## CAS 2017 <br> Vacuum simulations

INDIVIDUAL WORK - TUTORIAL GROUP \#1
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## Outline

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- Sticking factor \& outgassing rate
- Saturation time - analytical versus Monte Carlo approaches
- Transmission probability and pressure ratio as a function of sticking probability

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## Problem description

We have a NEG coated vacuum pipe connected to a vacuum system and two pressure gauges reading. A gas injection is performed and at steady state, the pressures measured in gauges 1 and 2 are:

- $P_{1}=1 \cdot 10^{-6} \mathrm{mbar}$
- $P_{2}=2.5 \cdot 10^{-9} \mathrm{mbar}$

What is the sticking factor of the NEG?

What is the flow rate of the inlet gas?


## Problem description

What do we know:

- Pipe geometry
- Pumping speed of the pump
- Pressure on gauges



## Problem description



Principle:

- Mass flow flowing through
a coated chamber
-Some molecules sticking
to the coating
-Some molecules pumped



## Molflow in a nutshell

MolFlow+ is a software developed at CERN in 1990 based on Monte Carlo method

The software allows to:
Draw a vacuum system

- Calculate pressure profiles for complex geometries in molecular flow regime
- In our case, evaluate the sticking probability $\alpha$ of NEG coating

All the results can be visualized in a user friendly way and
 shown in a real time

## Building the geometry



## Building the geometry




## Question 1: sticking probability and injection rate



Work out pressure ratio of two gauges

$$
P_{\text {ratio }}=\frac{P_{2}}{P_{1}}=2.5 * 10^{-3}
$$

Apply sticking probability to obtain the same pressure ratio in Molflow

- 0.052

Set the gas injection rate in the simulation to get the same pressures as given above

- $0.0001 \mathrm{mbar}{ }^{*} / \mathrm{s}$



## The complete system



## Question 2

NEG coating is an effective pump, but it can't pump gas forever: eventually it saturates. Its pumping ability drops quickly when the pumped gas forms one monolayer on the surface - corresponding to about 1E15 pumped molecules/cm²

In our setup, how much gas is that?
How much time does it take until our setup saturates?

## Question 2: time for complete saturation - analytical way



How much time does it take until our setup saturates?
$p_{1}=1 * 10^{-6} \mathrm{mbar}$
$p_{2}=2.5^{*} 10^{-7} \mathrm{mbar}$
S=300l/s
$A_{\text {neg }}=1971.1 \mathrm{~cm}^{2}$
$\mathrm{Q}_{\mathrm{s}}=10^{-4} \mathrm{mbar}{ }^{*} / \mathrm{s}$
$\mathrm{N}_{\text {sat }}=10^{15}$ molecules $/ \mathrm{cm}^{2}$


## Question 2: time for complete saturation - analytical way

As first we calculate the gas load $\mathrm{Q}_{2}$ after the NEG chamber:

$$
\begin{gathered}
p_{2}=\frac{Q_{2}}{S} \\
Q_{2}=p_{2} * S=8.4 * 10^{-7} \frac{\mathrm{mbar} * l}{\mathrm{~S}}
\end{gathered}
$$

To get the gas load absorbed by NEG coating we just subtract it from the total inlet gas:

$$
\Delta Q=Q s-Q_{2}=9.92 * 10^{-5} \frac{\mathrm{mbar} * l}{s}
$$

By dividing with the total surface area of NEG chamber we get the absorption rate of coating:

$$
z_{\text {abs }}=\frac{\Delta Q}{A_{\text {neg }}}=5.03 * 10^{-8} \frac{\mathrm{mbar} * l}{\mathrm{~cm}^{2} * \mathrm{~s}}
$$

## Question 2: time for complete saturation - analytical way

With the ideal gas equation we get number of molecules absorbed by NEG surface area in a second:

$$
\begin{gathered}
p * V=N * k_{b} * T \\
N_{a b s}=\frac{p * V}{k_{b} * T}=\frac{z_{a b s}}{k_{b} * T}=1.21 * 10^{12} \frac{\text { molecules }}{\mathrm{cm}^{2} * s}
\end{gathered}
$$

With division of number of absorbed molecules with total number of molecules needed to saturate the film we gate the time before pumping speed of NEG drops to zero:

$$
t_{a}=\frac{N_{s a t}}{N_{a b s}}=826 s
$$

In our setup, how much gas is that?

$$
N=N_{s a t} * A_{N E G}=1.97 * 10^{18} \mathrm{molecules}
$$



### 13.77 min

## Question 2- time for complete saturation in Molflow



Engineering way: Using Molflow+ to solve the problem

1) Select a facet of the NEG area and read impingement rate : $2.4 \times 10^{17}$ molecules* $\mathrm{m}^{-2 *} \mathrm{~s}^{-1}=2.4 \times 10^{13}$ molecules ${ }^{*} \mathrm{~cm}^{-2 *}{ }^{-1}$
2) The impingement rate times the sticking factor of the NEG of 0.05 gives us the number of absorbed particles per area $\mathrm{N}_{\text {abs }}=1.2 \times 10^{12}$ molecules* $\mathrm{cm}^{-2 *} \mathrm{~s}^{-1}$
3) We know that NEG coating is saturated at $\mathrm{N}_{\text {sat }}=10^{15}$ molecules* $\mathrm{cm}^{-2}$
4) The full saturation is reached at $t=N_{\text {sat }} / N_{\text {Abs }}$
$\mathrm{t}=10^{15}$ molecules* $\mathrm{cm}^{-2} / 2.4 \times 10^{13}$ molecules $\mathrm{cm}^{-2 *} \mathrm{~s}^{-1}=833 \mathrm{~s}$


### 13.88 min

## Question 3

What was the transmission ratio of the gas for the pressure ratio given in the task?

By changing the simulation parameters, make a "transmission ratio as a function of the sample's sticking factor" plot given that:
$X$ axis: different sticking factor values (around 5-7 different values)
$Y$ axis: gas transmission ratio

# Question 3: trans. probability and pressure ratio as a function of $\alpha$ 



$$
\begin{aligned}
& T_{\text {ratio }}=\frac{N_{\text {abs }}}{N_{\text {inj }}}=5 * 10^{-3} \\
& P_{\text {ratio }}=\frac{P_{2}}{P_{1}}=2.5 * 10^{-3}
\end{aligned}
$$

## Real life applications



## Reference paper

VACUUM

PERGAMON


Fig. 3. Pressure reduction factor as a function of the coating sticking probability obtained by Monte-Carlo simulation assuming a constant gas load before and after activation.

## Conclusions

Tutorial based on a real world application
The same problem was addressed analytically and numerically
With the basic knowledge of vacuum technology, Molflow becomes a very powerful tool

## Final conclusion Hard work \& Ice cream



19/06/2017

