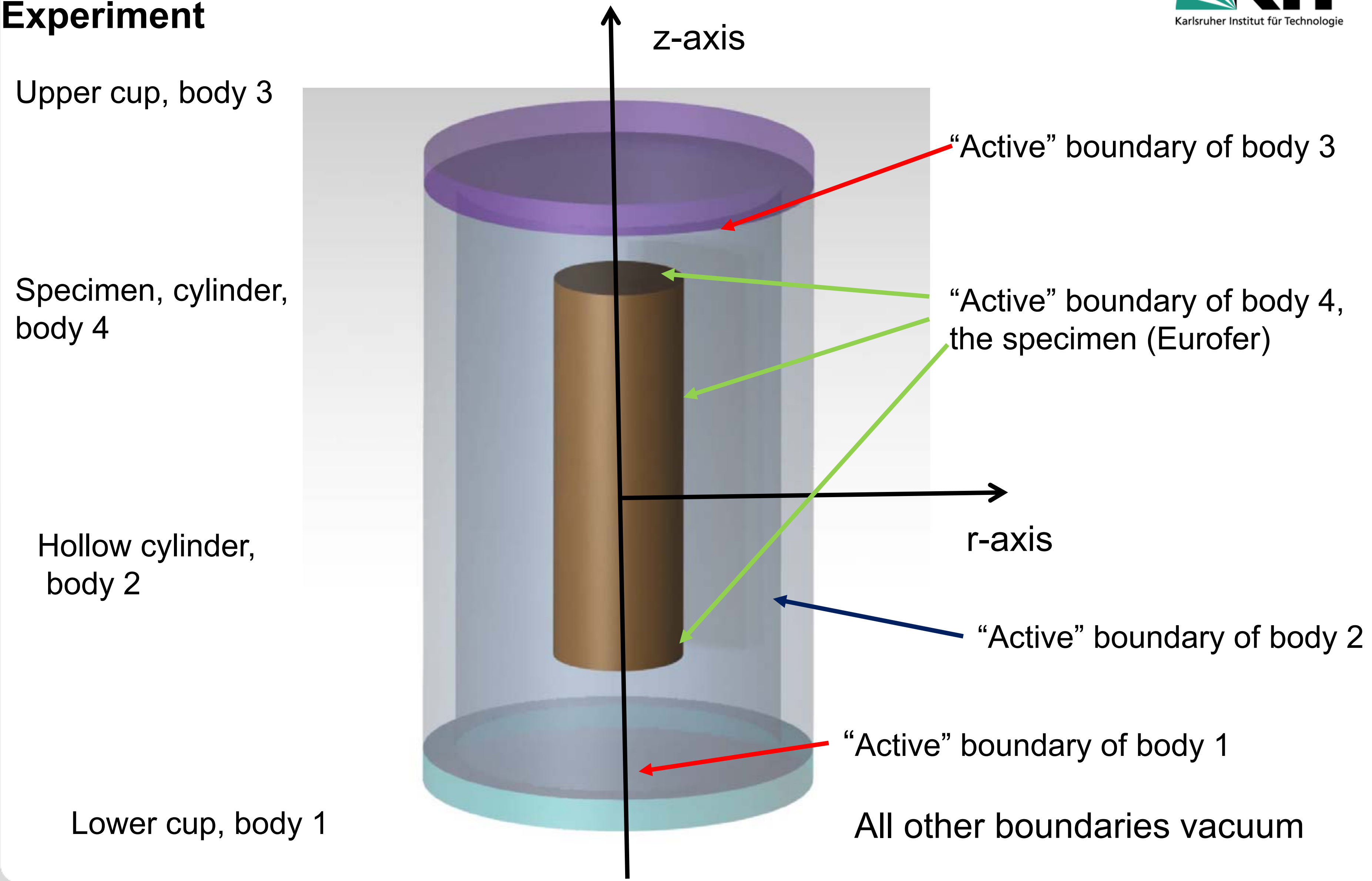
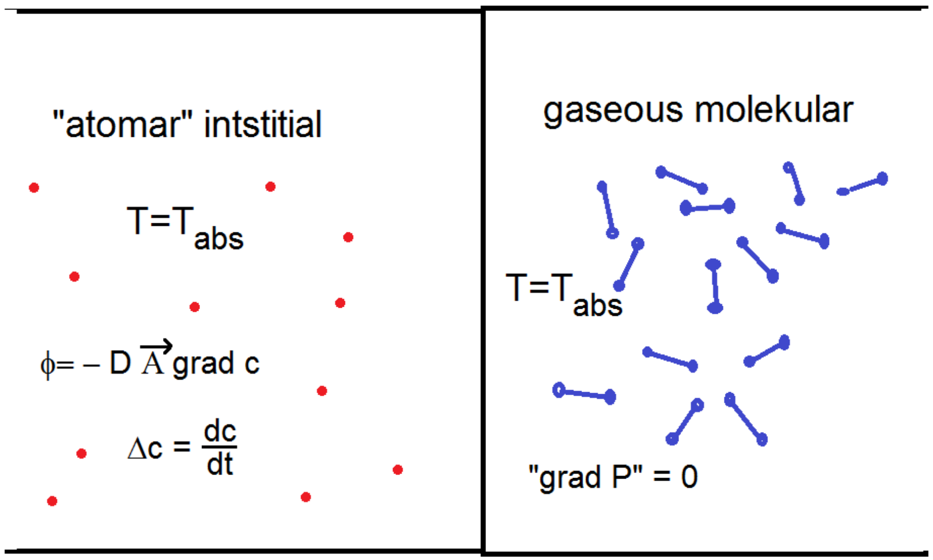
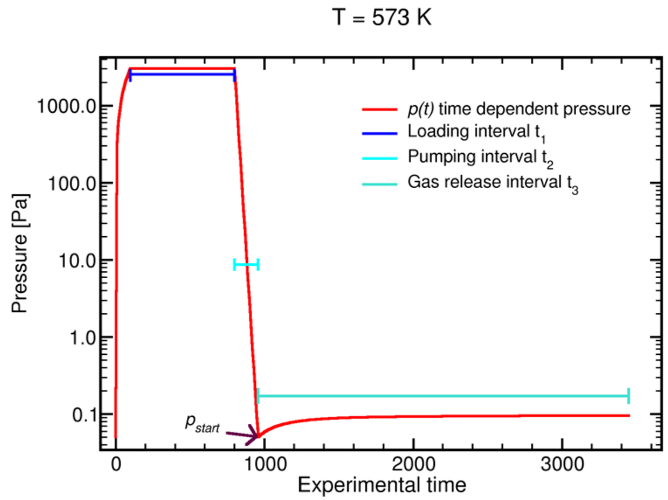
1.: Descripton of setup of an Isovoluminetric Thermal Desorption Experiment



2.: Physical descripton

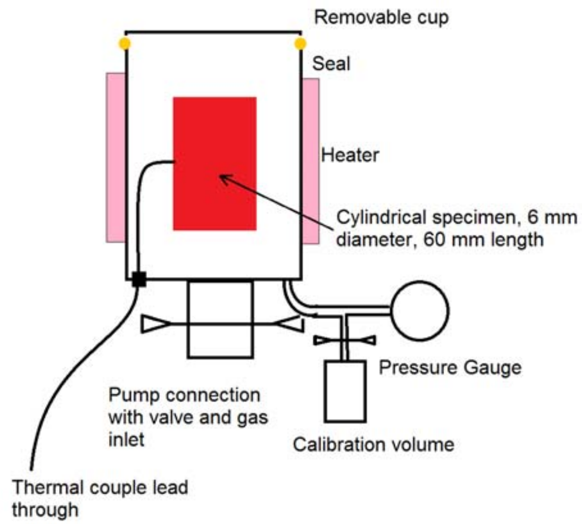




“Velocity” of mass transfer by diffusion constant D

Ratio of densities given by Sieverts´ law
(phase equilibrium)

$$c = k_s \sqrt{p_r}$$



Simple analytical Solutions

Without re-diffusion, complete outgasing:

$$\underbrace{p_r}_{t\to\infty} = \underbrace{p_{end}}_{switching\ off\ pump} + \frac{V_{sa}\, k_{s,sa}\, \sqrt{p_{load}}\; R\, T}{\Big(\underbrace{V_c}_{chamber} - \underbrace{V_{sa}}_{sample}\Big)^2}$$

With phase equilibrium, mass conservation (number of "hydrogens" in atomic interstitial and molecular gaseous state constant) and non interacting confinement condition:

$$0 = \frac{2\,(V_c - V_{sa})}{R\,T}\left(\sqrt{p_r}\right)^2 + V_s k_{s,sa} \underbrace{\sqrt{p_r}}_{="x"} - \left(V_s k_{s,sa}\sqrt{p_{end}} + \frac{2\, p_{end}\,(V_c - V_{sa})}{R\,T}\right)$$

$$\underbrace{p_r}_{t\to\infty} = \left(\frac{-1 \underbrace{+}_{neg.sqrt} \sqrt{1 + \left(\dfrac{8(V_c - V_{sa})\sqrt{p_{load}}}{R\,T\,V_s k_{s,sa}} + \dfrac{16\, p_{end}(V_c - V_{sa})^2}{\left(R\,T\,V_{sa} k_{s,sa}\right)^2} \right)}}{\left(\dfrac{V_{sa}\, k_{s,sa}\, R\,T}{4\,(V_c - V_{sa})}\right)^{-1}} \right)^2$$

3.: Structure of differential equations:

$$\frac{\partial c}{\partial t} = D_{sa}\Delta c \qquad \frac{\partial d}{\partial t} = D_{cu}\,\Delta d(i)\,, i = 1{,}2{,}3 \qquad \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}$$

$$c(0 \le r \le r_s, z = \pm z_s, \forall t) = k_{s,sa}\sqrt{p(t)}$$

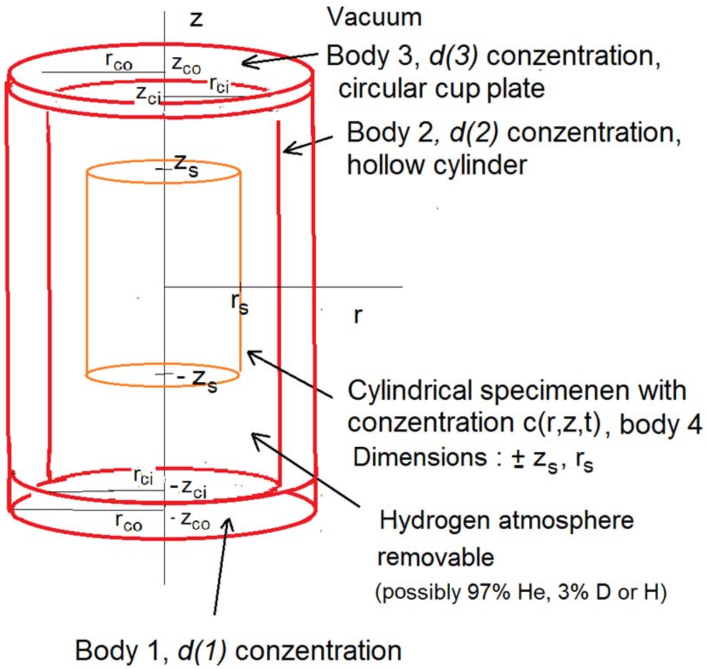
$$c(r = r_s, |z| \le z_s, \forall t) = k_{s,sa}\sqrt{p(t)}$$

$$d(1)(r \le r_{co}, z = -z_{ci}, \forall t) = k_{s,cu}\sqrt{p(t)}$$

$$d(2)(r = r_{ci}, -z_{ci} \le z \le z_{ci}, \forall t) = k_{s,cu}\sqrt{p(t)}$$

$$d(2)(r_{ci} \le r \le r_{co}, z = \pm z_{ci}, \forall t) = k_{s,cu}\sqrt{p(t)}$$

$$d(3)(r \le r_{co}, z = z_{ci}, \forall t) = k_{s,cu}\sqrt{p(t)}$$



3. Structure of differential equations

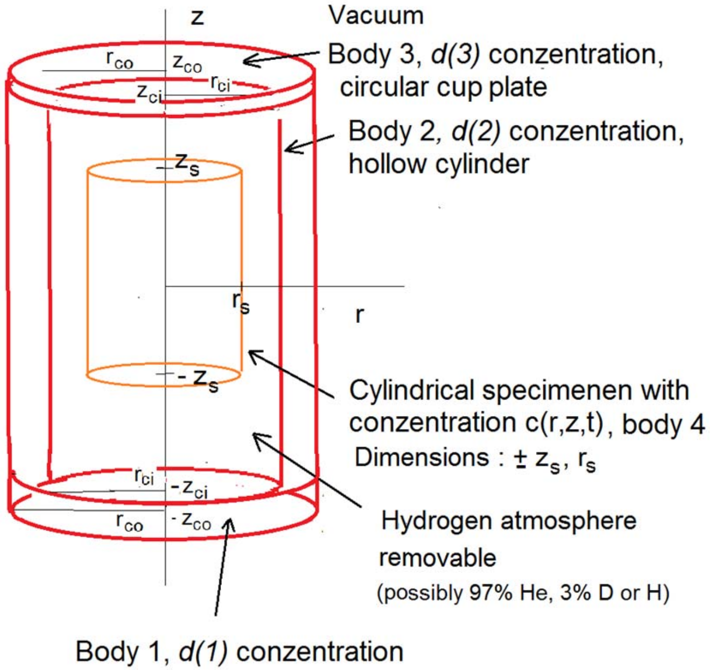
$$\frac{dm}{dt} = -2\,\pi\,D_{sa}\int_0^{r_s} \underbrace{2}_{symmetric}\; r\,\frac{\partial}{\partial z}\,c(r,z=z_s,t)\,dr$$

$$-\underbrace{2\,\pi\,r_s D_{sa}\int_{-z_s}^{z_s}\frac{\partial}{\partial r}\,c(r=r_s,z,t)\,dz}_{superficies\ surface\ of\ specimen}$$

$$-\underbrace{2\,\pi\,D_{cu}\int_0^{r_{co}} r\,\frac{\partial}{\partial z}\,d(1)(r,z=-z_{ci},t)\,dr}_{circular\ aerea\ of\ body\ 1}$$

$$-\underbrace{2\,\pi\,r_{ci}D_{cu}\int_{-z_{ci}}^{z_{ci}}\frac{\partial}{\partial r}\,d(2)(r=r_{ci},z,t)\,dz}_{superficies\ surface\ of\ body\ 2}$$

$$-\underbrace{2\,\pi\,D_{cu}\int_0^{r_{co}} r\,\frac{\partial}{\partial z}\,d(3)(r,z=z_{ci},t)\,dr}_{circular\ area\ of\ body3}$$



$$p(t) = p_{start} + \underbrace{k_v}_{RT_{abs}/V_{gas}}\int_{t_1+t_2}^{t}\underbrace{0.5}_{gaseous \leftrightarrow interstitial}\frac{dm}{dt}\,dt$$

4. Outlook to analytical solution

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Die Lösung für die Diffusionsgleichung mit Zylinderkoordinaten $(\varphi$-unabhängig$)$

$$\frac{dc}{dt} = D_{sa}\left\{\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial z^2}\right\}$$

mit Randbedingung $K_{s,sa}\sqrt{p}$ (Konstante) für

$r = r_s,\ |z| \le z_s$

und

$0 \le r \le r_s,\ z = \pm z_s$

ist

$$c(r,z,t) = \sum_{k=1}^{\infty}\sum_{n=0}^{\infty} B_{kn} e^{-\mu_{kn} t} \cos\left(\frac{n\pi z}{2z_s}\right) J_0\left(\sqrt{\frac{\mu_{kn}}{D_{sa}} - \left(\frac{n\pi}{2z_s}\right)^2}\, r\right) + K_{s,sa}\sqrt{p},$$

wobei

$$B_{kn} = \frac{\int_{-z_s}^{z_s}\int_0^{r_s}\left(u(r,z,0) - K_{s,sa}\sqrt{p}\right)\cos\left(\frac{n\pi z}{2z_s}\right) J_0\left(\sqrt{\frac{\mu_{kn}}{D_{sa}} - \left(\frac{n\pi}{2z_s}\right)^2}\, r\right) r\,dr\,dz}{\int_{-z_s}^{z_s}\int_0^{r_s}\cos^2\left(\frac{n\pi z}{2z_s}\right) J_0\left(\sqrt{\frac{\mu_{kn}}{D_{sa}} - \left(\frac{n\pi}{2z_s}\right)^2}\, r\right)^2 r\,dr\,dz}$$

und

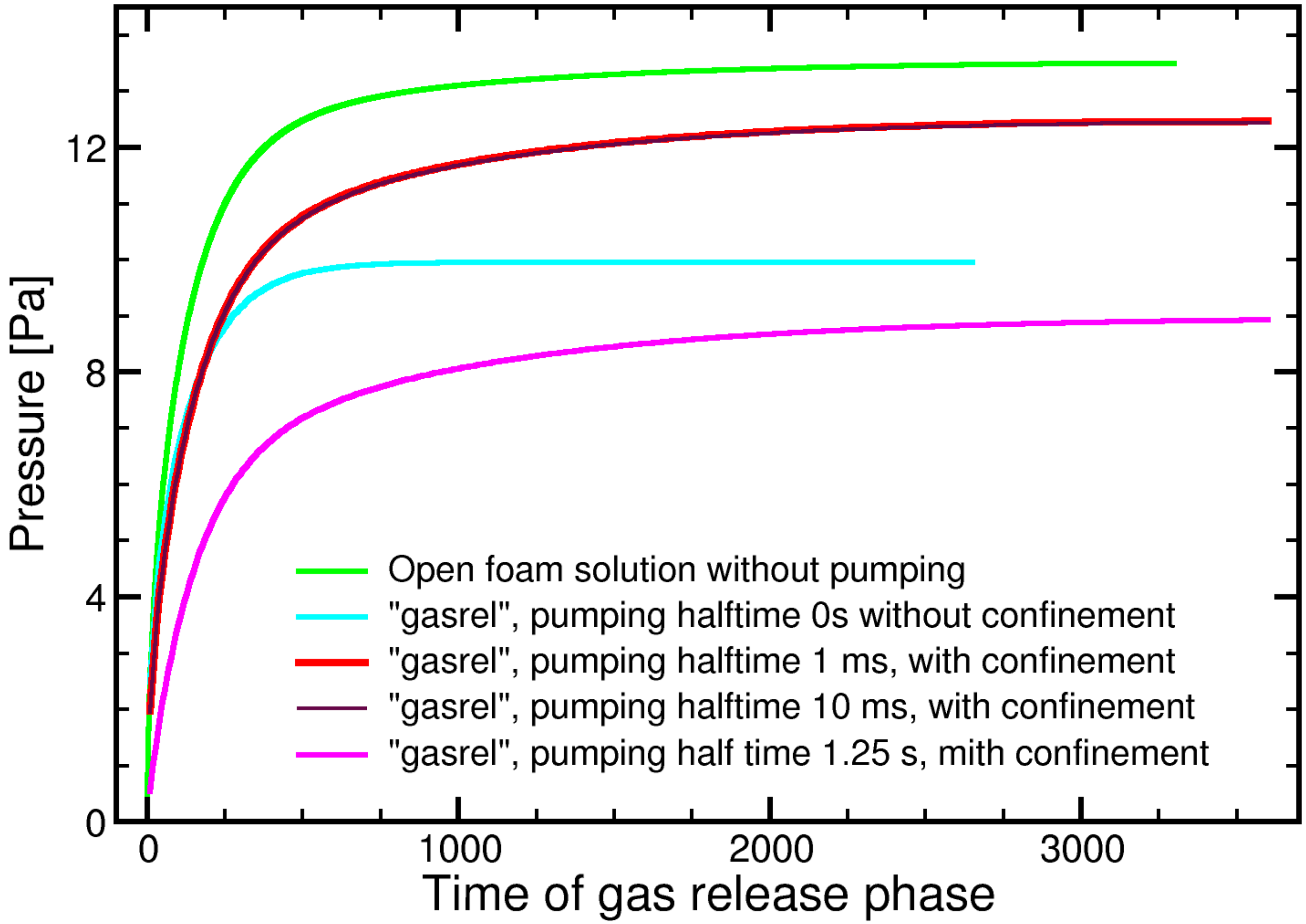
$$\mu_{kn} = D_{sa}\left\{\left(\frac{\alpha_k}{r_s}\right)^2 + \left(\frac{n\pi}{2z_s}\right)^2\right\}$$

mit α_k: k-te Nullstelle von Besselfunktion J_0.
Eine Symmetrie für z-Achse wurde vorausgesetzt.
Um Konstante B_{kn} zu berechnen, muss $u(r,z,0)$ durch eine gegebene Funktion (Anfangsbedingung) ersetzt werden.

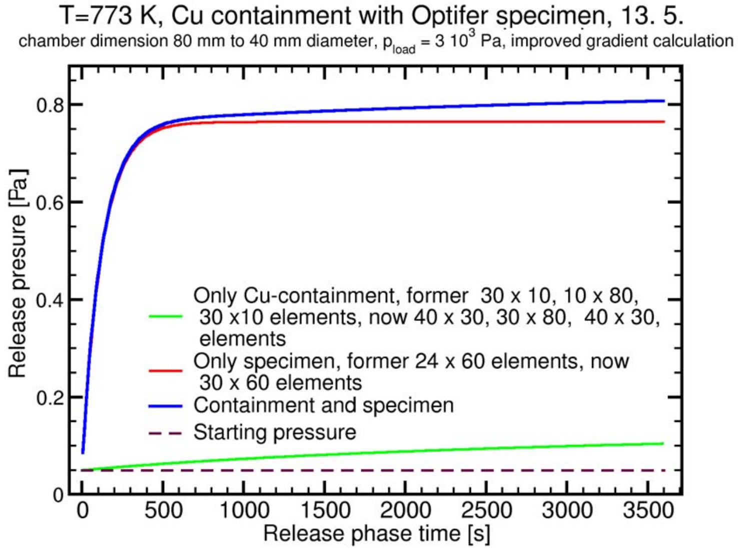
5. Outlook to open foam results

"gasrel" calculation with 6400 specimen element and 1800 elements

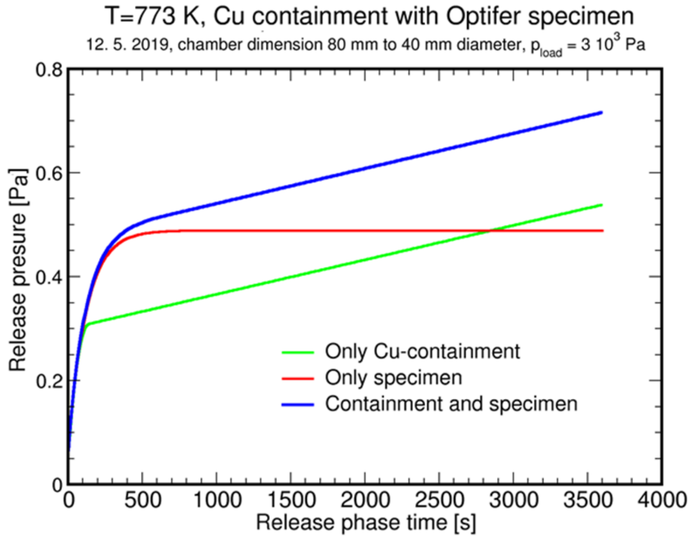
14 halftimes reaching endpresure (0.1 Pa)



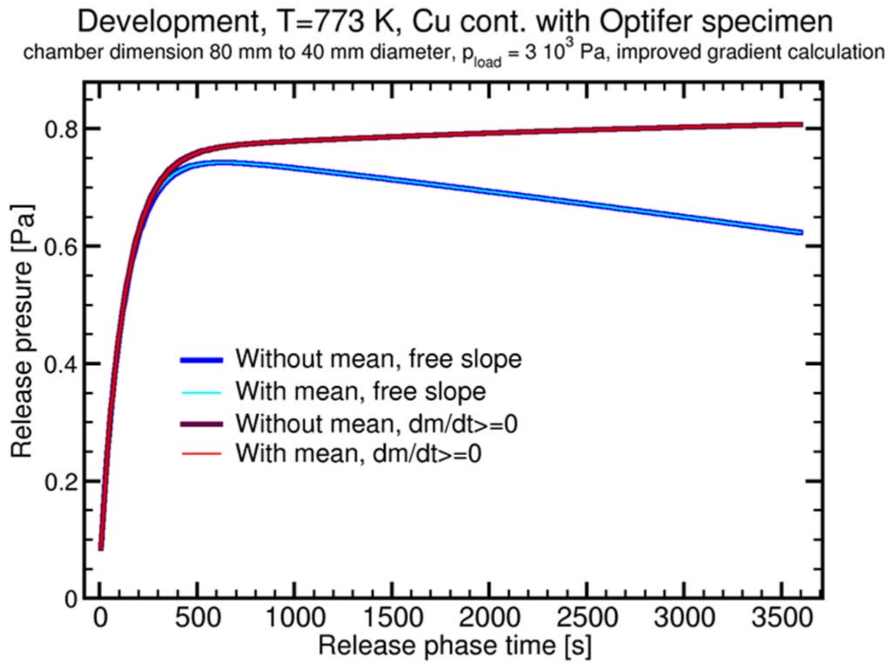
6.: Results of numerical solution



Simple numerical gradient calculation



Numerical artefacts



Gas release Experiment, current status

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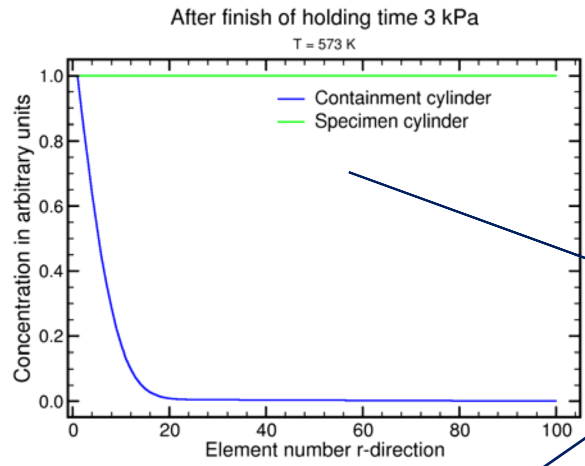
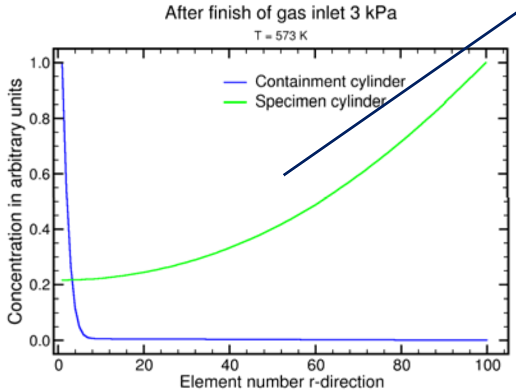
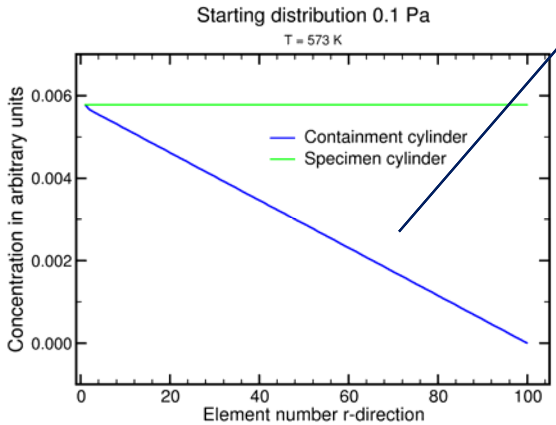
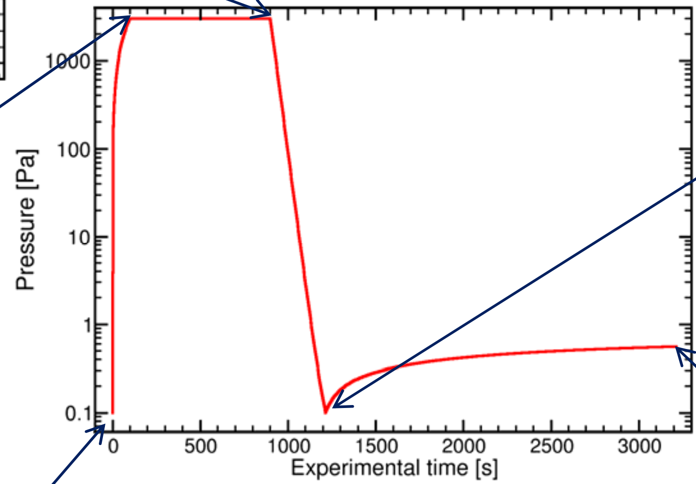
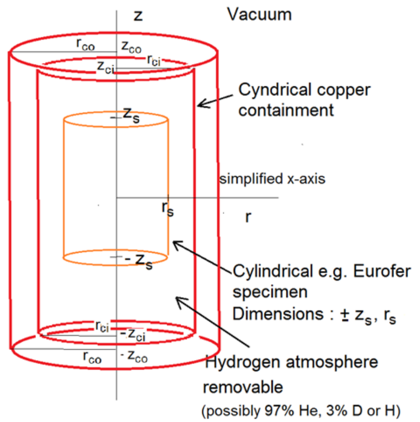
Result of 1D solver r-dependency.

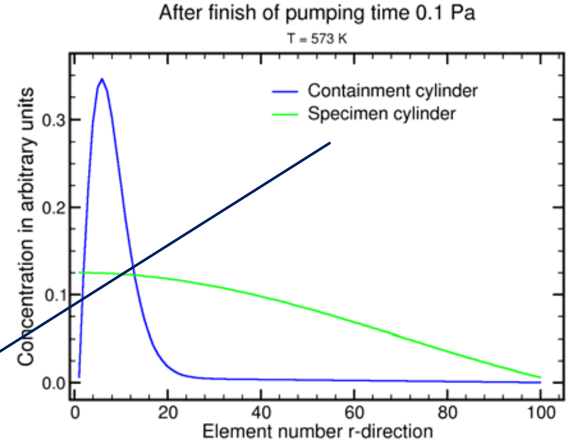


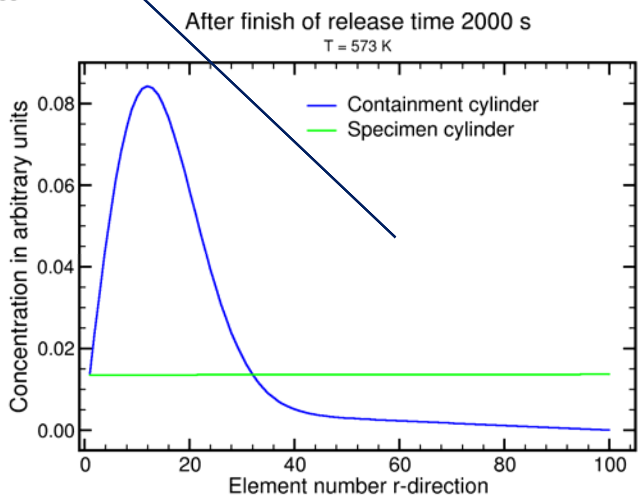












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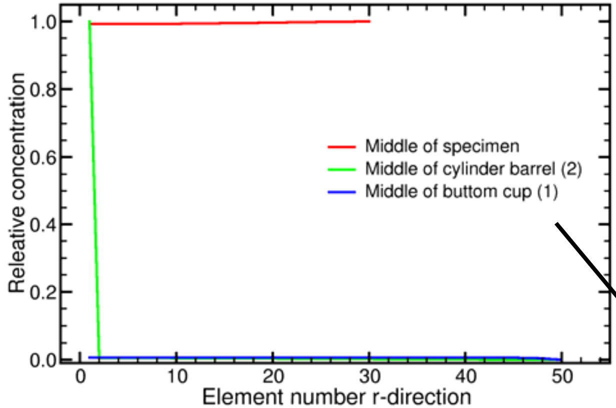
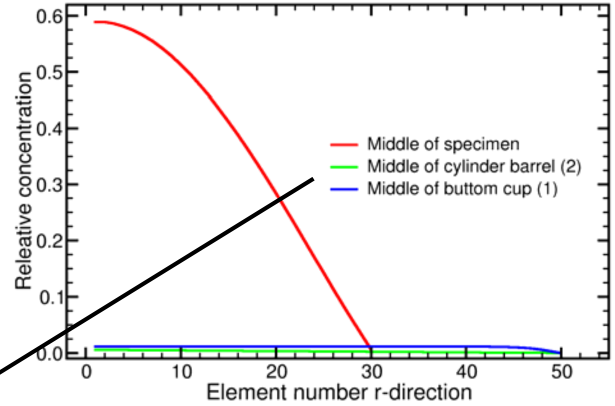
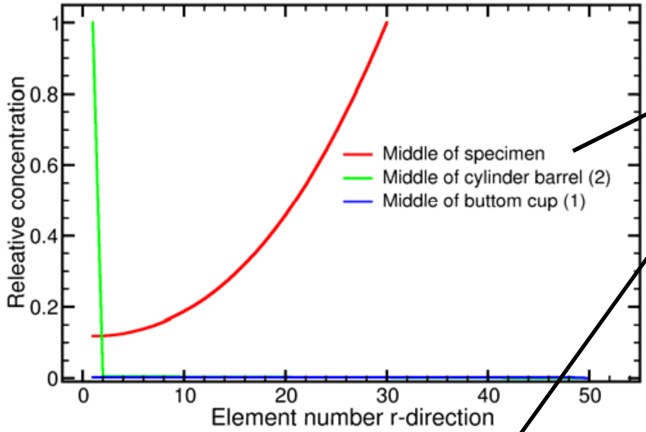
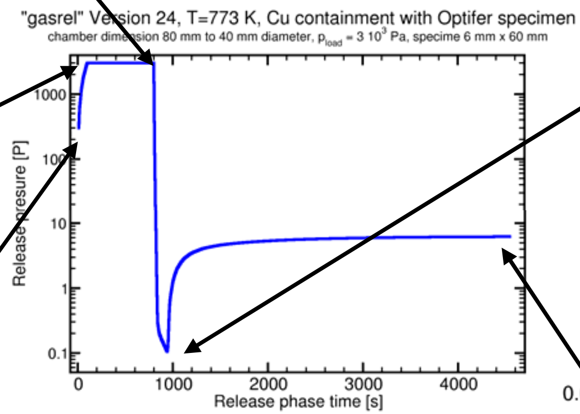
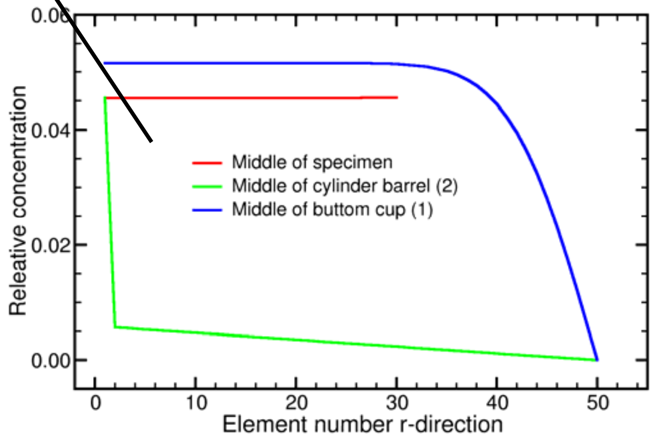


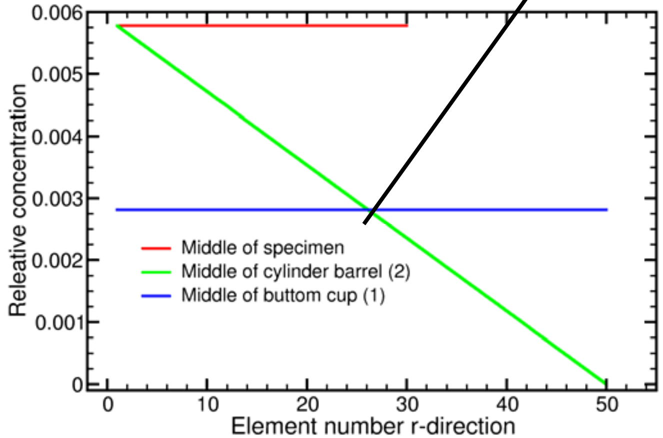
Calculation time 2D
2 h, inverse problem
approx. 920 h Uc1



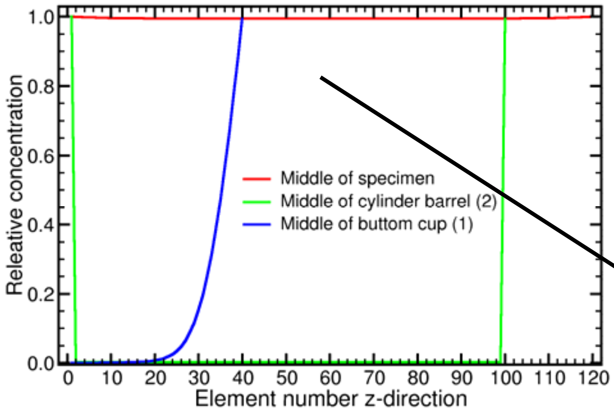


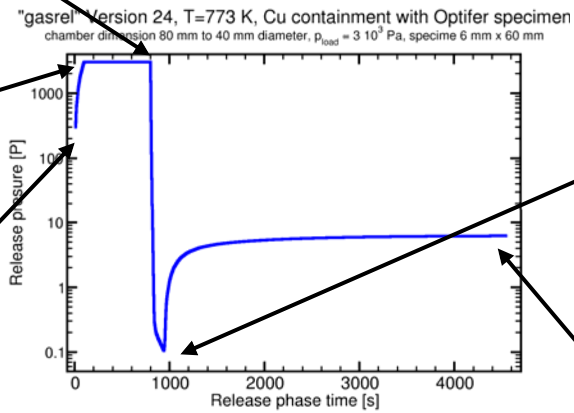


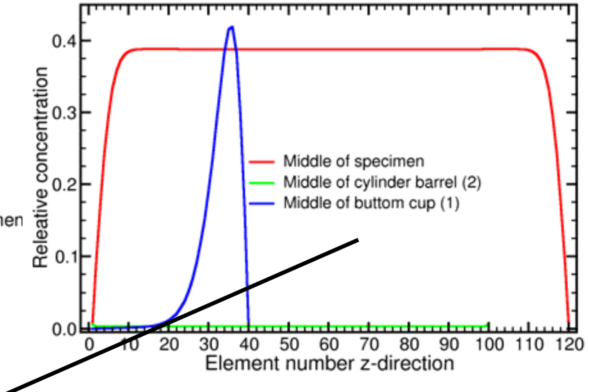


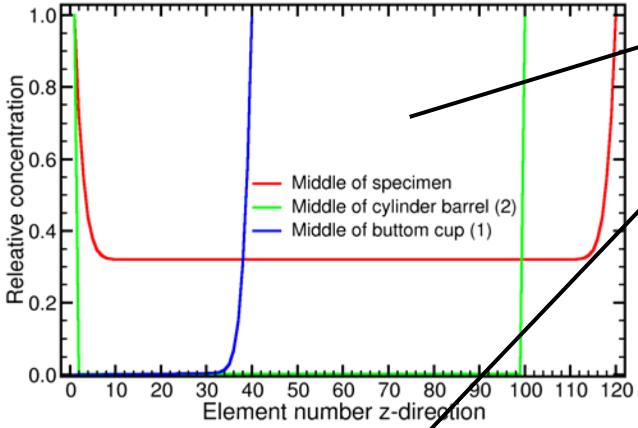


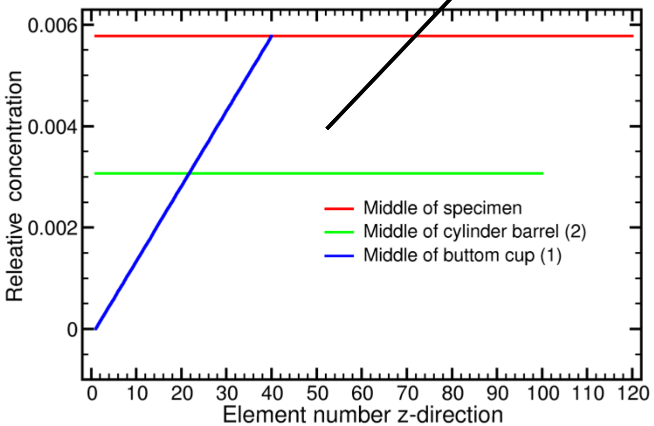
Calculation with 2D Version 24 with 12600 elements



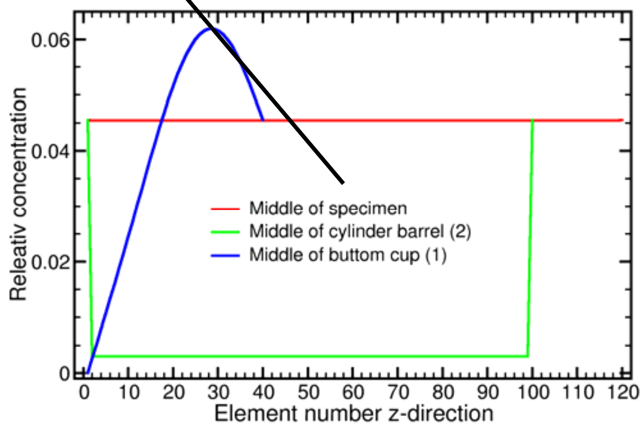




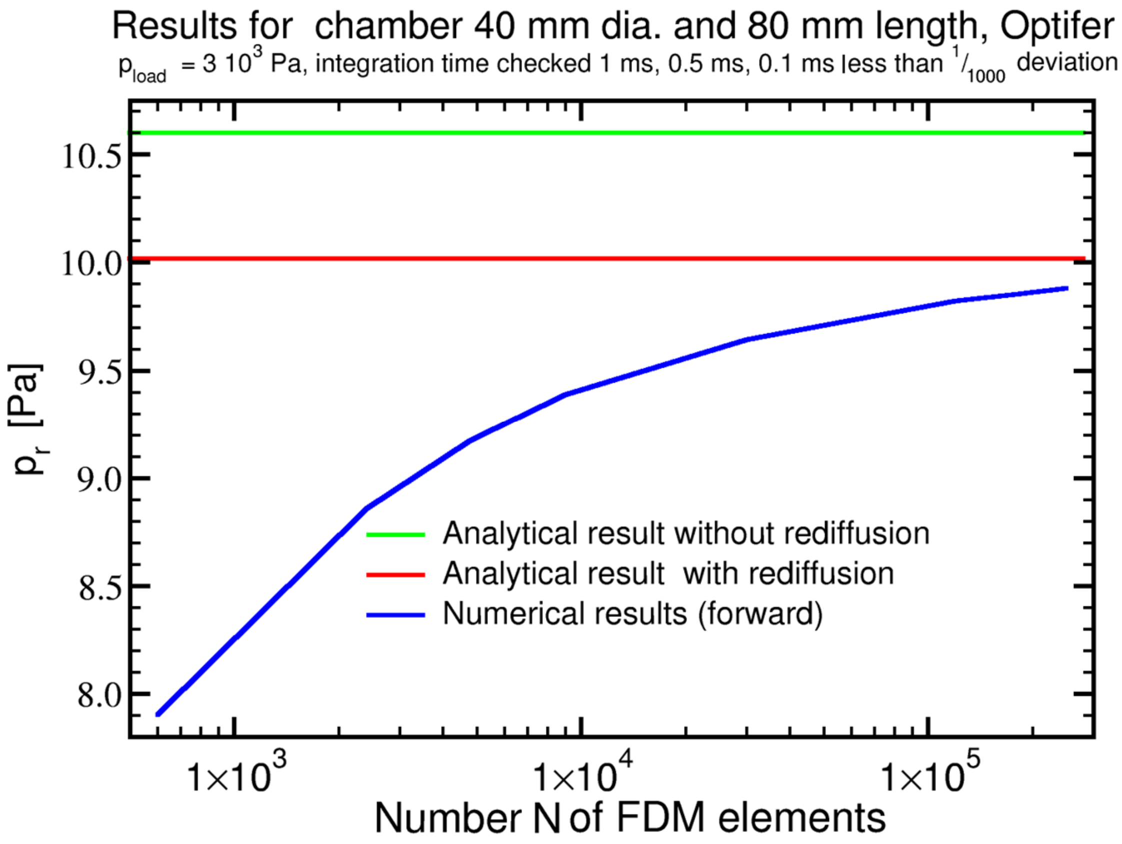


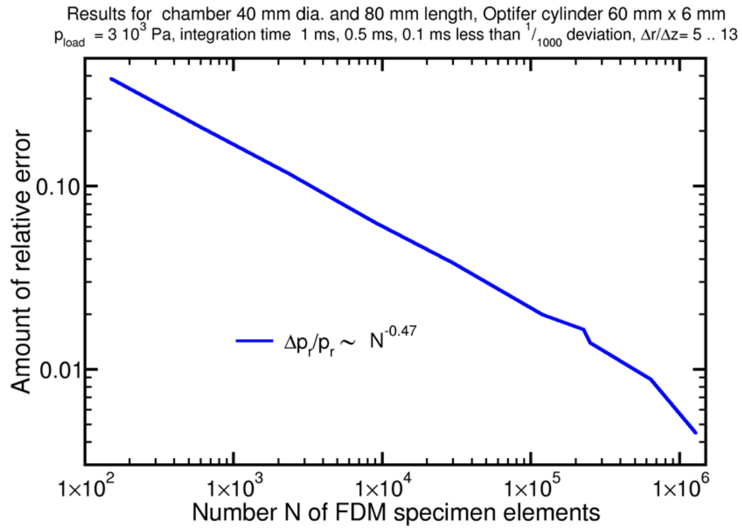


Body	R-elem	Z-elem
Speci men	30	120
1	50	40
2	50	100
3	50	40



Comparison with analytical solution:

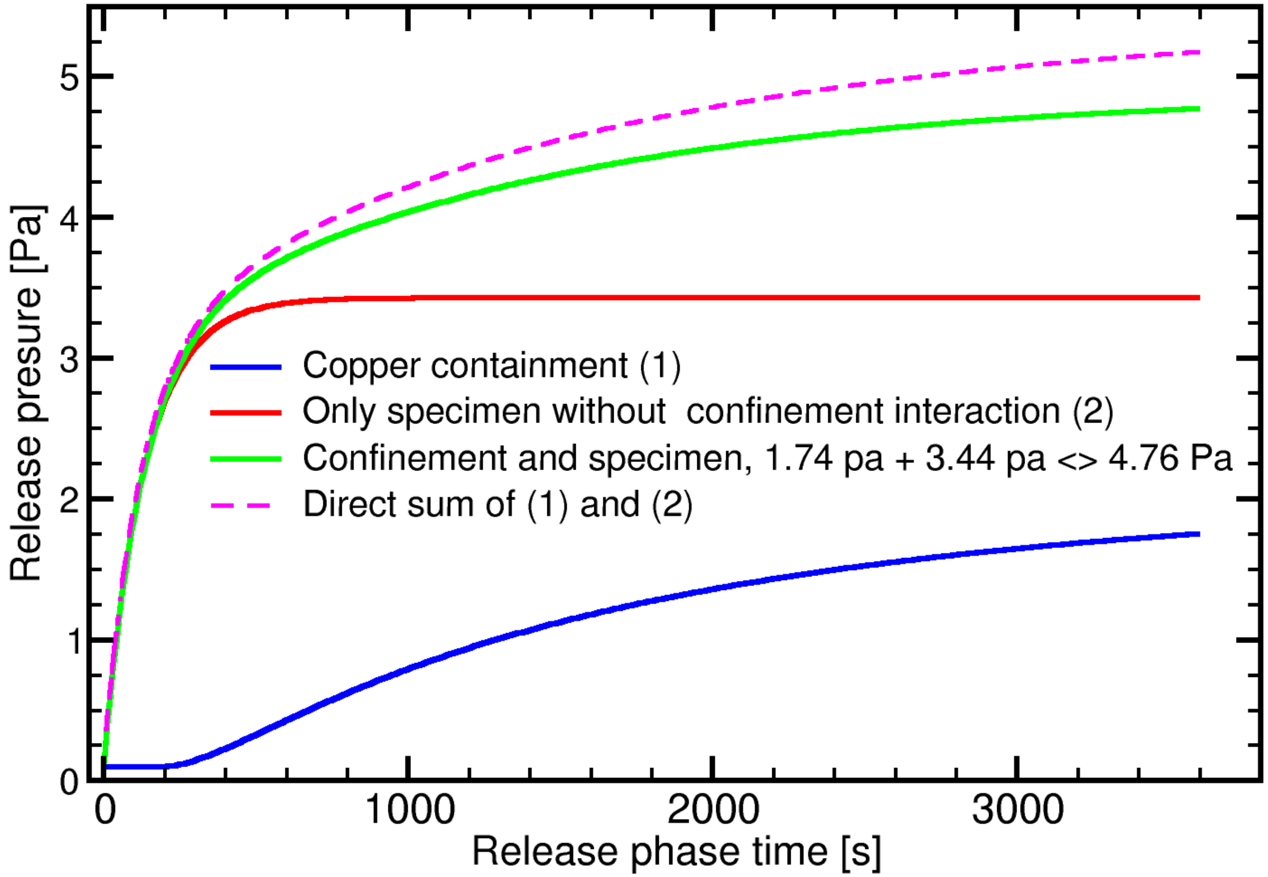


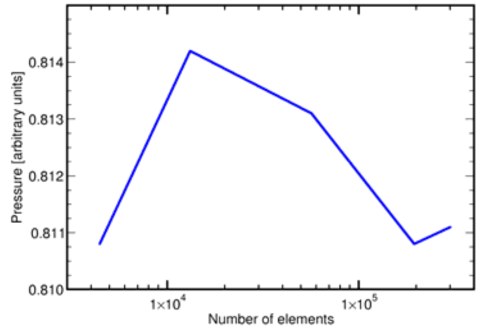


Comparison to analytical solution

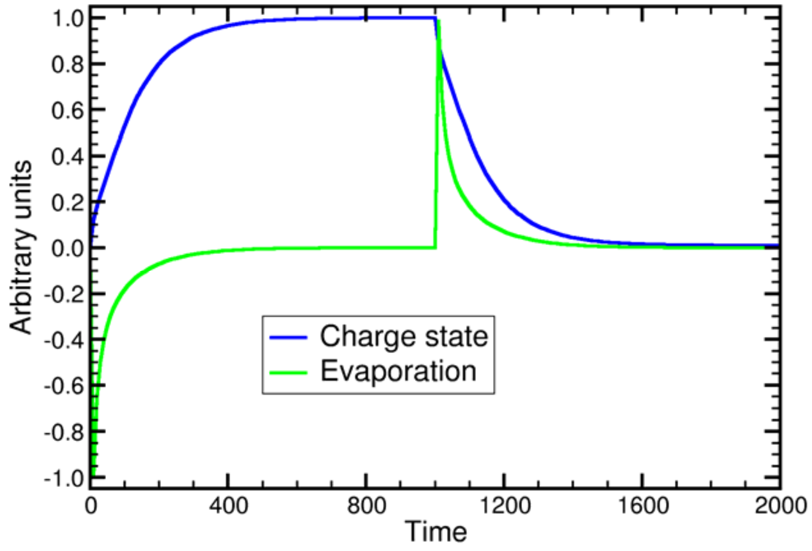
"gasrel24", T=773 K, Cu containment with Optifer specimen, 24. 5.

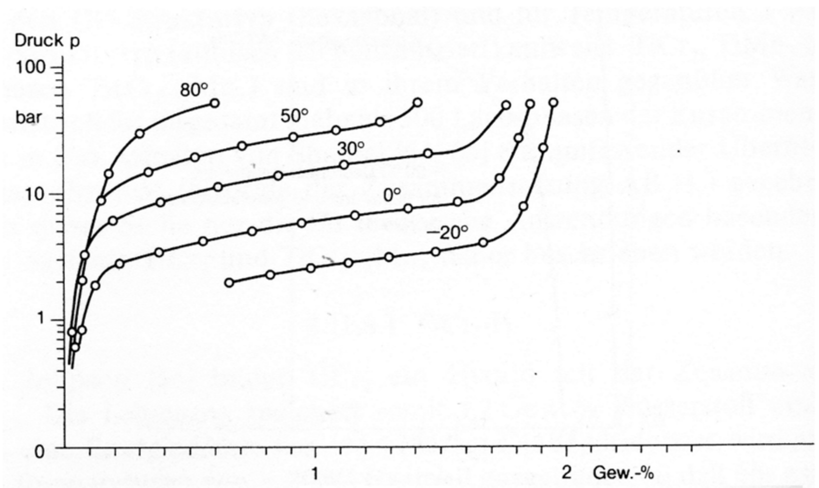
chamber dimension 80 mm to 40 mm diameter, $p_{load} = 3\ 10^3$ Pa, interstitial-molecular





7. Thermal desorption experiment as possible automotive application (energy storage)





Konzentrations-Druck-Isothermen der Legierung $Ti_{0,9}Zr_{0,1}CrMn$-H

	Thermal desorption, GR	Metal hydride storage	Lithiumorthosilicate tritium extraction
Pressure	3 kPa	5 10^5 – 10^6 Pa	1 Pa
Extraction to	Hydrogen atmosphere		
Material	Sieverts´	Non linear	Isotope exchange
Temperature	300°C-500°C	20°C-30°C	> 500°C

Acknowledgement:

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The current talk summarizes results of two running projects:

Main goal of the first one is the determination of transport parameters of hydrogen in structural metallic materials used for components in fusion power stations:

This work has been carried out within the framework of the EUROfusion Consortium, and has received funding from the Euratom research and training program 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission

The authors further acknowledge support and founding by the KIT center MathSEE in the frame of a second project:
Neue Lösungen der Kontinuitätsdifferentialgleichung mit Phasengleichgewicht zur Verbesserung der Ergebnisse bei der Auswertung von Experimenten.