Karlsruher Institut für Technologie

NUMERICAL ANALYSIS OF AN ISOVOLUMETRIC THERMAL DESORPTION EXPERIMENT

A. von der Weth, K. Nagatou,
F. Arbeiter, R. Dagan, D. Klimenko, V. Pasler, M. Schulz,
INR, KIT, CN, Athens, 25th June, 2019

IKIT/INR/MET (Maschinenbau)

1.: Description of setup
2.: Simple analytical solutions
3.: Structure of Differential Equations
4.: Results of numerical optimization
5.: Outlook to analytical solution

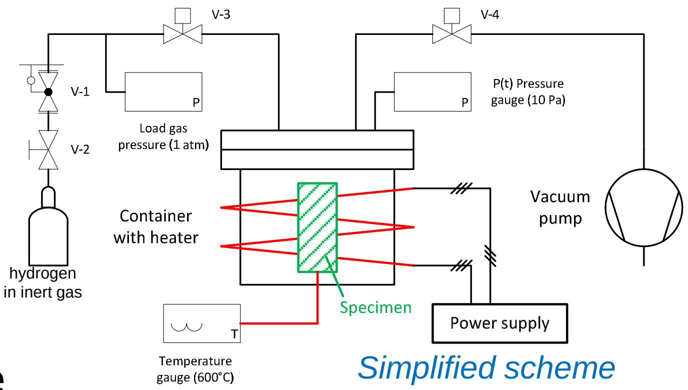
E-mail: axel.vonderWeth@kit.edu

Reminder: gas release diffusion experiments

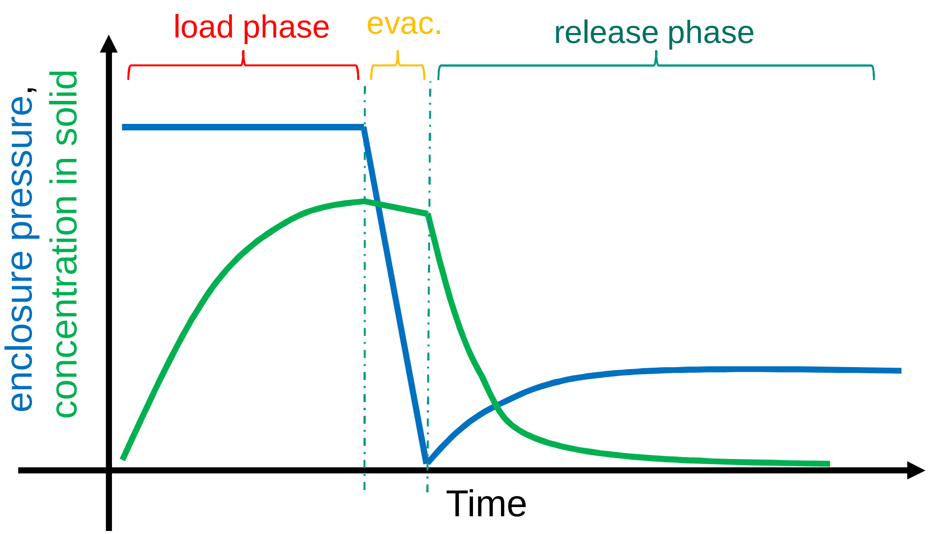
Procedure:

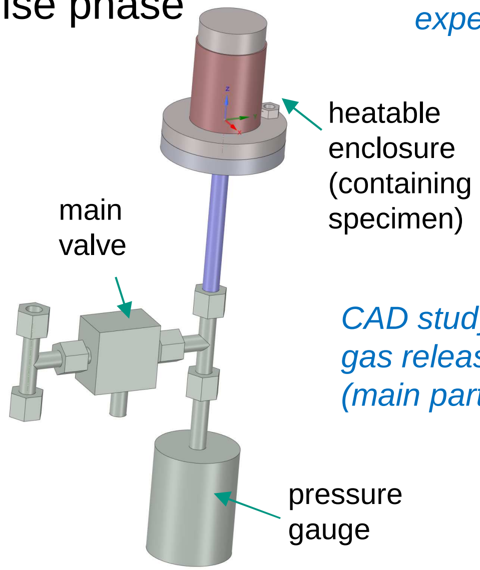
1. Specimen placed in defined volume enclusure
2. Load specimen with hydrogen at defined conditions (T, p_{H2})
3. Swiftly evacuate gases from enclosure
4. Measure pressure increase p(t) in enclosure

➔ Sieverts' constant can be deduced from final pressure
➔ Diffusion constant can be deduced from pressure rise phase



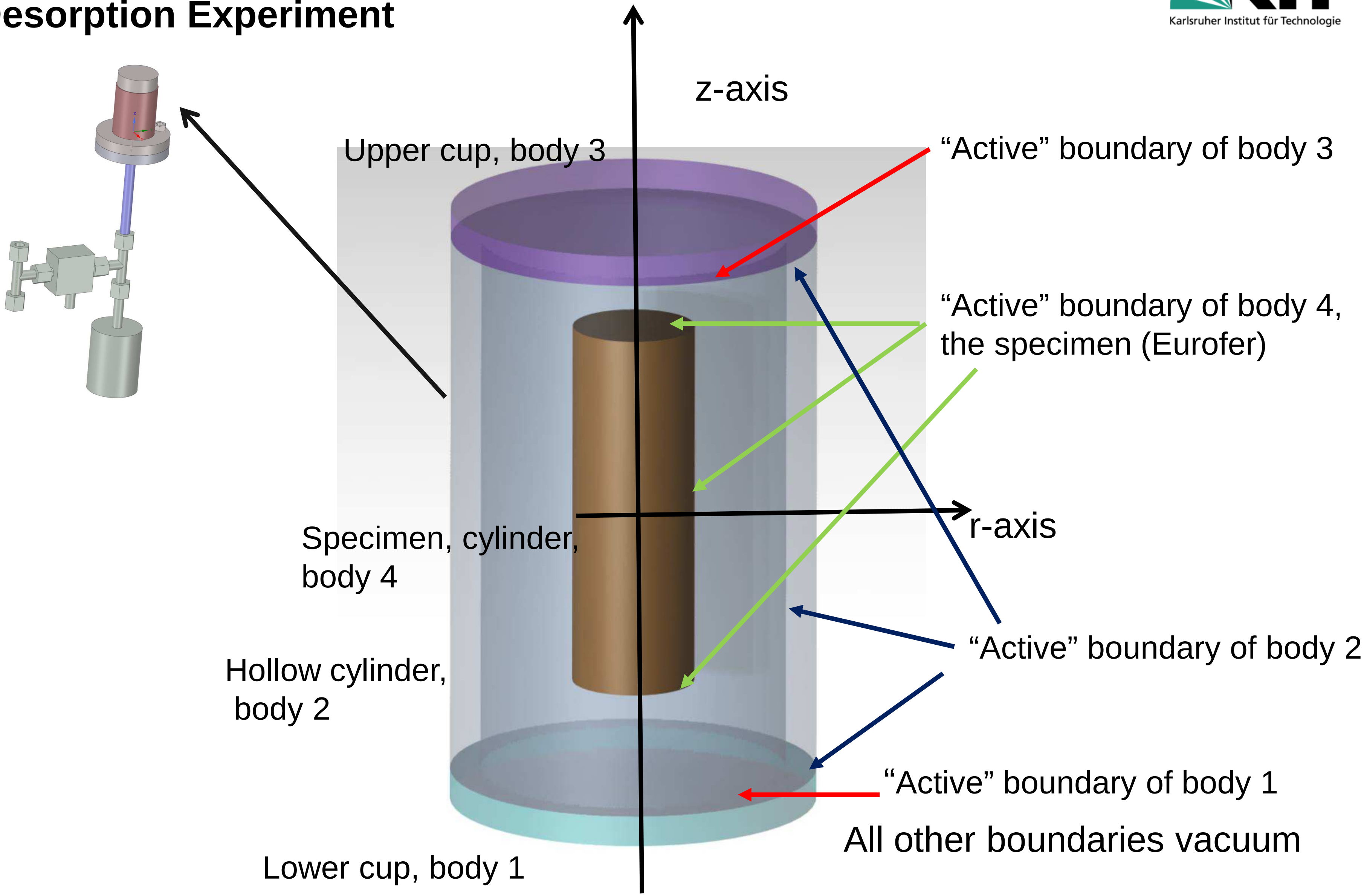
Simplified scheme of gas release experimental setup



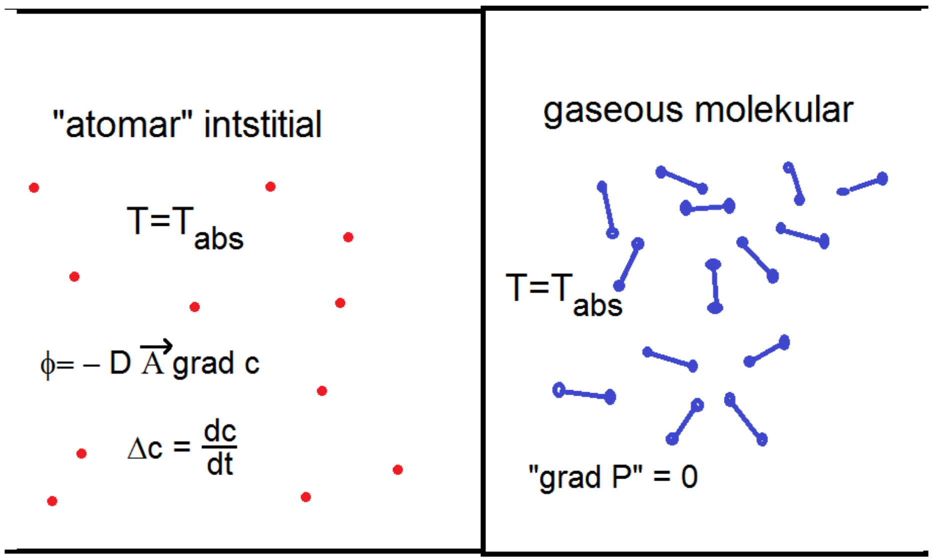


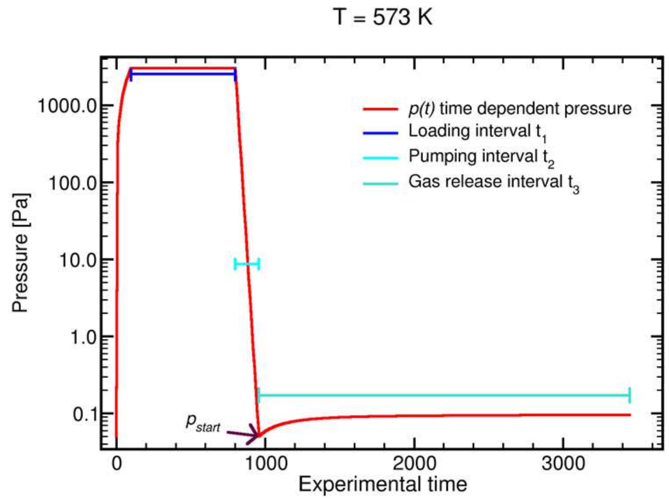
CAD study of gas release setup (main parts)

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



1.: Physical description

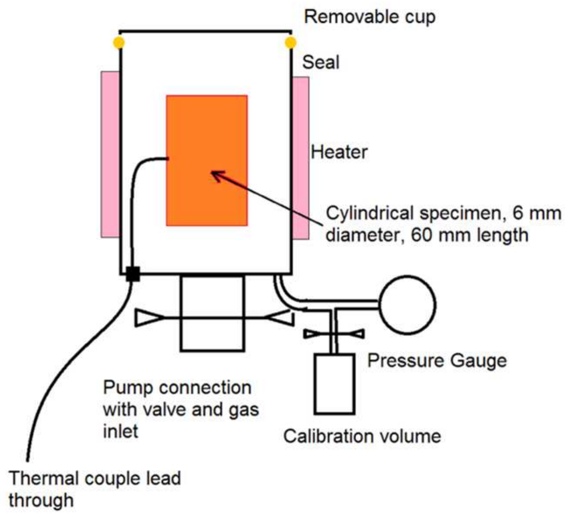




“Velocity” of mass transfer by diffusion constant D

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

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



2.: Simple analytical Solutions

Without re-diffusion, complete outgassing, $c_{sample} = 0$:

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

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

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

$$k_{s,sa} = \frac{2\,(V_c - V_{sa})}{R\,T\,V_{sa}}\,\frac{(p_r - p_{end})}{\sqrt{p_{load}} - \sqrt{p_r}}$$

Experimentally difficult realization of boundaries, no statement about diffusion constant

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

3.: Structure of differential equations:

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

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} + \underbrace{\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}}_{=0}$$

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

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

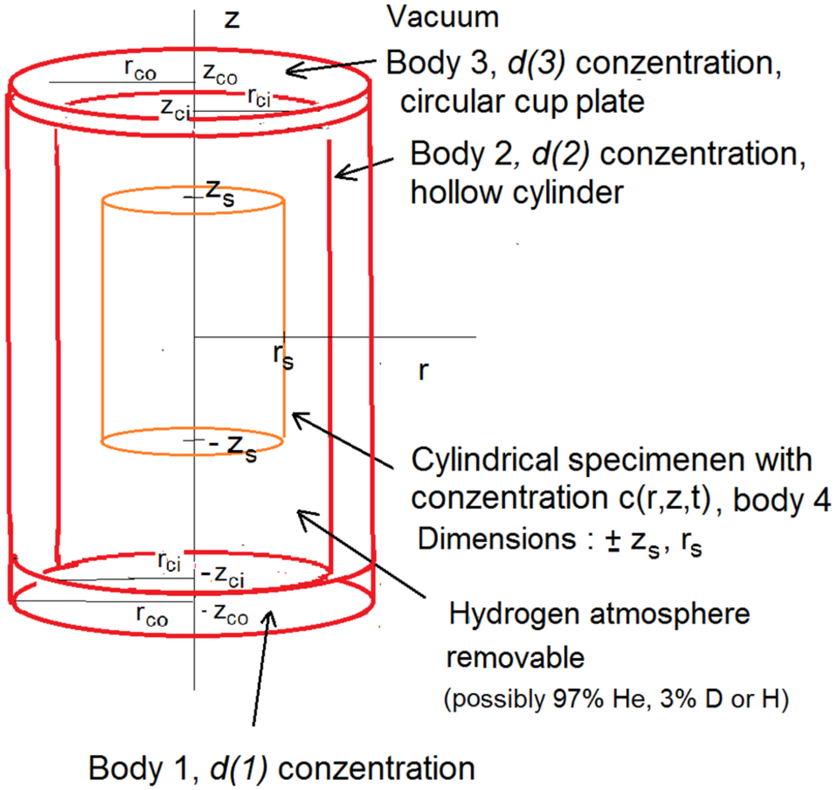
$$d(1)(r \leq r_{co}, z = -z_{ci}, \forall t) = k_{s,cu}\sqrt{p(t)}$$

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

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

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

Analytical 1d: Sedano, Perujo (1999), Esteban Douglas (2001) , Eichenauer Pebler (1957) Hattenbach (1961)
Analytical 2d: Eichenauer, Pebler, Witte 1965



3. Structure of differential equations

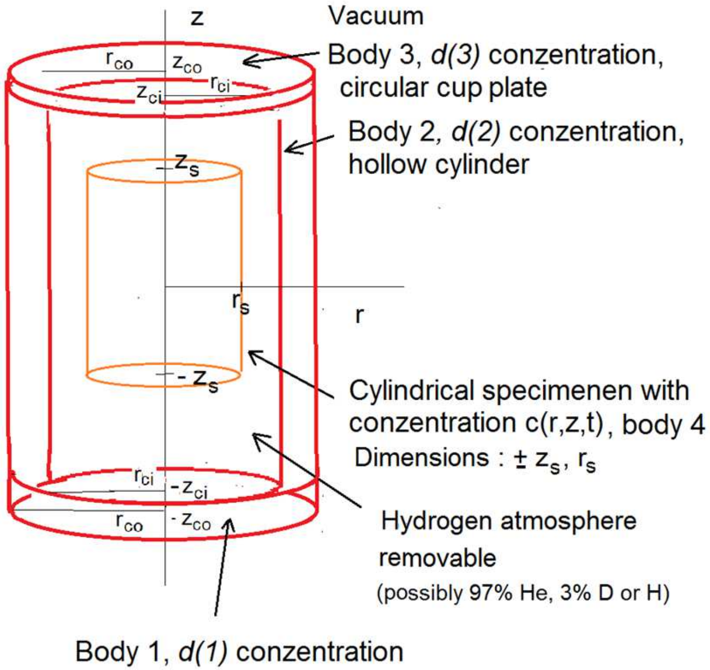
$$\frac{dm}{dt} = -2\,\pi\,D_{sa}\int_0^{r_s} \underbrace{2}_{symmetric}\; r\,\frac{\partial}{\partial z}\,c(r,z=z_s,t)\,dr$$

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

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

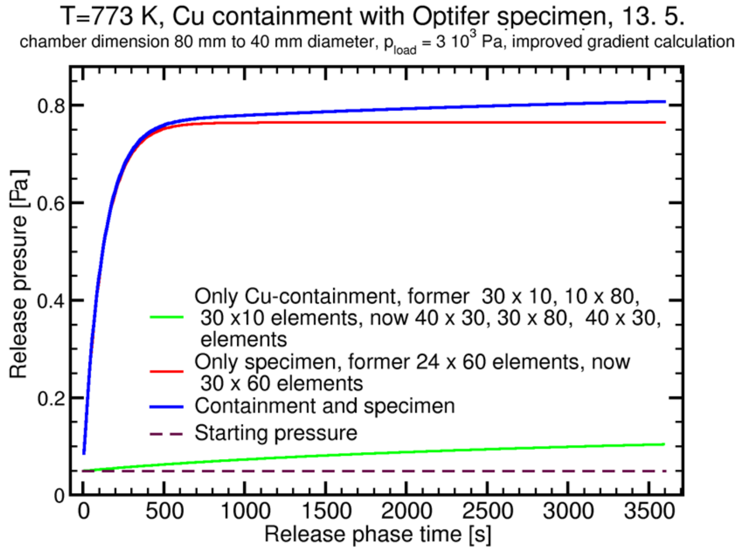
$$-\;2\,\pi\,r_{ci}D_{cu}\int_{-z_{ci}}^{z_{ci}}\frac{\partial}{\partial r}\,d(2)(r=r_{ci},z,t)\,dz$$
$$superficies\ surface\ of\ body\ 2$$

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

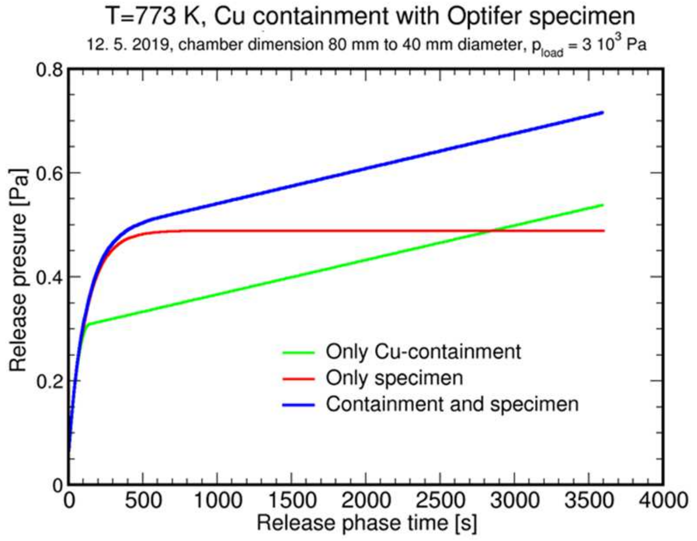


$$p(t) = p_{start} + \underbrace{k_v}_{RT_{abs}/V_{gas}} \int_{t_1+t_2}^{t} \underbrace{0.5}_{gaseous\leftrightarrow interstitial}\;\frac{dm}{dt}\,dt$$

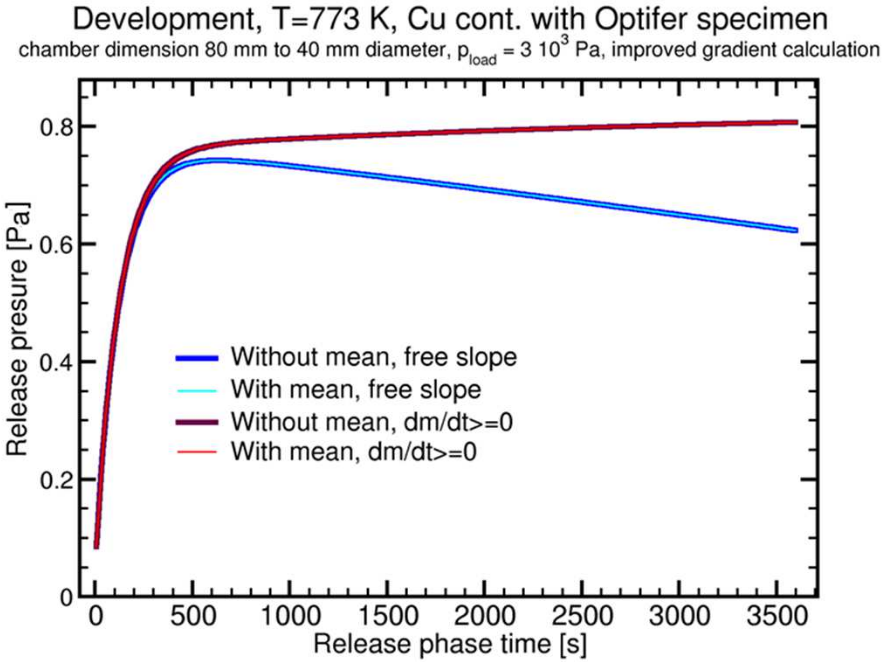
4.: Results of numerical solution



Simple numerical gradient calculation

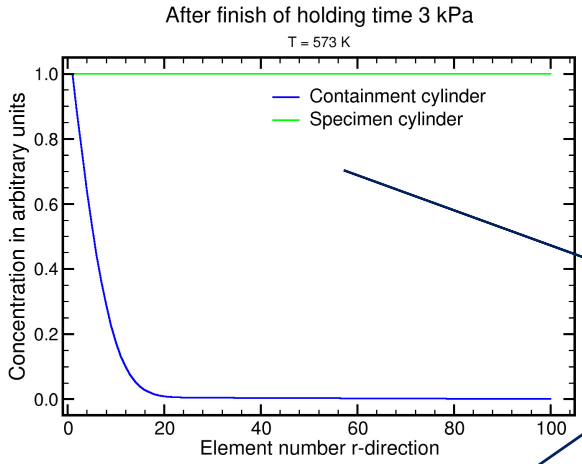


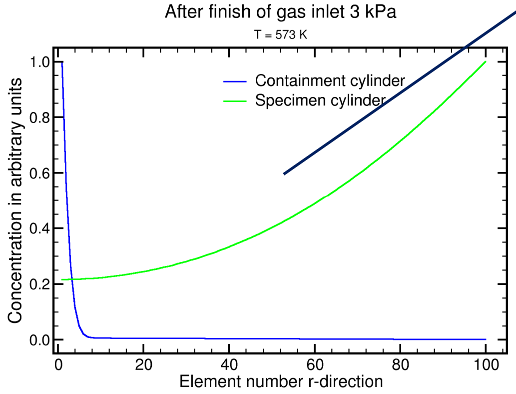
Numerical artefacts

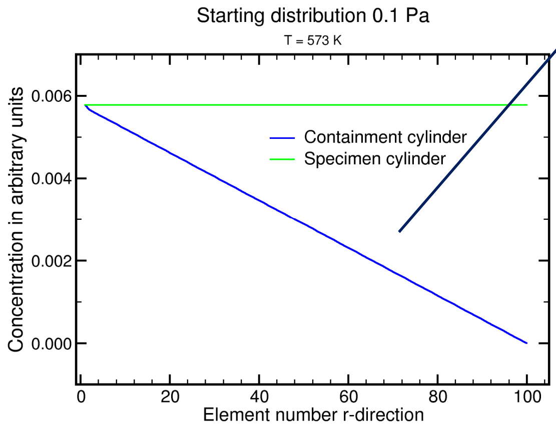


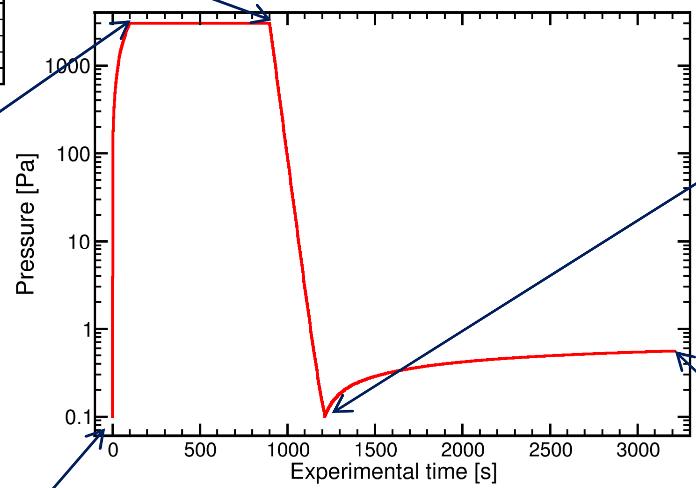
Gas release Experiment:

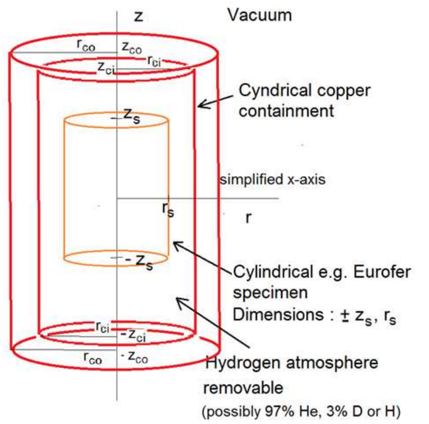
Result of 1D solver r-dependency.

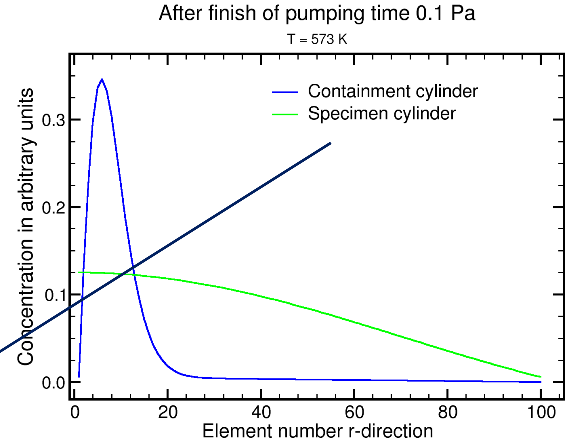


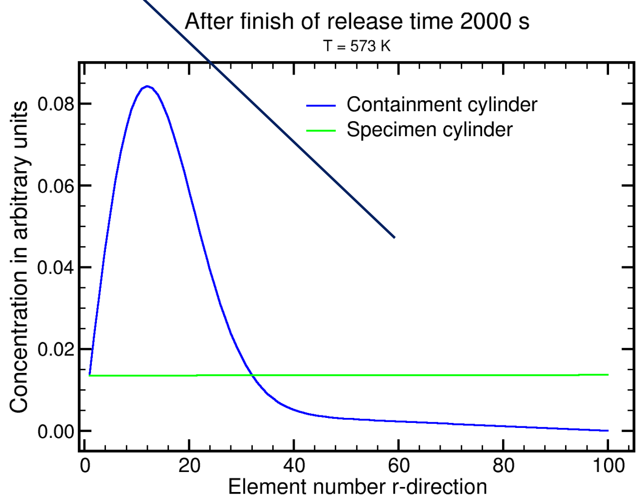












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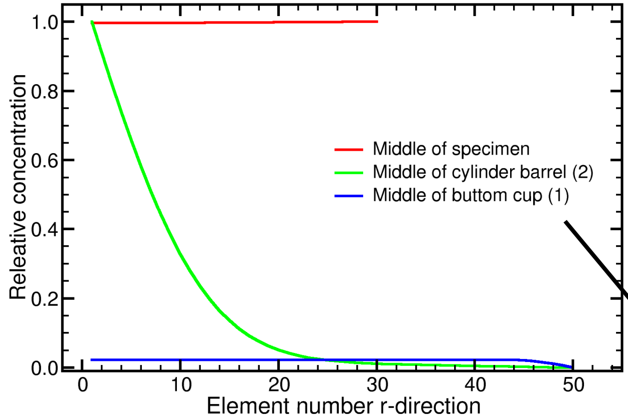
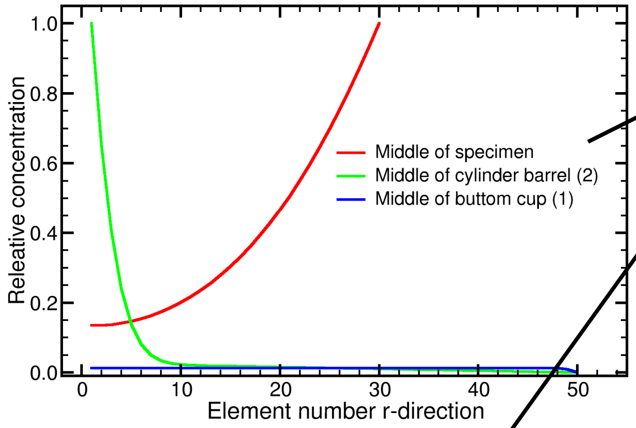
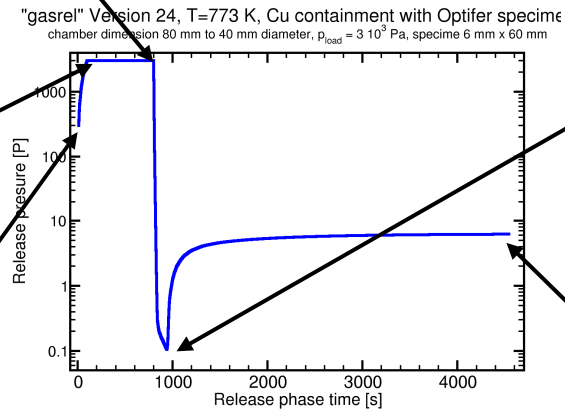
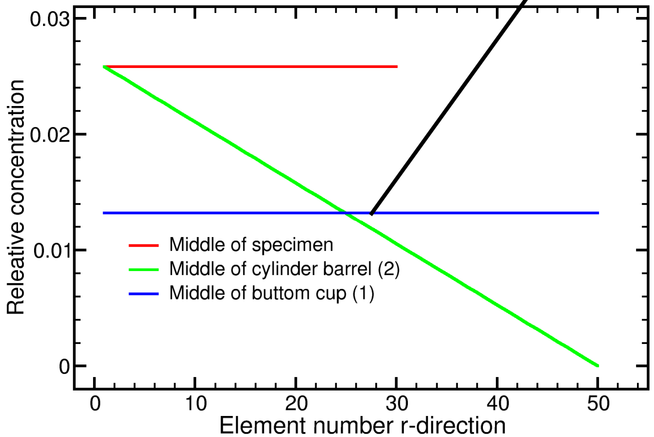
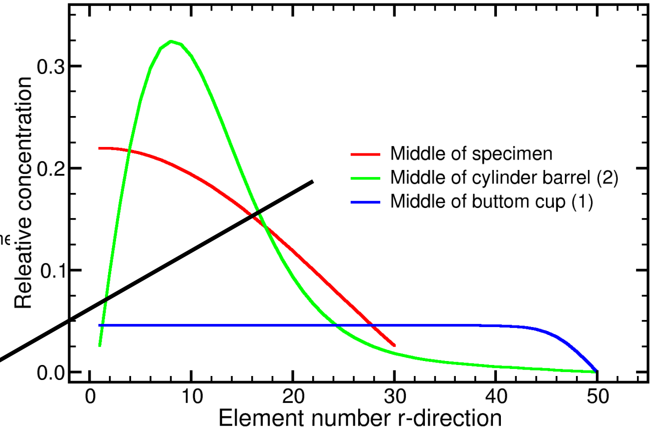


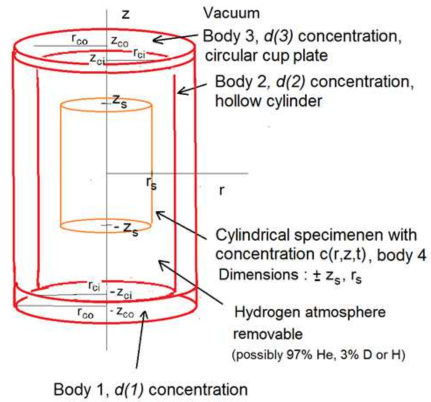
Calculation time 2D
35´, inverse problem
approx. 440 days
Uc1 accuracy ≈ 10 %

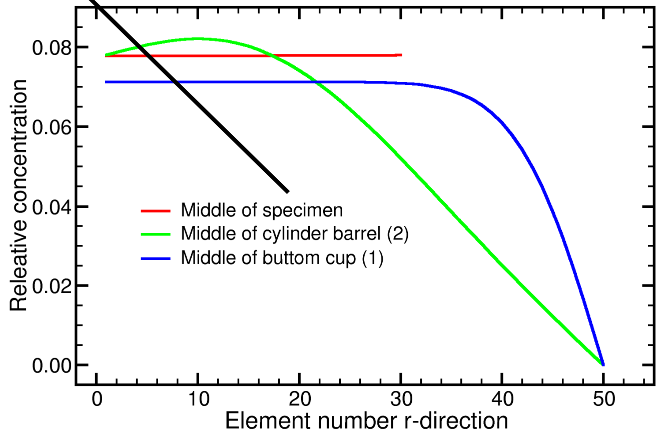




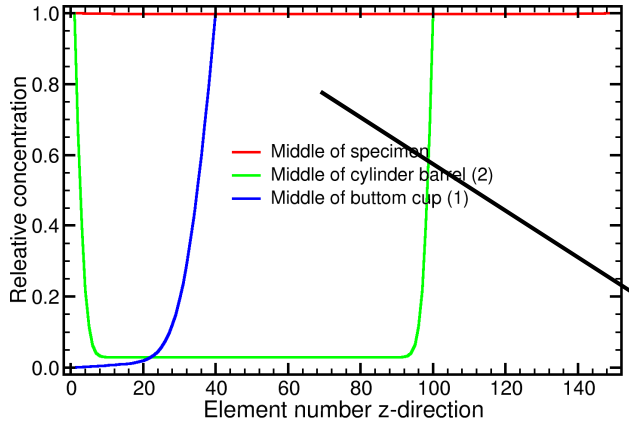


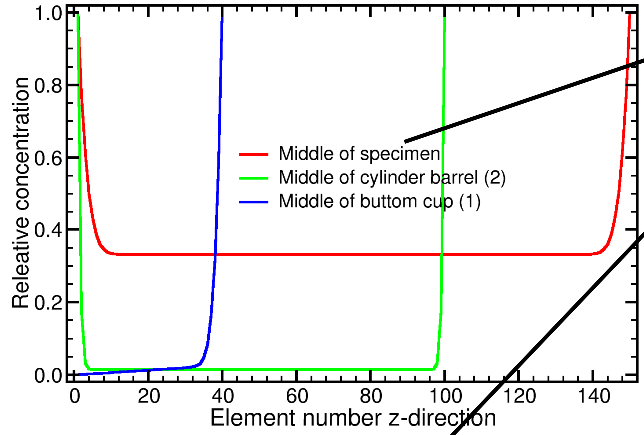


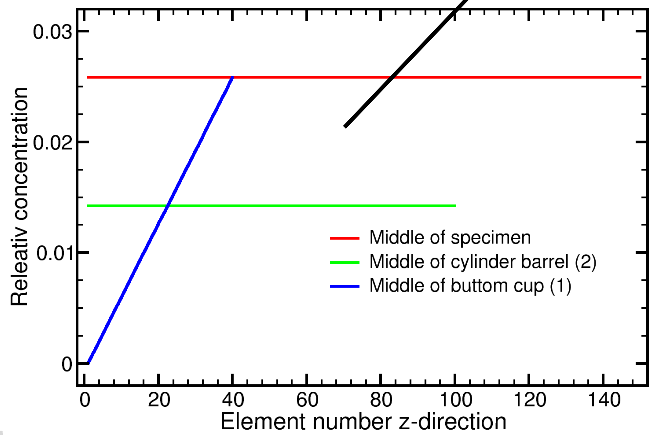


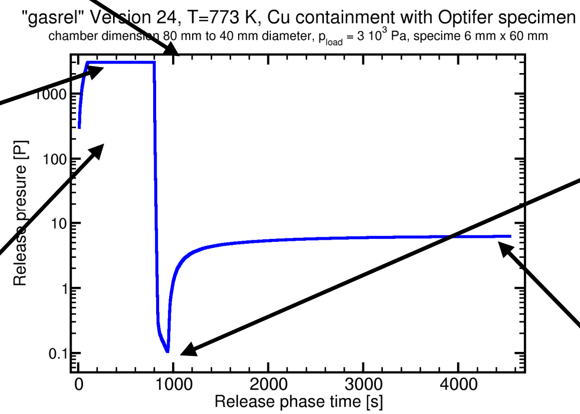


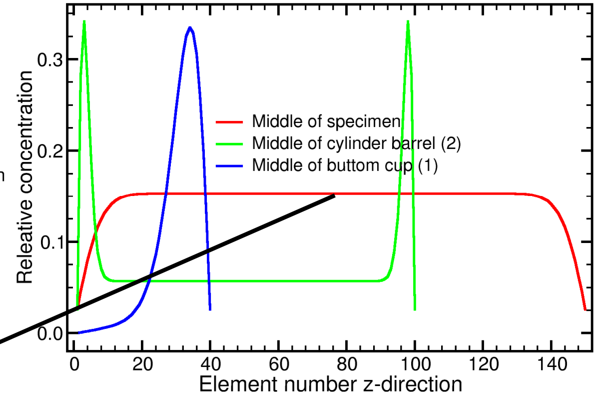
Calculation with 2D Version 24 with 13500 elements

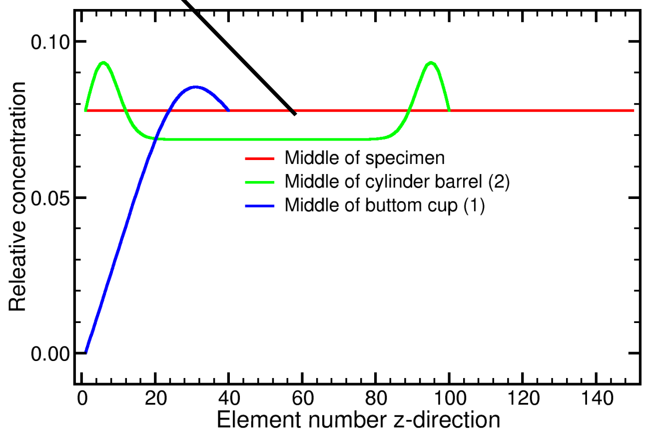










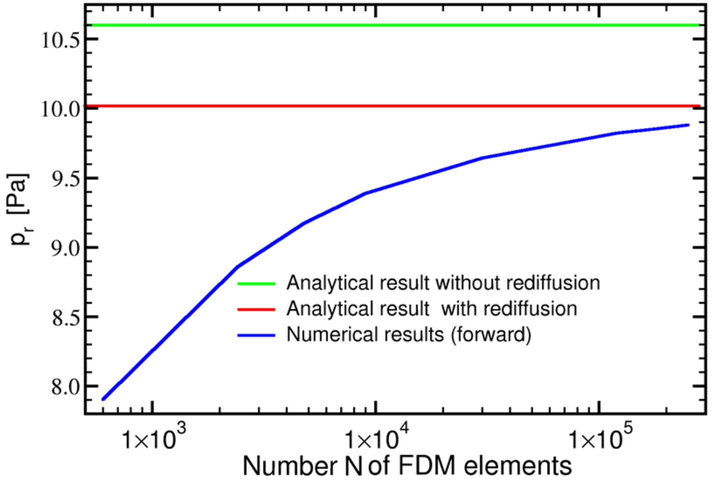


Body	R	Z
Specimen	30	150
1	50	40
2	50	100
3	50	40

Comparison with analytical solution:

Results for chamber 40 mm dia. and 80 mm length, Optifer

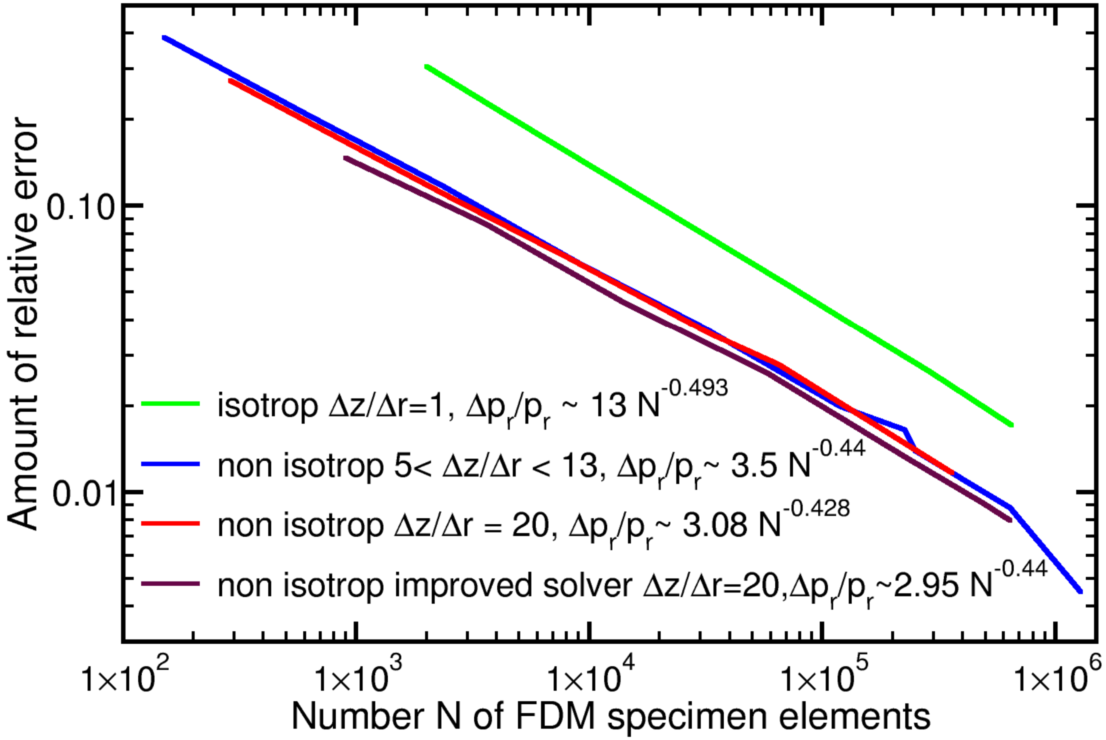
p_{load} = 3 10^3 Pa, integration time checked 1 ms, 0.5 ms, 0.1 ms less than $^1/_{1000}$ deviation



$$10^{-11} < \frac{D_{sa}\Delta t}{\Delta z^2} < 10^{-6}$$

Results for chamber 40/20 mm dia. and 80 mm length, Optifer cylinder 60 mm x 6 mm

p_{load} = 3 10^3 Pa, integration time 1 ms, 0.5 ms, 0.1 ms less than $^1/_{1000}$ deviation



Small excurse to solver algorithms:

1D forward Euler

$$c(i,t+\Delta t) = c(i,t) + \frac{D\,\Delta t}{\Delta r^2}\left(c(i+1,t) + c(i-1,t) - 2c(i,t)\right) + \frac{D\,\Delta t}{2\,r\,\Delta r}\left(\left(c(i+1,t)\right) - c(i-1,t)\right)$$

2D improved forward Euler:

$$c(i,j,t+\Delta t) = c(i,j,t) + \frac{D\,\Delta t}{2\,i\,\Delta r^2}\left((2i+1)c(i+1,j,t) + (2i-1)c(i-1,j,t) - (4i)c(i,t)\right) + \frac{D\,\Delta t}{\Delta z^2}\left(\left(c(i,j+1,t)\right) + c(i,j-1,t) - 2c(i,j)\right)$$

Desired: Backward Euler solver, e. g. 1D cartesian:

$$\vec{c}_{k+1} = \vec{c}_k + \begin{vmatrix} 0 & & & & & \\ D^* & -2D^* & D^* & & & \\ & D^* & -2D^* & D^* & & \\ & & D^* & -2D^* & D^* & \\ & & & \ddots & & \\ & & & D^* & -2D^* & D^* \\ & & & & & 0 \end{vmatrix} \vec{c}_{k+1} \qquad \vec{c}_{k+1} = \begin{vmatrix} 1 & & & & & \\ -D^* & 1+2D^* & -D^* & & & \\ & -D^* & 1+2D^* & -D^* & & \\ & & -D^* & 1+2D^* & -D^* & \\ & & & -D^* & 1+2D^* & -D^* \\ & & & & \ddots & \\ & & & -D^* & 1+2D^* & -D^* \\ & & & & & 1 \end{vmatrix}^{-1} \vec{c}_k$$

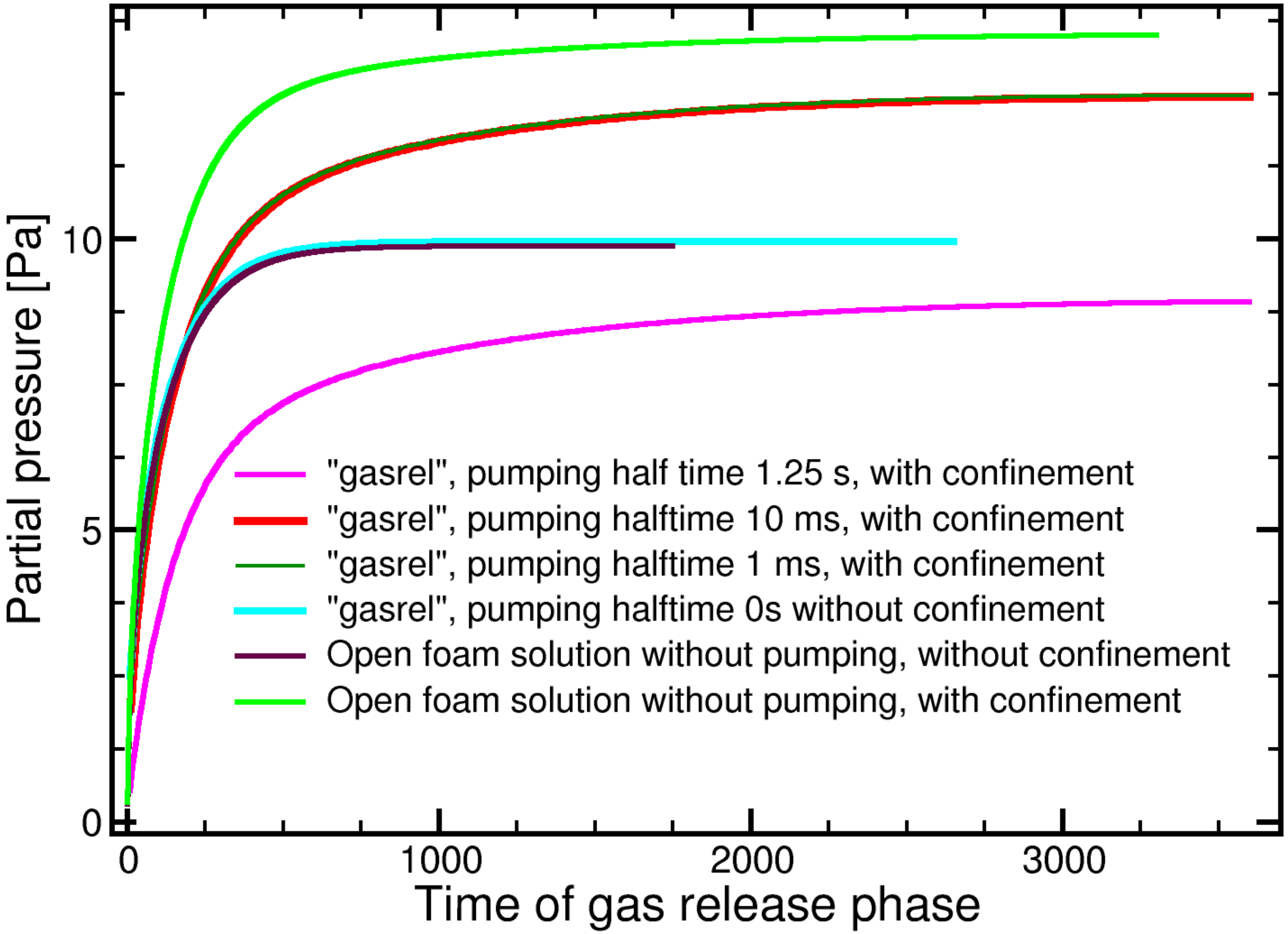
$$D^* = \frac{D\,\Delta t}{\Delta x^2}$$

2D n x n x m tensor ?

4.: Results

"gasrel" calculation with 6400 specimen element and 1800 conf. elements

14 halftimes reaching endpresure (0.1 Pa)



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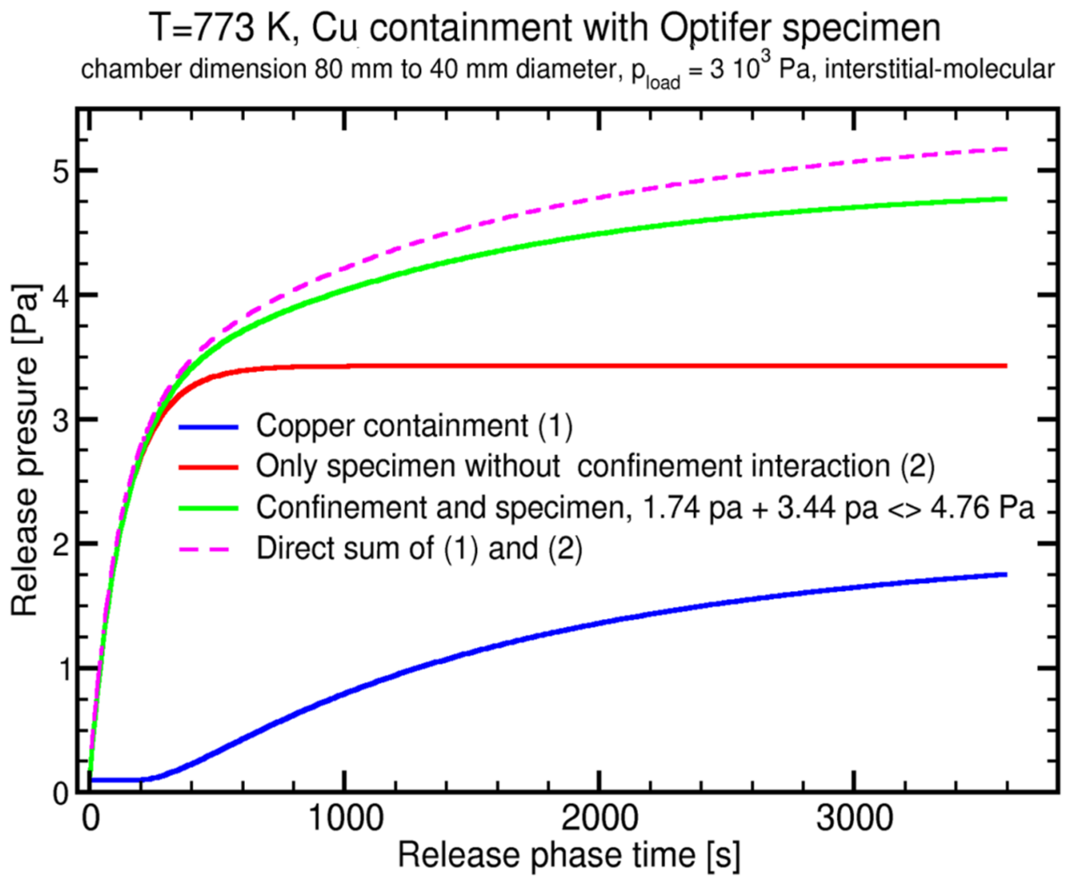
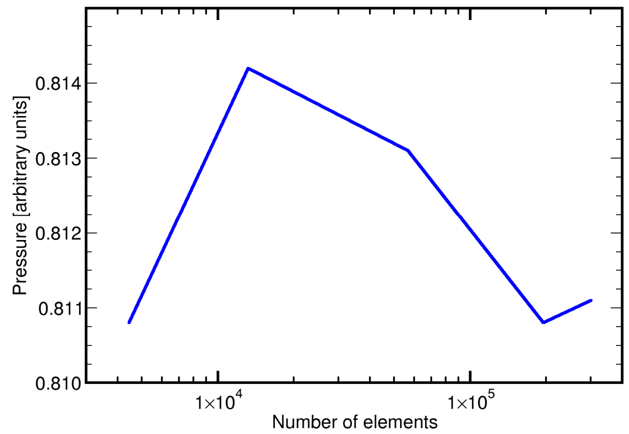
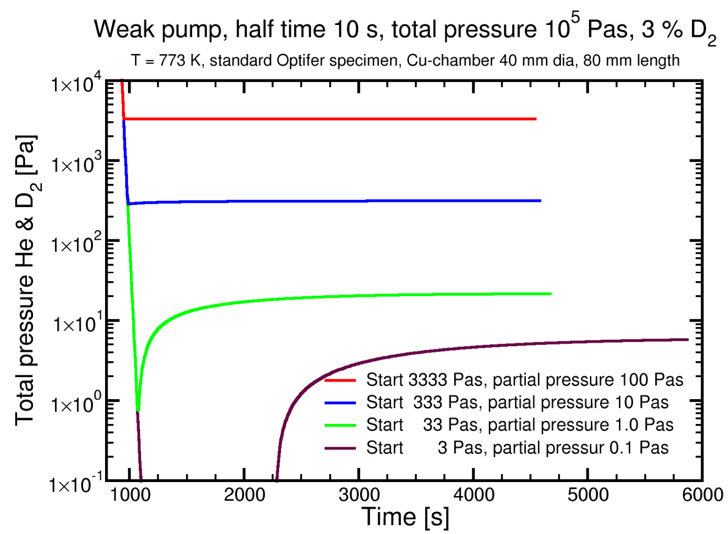
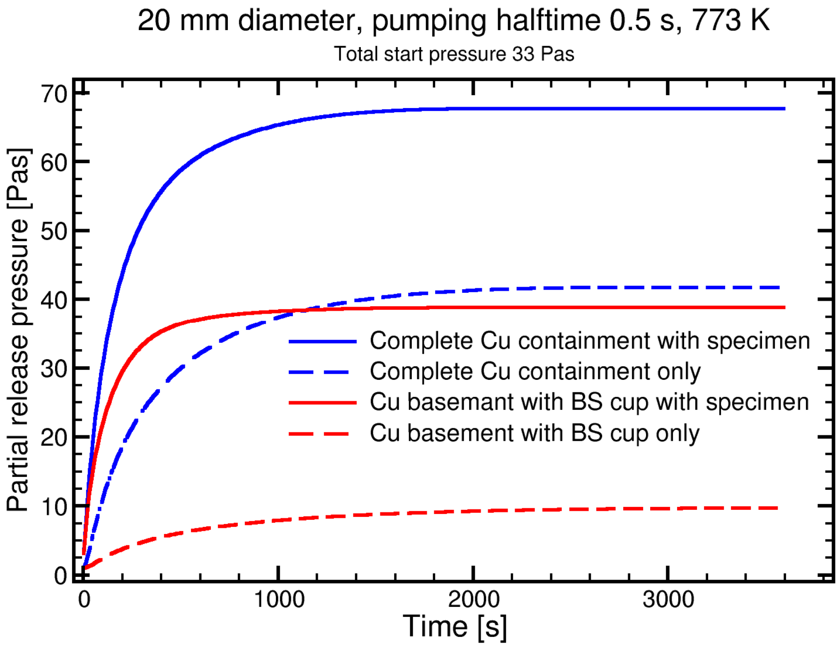


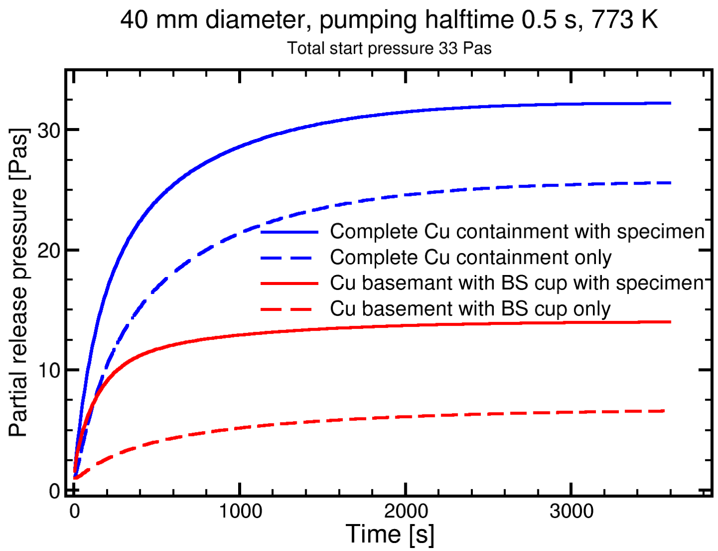


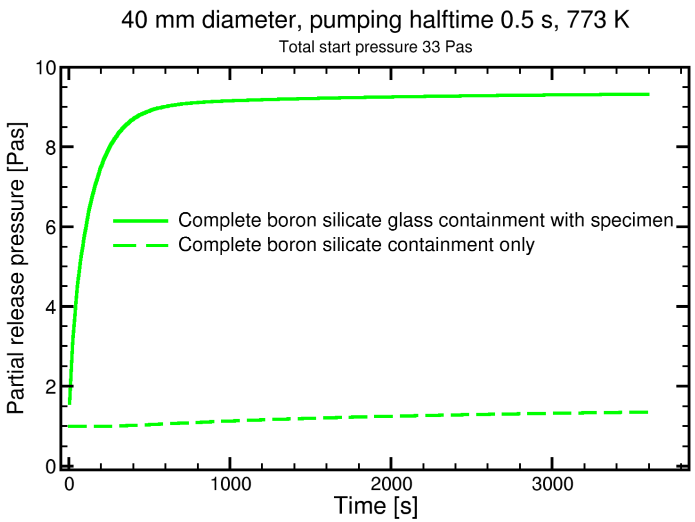
Choosing starting pressure:

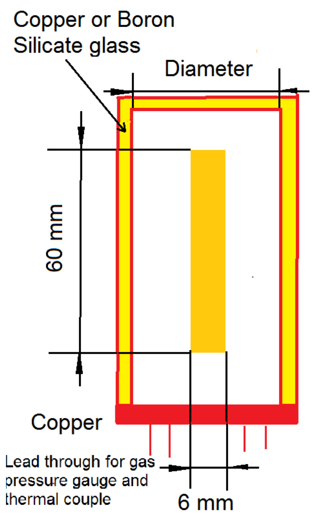


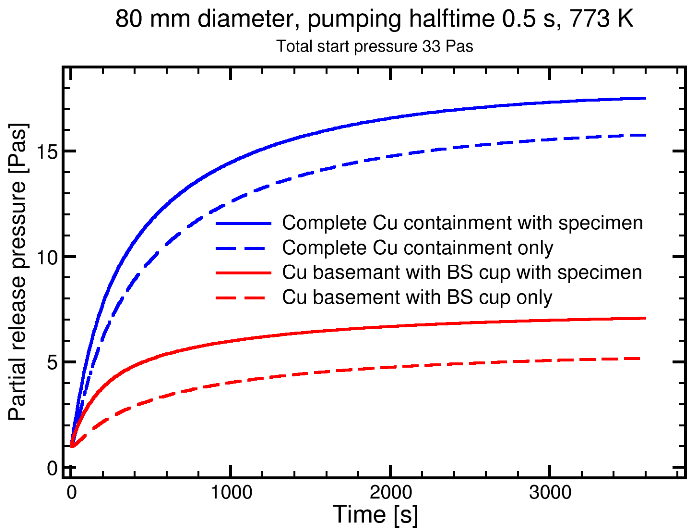
Results for conception of experiments











5.: Outlook to analytical solution

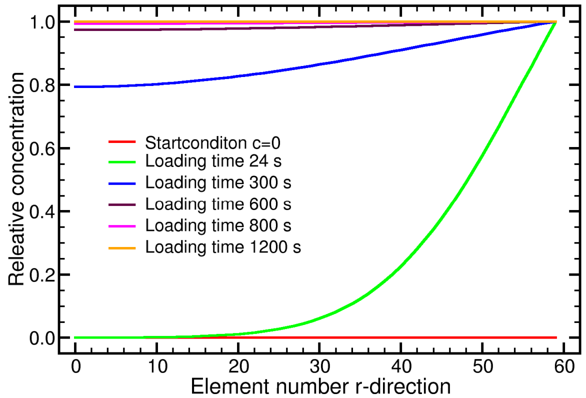
Solution in the charging interval

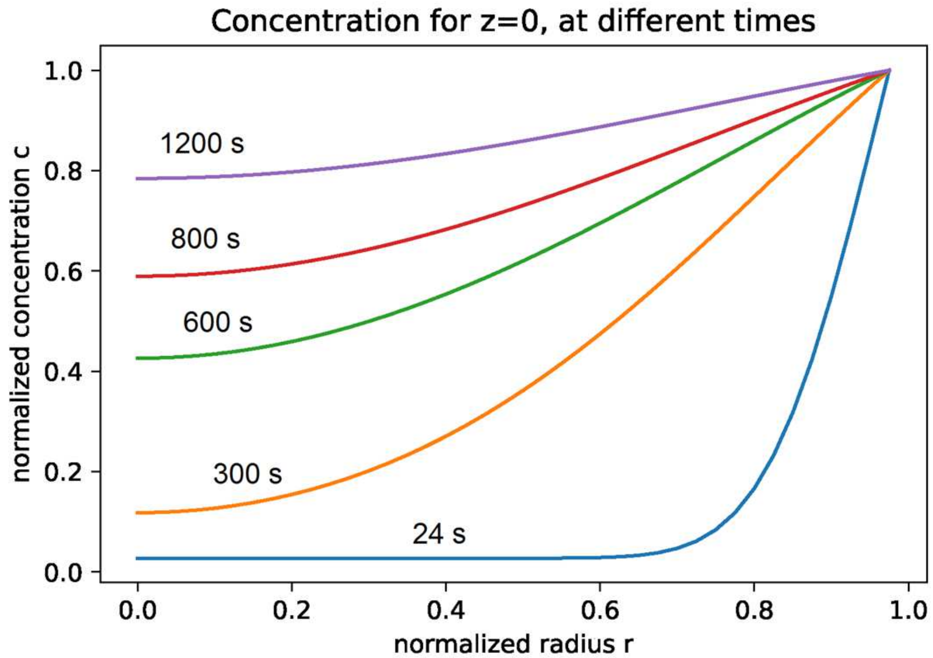
$$c(r,z,t) = k_{s,sa}\sqrt{p_{load}}\sum_{n,m}\frac{8(-1)^{n+1}}{\pi(2n+1)x_m J_1(x_m)}\exp\left(-\gamma_{n,m}^2 t\right)\cos\left((2n+1)\frac{\pi}{2}z\right)J_0(x_m r)$$

where

$$\gamma_{n,m}^2 = D_{sa}\left(\frac{x_m^2}{r_s^2}+\frac{(2n+1)^2\pi^2}{4z_s^2}\right),$$ $J_\alpha(x)$ (α=0,1) Bessel functions of the first kind,

x_m the m-th roots of $J_0(x)$.





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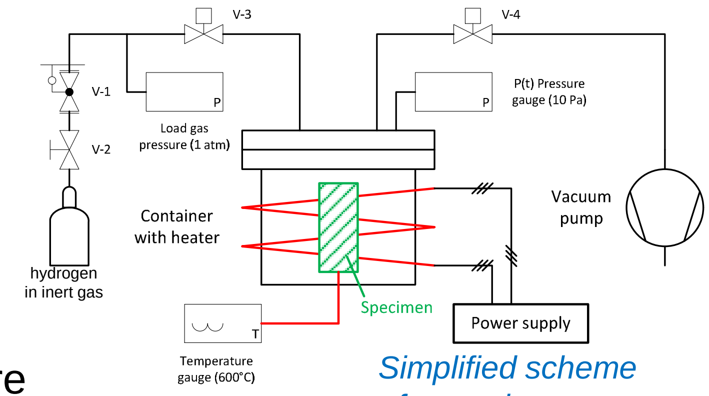
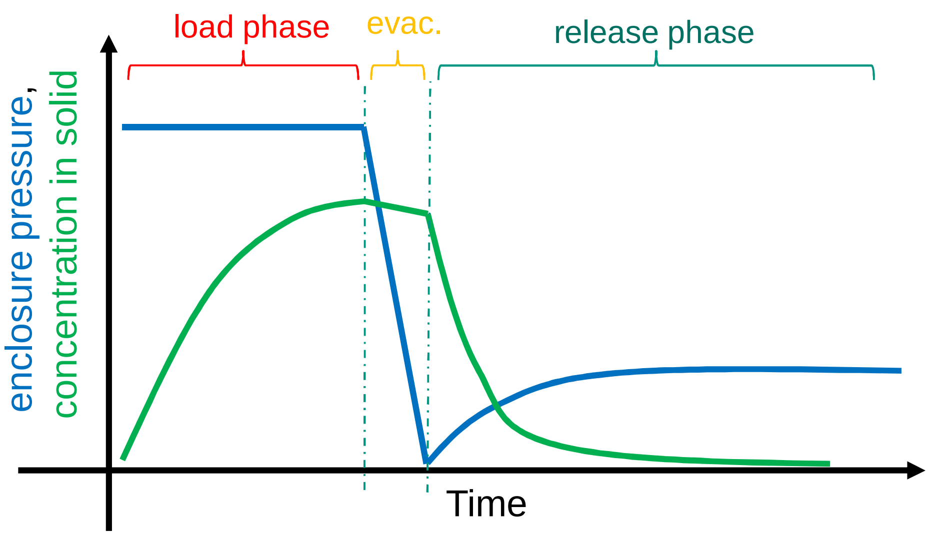
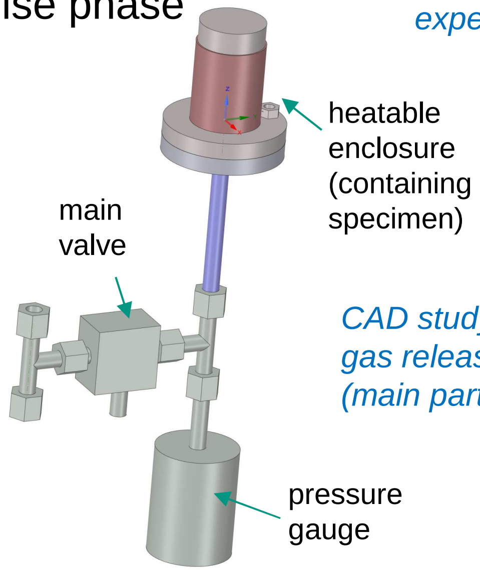
➔ Sieverts' constant can be deduced from final pressure
➔ Diffusion constant can be deduced from pressure rise phase



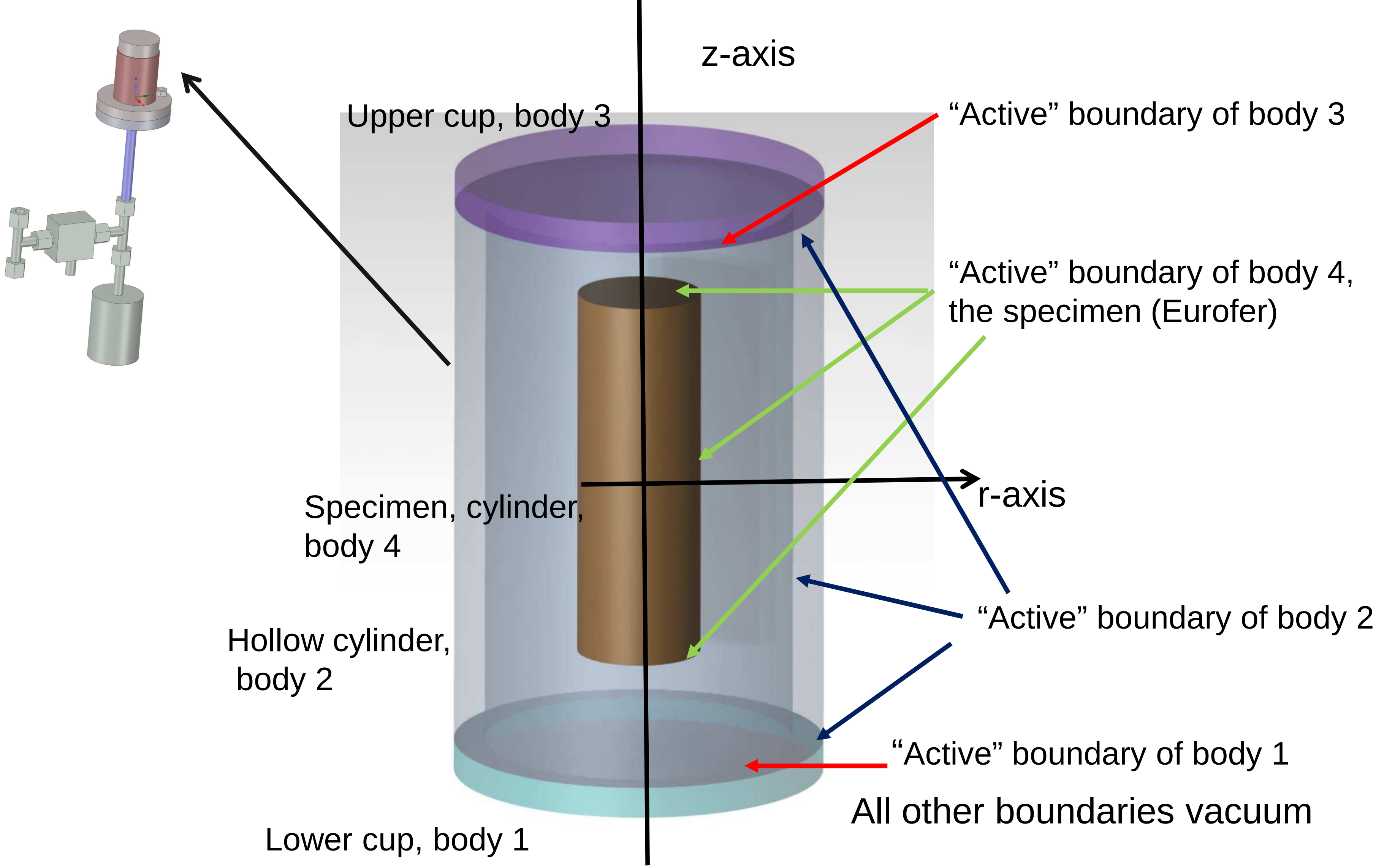
Simplified scheme of gas release experimental setup



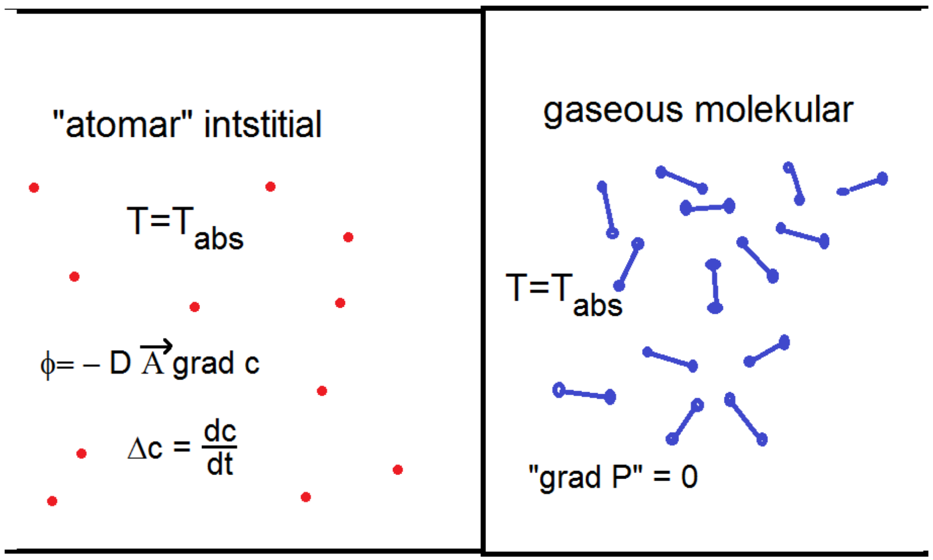


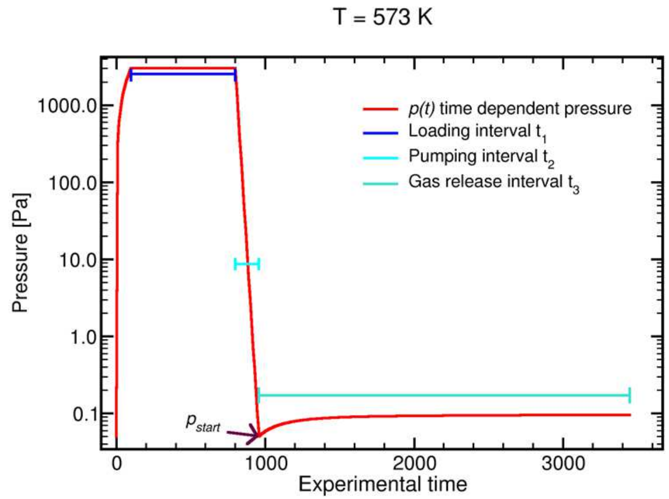
CAD study of gas release setup (main parts)

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



1.: Physical description

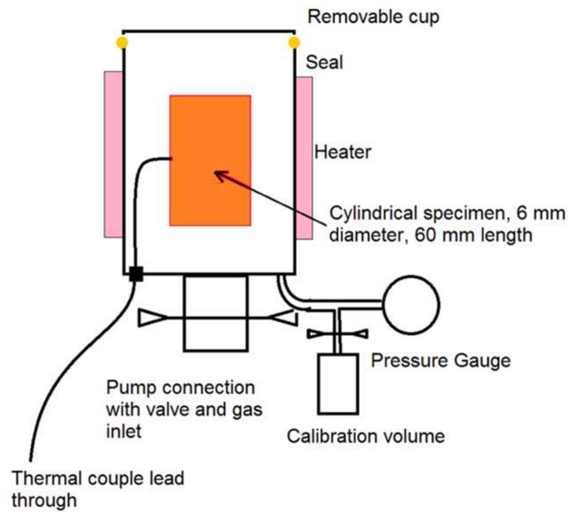




"Velocity" of mass transfer by diffusion constant D

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

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



2.: Simple analytical Solutions

Without re-diffusion, complete outgassing, $c_{sample} = 0$:

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

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

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

$$k_{s,sa} = \frac{2\,(V_c - V_{sa})}{R\,T\,V_{sa}}\,\frac{(p_r - p_{end})}{\sqrt{p_{load}} - \sqrt{p_r}}$$

Experimentally difficult realization of boundaries, no statement about diffusion constant

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

3.: Structure of differential equations:

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

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} + \underbrace{\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}}_{=0}$$

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

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

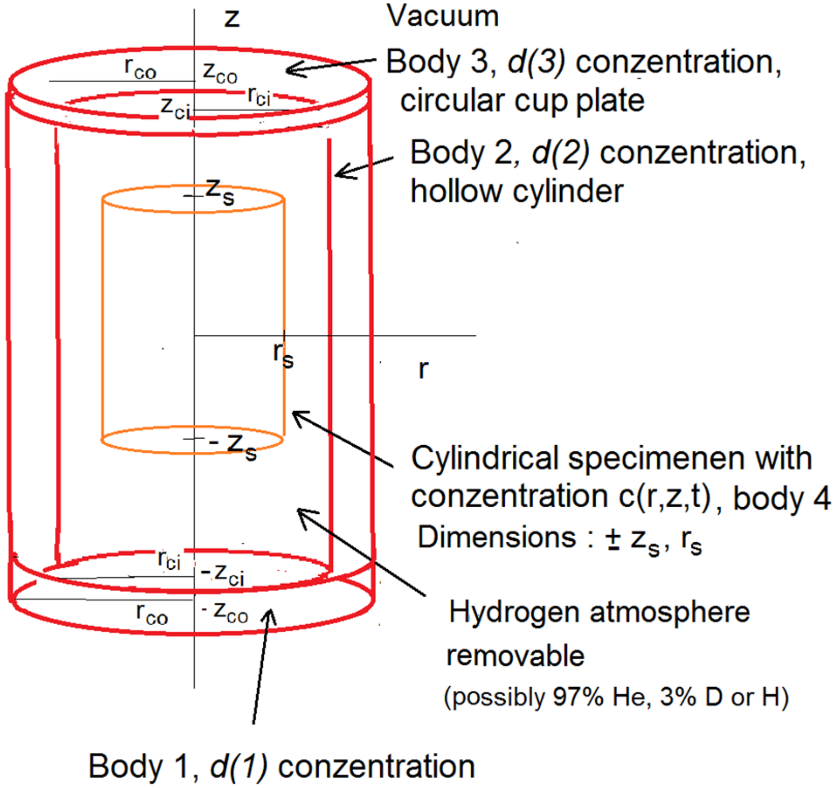
$$d(1)(r \le r_{co}, z = -z_{ci}, \forall t) = k_{s,cu}\sqrt{p(t)}$$

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

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

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

Analytical 1d: Sedano, Perujo (1999), Esteban Douglas (2001) , Eichenauer Pebler (1957) Hattenbach (1961)
Analytical 2d: Eichenauer, Pebler, Witte 1965



3. Structure of differential equations

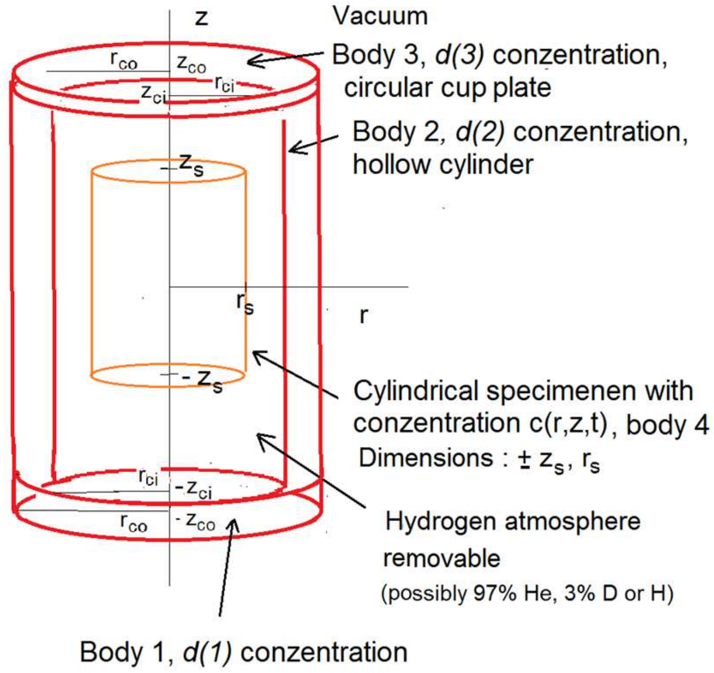
$$\frac{dm}{dt} = -2\,\pi\, D_{sa} \int_0^{r_s} \underbrace{2}_{symmetric}\; r\, \frac{\partial}{\partial z}\, c(r, z = z_s, t)\, dr$$

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

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

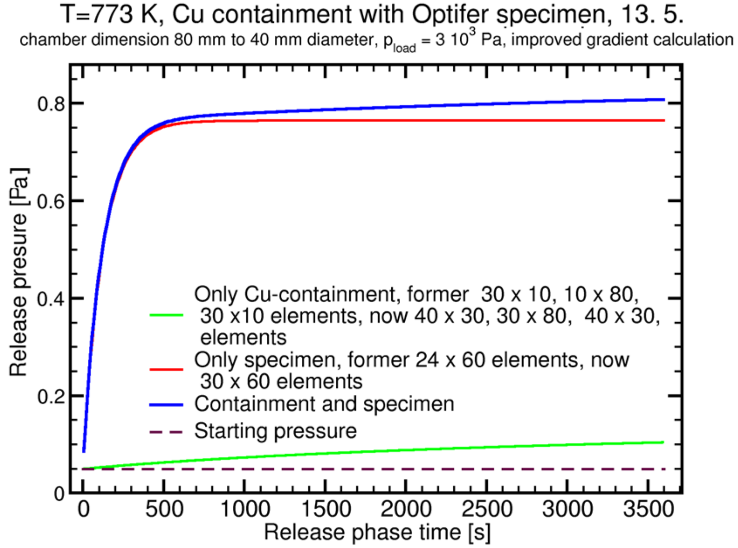
$$- \underbrace{2\,\pi\, r_{ci} D_{cu} \int_{-z_{ci}}^{z_{ci}} \frac{\partial}{\partial r}\, d(2)(r = r_{ci}, z, t)\, dz}_{superficies\ surface\ of\ body\ 2}$$

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

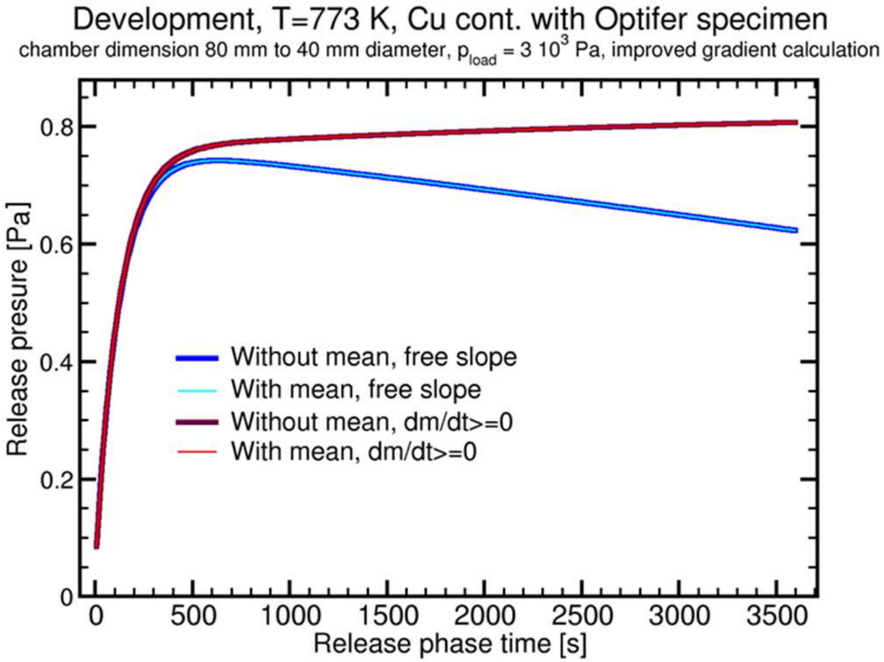


$$p(t) = p_{start} + \underbrace{k_v}_{RT_{abs}/V_{gas}} \int_{t_1+t_2}^{t} \underbrace{0.5}_{gaseous \leftrightarrow interstitial} \frac{dm}{dt}\, dt$$

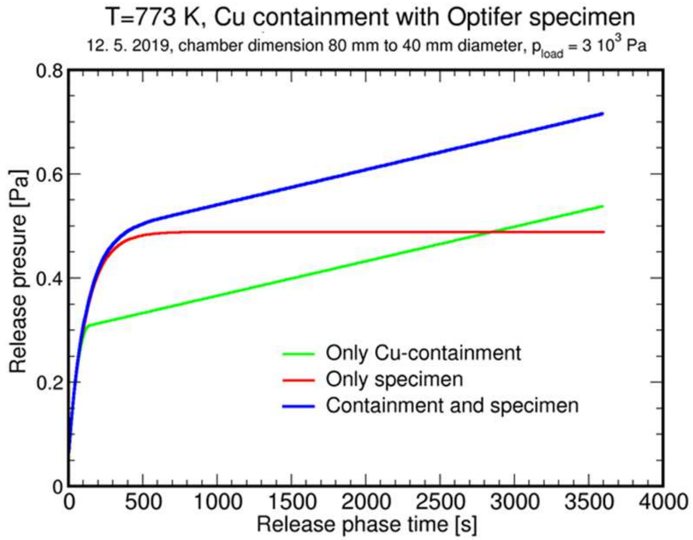
4.: Results of numerical solution



Numerical artefacts

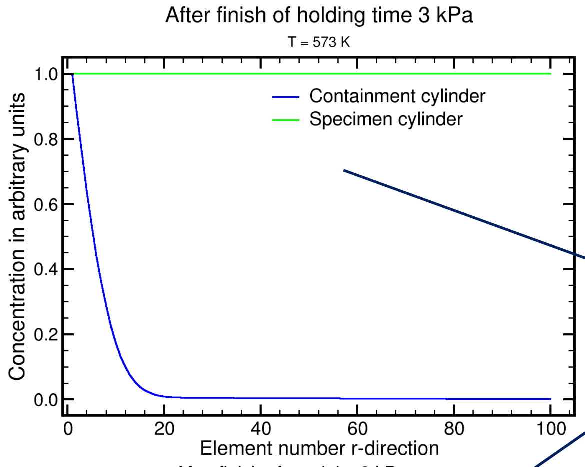


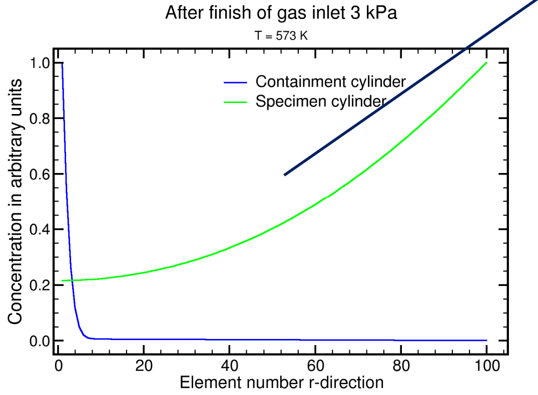
Simple numerical gradient calculation

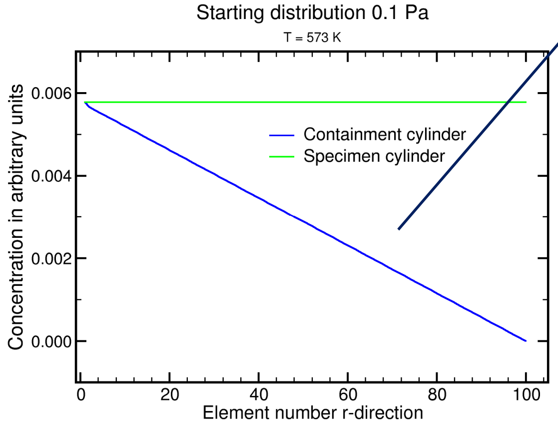


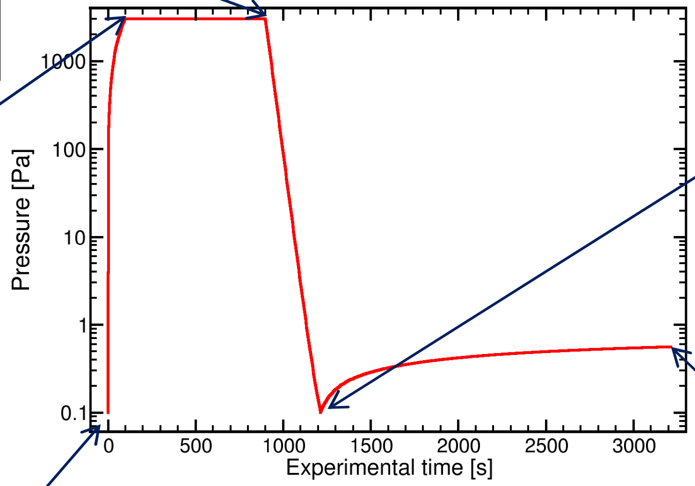
Gas release Experiment:

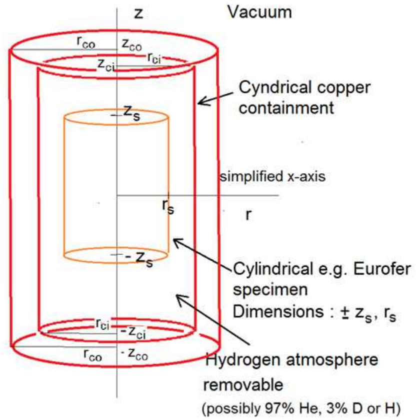
Result of 1D solver r-dependency.

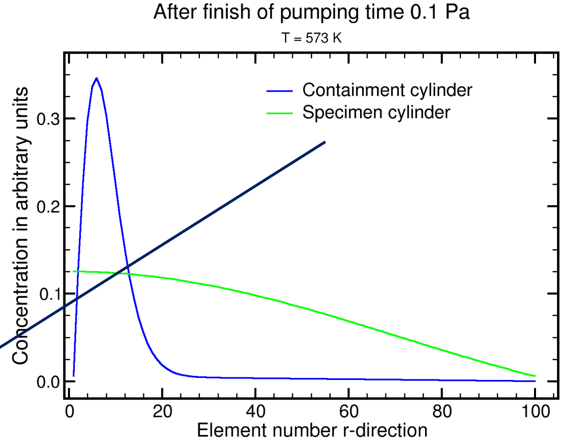


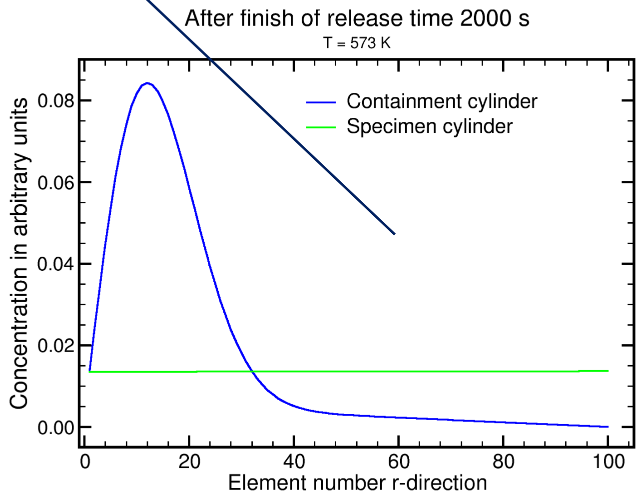


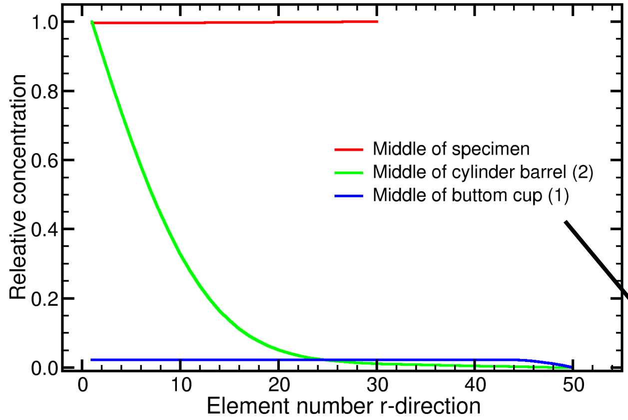




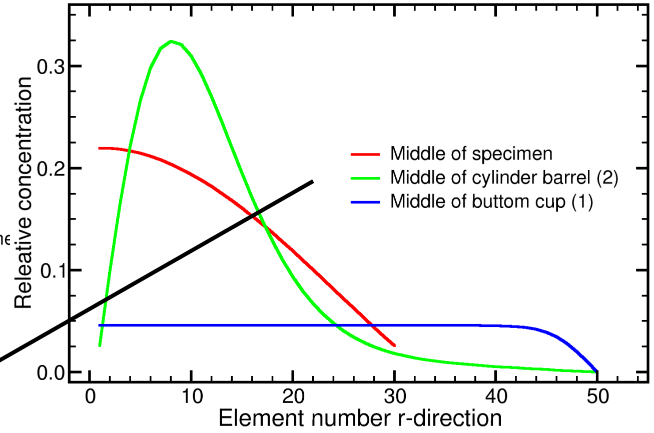


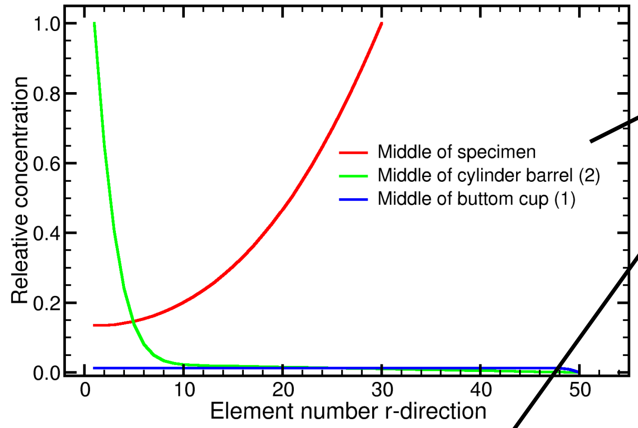


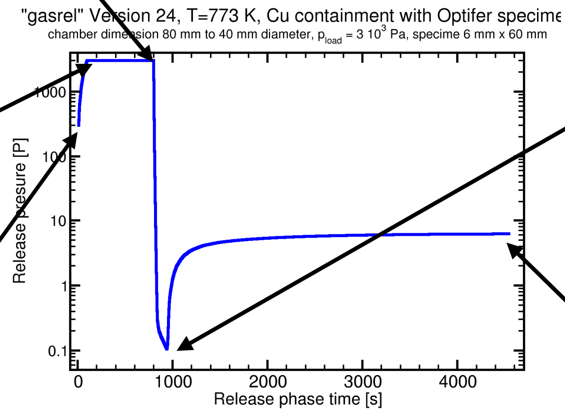


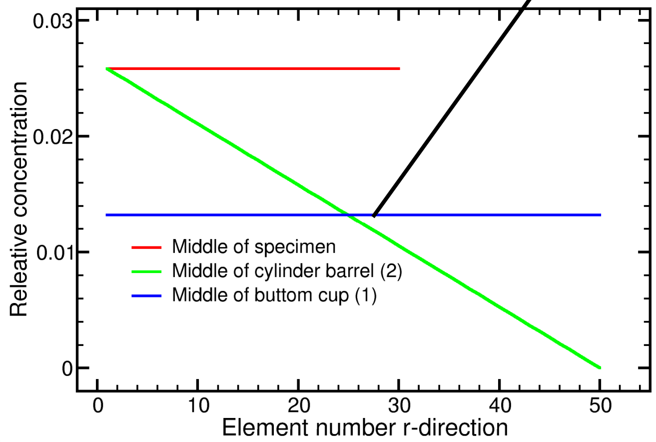


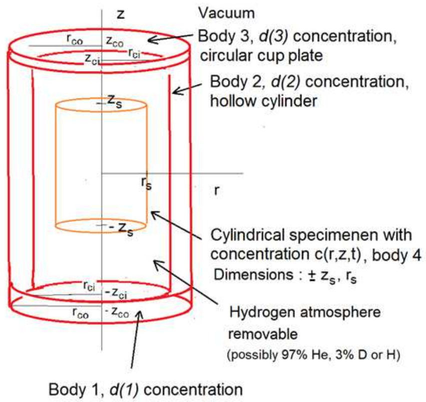
Calculation time 2D
35´, inverse problem
approx. 440 days
Uc1 accuracy ≈ 10 %

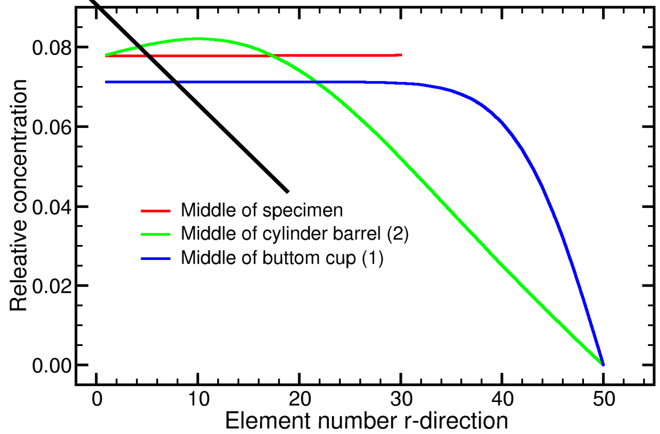




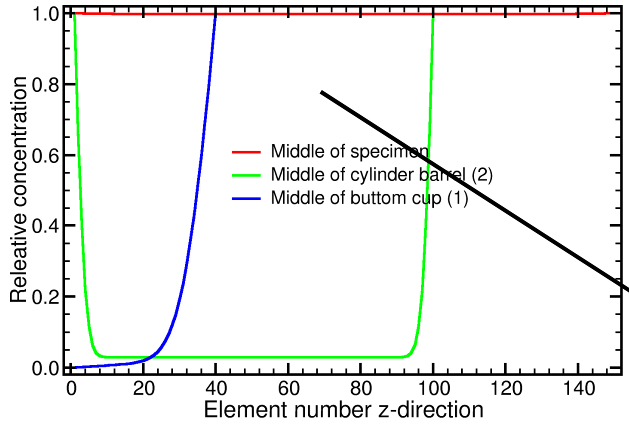


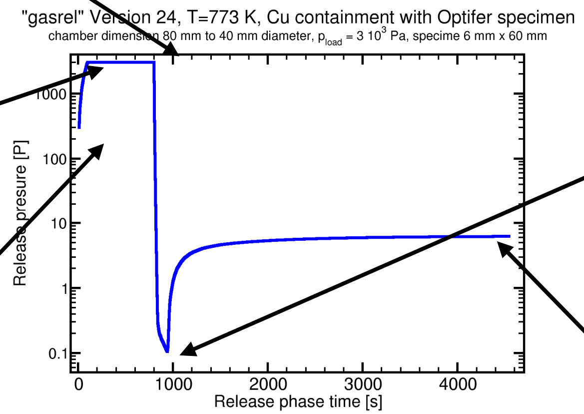


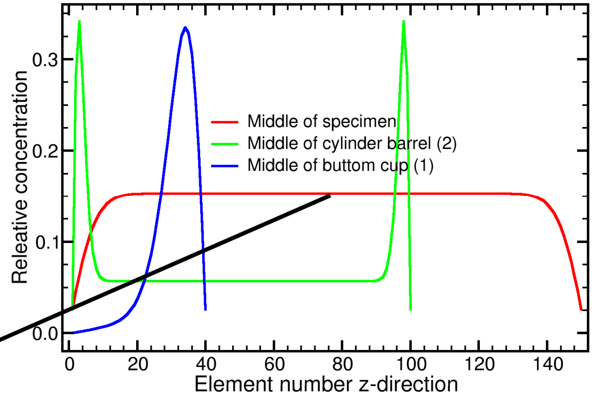


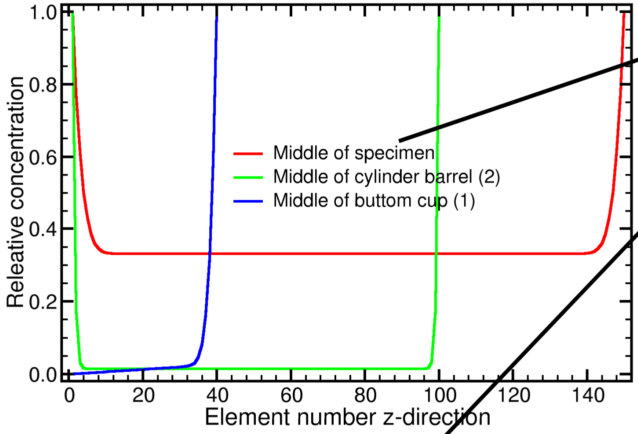


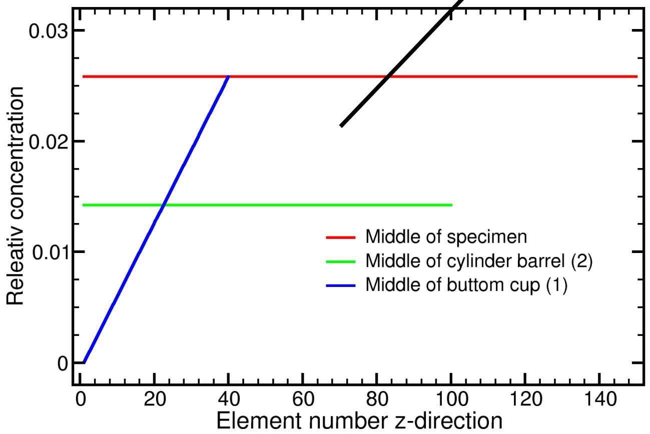
Calculation with 2D Version 24 with 13500 elements



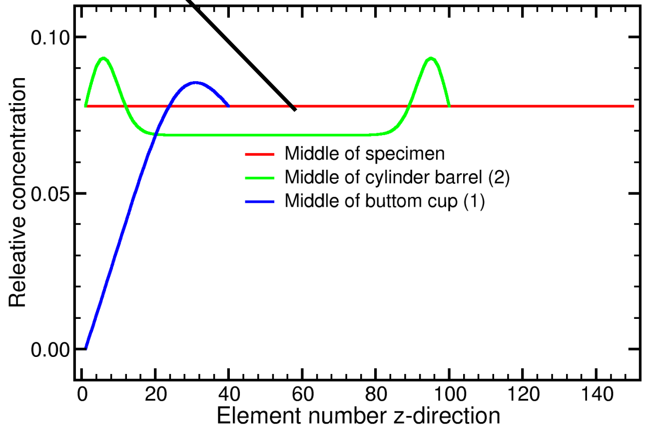








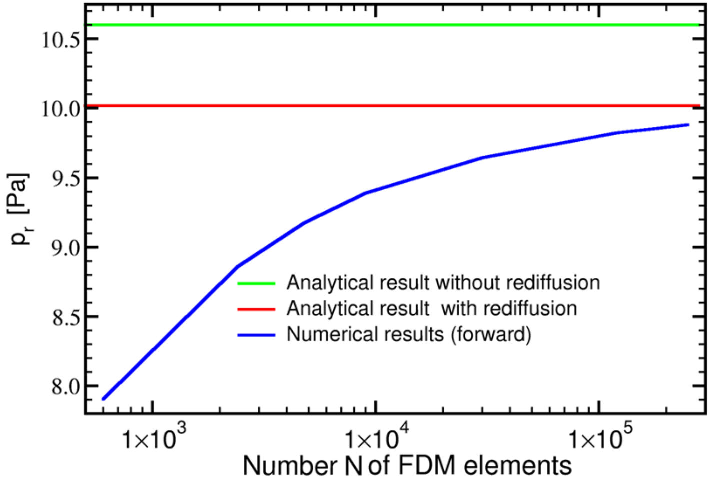
Body	R	Z
Specimen	30	150
1	50	40
2	50	100
3	50	40



Comparison with analytical solution:

Results for chamber 40 mm dia. and 80 mm length, Optifer

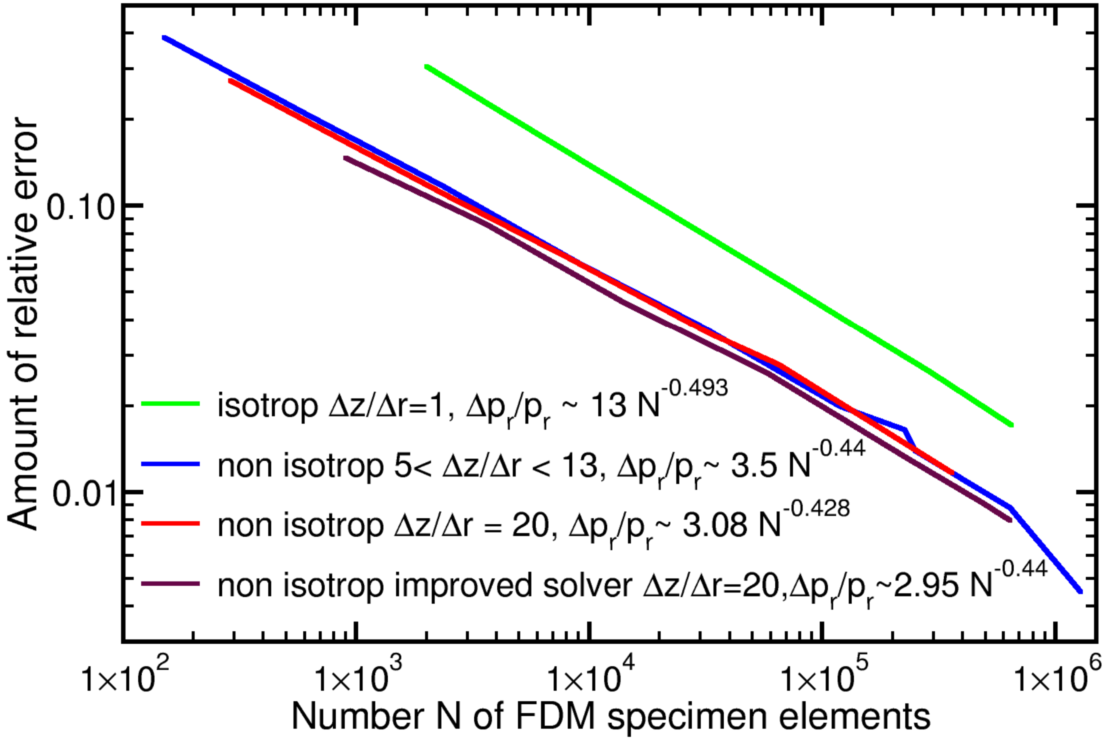
p_{load} = 3 10^3 Pa, integration time checked 1 ms, 0.5 ms, 0.1 ms less than $^1/_{1000}$ deviation



$$10^{-11} < \frac{D_{sa}\Delta t}{\Delta z^2} < 10^{-6}$$

Results for chamber 40/20 mm dia. and 80 mm length, Optifer cylinder 60 mm x 6 mm

p_{load} = 3 10^3 Pa, integration time 1 ms, 0.5 ms, 0.1 ms less than $^1/_{1000}$ deviation



Small excurse to solver algorithms:

1D forward Euler

$$c(i,t+\Delta t) = c(i,t) + \frac{D\,\Delta t}{\Delta r^2}\big(c(i+1,t) + c(i-1,t) - 2c(i,t)\big) + \frac{D\,\Delta t}{2\,r\,\Delta r}\Big(\big(c(i+1,t)\big) - c(i-1,t)\Big)$$

2D improved forward Euler:

$$c(i,j,t+\Delta t) = c(i,j,t) + \frac{D\,\Delta t}{2\,i\,\Delta r^2}\big((2i+1)c(i+1,j,t) + (2i-1)c(i-1,j,t) - (4i)c(i,t)\big) + \frac{D\,\Delta t}{\Delta z^2}\Big(\big(c(i,j+1,t)\big) + c(i,j-1,t) - 2c(i,j)\Big)$$

Desired: Backward Euler solver, e. g. 1D cartesian:

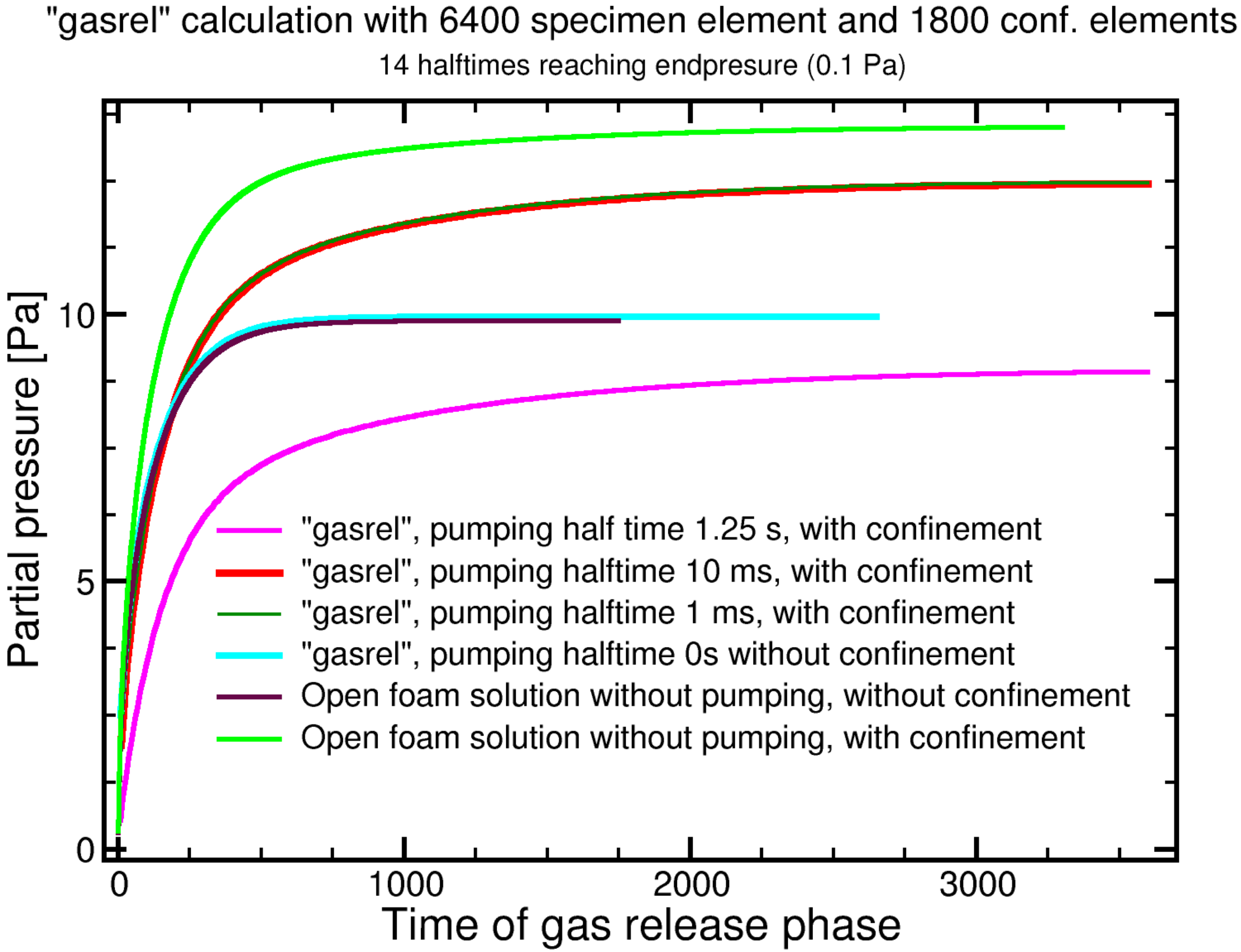
$$\vec{c}_{k+1} = \vec{c}_k + \begin{vmatrix} 0 & & & & & \\ D^* & -2D^* & D^* & & & \\ & D^* & -2D^* & D^* & & \\ & & D^* & -2D^* & D^* & \\ & & & \ddots & & \\ & & & D^* & -2D^* & D^* \\ & & & & & 0 \end{vmatrix} \vec{c}_{k+1}$$

$$D^* = \frac{D\,\Delta t}{\Delta x^2}$$

$$\vec{c}_{k+1} = \begin{vmatrix} 1 & & & & & \\ -D^* & 1+2D^* & -D^* & & & \\ & -D^* & 1+2D^* & -D^* & & \\ & & -D^* & 1+2D^* & -D^* & \\ & & & -D^* & 1+2D^* & -D^* \\ & & & & \ddots & \\ & & & -D^* & 1+2D^* & -D^* \\ & & & & & 1 \end{vmatrix}^{-1} \vec{c}_k$$

2D n x n x m tensor ?

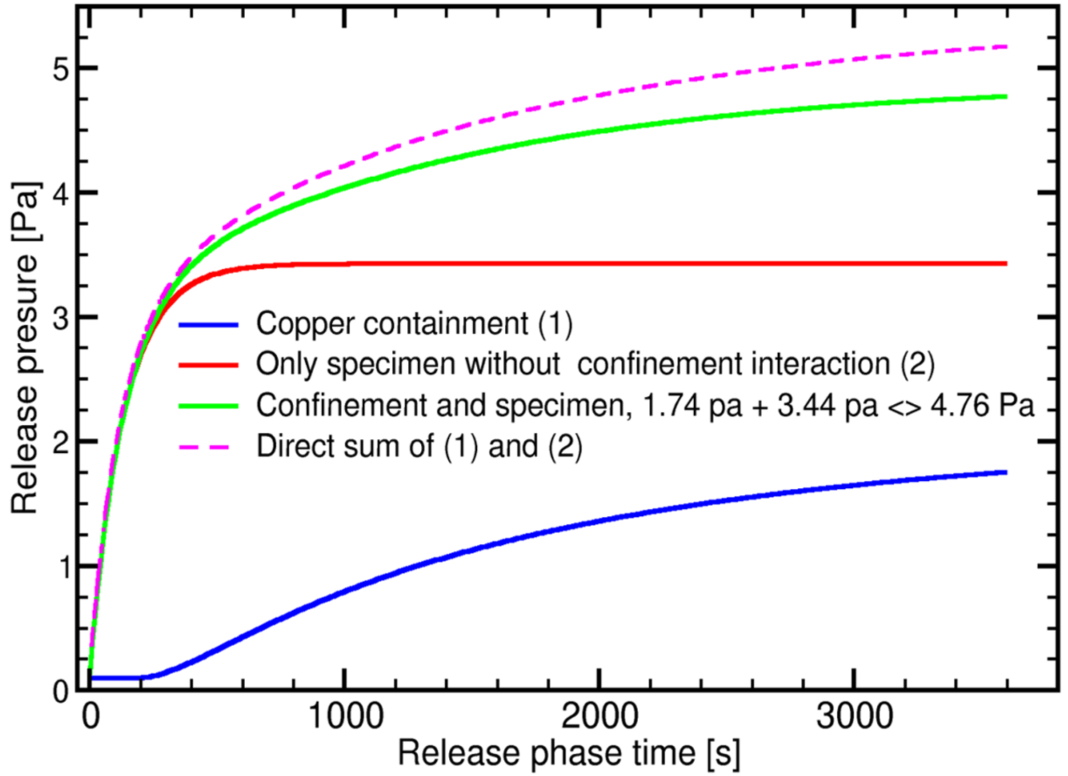
4.: Results



"gasrel" calculation with 6400 specimen element and 1800 conf. elements
14 halftimes reaching endpresure (0.1 Pa)
Partial pressure [Pa]
Time of gas release phase
0
5
10
0
1000
2000
3000
"gasrel", pumping half time 1.25 s, with confinement
"gasrel", pumping halftime 10 ms, with confinement
"gasrel", pumping halftime 1 ms, with confinement
"gasrel", pumping halftime 0s without confinement
Open foam solution without pumping, without confinement
Open foam solution without pumping, with confinement

T=773 K, Cu containment with Optifer specimen

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



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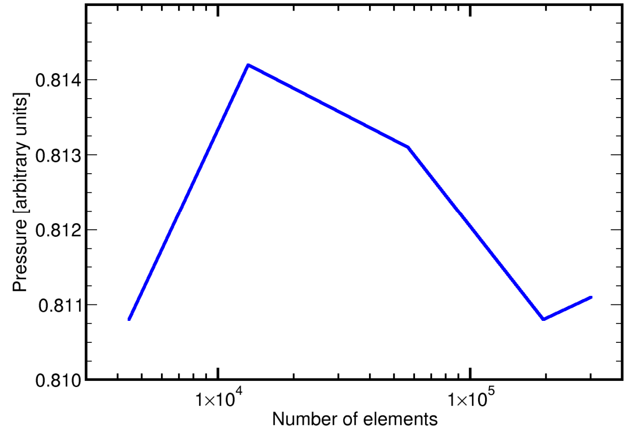
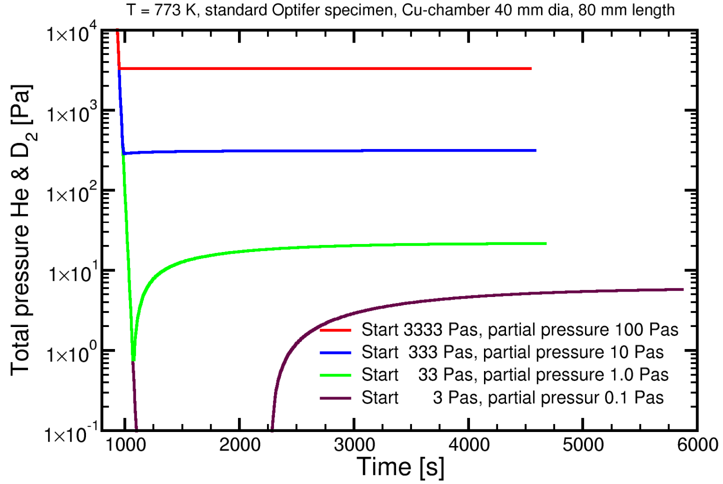


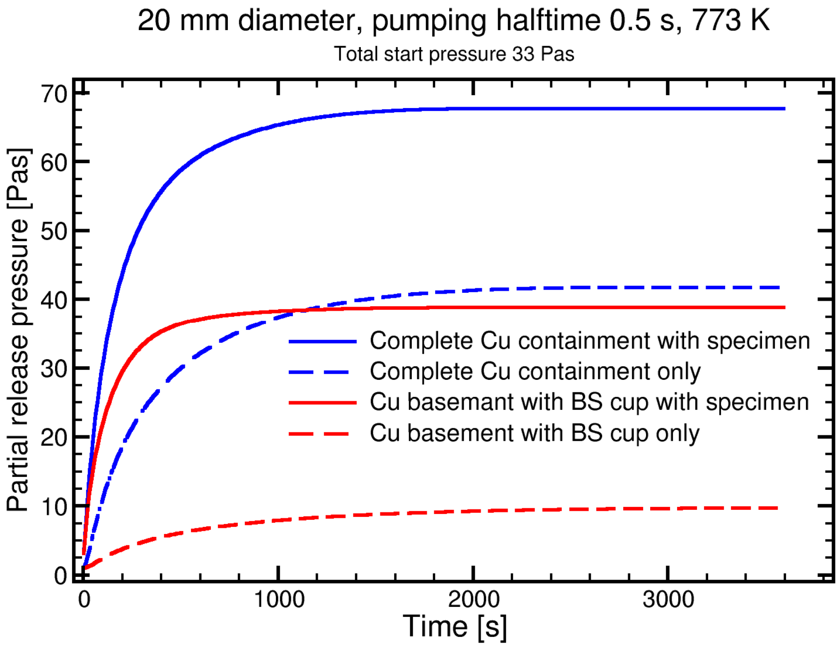
Choosing starting pressure:

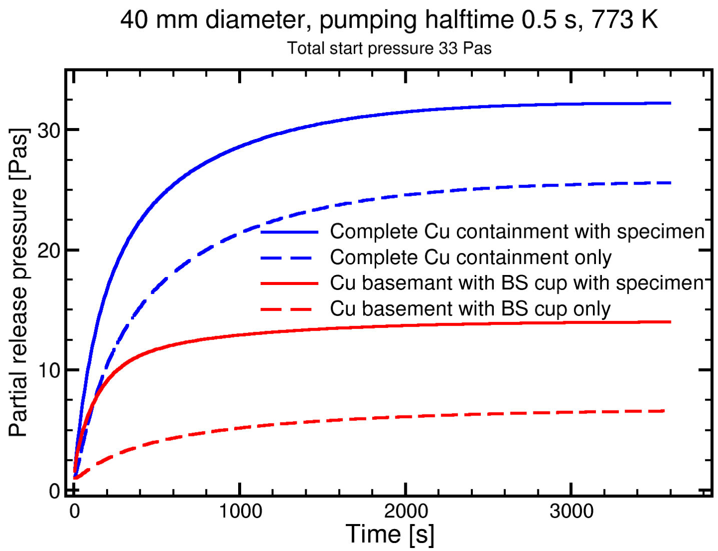
Weak pump, half time 10 s, total pressure 10^5 Pas, 3 % D_2

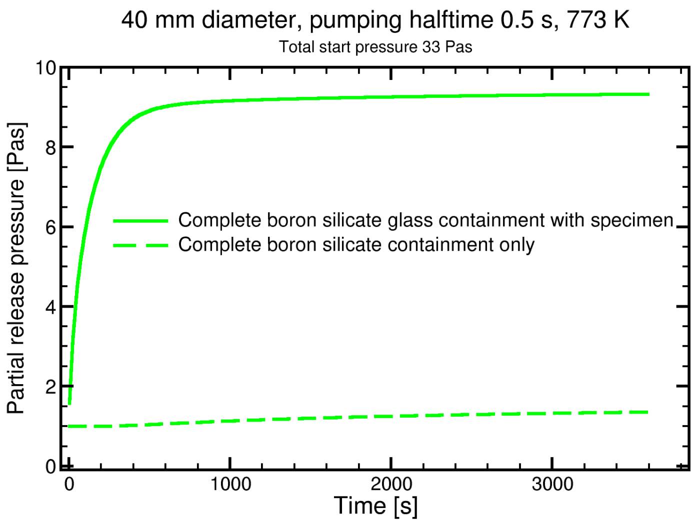
T = 773 K, standard Optifer specimen, Cu-chamber 40 mm dia, 80 mm length

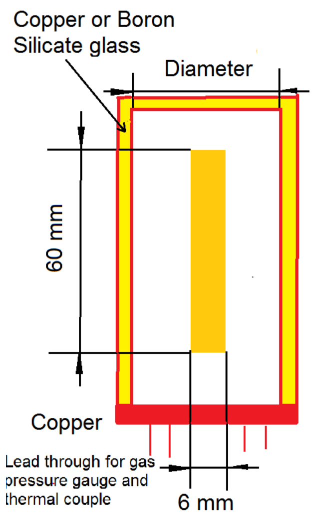


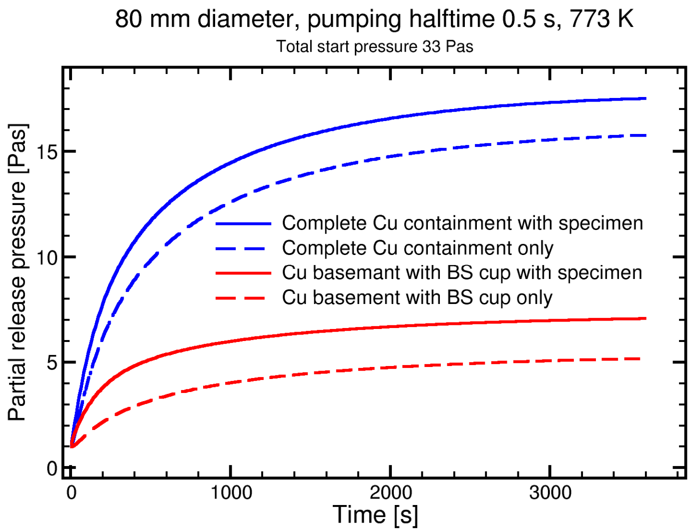
Results for conception of experiments











5.: Outlook to analytical solution

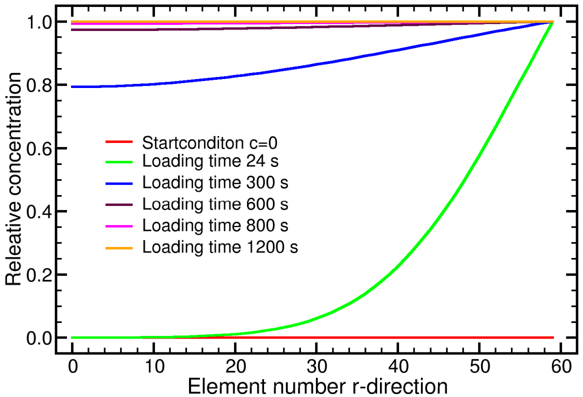
Solution in the charging interval

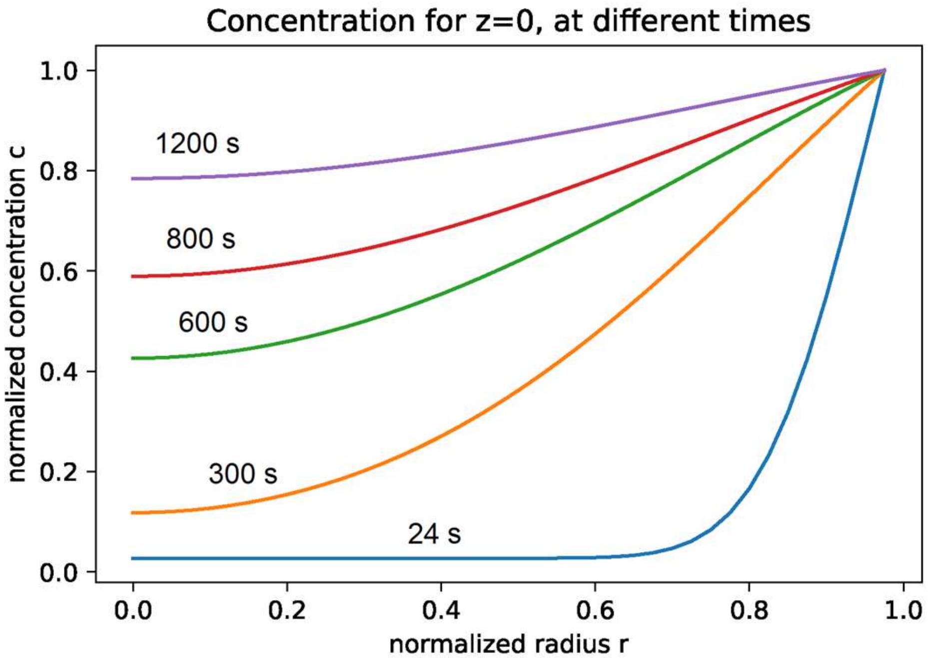
$$c(r,z,t) = k_{s,sa}\sqrt{p_{load}}\sum_{n,m}\frac{8(-1)^{n+1}}{\pi(2n+1)x_m J_1(x_m)}\exp\left(-\gamma_{n,m}^2 t\right)\cos\left((2n+1)\frac{\pi}{2}z\right)J_0(x_m r)$$

where

$$\gamma_{n,m}^2 = D_{sa}\left(\frac{x_m^2}{r_s^2}+\frac{(2n+1)^2\pi^2}{4z_s^2}\right),$$ $J_\alpha(x)$ (α=0,1) Bessel functions of the first kind,

x_m the m-th roots of $J_0(x)$.





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NUMERICAL ANALYSIS OF AN ISOVOLUMETRIC THERMAL DESORPTION EXPERIMENT

A. von der Weth, K. Nagatou,
F. Arbeiter, R. Dagan, D. Klimenko, V. Pasler, M. Schulz,
INR, KIT, CN, Athens, 25th June, 2019

IKIT/INR/MET (Maschinenbau)

1.: Description of setup
2.: Simple analytical solutions
3.: Structure of Differential Equations
4.: Results of numerical optimization
5.: Outlook to analytical solution

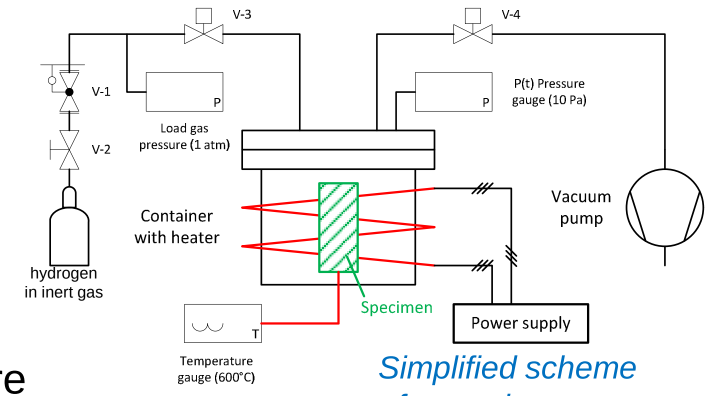
E-mail: axel.vonderWeth@kit.edu

Reminder: gas release diffusion experiments

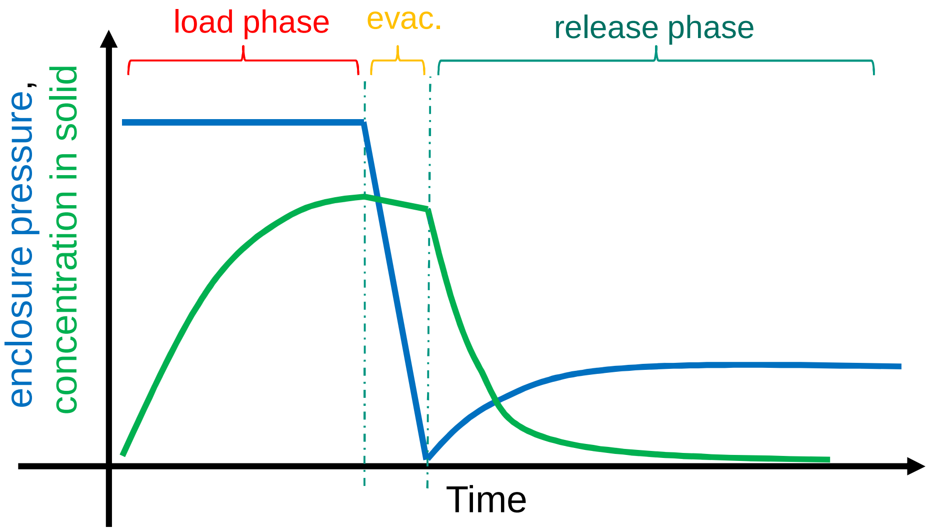
KIT Karlsruher Institut für Technologie

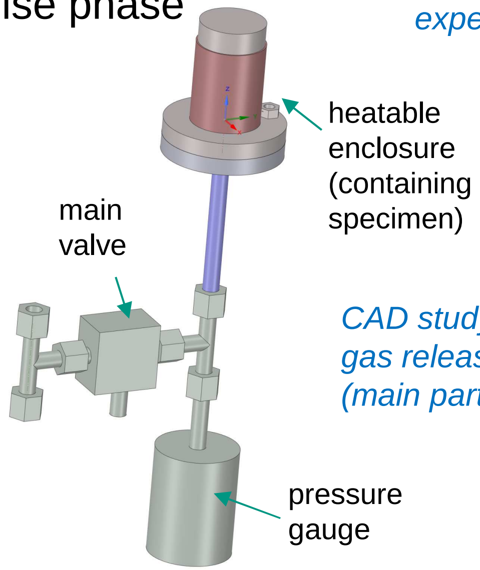
Procedure:
1. Specimen placed in defined volume enclusure
2. Load specimen with hydrogen at defined conditions (T, p_{H2})
3. Swiftly evacuate gases from enclosure
4. Measure pressure increase p(t) in enclosure

➔ Sieverts' constant can be deduced from final pressure
➔ Diffusion constant can be deduced from pressure rise phase



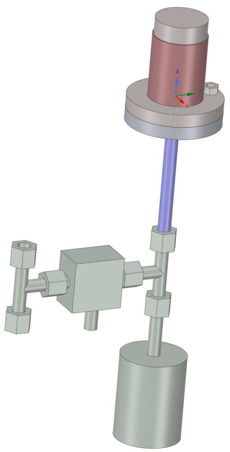
Simplified scheme of gas release experimental setup

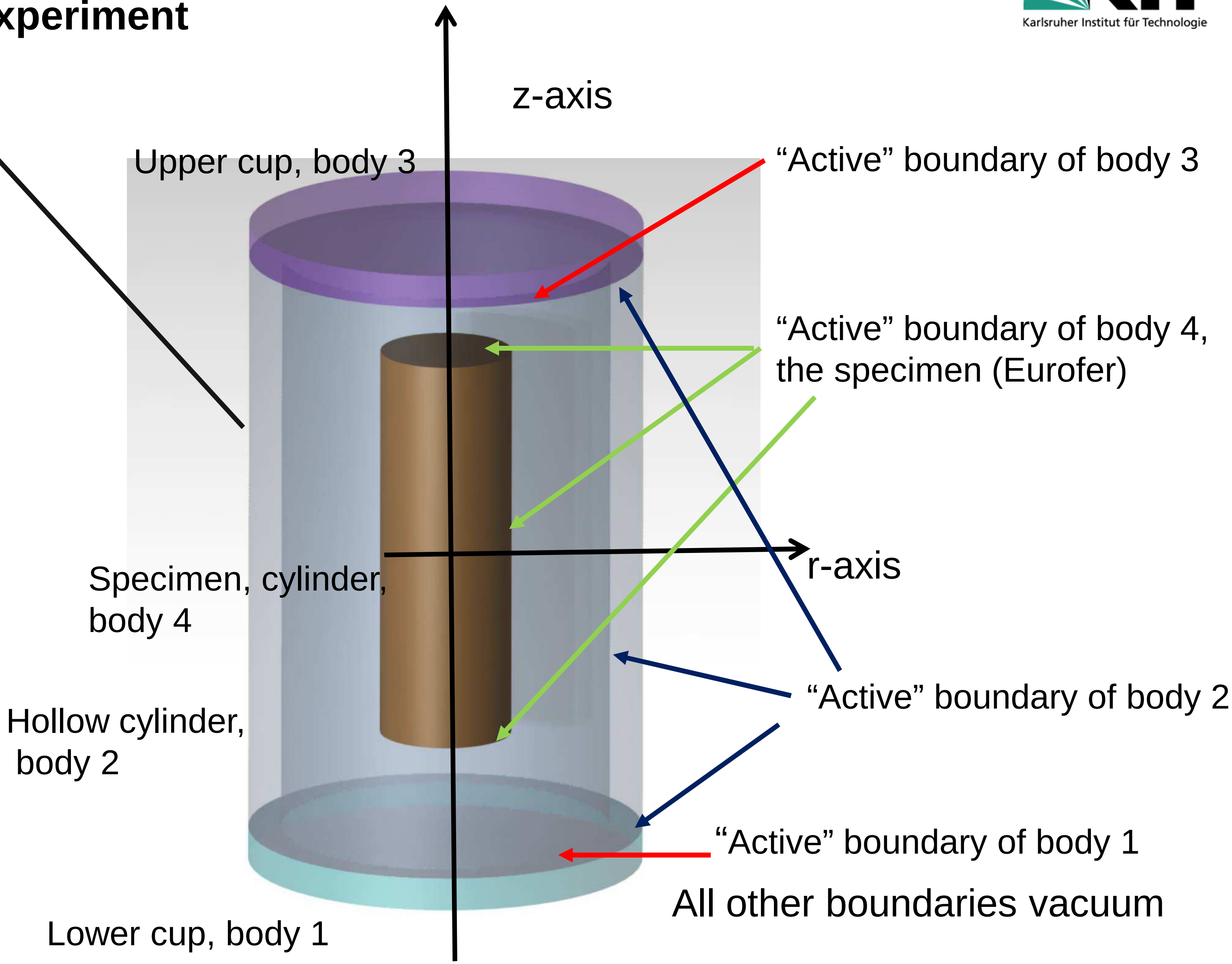




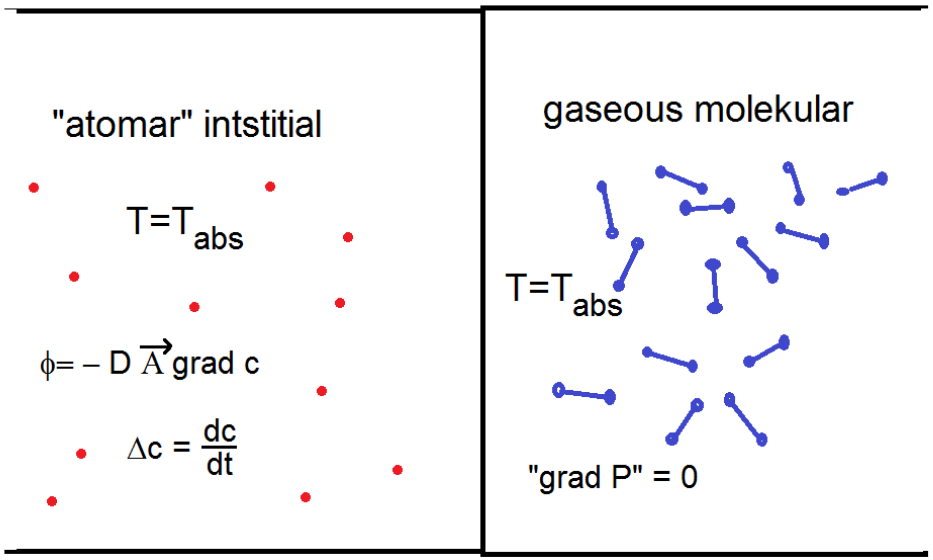
CAD study of gas release setup (main parts)

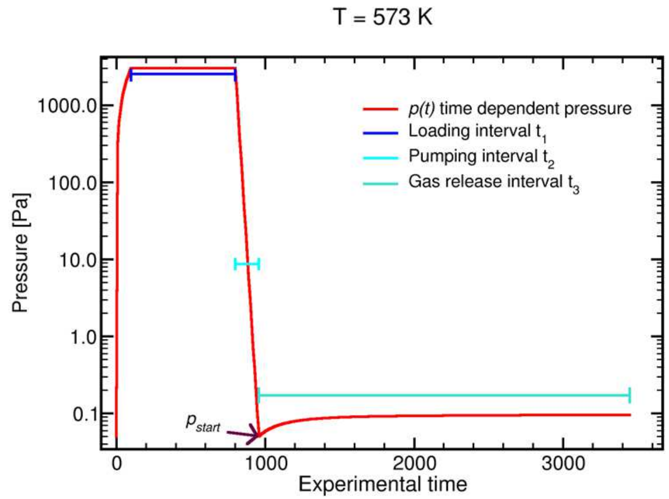
1.: Description of setup of an Isovoluminetric Thermal Desorption Experiment





1.: Physical description

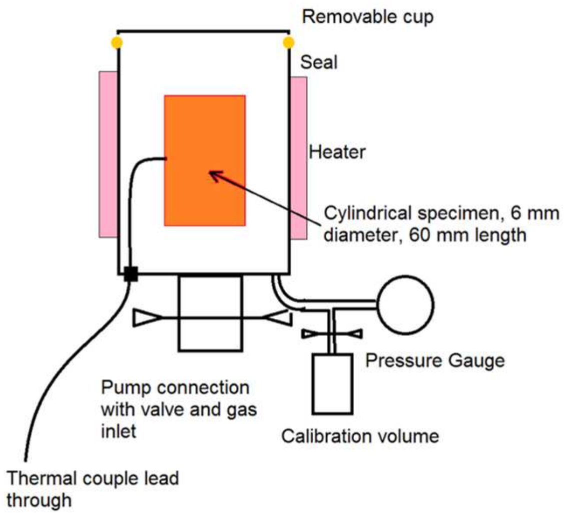




“Velocity” of mass transfer by diffusion constant D

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

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



2.: Simple analytical Solutions

Without re-diffusion, complete outgassing, $c_{sample} = 0$:

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

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

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

$$k_{s,sa} = \frac{2\,(V_c - V_{sa})}{R\,T\,V_{sa}}\,\frac{(p_r - p_{end})}{\sqrt{p_{load}} - \sqrt{p_r}}$$

Experimentally difficult realization of boundaries, no statement about diffusion constant

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

3.: Structure of differential equations:

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

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} + \underbrace{\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}}_{=0}$$

Analytical 1d: Sedano, Perujo (1999), Esteban Douglas (2001) , Eichenauer Pebler (1957) Hattenbach (1961)
Analytical 2d: Eichenauer, Pebler, Witte 1965

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

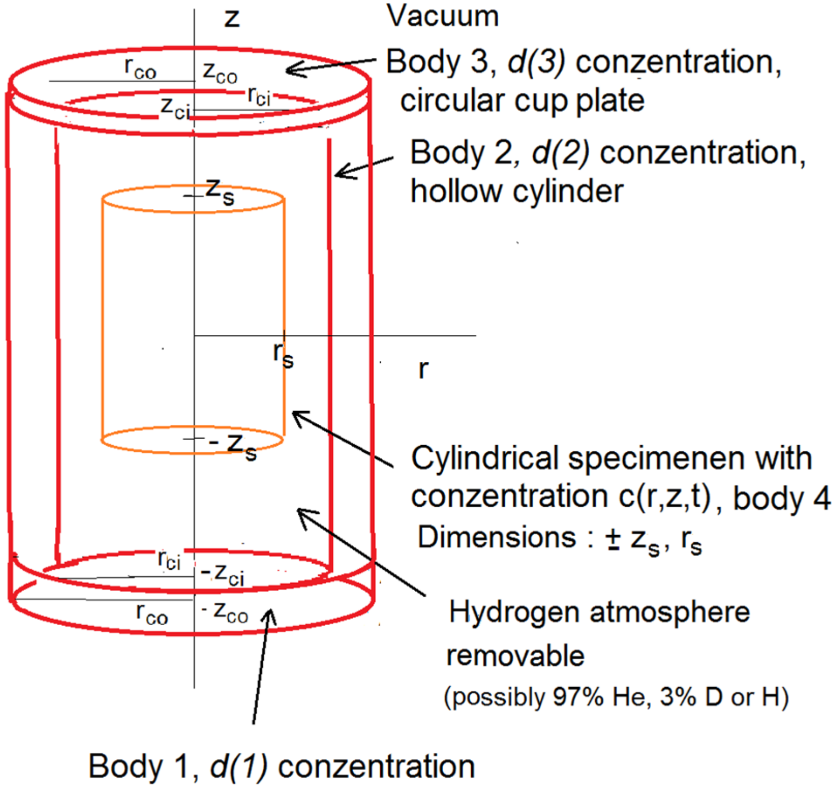
$$\mathrm{c}(r = r_s, |z| \le z_s, \forall t) = k_{s,sa}\sqrt{p(t)}$$

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

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

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

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



3. Structure of differential equations

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

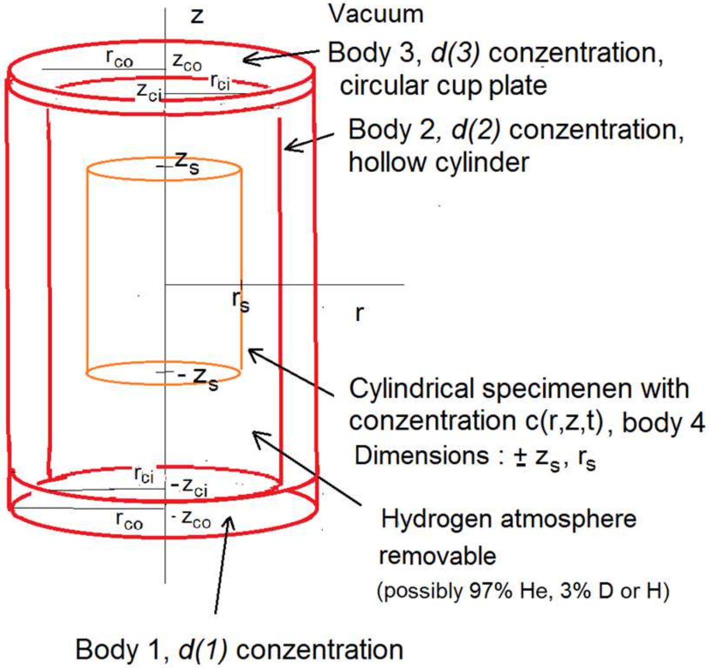
$$-\;\underbrace{2\,\pi\,r_s D_{sa}\int_{-z_s}^{z_s}\frac{\partial}{\partial r}\,c(r = r_s, z, t)\,dz}_{superficies\ surface\ of\ specimen}$$

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

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

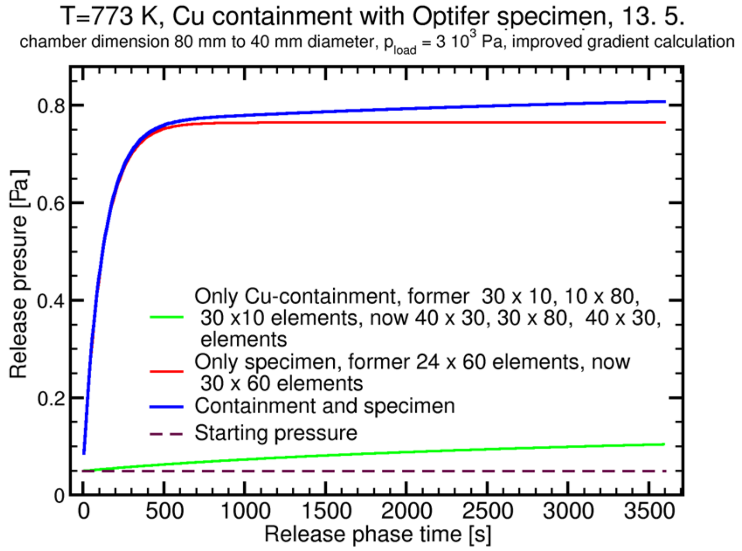
$superficies\ surface\ of\ body\ 2$

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

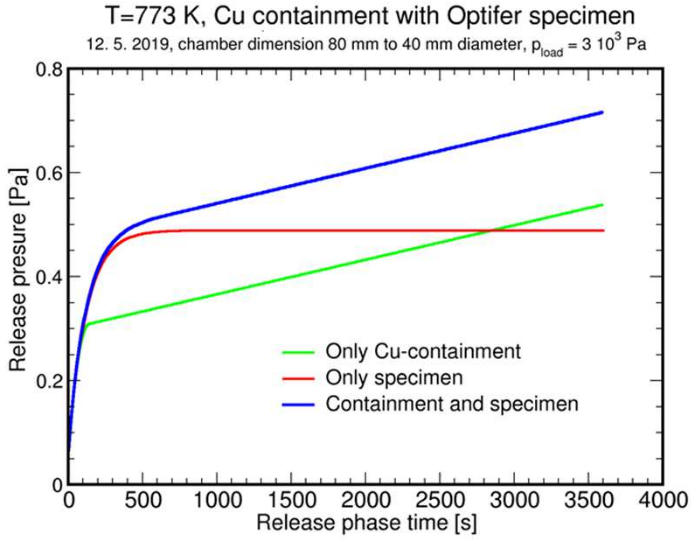


$$p(t) = p_{start} + \underbrace{k_v}_{RT_{abs}/V_{gas}} \int_{t_1+t_2}^{t} \underbrace{0.5}_{gaseous\leftrightarrow interstitial}\;\frac{dm}{dt}\,dt$$

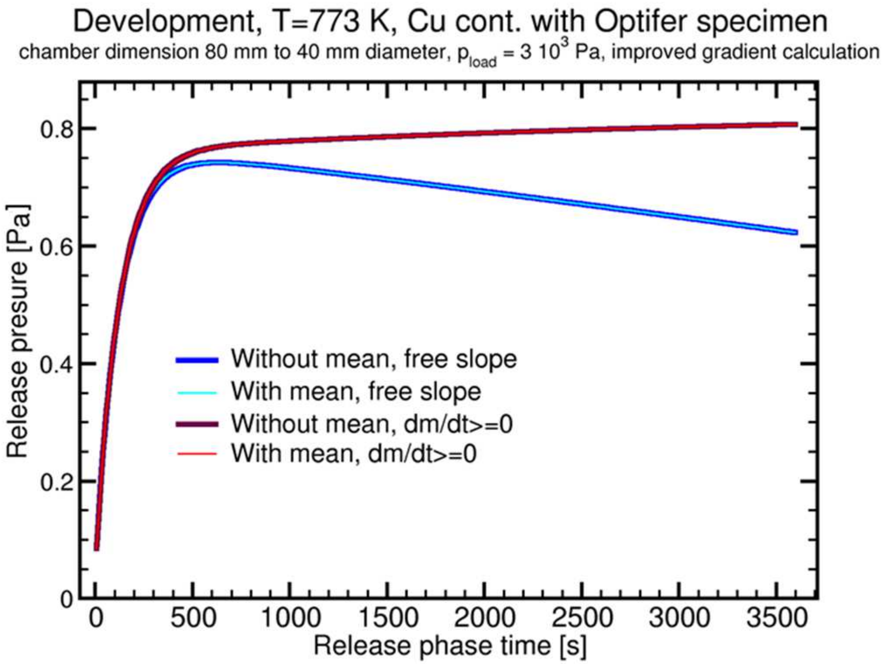
4.: Results of numerical solution



Simple numerical gradient calculation

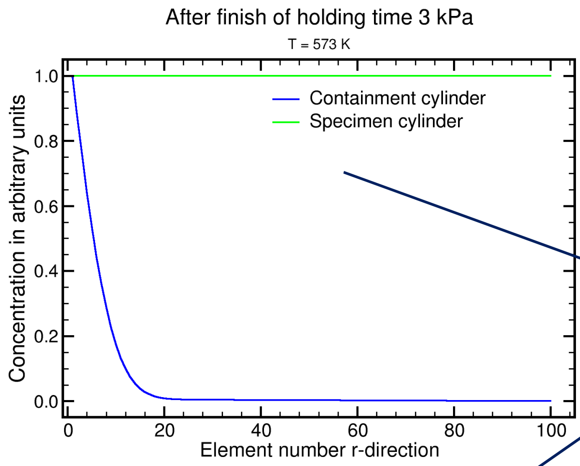


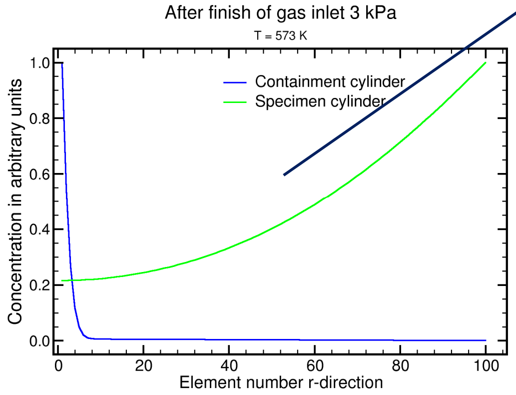
Numerical artefacts

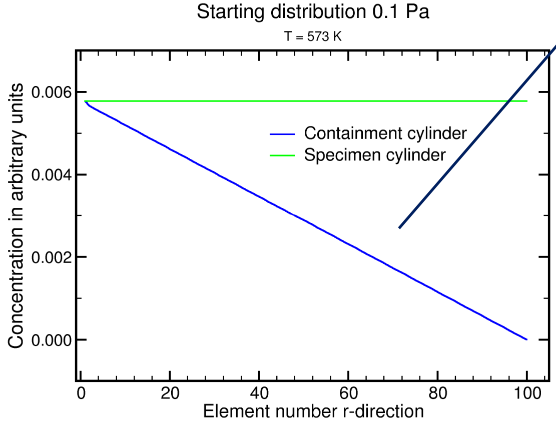


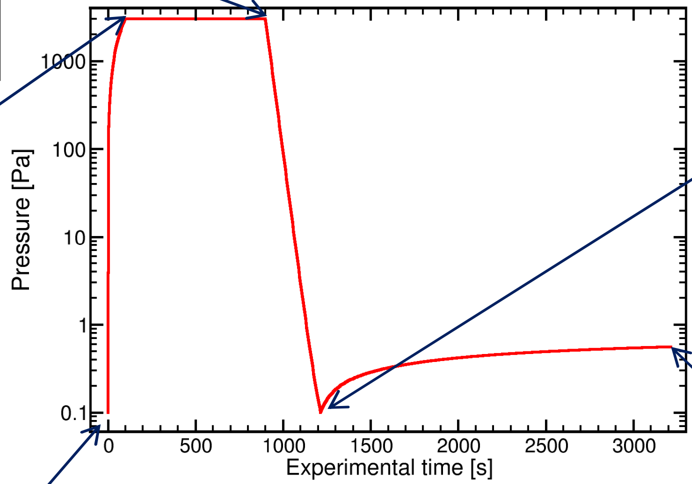
Gas release Experiment:

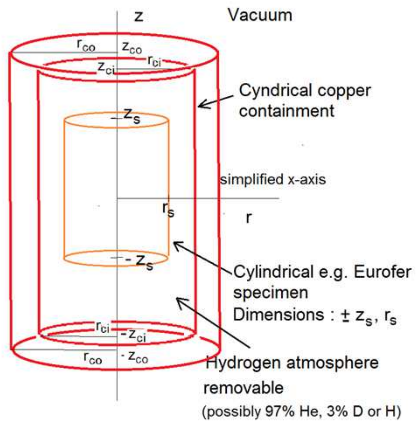
Result of 1D solver r-dependency.

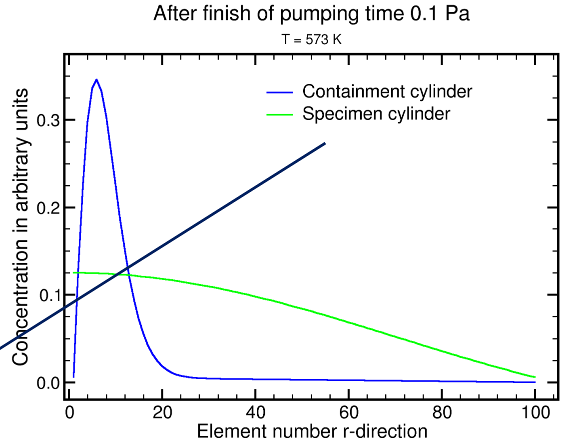


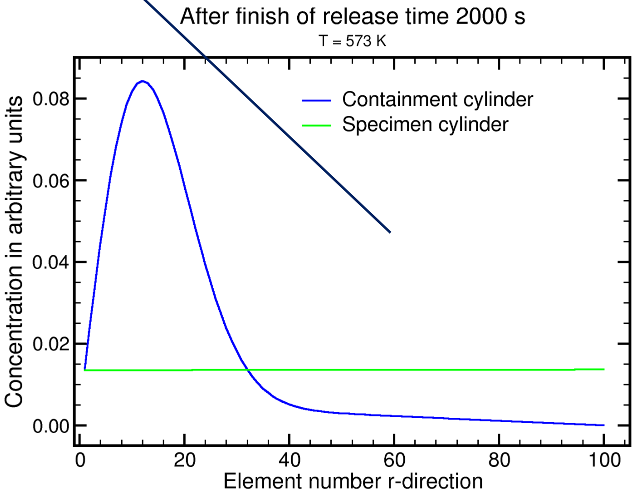




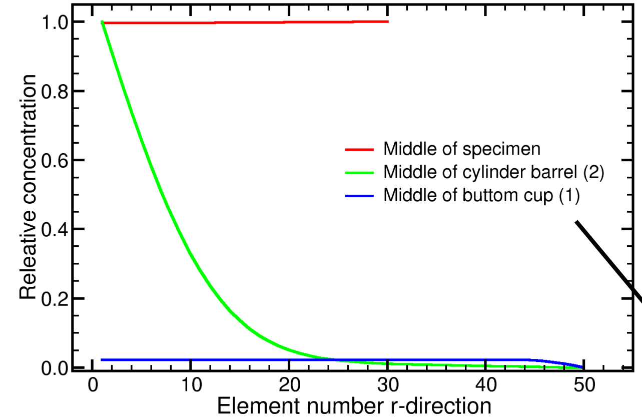


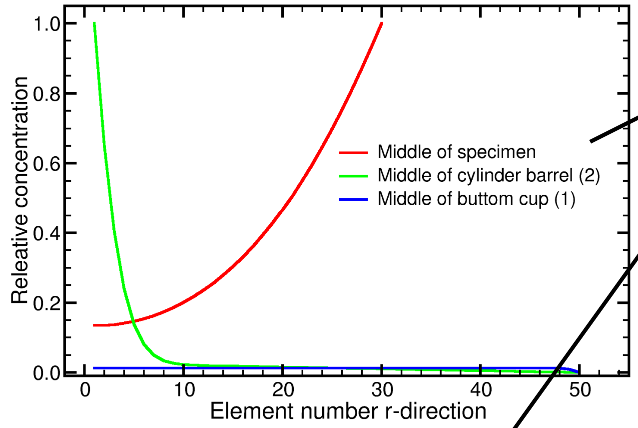


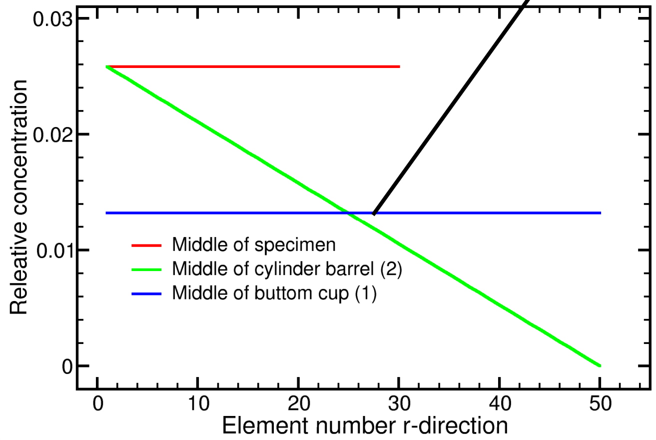


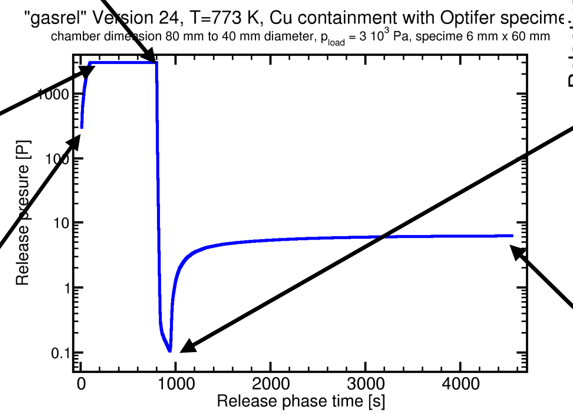


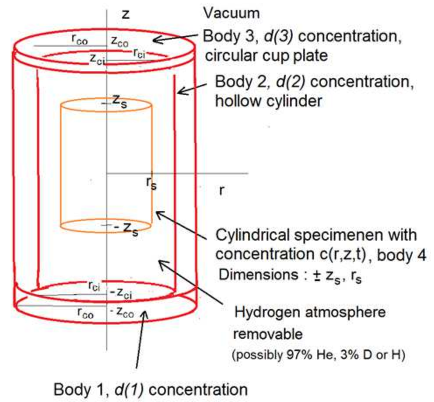
Calculation time 2D
35´, inverse problem
approx. 440 days
Uc1 accuracy ≈ 10 %

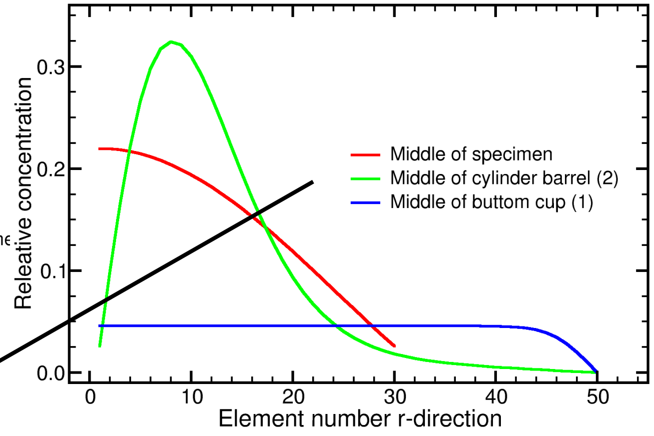


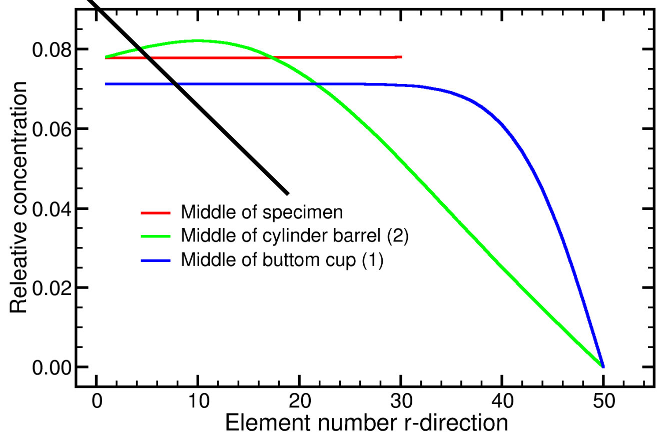




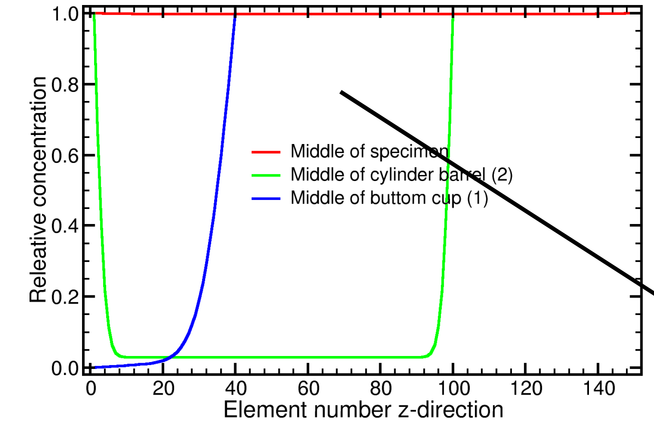


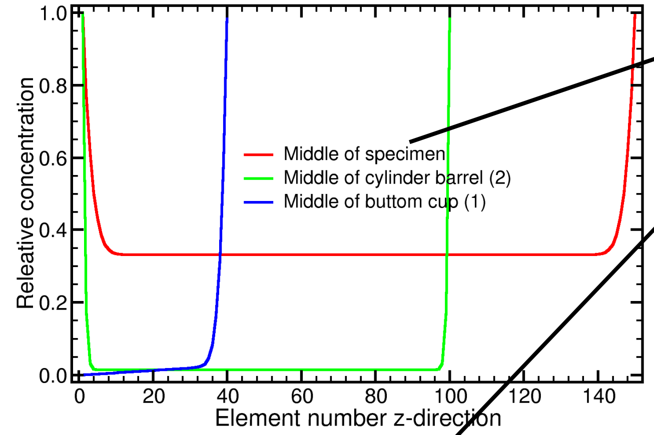


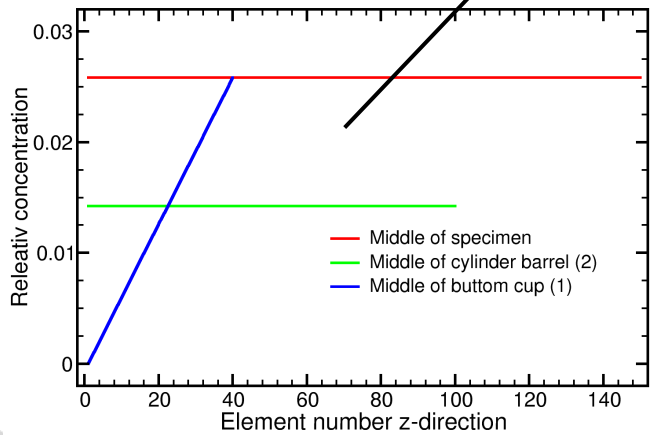


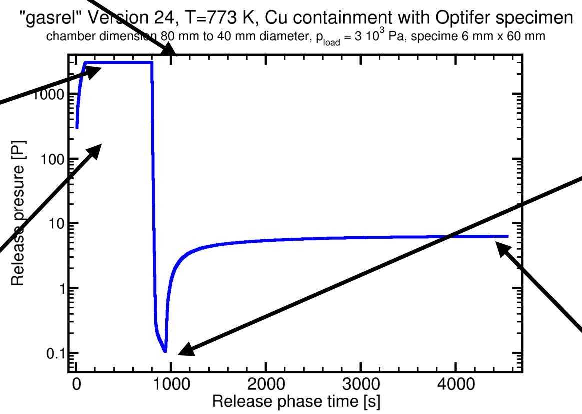


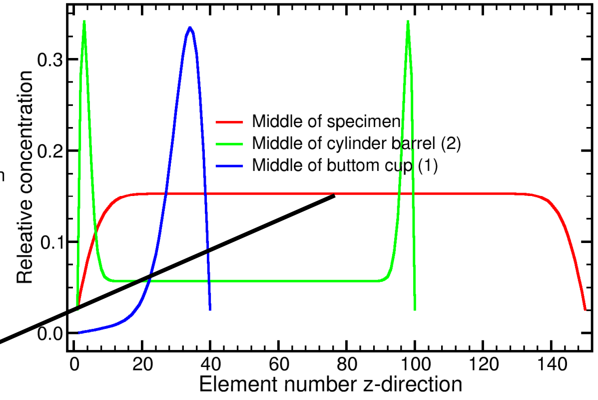
Calculation with 2D Version 24 with 13500 elements

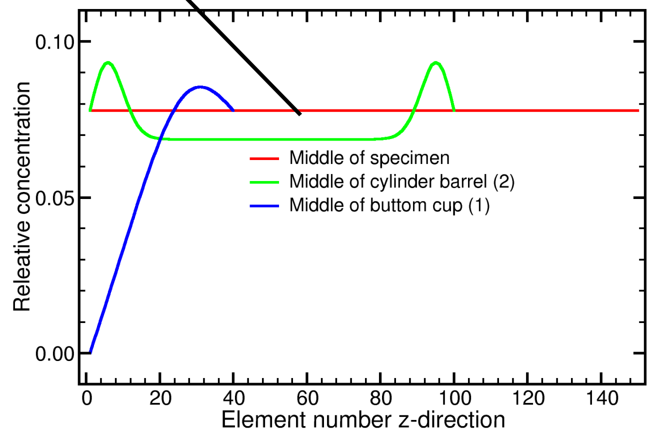






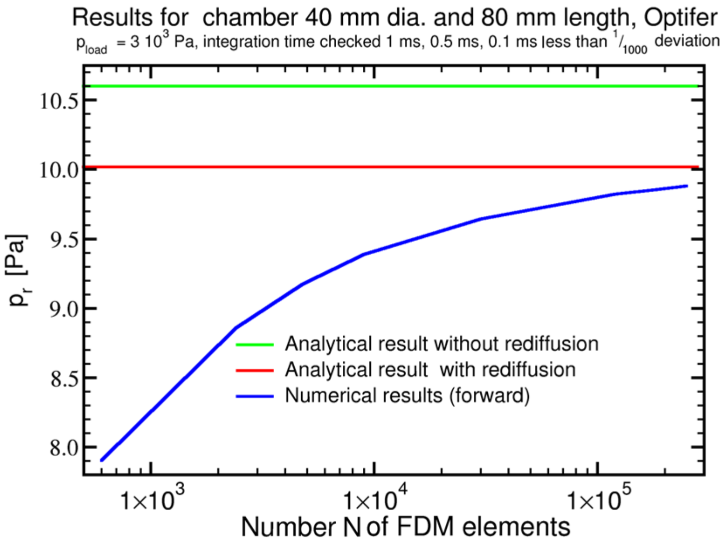




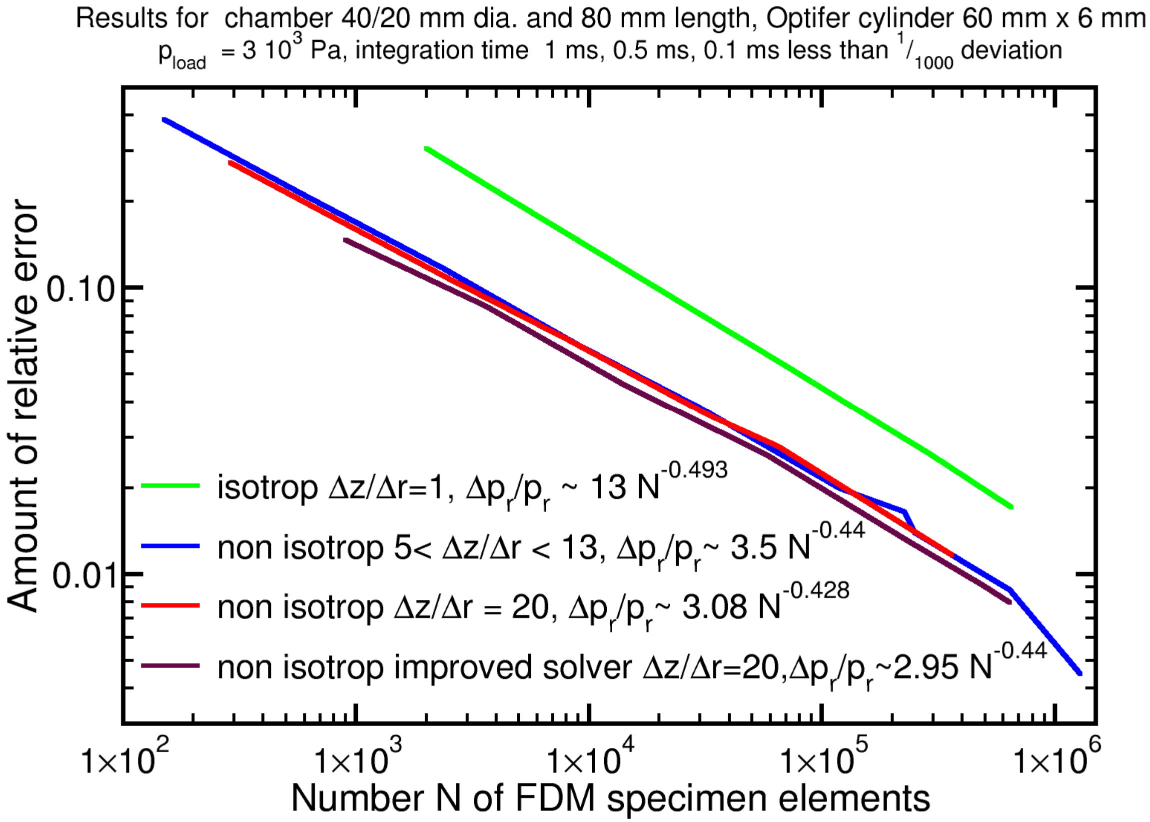


Body	R	Z
Specimen	30	150
1	50	40
2	50	100
3	50	40

Comparison with analytical solution:



$$10^{-11} < \frac{D_{sa}\Delta t}{\Delta z^2} < 10^{-6}$$



Small excurse to solver algorithms:

1D forward Euler

$$c(i,t+\Delta t) = c(i,t) + \frac{D\,\Delta t}{\Delta r^2}\left(c(i+1,t) + c(i-1,t) - 2c(i,t)\right) + \frac{D\,\Delta t}{2\,r\,\Delta r}\left(\left(c(i+1,t)\right) - c(i-1,t)\right)$$

2D improved forward Euler:

$$c(i,j,t+\Delta t) = c(i,j,t) + \frac{D\,\Delta t}{2\,i\,\Delta r^2}\left((2i+1)c(i+1,j,t) + (2i-1)c(i-1,j,t) - (4i)c(i,t)\right) + \frac{D\,\Delta t}{\Delta z^2}\left(\left(c(i,j+1,t)\right) + c(i,j-1,t) - 2c(i,j)\right)$$

Desired: Backward Euler solver, e. g. 1D cartesian:

$$\vec{c}_{k+1} = \vec{c}_k + \begin{vmatrix} 0 & & & & & \\ D^* & -2D^* & D^* & & & \\ & D^* & -2D^* & D^* & & \\ & & D^* & -2D^* & D^* & \\ & & & \ddots & & \\ & & & D^* & -2D^* & D^* \\ & & & & & 0 \end{vmatrix} \vec{c}_{k+1} \qquad \vec{c}_{k+1} = \begin{vmatrix} 1 & & & & & \\ -D^* & 1+2D^* & -D^* & & & \\ & -D^* & 1+2D^* & -D^* & & \\ & & -D^* & 1+2D^* & -D^* & \\ & & & -D^* & 1+2D^* & -D^* \\ & & & & \ddots & \\ & & & -D^* & 1+2D^* & -D^* \\ & & & & & 1 \end{vmatrix}^{-1} \vec{c}_k$$

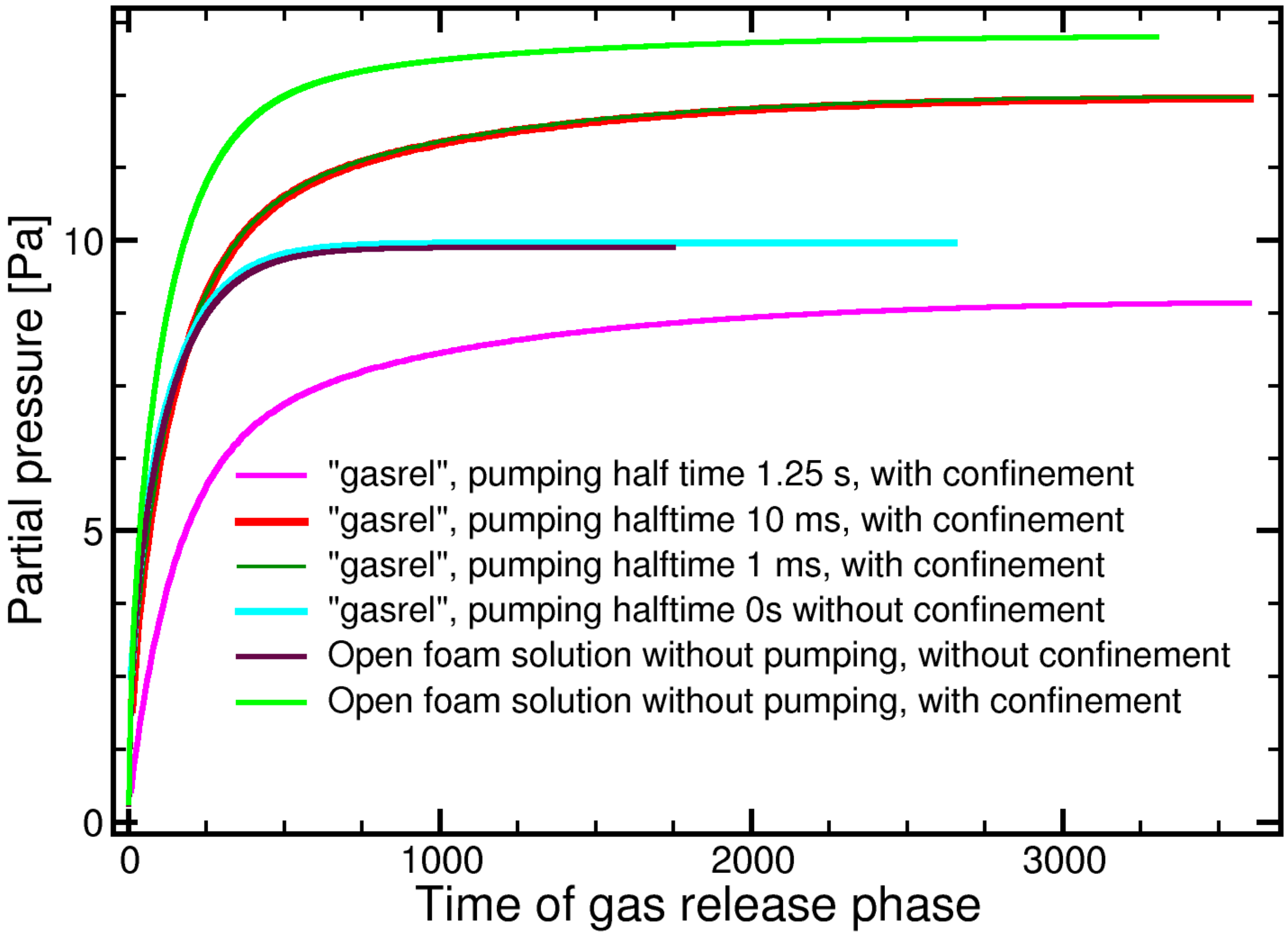
$$D^* = \frac{D\,\Delta t}{\Delta x^2}$$

2D n x n x m tensor ?

4.: Results

"gasrel" calculation with 6400 specimen element and 1800 conf. elements

14 halftimes reaching endpresure (0.1 Pa)



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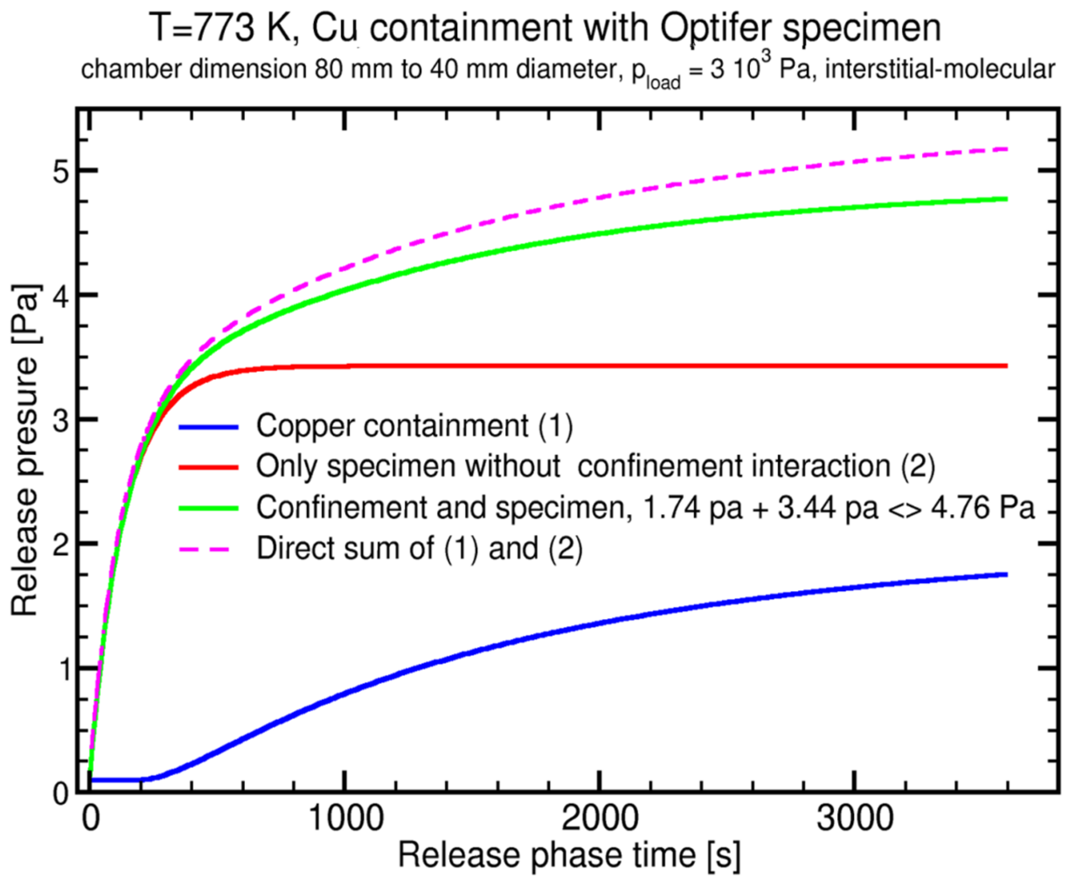
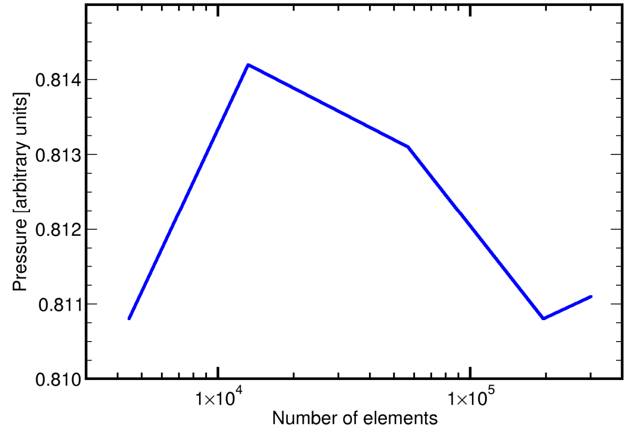
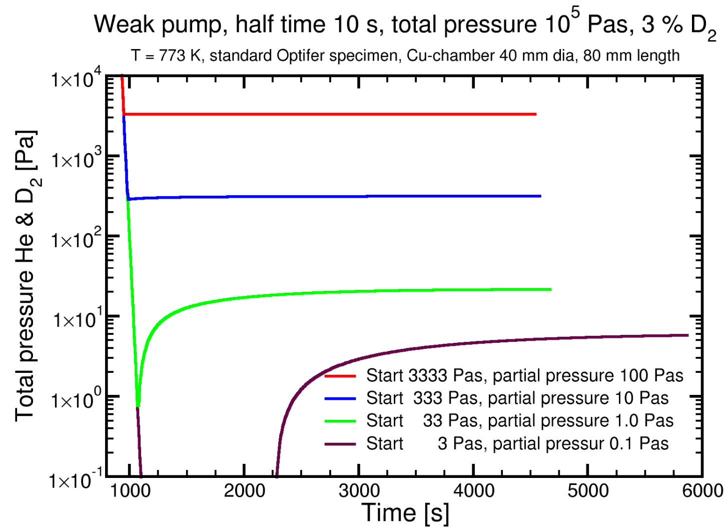




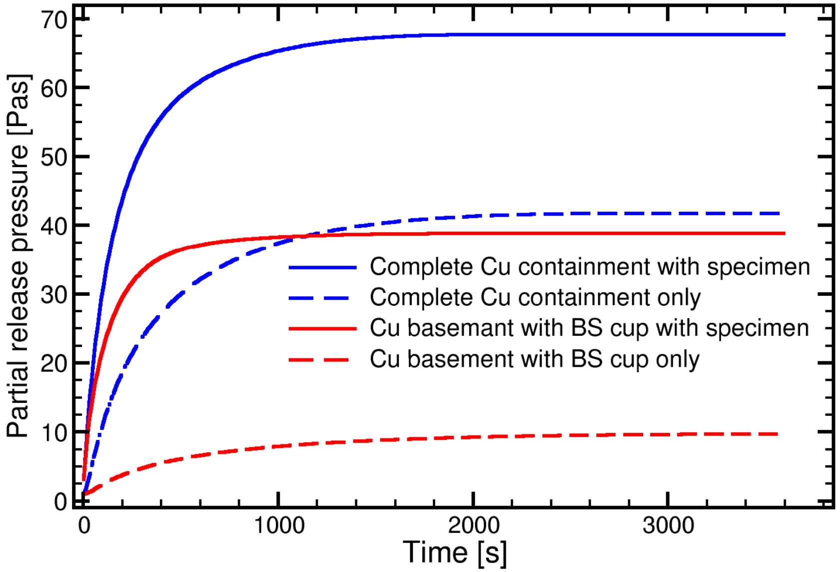
Choosing starting pressure:



Results for conception of experiments

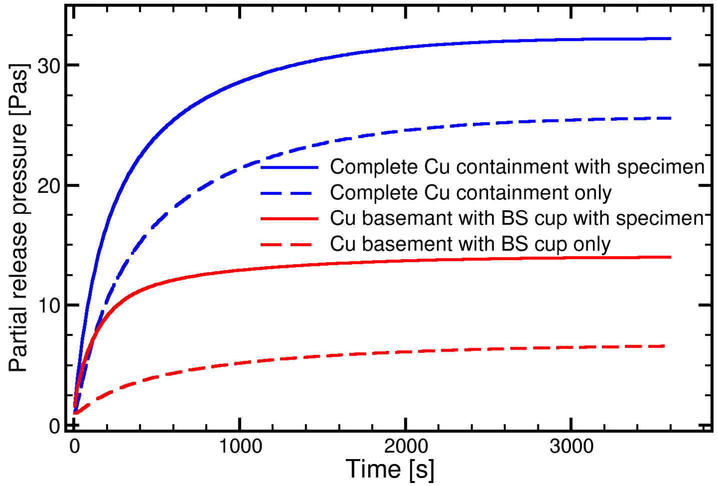
20 mm diameter, pumping halftime 0.5 s, 773 K

Total start pressure 33 Pas



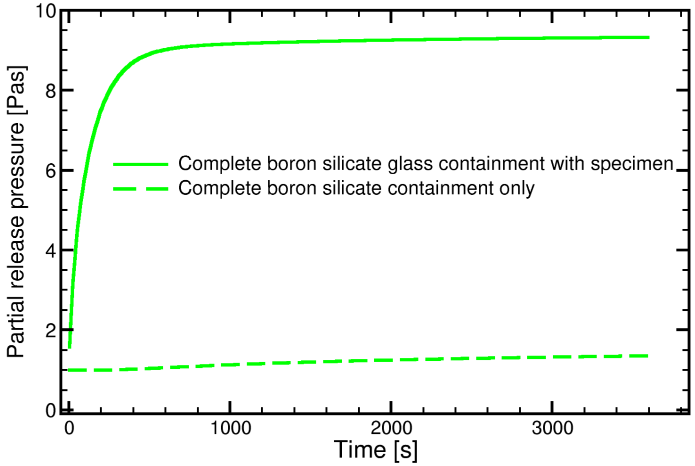
40 mm diameter, pumping halftime 0.5 s, 773 K

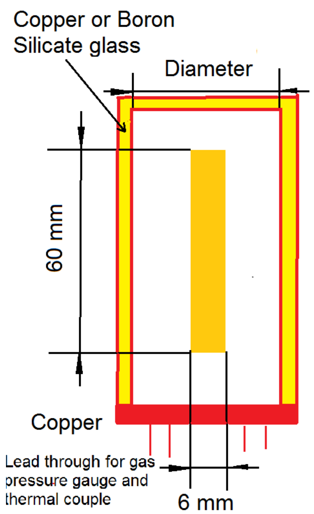
Total start pressure 33 Pas



40 mm diameter, pumping halftime 0.5 s, 773 K

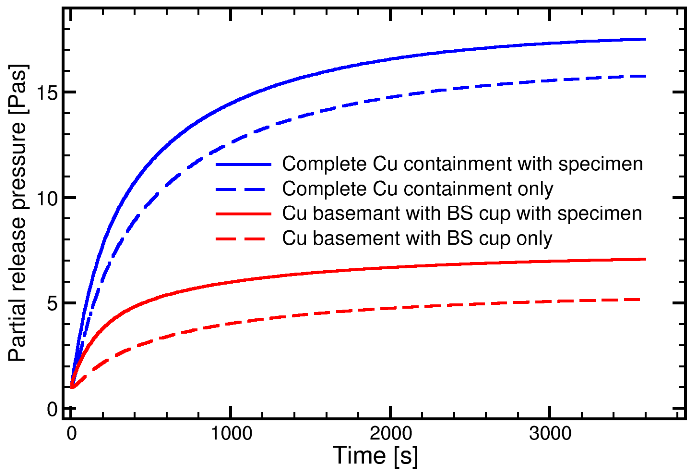
Total start pressure 33 Pas





80 mm diameter, pumping halftime 0.5 s, 773 K

Total start pressure 33 Pas



5.: Outlook to analytical solution

Solution in the charging interval

$$c(r,z,t) = k_{s,sa}\sqrt{p_{load}}\sum_{n,m}\frac{8(-1)^{n+1}}{\pi(2n+1)x_m J_1(x_m)}\exp\left(-\gamma_{n,m}^2 t\right)\cos\left((2n+1)\frac{\pi}{2}z\right)J_0(x_m r)$$

where

$$\gamma_{n,m}^2 = D_{sa}\left(\frac{x_m^2}{r_s^2}+\frac{(2n+1)^2\pi^2}{4z_s^2}\right),\ J_\alpha(x)\ (\alpha=0,1)\text{ Bessel functions of the first kind,}$$

x_m the m-th roots of $J_0(x)$.