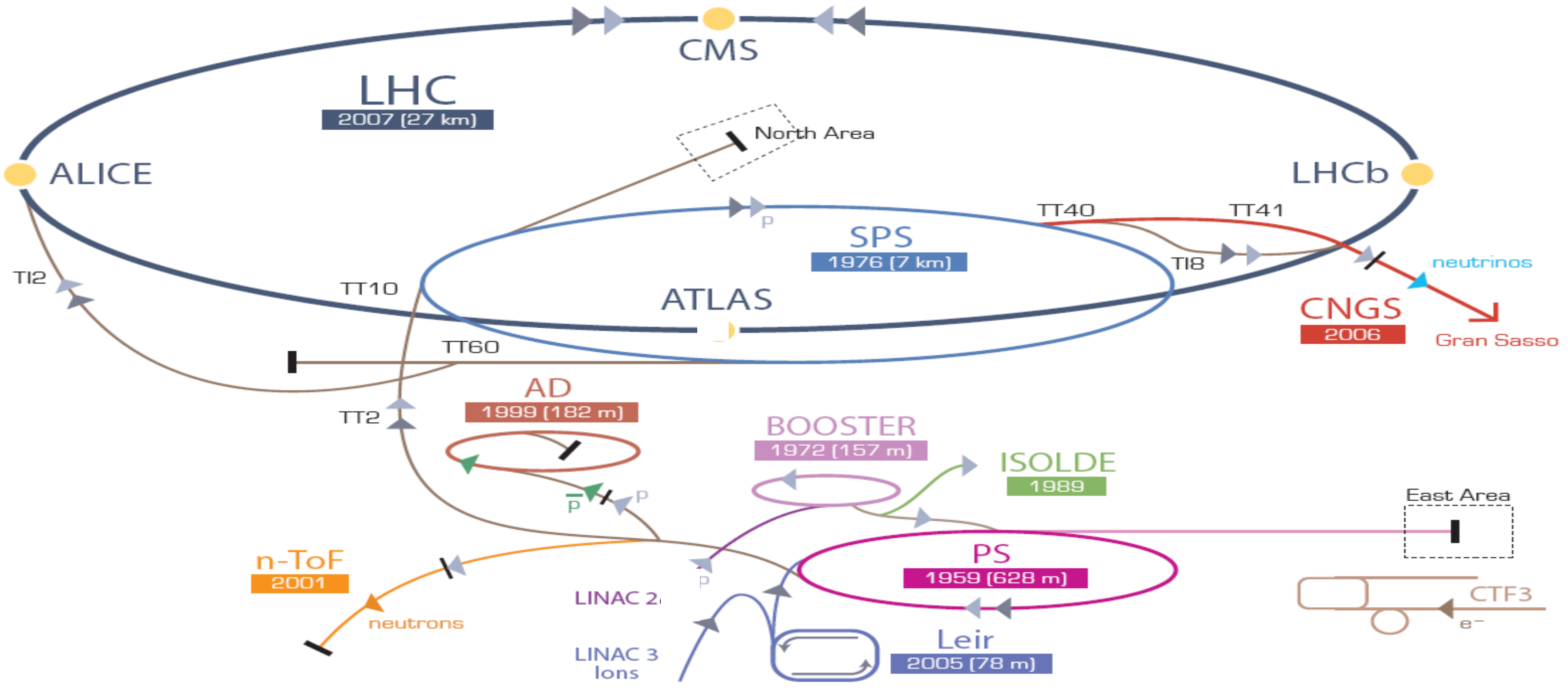
COMSOL CONFERENCE
2016 MUNICH

Simulation of Non-Evaporable Getter saturation with COMSOL®

Outline

1. Vacuum systems @ CERN;
2. NEG pumps and saturation mechanism;
3. Free molecular flow: COMSOL simulations;
4. Results and experimental benchmark;
5. Summary.

CERN Accelerator Complex



▸ p (proton) ▸ ion ▸ neutrons ▸ p̄ (antiproton) proton/antiproton conversion ▸ neutrinos ▸ electron

LHC Large Hadron Collider SPS Super Proton Synchrotron PS Proton Synchrotron

AD Antiproton Decelerator CTF3 Clic Test Facility CNGS Cern Neutrinos to Gran Sasso ISOLDE Isotope Separator OnLine DEvice

LEIR Low Energy Ion Ring LINAC LINear ACcelerator n-ToF Neutrons Time Of Flight

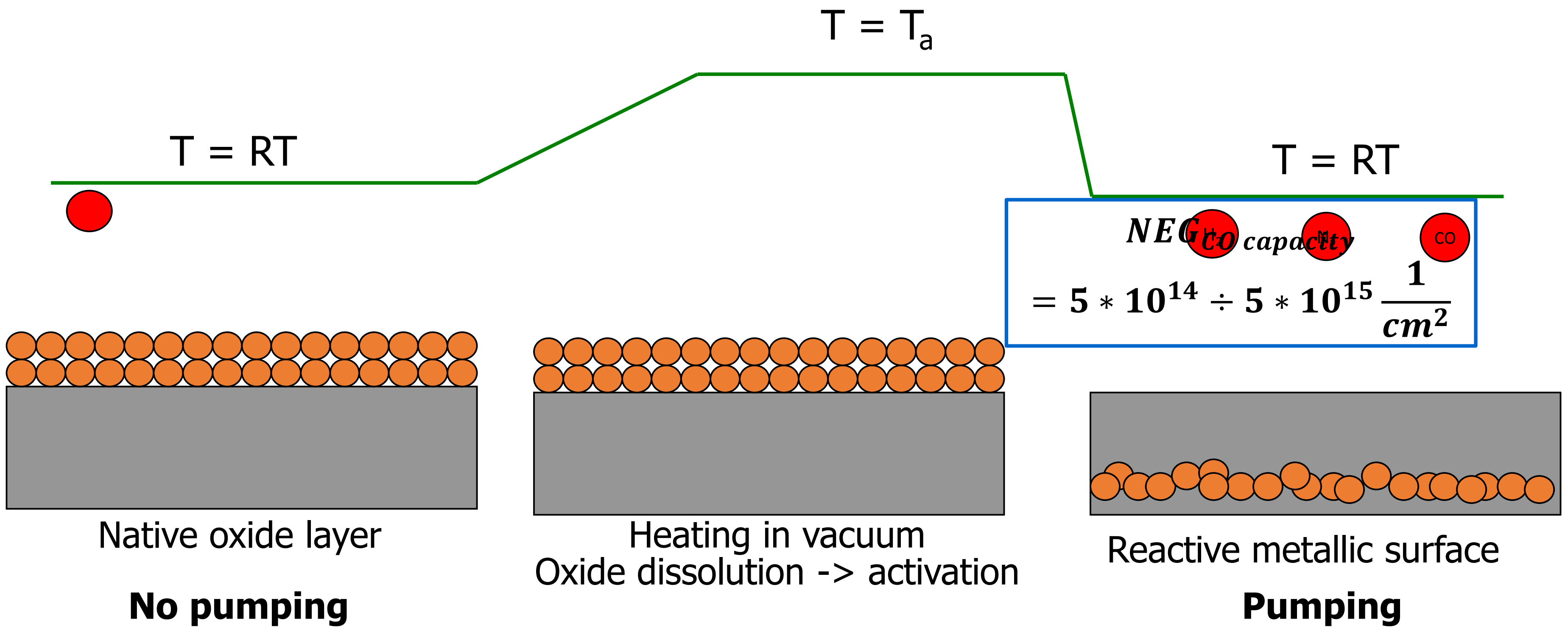
…and some numbers

Machine	Type	Year	Energy	Bakeout	Pressure (Pa)	Length	Particles
Linac, Booster, ISOLDE, PS, n-TOF and AD Complex						**2.6 km !**	
LINAC 2	linac	1978	50 MeV	Ion pumps	10^{-7}	40 m	p
ISOLDE	electrostatic	1992	60 keV	-	10^{-4}	150 m	ions: 700 isotopes and 70 (92) elements
REX-ISOLDE	linac	2001	3 Mev/u	partly	10^{-5} - 10^{-10}	20 m	
LINAC 3	linac	1994	4.2 MeV/u	Ion pumps	10^{-7}	30 m	ions
LEIR	accumulator	1982/2005	72 MeV/u	complete	10^{-10}	78 m	pbar, ions
PSB	synchrotron	1972	1-1.4 GeV	Ion pumps	10^{-7}	157 m	P, ions
PS	synchrotron	1959	28 GeV	Ion pumps	10^{-7}	628 m	P, ions
AD	decelerator	?	100 MeV	complete	10^{-8}	188 m	pbar
CTF3 complex	linac/ring	2004-09		partly	10^{-8}	300 m	e
PS to SPS TL	Transfer line	1976	26 GeV	-	10^{-6}	~1.3 km	P, ions
SPS Complex						**15.7 km !**	
SPS	synchrotron	1976	450 GeV	Extractions	10^{-7}	7 km	p, ions
SPS North Area	Transfer line	1976		-	10^{-6} - 10^{-7}	~1.2 km	
SPS West Area	Transfer line	1976				~ 1.4 km	
SPS to LHC TI2/8 Line	Transfer line	2004/2006				2 x 2.7 km	
CNGS Proton Line	Transfer line	2005				~730 m	
LHC Accelerator						***~109 km !***	
LHC Arcs (Beam x2, Magnets & QRL insul.)	collider	2007	2 × 7 TeV	-	< 10^{-8}	2 x (2 x 25 km)	p, ions
LSS RT separated beams				complete		2 × 3.2 km	
LSS RT recombination						~ 570 m	
Experimental areas						~ 180 m	
Beam Dump Lines TD62/68	Transfer line	2006	7 TeV	-	10^{-6}	2 × 720 m	
				High Vacuum		~20 km	**~128 km !**
				UHV w/wo NEG		~ 57.5 km	
				Insulation vacuum		~ 50 km	

Based on NEG pumping system

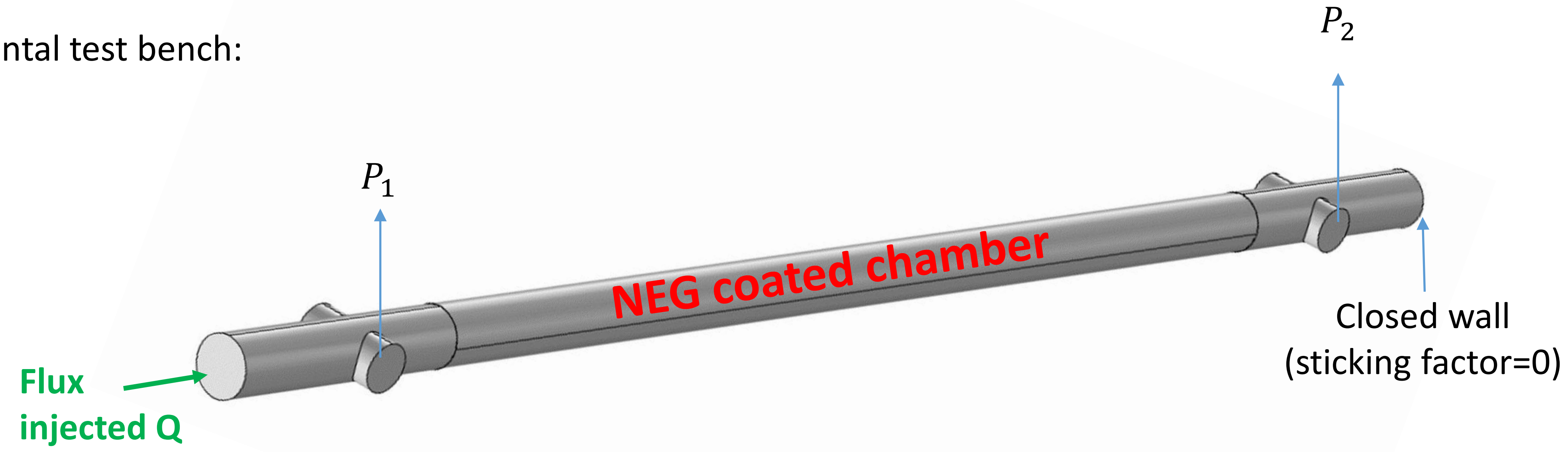
NEG Alloy: Pumping Mechanism

A NEG coating is a metallic alloy that can pump most of the gases present in a vacuum system after thermal dissolution of its native oxide layer (activation process).



Evaluation of NEG performance

Experimental test bench:

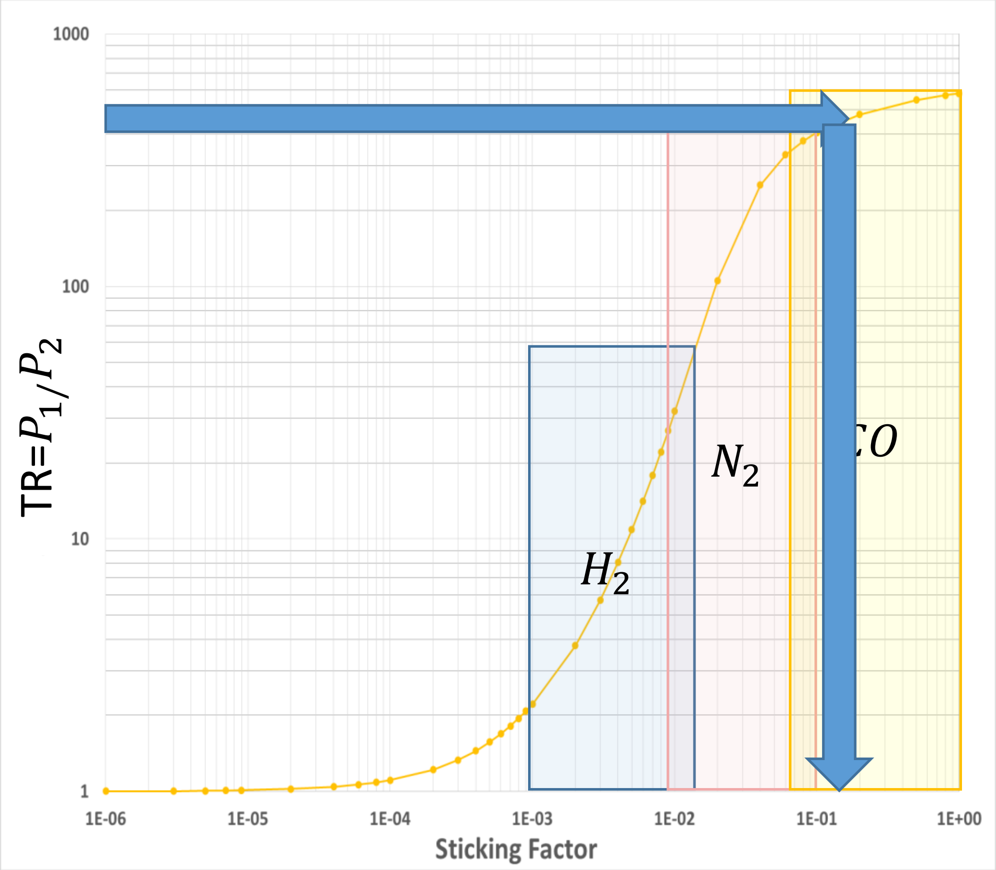


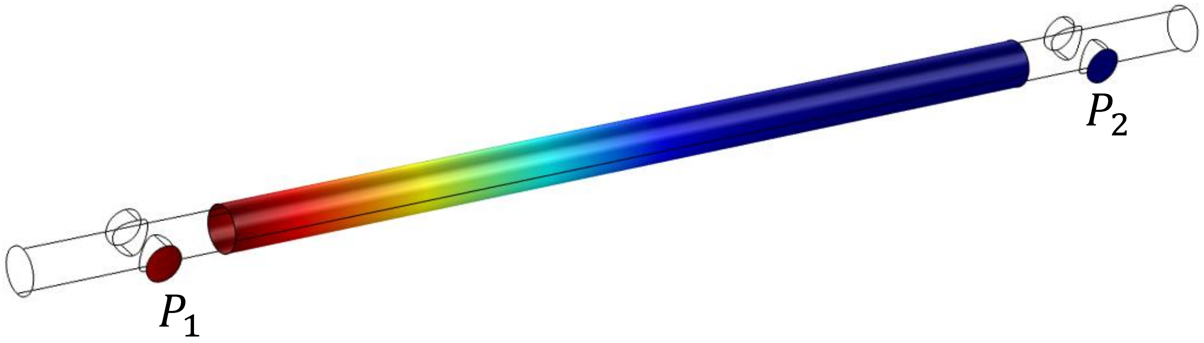
- Pumping speed: $S = \frac{Q}{P_1}$ $[{}^{l}/_{s}]$

- Transmission ratio: $Tr = \frac{P_1}{P_2}$

Sticking coefficient evaluation by transmission method

First simulations in COMSOL are used to calculate the transmission trends





Then, using the TR carried out experimentally, is possible to extract the sticking coefficient for each gas injected.

***CO* has the highest SF**:
Highest transmission ratios mean lowest P_2.

Limitation of the CO transmission methods

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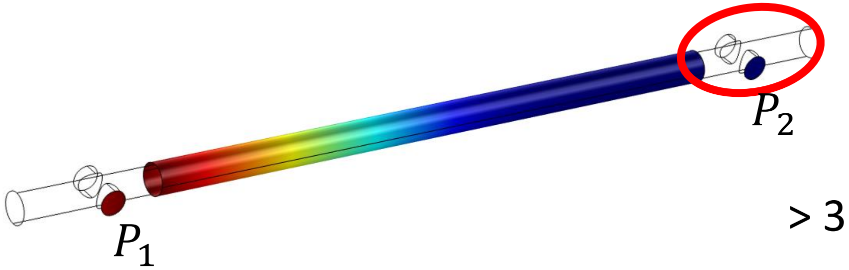


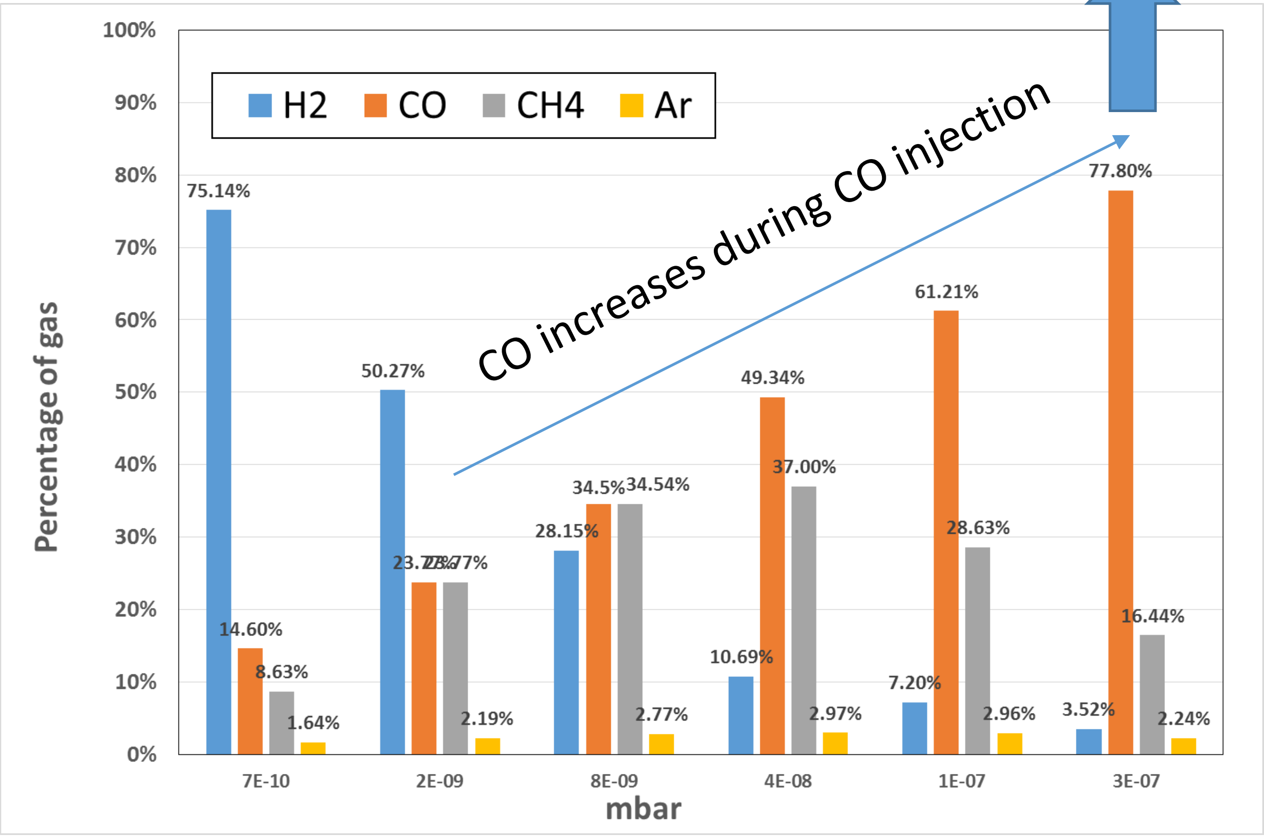
$>$ 3E-7 mbar

≈ 1e17 CO molecules injected

A saturation of the NEG pumping sites is expected

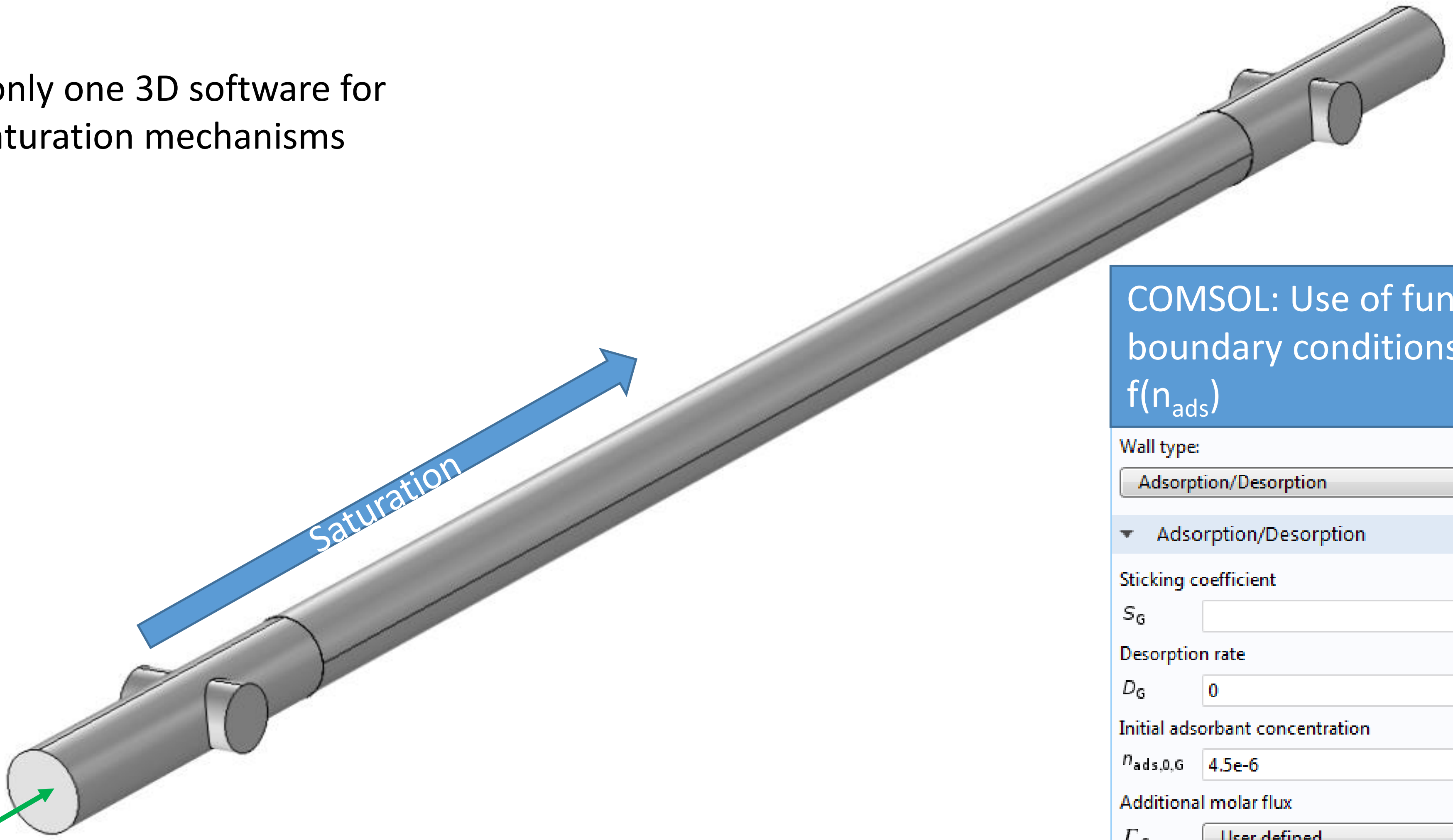
$$(NEG_{CO\ capacity} = 5 * 10^{14} \div 5 * 10^{15} \frac{1}{cm^2})$$

NEED
Dynamic simulation of NEG pumping



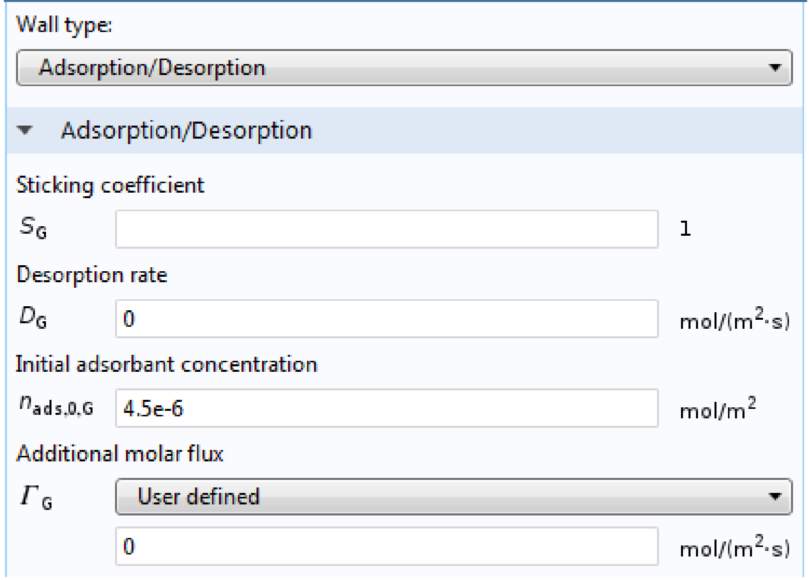
Why COMSOL?

The only one 3D software for
3D saturation mechanisms



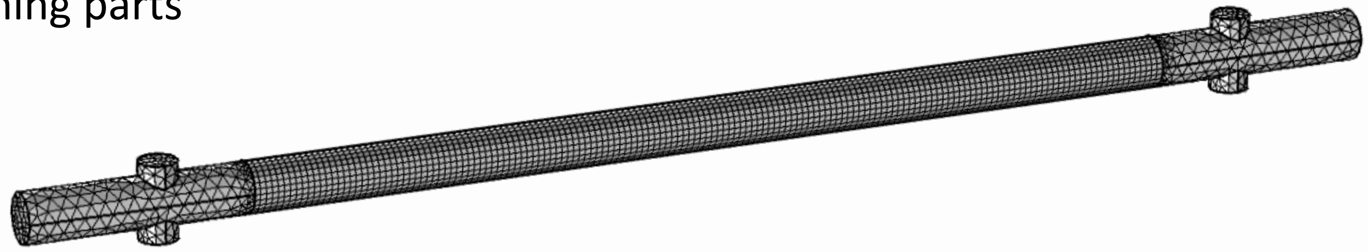
Flux injected Q

COMSOL: Use of functions as boundary conditions → Sticking Factor $f(n_{ads})$

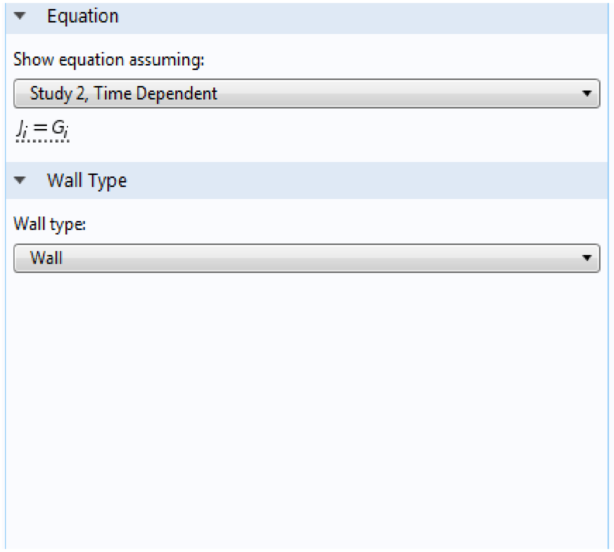


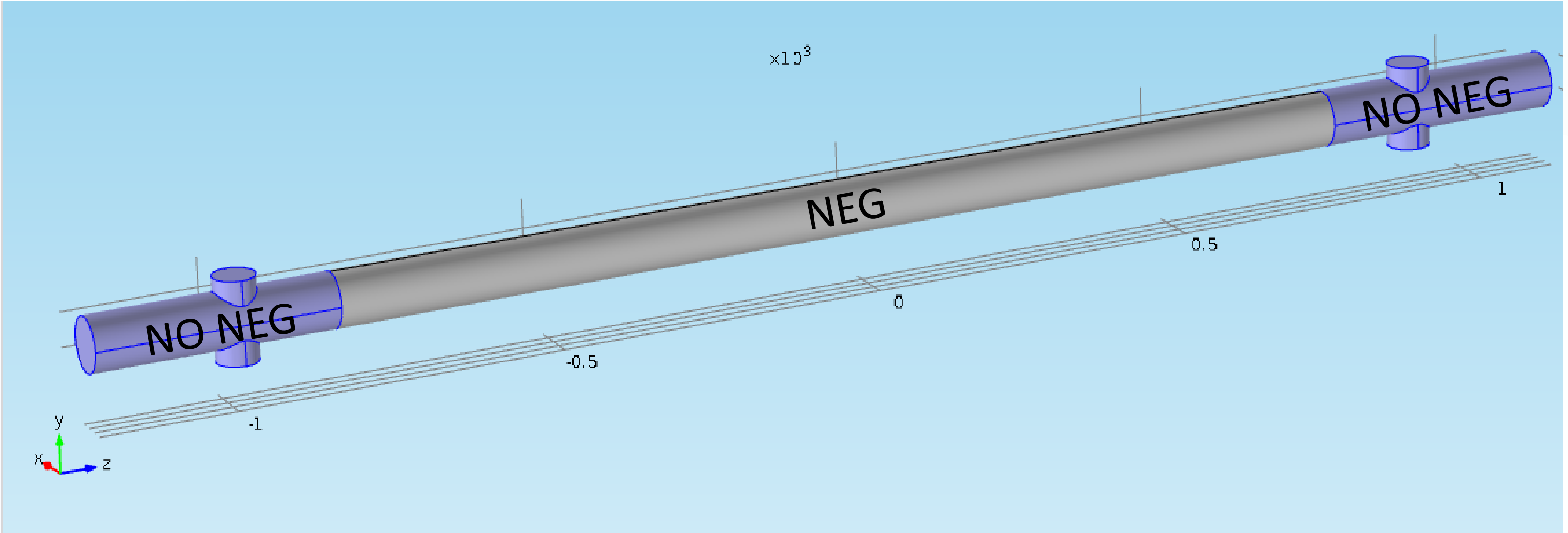
Building the simulation

1) Mapped mesh with $1cm^2$ square elements for the NEG surface, less refined on the remaining parts



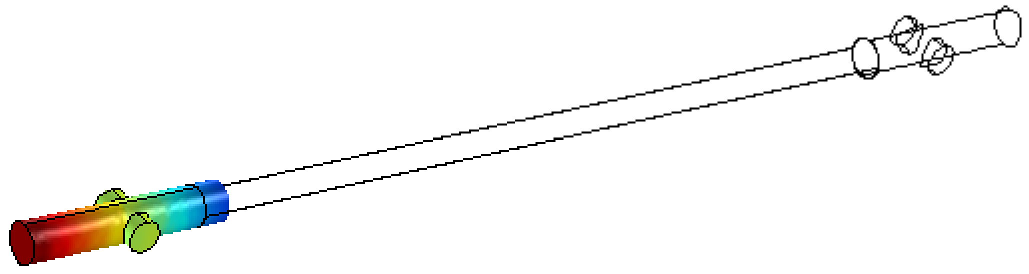
2) Wall type definition





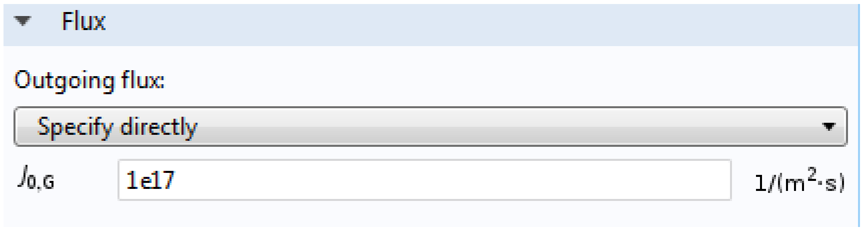
Building the simulation

3) Outgassing wall type for the inlet facet

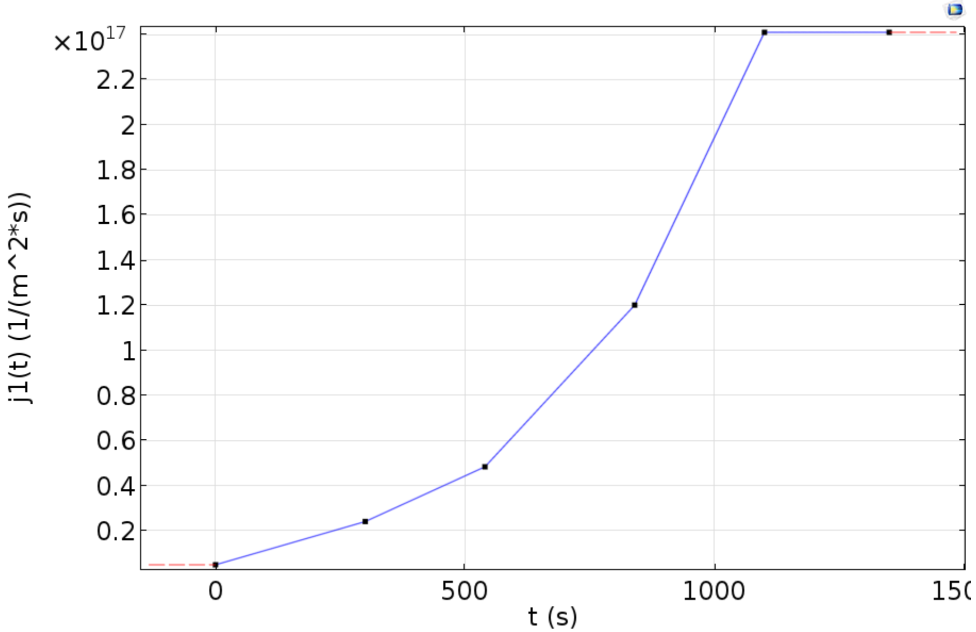


$J_i = G_i + J_{0,j}$

Constant emitted flux



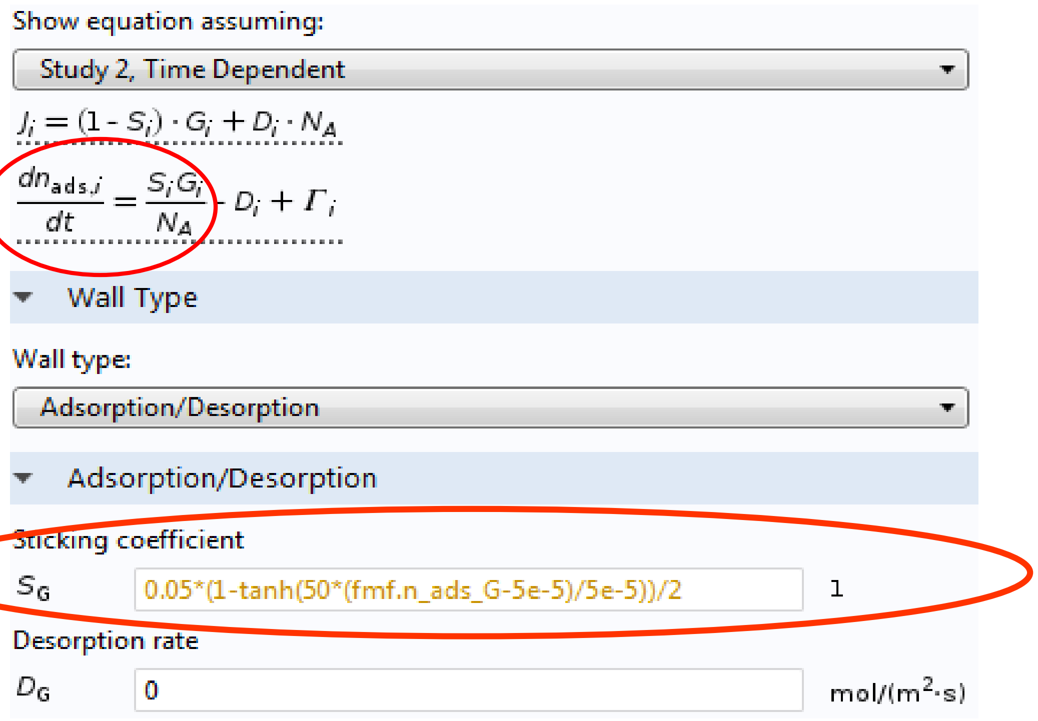
Interpolating function recreating the experimental injected flux of molecules



Building the simulation

4) <u>Adsorption wall type</u> for the NEG surface

The sticking coefficient needs to be related to the adsorbed molecules per surface unit (defined on the mesh)



Model for the Sticking coefficient decrease to 0 has been selected: a $tanh$ function results easier processable than a $Sticking\ factor \rightarrow 0$ step function. Not reaching of convergence and numerical oscillations in the results were the most common problems.

Building the simulation

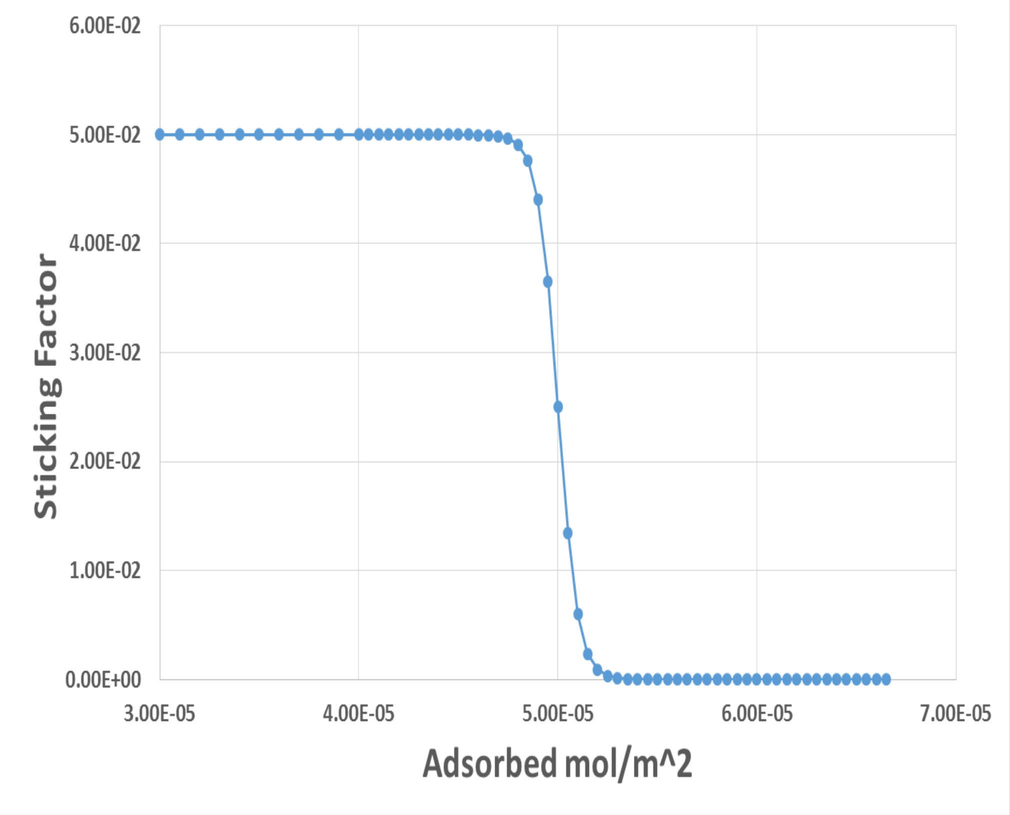
4) <u>Adsorption wall type</u> for the NEG surface

$$\text{SF} = SFco * \frac{1 - tanh\left(\alpha * \frac{(Mol.ads - NEG\ capacity)}{NEG\ capacity}\right)}{2}$$

$SFco$= 0.05 (experimental value)

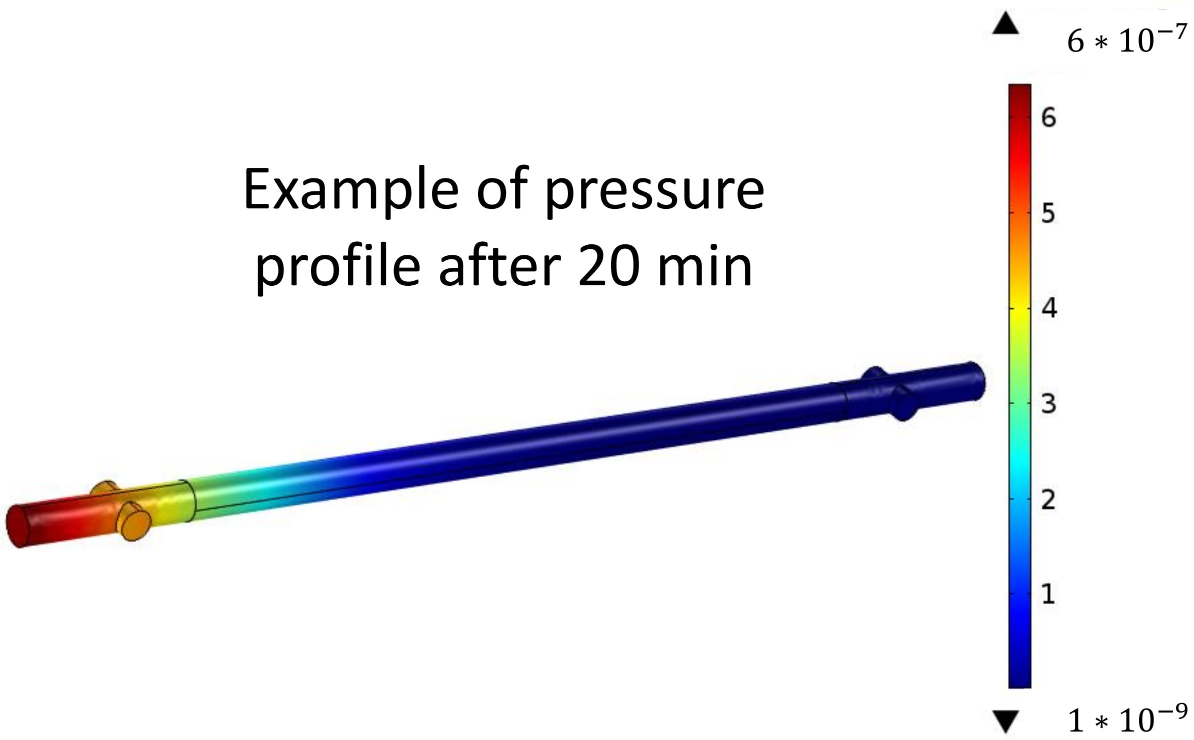
Tuning factor: slope

The # of adsorbed molecules has been normalized to the adsorbent capacity $(1 \cdot 10^{15}\ \frac{molecules}{cm^2}$ expressed as $5 \cdot 10^{-5}\ \frac{mol}{m^2})$

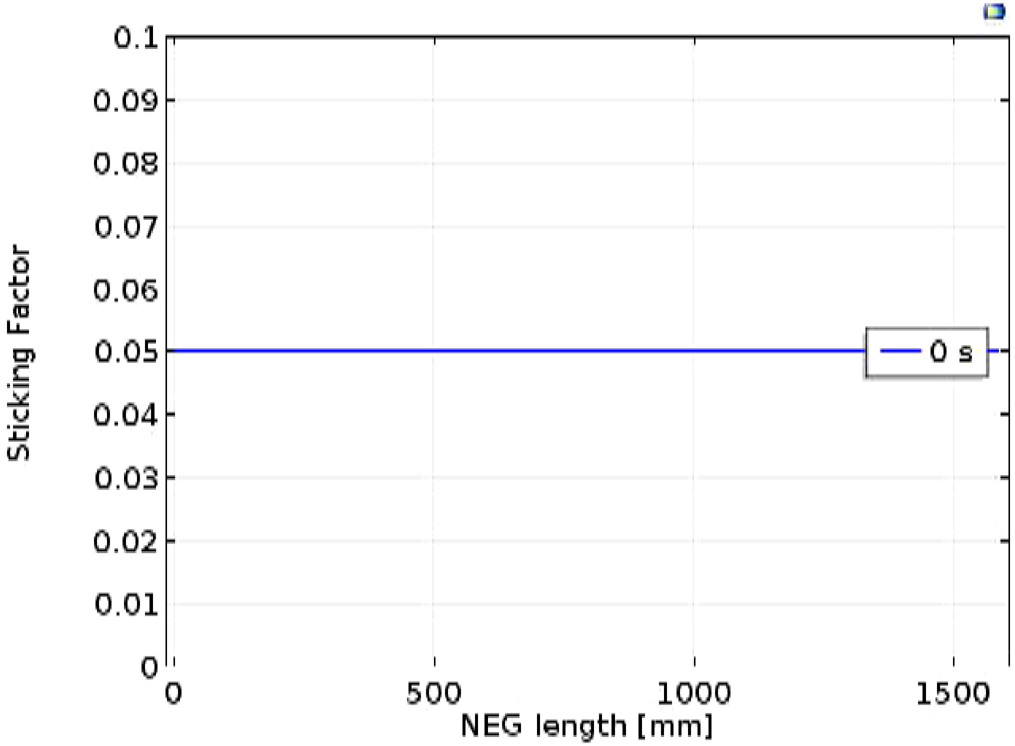


Simulated saturation process: Pressure evolution

Example of pressure profile after 20 min

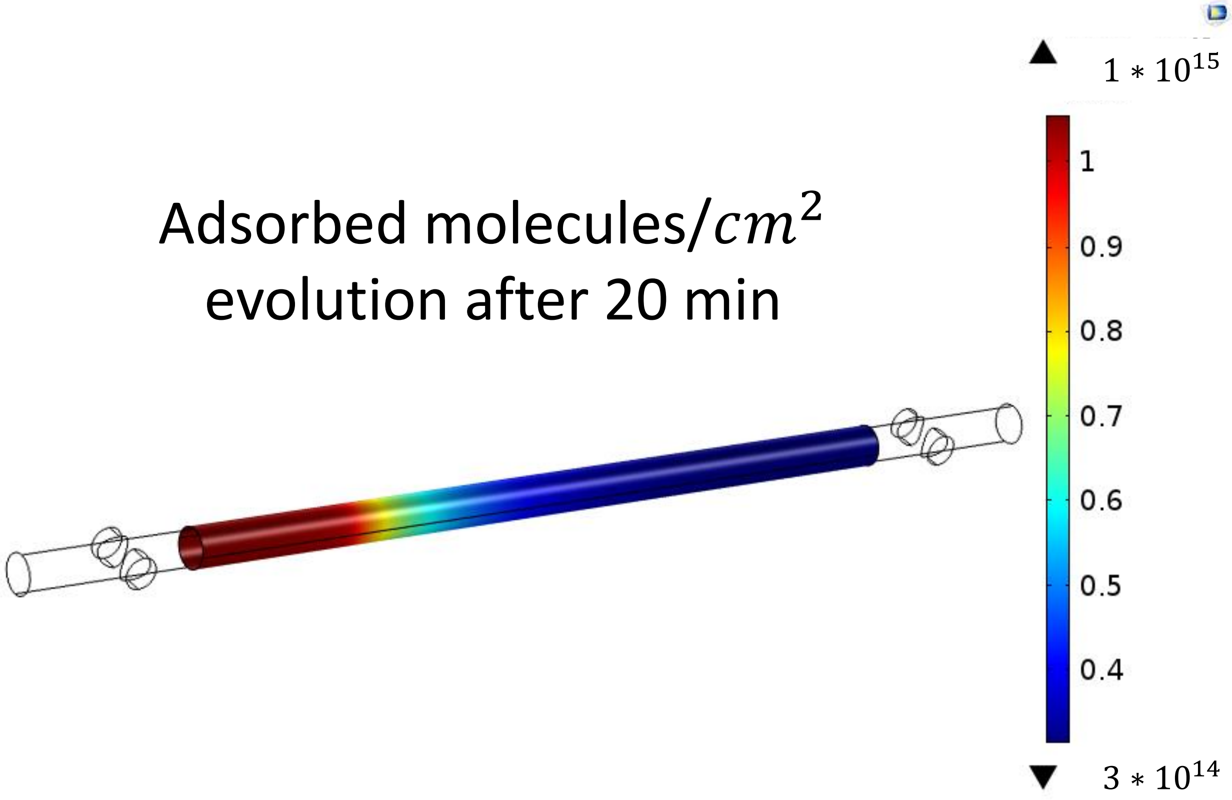


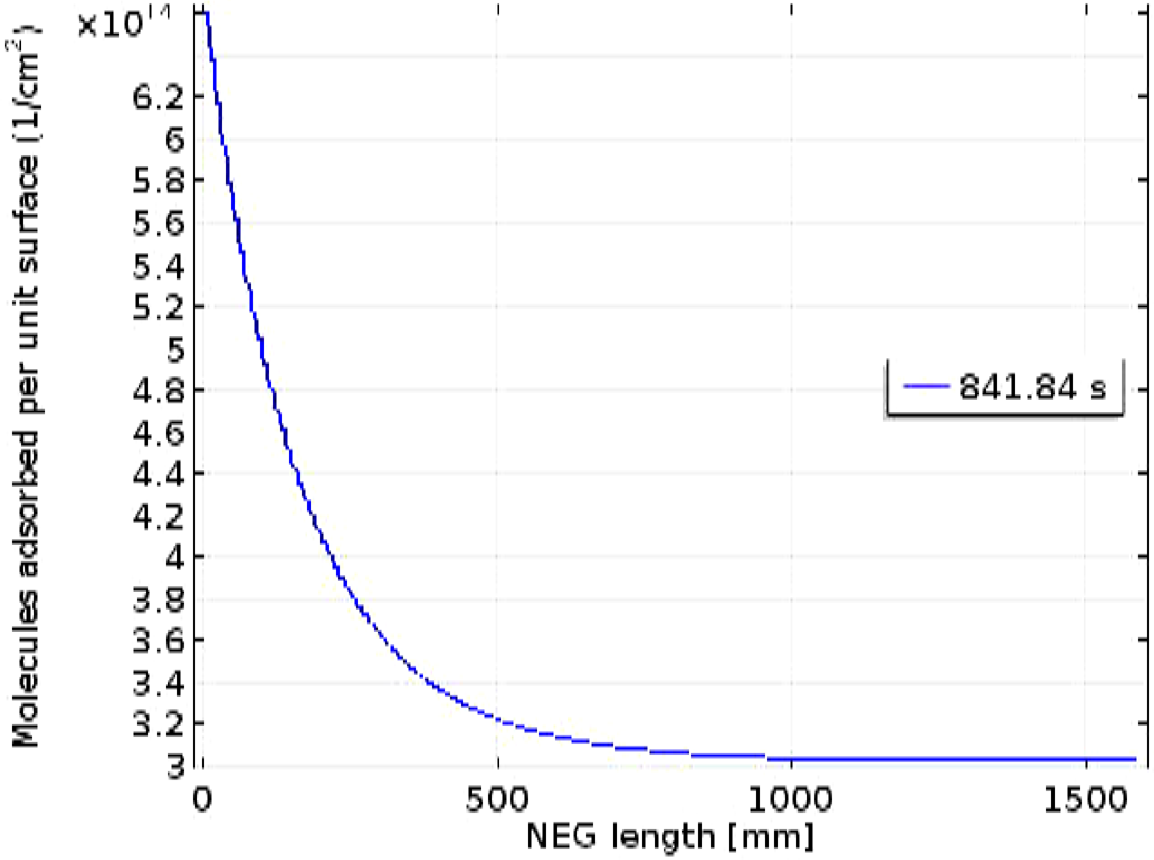
Saturation proceeds as a wave:
NEG adsorbent sites lose their properties behaving as simple stainless steel.



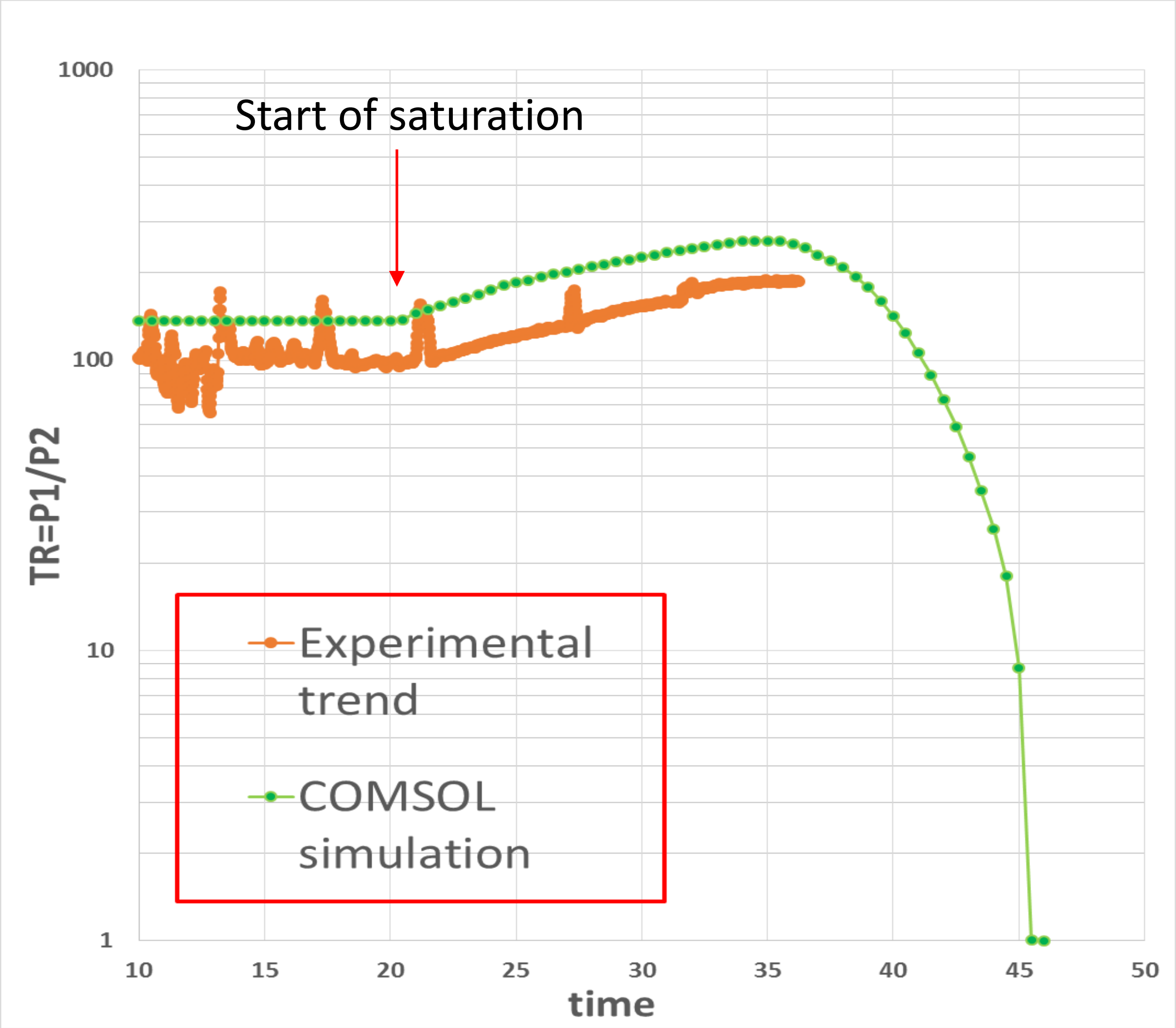
Simulated saturation process: Adsorbed molecules

Adsorbed molecules/cm^2 evolution after 20 min



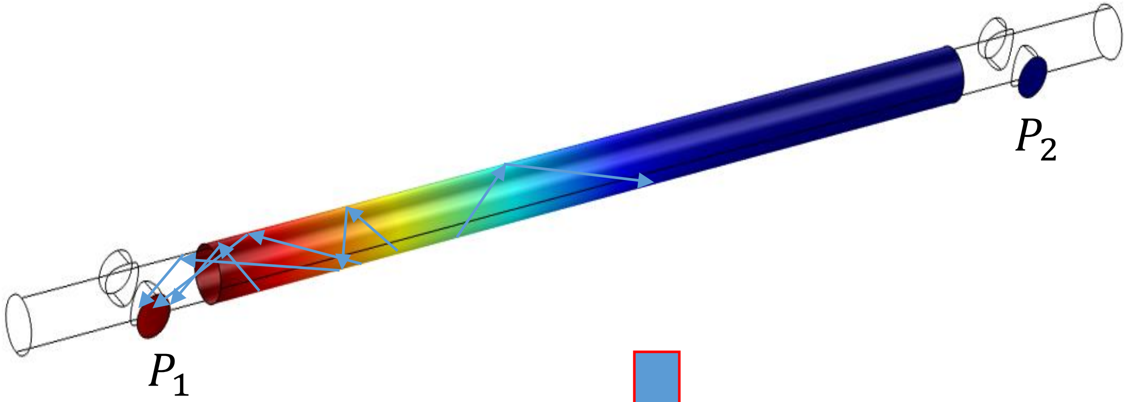


Experimental bench mark



Simulation transmission ratio trend follows the experimental one.

Transmission rises at first: molecules have a higher probability to be recorded at the entrance gauge.



Full saturation → Equilibrium P_1=P_2

Summary

- 3D dynamic saturation of a NEG coated chamber has been simulated with COMSOL. No other software available for 3D dynamic molecular flow simulation with variable sticking factors and absorption.
- The simulation agrees with the experimental data.
- Simulations can estimate the amount of gas to be injected before saturation.
- Potential uses of COMSOL:
  - Pressure evolution with NEG saturation in complex 3D geometries.
  - Reverse problem → Known transmission ratio calculate sticking factor through optimization in complex 3D geometries.

Thanks for your attention!