Analytical solution of a gas release problem considering permeation with time dependent boundary conditions

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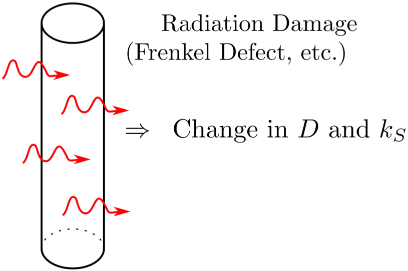
Motivation

- Influence of radiation damage on Diffusion and Sieverts' constant



- Setup-Material?
- Heating heals defects!
- How to recover D and k_s from data?

Experiments like this are relevant for:

- Reactor and Fusion-technology,
- Green energy: Storage and transport of H_2,
- repository exploration, ...

Outline

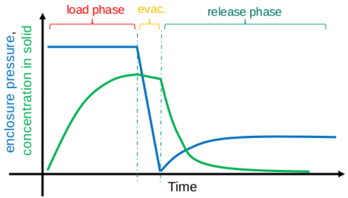
- Motivation
- Experiment, Setup
- Diffusion-Equation with time dependent boundary-conditions
- Explicit Solution for each time interval [Sample]
- Partial pressure of Hydrogen during Release-Interval

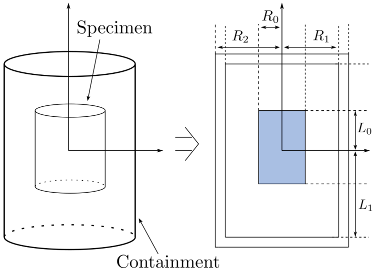
Experimental Setup

- Cylinder geometric isovolumetric setup
- Loading with Hydrogen at defined pressure p_L (and Temperature T)
- Evacuate the System $\rightarrow p(t) = p_L \exp[-\lambda t]$
- Recover Sieverts' and Diffusion Constant

$$R_0 = 3.0\,10^{-3}\,\mathrm{m},\; L_0 = 3.0\,10^{-2}\,\mathrm{m}$$

$$R_1 = 0.01\,\mathrm{m},\; R_2 = 0.02\,\mathrm{m},\; L_1 = 0.04\,\mathrm{m}$$





Boundary Conditions

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Note: (Sieverts' Law)

On the surfaces the Concentration of (Mono-atomic)-Hydrogen is given by

$$c \equiv k\sqrt{p(t)} \quad \forall t \geq 0$$

$$p(t) = \begin{cases} p_L, t \in [t_0 = 0, t_1] \\ p_L \exp[-\lambda t], t \in [t_1, t_2] \\ \text{unclear}, t \in [t_2, t_3] \end{cases}$$

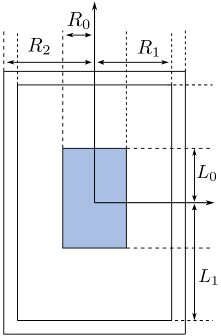
Note: (Diffusion-Equation)

$$\partial_t c^{(n)} - D_j \Delta c^{(n)} = 0, j \in \{s, c\}\; t \in [t_n, t_{n+1}]$$

$$c^{(n)}(r, z, t) = k_j\sqrt{p(t)} \text{ for } \begin{cases} r \in \{R_0, R_1\} \\ z \in \{\pm L_0, \pm L_1\} \end{cases}$$

$$c^{(n)}(R_2, z, t) \equiv 0$$

$$c^{(n)}(r, z, t_n) = c^{(n-1)}(r, z, t_{n-1}), c^{(-1)} \equiv 0$$



Solving These Equations

Zero-Boundary condition [Sample]

$$g_S(r,z,t) := c(r,z,t) - k_s\sqrt{p(t)}, r \in [0, R_0], z \in [-L_0, L_0]$$
$$\Rightarrow \partial_t g_S - D_s \Delta g_S = k_s \partial_t \sqrt{p}$$

Zero-Boundary condition [Containment, neglecting z]

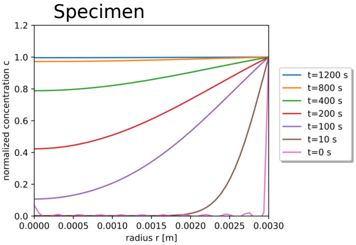
$$g_C(r,t) := c(r,t) - \tau(r) k_c \sqrt{p(t)}, \tau(r) = \frac{\log[r] - \log[R_2]}{\log[R_1] - \log[R_2]}, r \in [R_1, R_2]$$
$$\Rightarrow \partial_t g_C - D_c \Delta g_C = \tau k_s \partial_t \sqrt{p}$$

Hom. PDE $\underset{\text{Separation of variables}}{\rightarrow}$ **ODEs** $\underset{\text{Solvable}}{\rightarrow}$ **Fundamental Solutions**

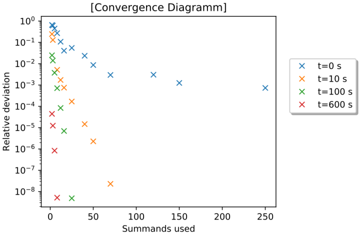
$\underset{\text{Variation of Constants}}{\rightarrow}$ **Full Solution**

Sample: Analytical Solution

$t \in [0, t_1]$, $p(t) \equiv 3\,\text{kPa}$, $k_s = 1.829\,10^{-3}\,\frac{\text{mol}}{\sqrt{\text{Pam}^3}}$, $D_s = 7.879\,10^{-9}\,\frac{\text{m}^2}{\text{s}}$



Concentration Profile for $z = 0$.

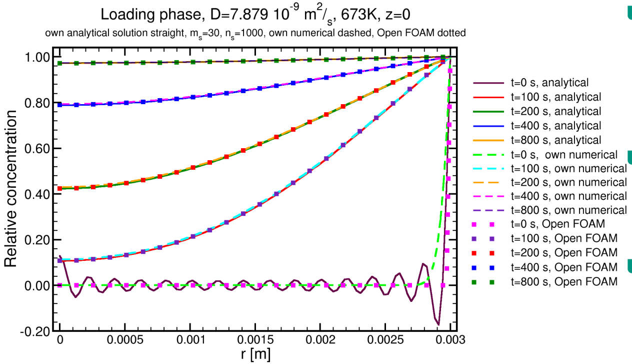


Relative error of approximation.

$$g_S(r,z,t) = \sum_{n,m} b_{n,m} \exp[-\gamma_{m,n}^2 t] \cos\left((2n+1)\frac{\pi}{2L_0} z\right) J_0\left(x_m \frac{r}{R_0}\right),$$

$$\gamma_{m,n}^2 = D_s\left(\frac{x_m^2}{R_0^2} + \frac{(2n+1)^2\pi^2}{4L_0^2}\right), \quad b_{m,n} = 8\frac{(-1)^{n+1} k_s \sqrt{p_L}}{\pi(2n+1)x_m J_1(x_m)}$$

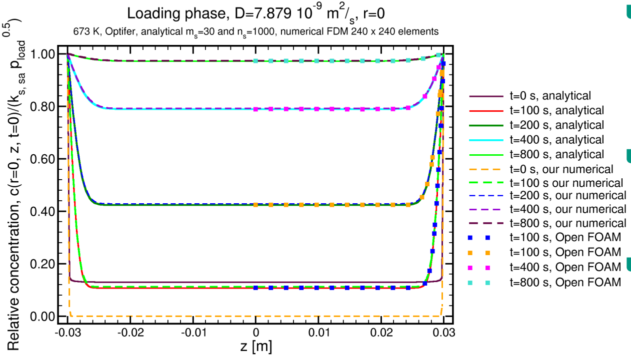
Compare: Numerical (Fortran), Analytical (Python), OpenFOAM



- Analytical Solution **Python + Fortran**
- Numerical Solution **Fortran**
- Numerical Simulation **OpenFOAM**

Different approaches show similar results!

Compare: Numerical (Fortran), Analytical (Python), OpenFOAM

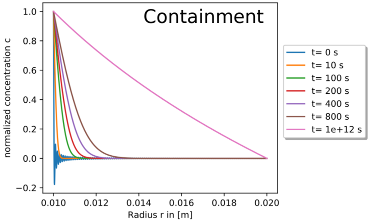


- Analytical Solution **Python + Fortran**
- Numerical Solution **Fortran**
- Numerical Simulation **OpeanFOAM**

Different approaches show similar results!

Containment: Analytical Solution

$t \in [0, t_1]$, $p(t) \equiv 3\,\text{kPa}$, $k_c = 5.941\,10^{-4}\,\frac{\text{mol}}{\sqrt{\text{Pa}}\text{m}^3}$, $D_c = 8.257\,10^{-10}\,\frac{\text{m}^2}{\text{s}}$



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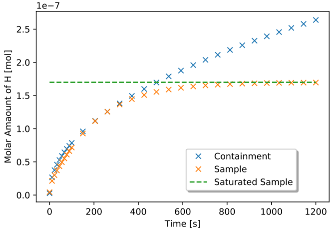


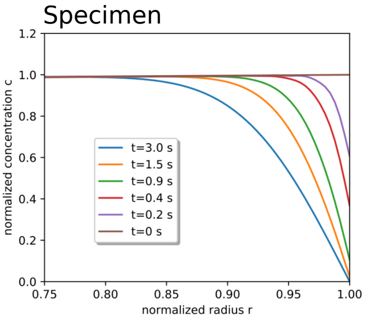
Stored amount of Hydrogen.

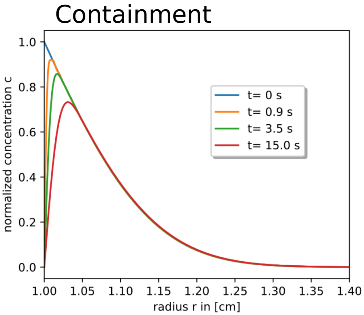
$$g_c(r,z,t) = \sum_{n=1}^{\infty} A_n \exp[-\lambda_n^2 \frac{D}{R_1^2} t] \left(\frac{-Y_0(\lambda_n)}{J_0(\lambda_n)} J_0(\lambda_n \frac{r}{R_1}) + Y_0(\lambda_n \frac{r}{R_1}) \right)$$

$$\det \begin{pmatrix} J_0(\lambda_n) & Y_0(\lambda_n) \\ J_0(\lambda_n \frac{R_1}{R_2}) & Y_0(\lambda_n \frac{R_1}{R_2}) \end{pmatrix} = 0, A_n = -k\sqrt{p_L} \frac{\int_{R_1}^{R_2} \tau(r) u_n(r) r dr}{\int_{R_1}^{R_2} u_n(r)^2 r dr}$$

Pumping Interval

Fick's Law $\rightarrow c(r, z, t) = p_L \exp[-\lambda t]$, for $r \in \{R_0, R_1\}, z \in \{L_0, L_1\}$
Fixed Ratio: 97 % He and 3 % H_2
Remaining Partial Pressure: $\Rightarrow p_{H_2}(0.9s) = 1\text{Pa}$





$$\frac{m_H^s(800\,\text{s}+0.9\,\text{s})}{k_s\sqrt{P_L}V_{sample}} \approx 96\% \qquad \frac{m_H^c(800\,\text{s}+0.9\,\text{s})}{k_s\sqrt{P_L}V_{sample}} \approx 124\%$$

Release Interval

Problem: $p(t)$ in gaseous phase unknown $\Rightarrow$ No Boundary Conditions

Note: (Initial Guess)

$$\sqrt{p(t)} = \frac{\sqrt{p_f} - \sqrt{p_0}}{1 - \exp[-\beta T]} \left(1 - \exp[-\beta t]\right) + \sqrt{p_0} \tag{1}$$

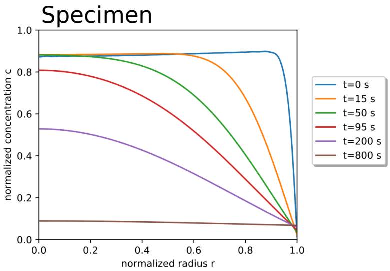
[Sedano et al., J. Nucl. Mater. (1999)]

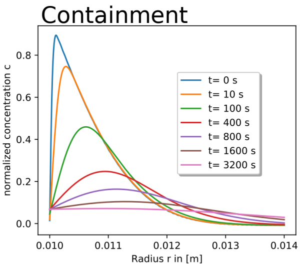
$$\partial_t g_S - D_s \Delta g_S = k_s \underbrace{\partial_t \sqrt{p}}_{\text{Now Easy}}\,, \qquad \partial_t g_C - D_c \Delta g_C = \tau k_c \partial_t \sqrt{p}$$

Note:

- β, T and p_f free parameters,
- Sieverts' Law still holds for the pressure above.

Release Interval Graphics





$$j_1^s(t) = -2\pi\, D_s \int_{-L}^{L} R_0 \partial_r c(R_0, z, t) dz$$

$$j_2^s(t) = -4\pi\, D_s \int_{0}^{R_0} \partial_z c(r, L_0, t) r dr$$

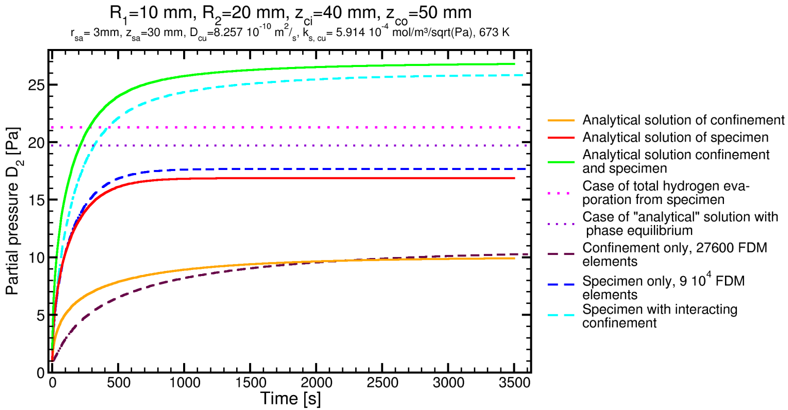
$$j_3^c(t) = -2\pi\, D_c \int_{-L_1}^{L_1} R_1 \partial_r c(R_1, z, t) dz$$

Flux of Hydrogen:

- Coat Containment j_3^c,
- (2x Caps Containment),
- Coat Specimen j_1^s,
- Caps Specimen j_2^s.

Pressure Increase

$$m(t) = \sum_k \int_0^t j_k(\tau) d\tau, \quad p_{H_2}(t) = \frac{(m_H^s(t) + m_H^c(t))\, RT}{2\,(V_0 - V_S)}.$$



Conclusion

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- Fortran FDM and analytic (Python) model show similar results,
- Measure containment effect,
- Recover D and k with B&B (fast evaluation -> analytic solution),
- Estimate: Duration of Experiment,

copper containment may be usable

Open Problems:

- Guess function $\sqrt{p(t)}$ does not exactly fit. (Fixed-point Iteration),
- Melting Point of copper $\approx 1.300\ \mathrm{K}$.

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 under grant agreement No. 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission

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