Vacuum chamber conditioning and saturation simulation tool (VacuumCOST)

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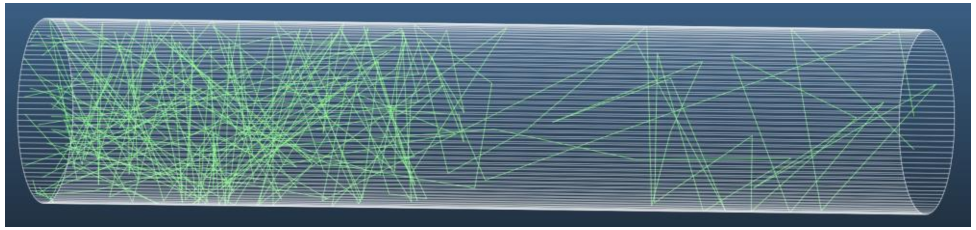
13/06/2023

Objective of this talk

- <u>Not</u> exactly NEG coating saturation despite what the seminar invitation said...
- Demonstration of a <u>tool</u> for time-dependent vacuum simulations (using MolFlow).
  1. How it functions.
  2. Testing/benchmarking
  3. Demonstration of results

Quick MolFlow reminder

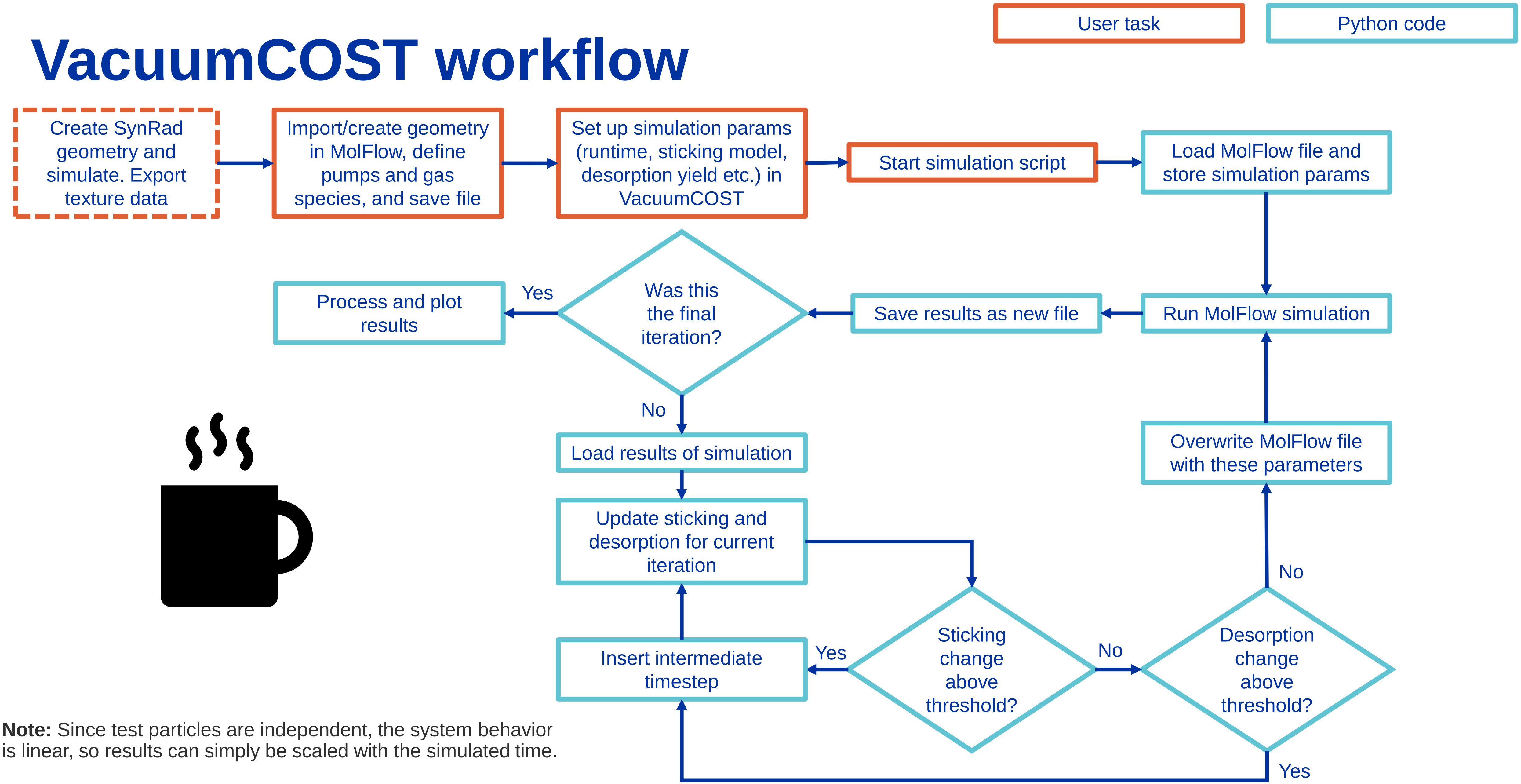


- **Molecular flow simulations using TPMC method.**
- **Simulate different gas species in more or less any geometry.**
- **Define desorption and pumping speed (sticking factor) for individual facets.**
  - Possible to import textured desorption from SynRad.

... so why VacuumCOST?

- **MolFlow is highly suitable for steady-state simulations.**
  - In time-dependent mode, parameters must be pre-defined. Does not update simulation parameters based on results of earlier moments.
- **VacuumCOST calls MolFlow iteratively to simulate using a time marching method.**
  - Updating parameters automatically between each step.

VacuumCOST workflow

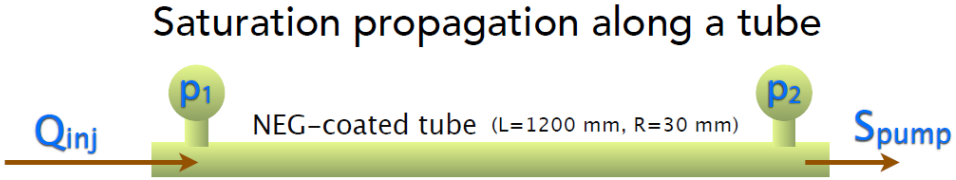


Note: Since test particles are independent, the system behavior is linear, so results can simply be scaled with the simulated time.

Initial test – benchmarking with similar code

Reproduce results from one of our colleagues in Japan:

- **Simple model of gas injection into NEG-coated tube.**
- **Assume initial sticking coefficient 1 and linear decrease as function of surface coverage.**
- **Fixed quasi-linear time step spacing (~100 s resolution).**

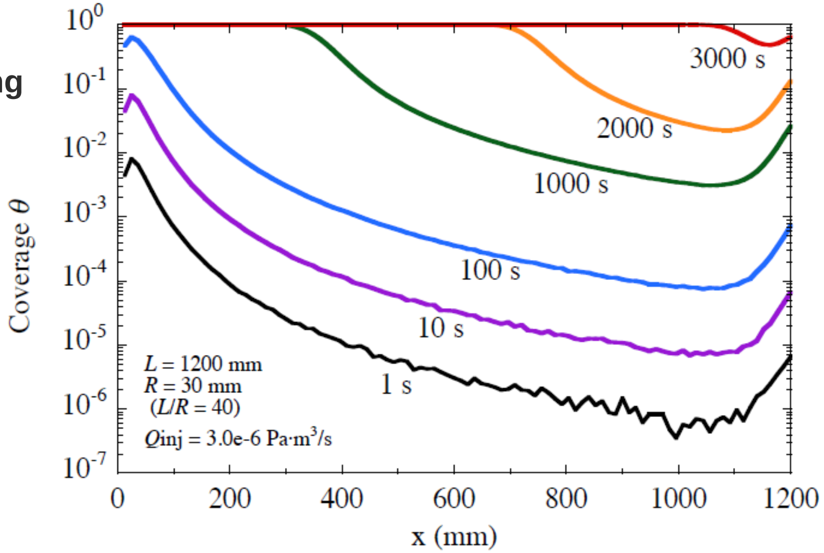


s_0 (initial sticking probability) = 1

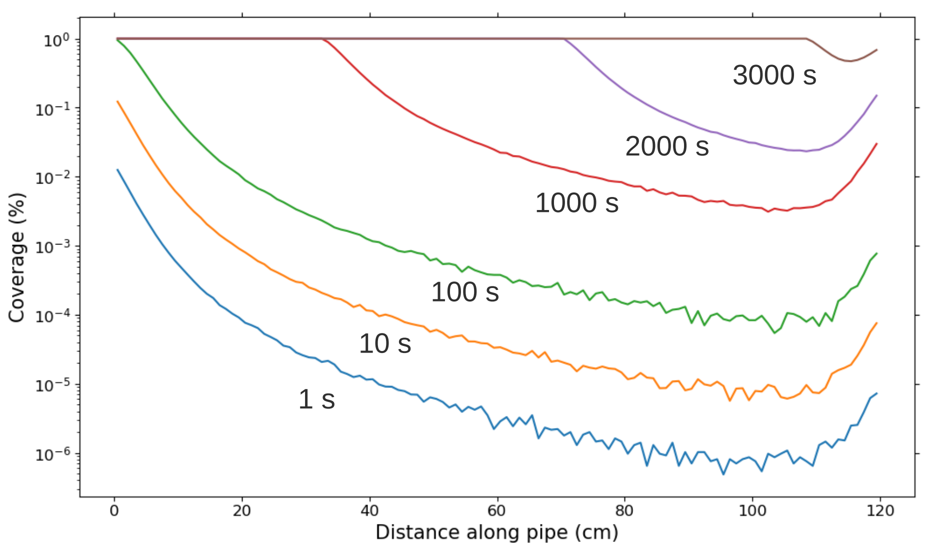
$Q_{inj} = 3.0\times10^{-6}$ Pa·m³/s (= 7.23×10^{6} MCP/s × 10^{8} molecules/MCP × kT), S_{pump} = 7 L/s

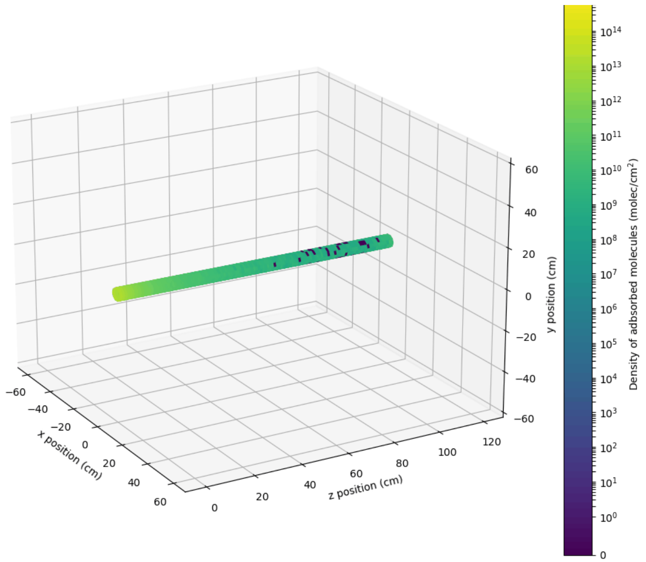
$\sigma_{ML} = 1.0\times10^{19}$ molecules/m²

Credit: Yasunori Tanimoto [1]



VacuumCOST result





Importance of temporal resolution

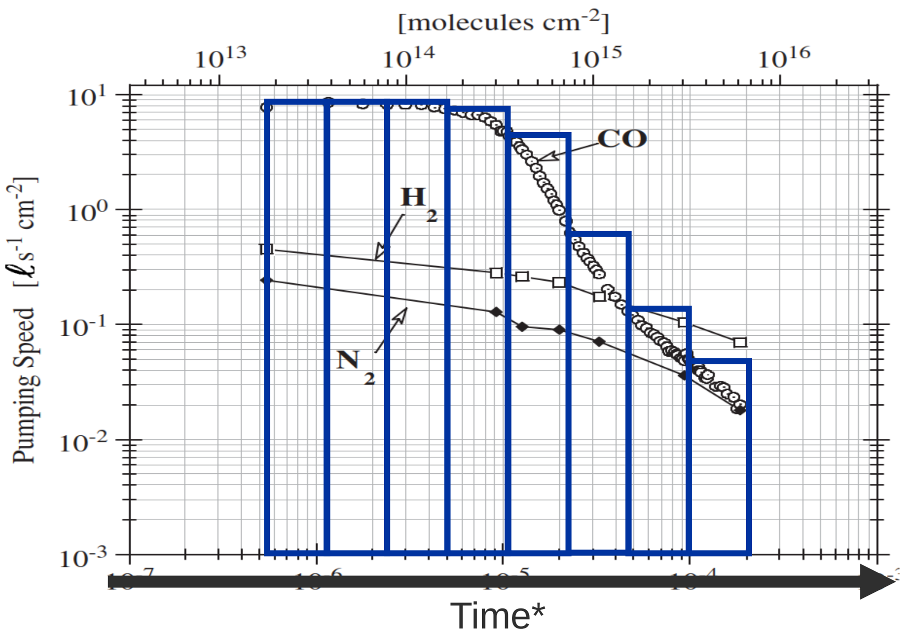
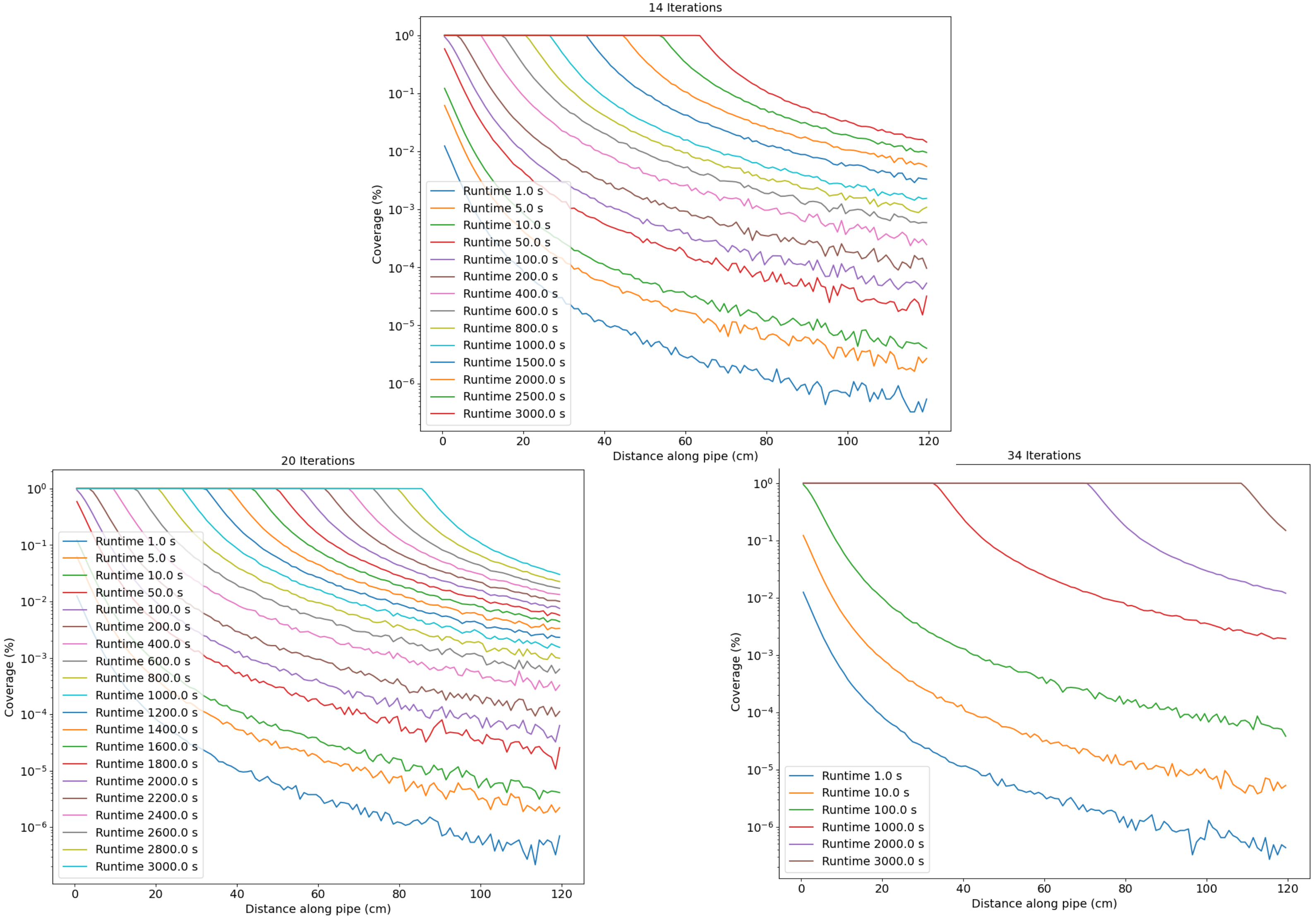


Figure adapted from [2]

*Assuming continuous presence of gas.

Effect on simulated NEG saturation in tube

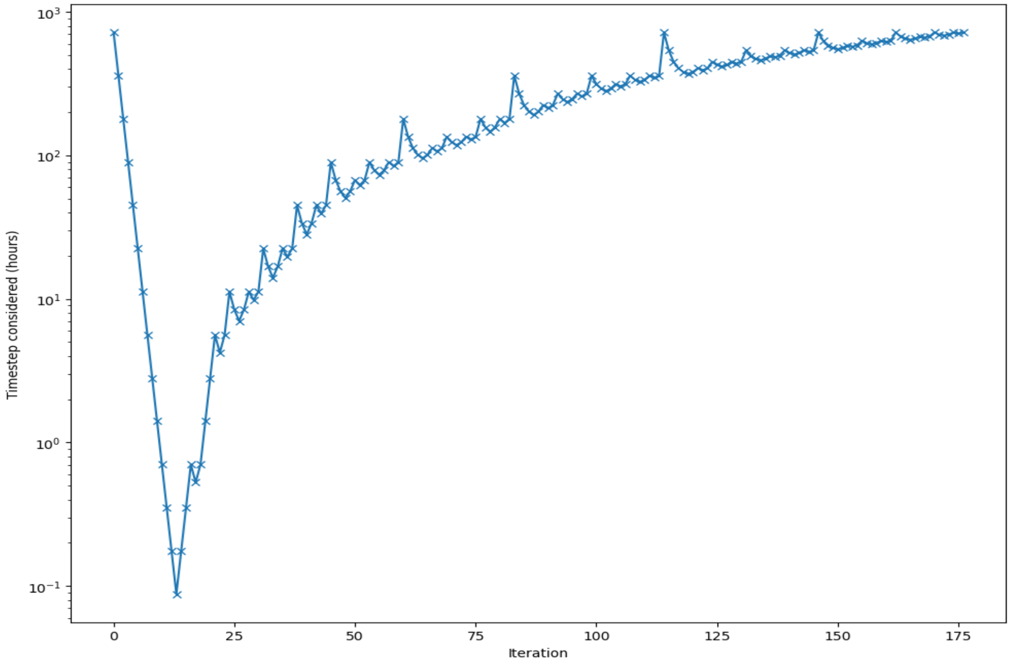


Determining required temporal resolution

- **Temporal resolution affects simulation results!**
  - The simulation is always lagging behind physical time both for saturation and desorption.
- **What is “sufficient” temporal resolution to minimize this discrepancy?**
  - May be difficult to know beforehand.
  - Steps can be pre-defined (linear, log, user-defined spacing).
- **VacuumCOST can also determine required resolution for you.**
  - Benefits:
    - Dynamic resolution only as good as required.
    - Automatically adapts to sudden changes in vacuum environment.
  - Drawbacks:
    - Non-uniform step spacing throughout simulation.
    - Total simulation time not known beforehand.

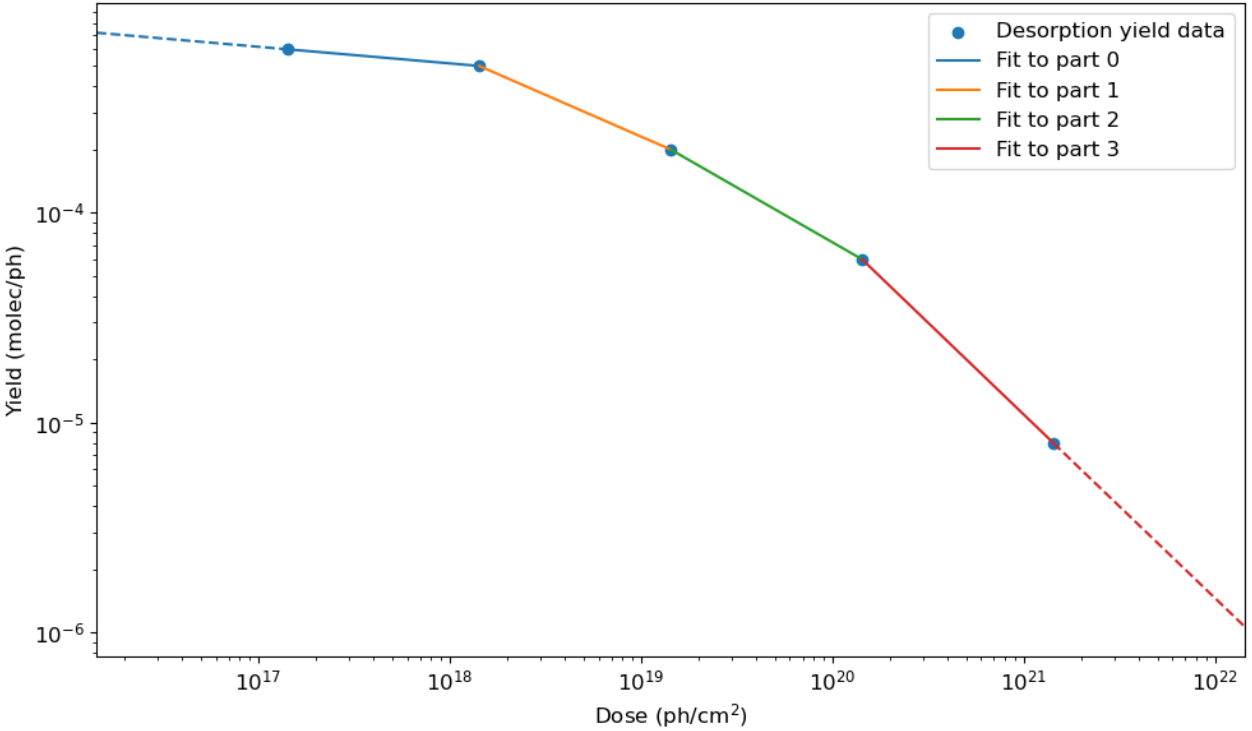
Automatic insertion of time steps

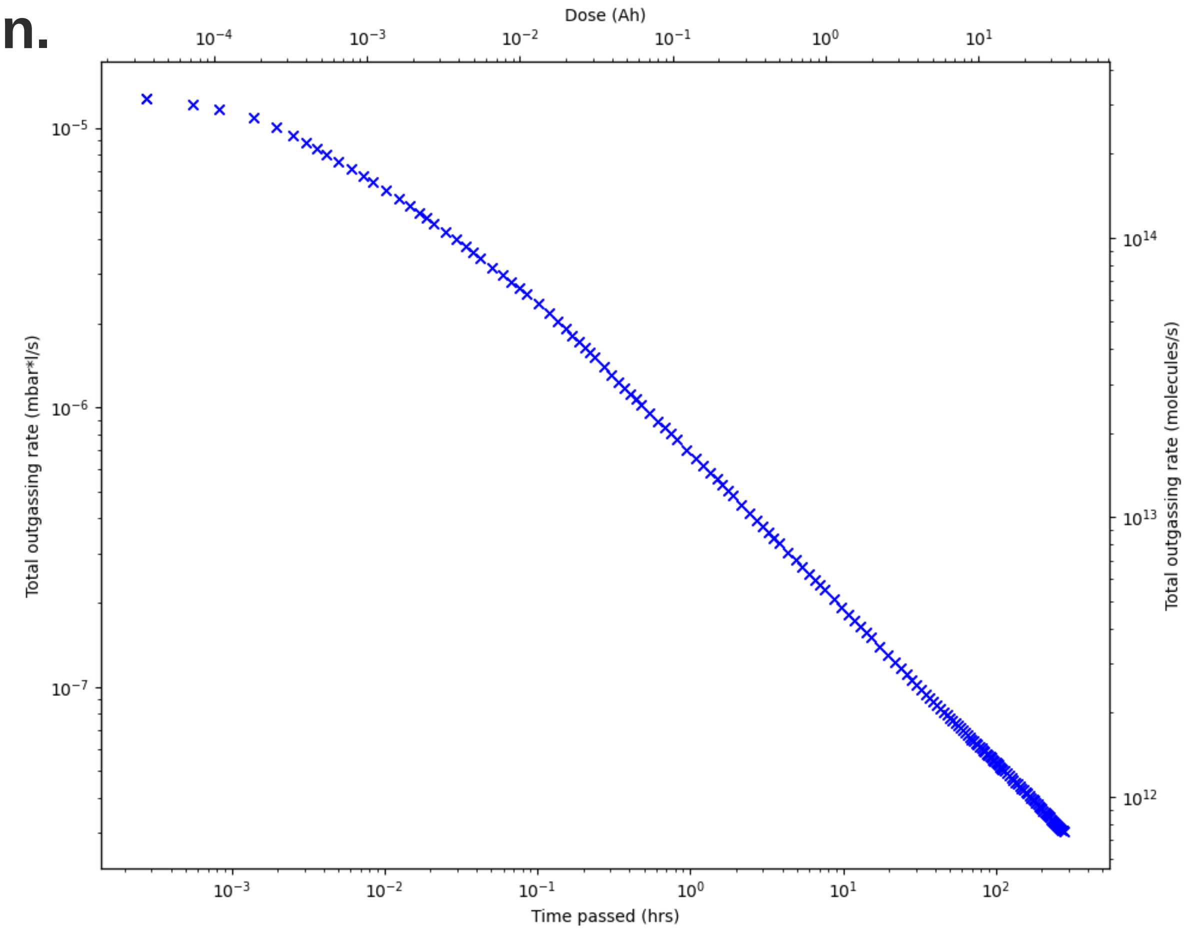
1. Start with only initial and final time steps.
2. After simulating a step, calculate the change in sticking across subset of facets*.
3. If change is above user-defined threshold, insert intermediate time step.



Dynamic desorption from SynRad

Calculate SR flux density and integrate to find dose.
SR flux is then used to determine PSD evolution.





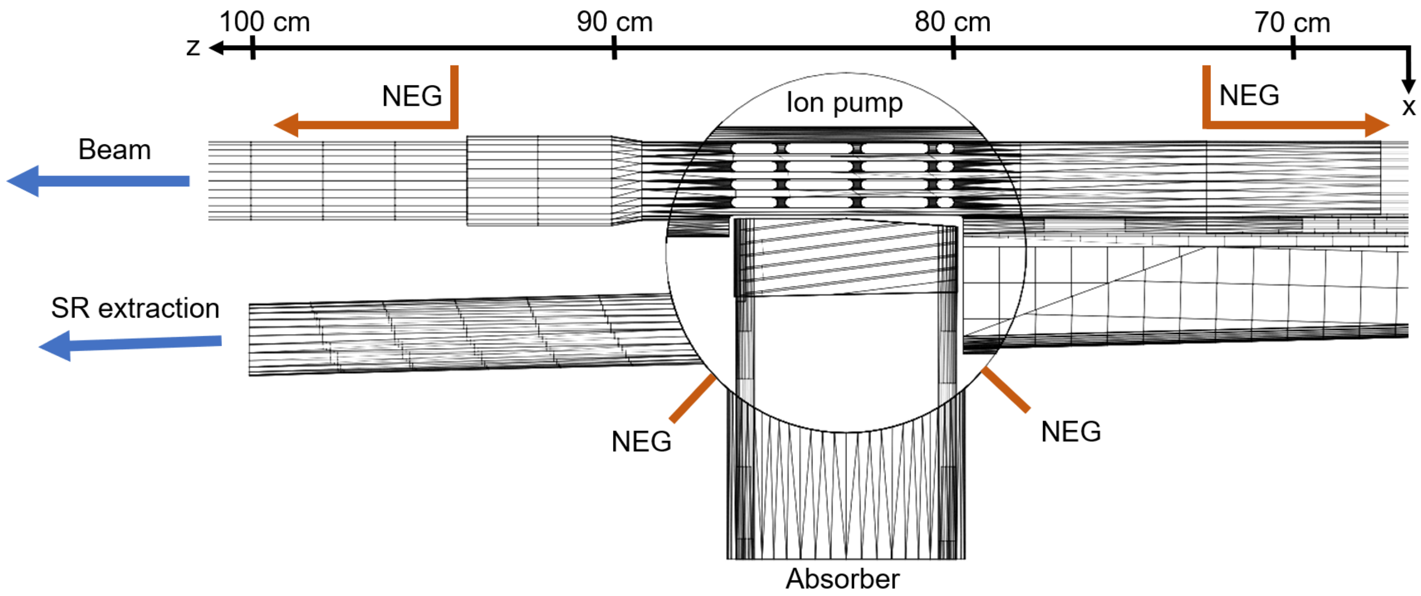
- Also criteria for injection of time step.
- Possibility of using multiple different desorption yield maps and pre-conditioning.

Code validation: MAX IV crotch absorber simulation

Real-world example of NEG-coated region in a light source.

1. **Get photon flux density from SynRad.**

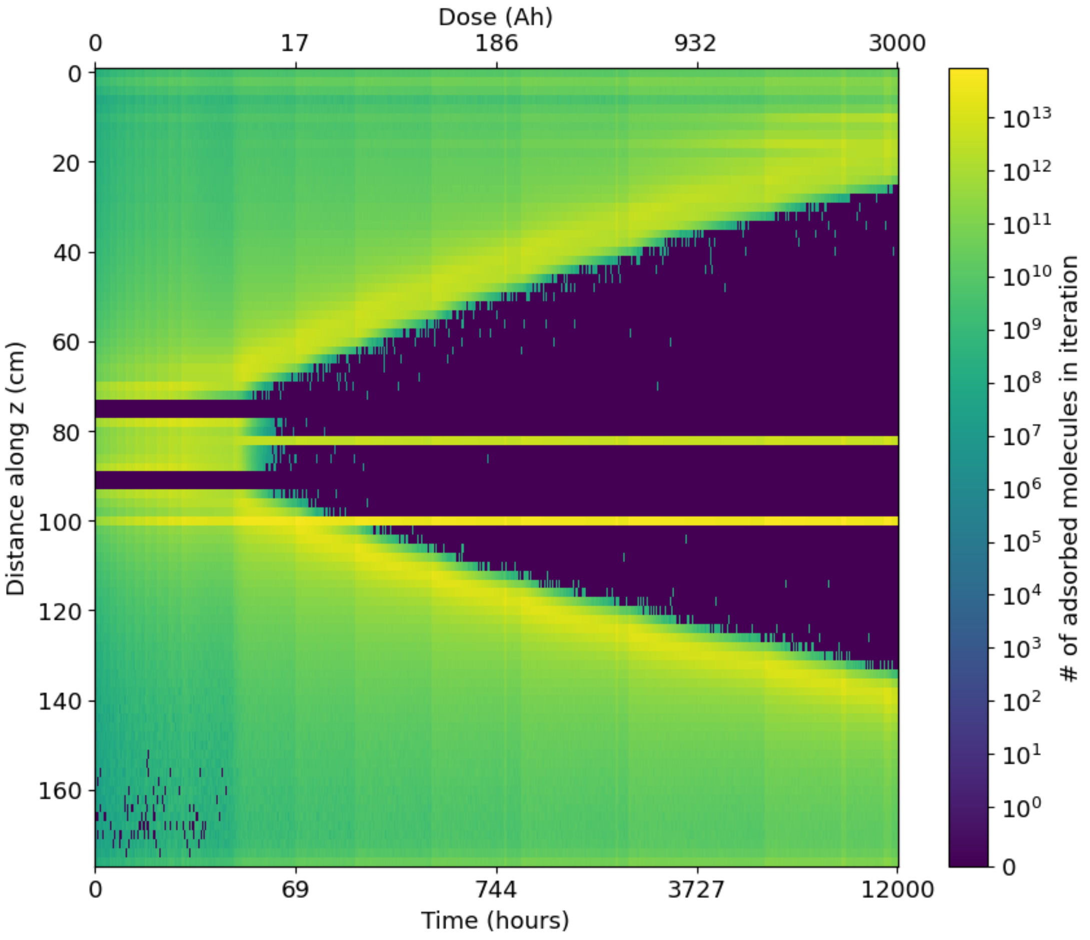
2. **Simulate using MolFlow/VacuumCOST.**

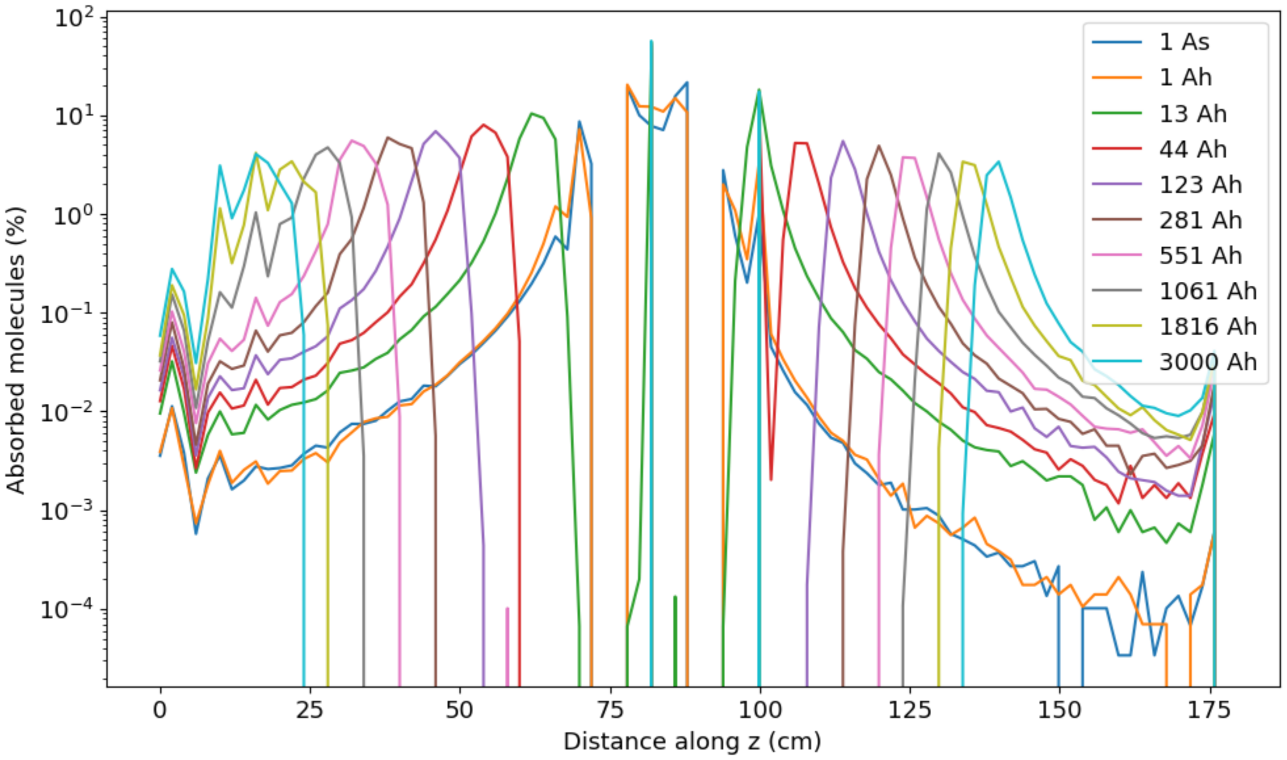


About 1600 time steps tested for a final of ~700 steps used to simulate the system until 3k Ah.

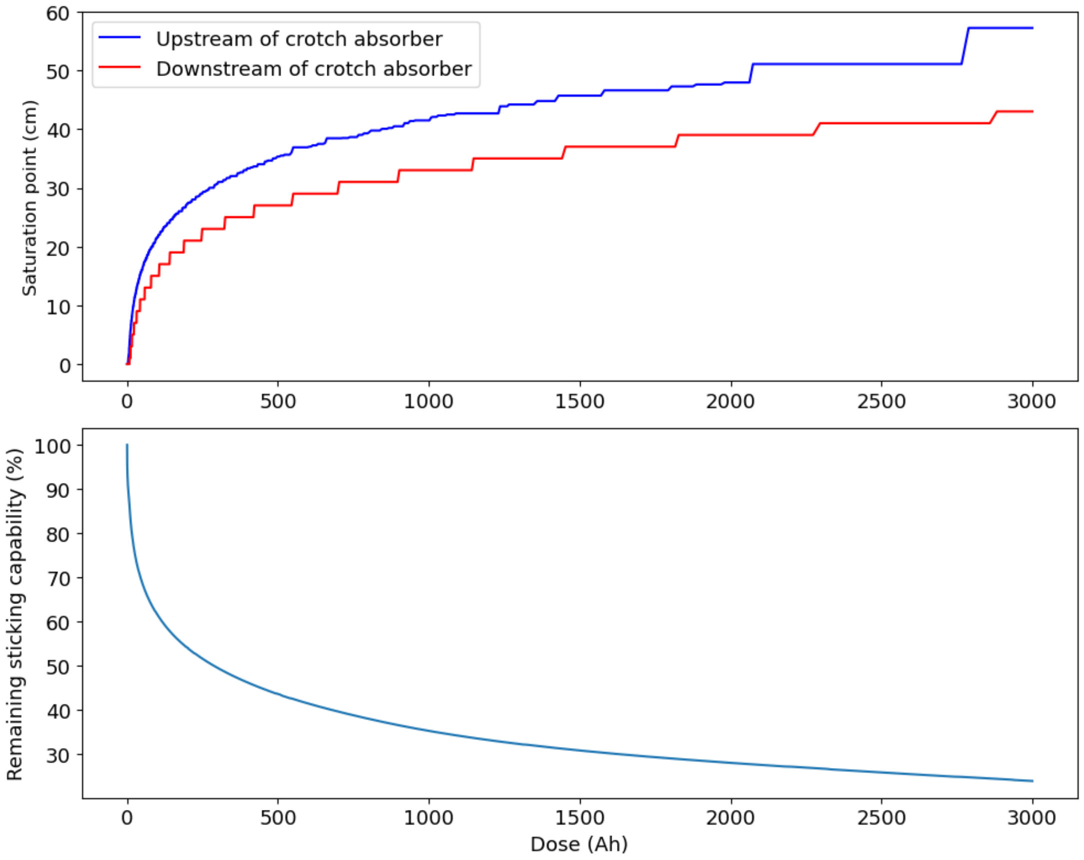
Code validation: MAX IV crotch absorber simulation

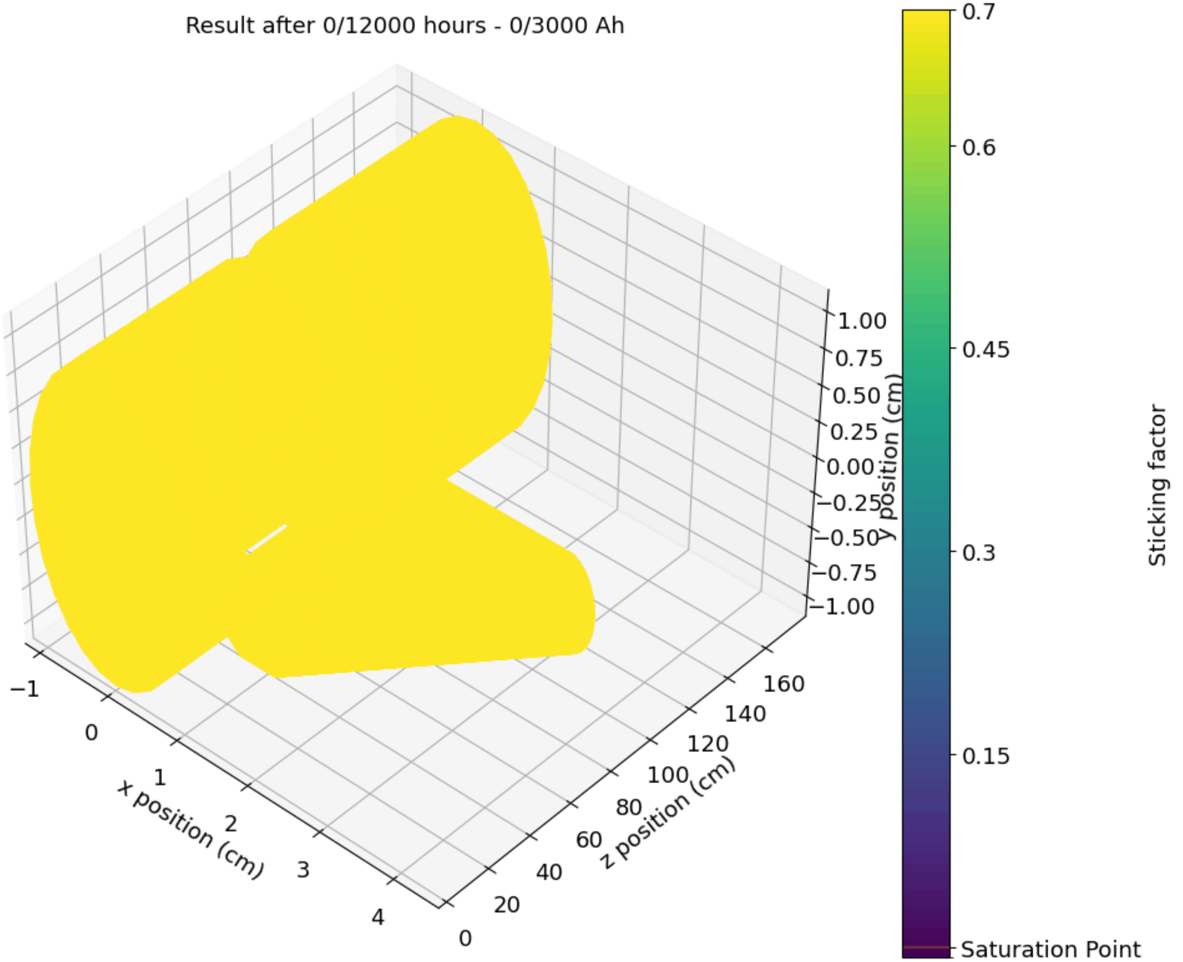
Location of molecule absorption as function of time.



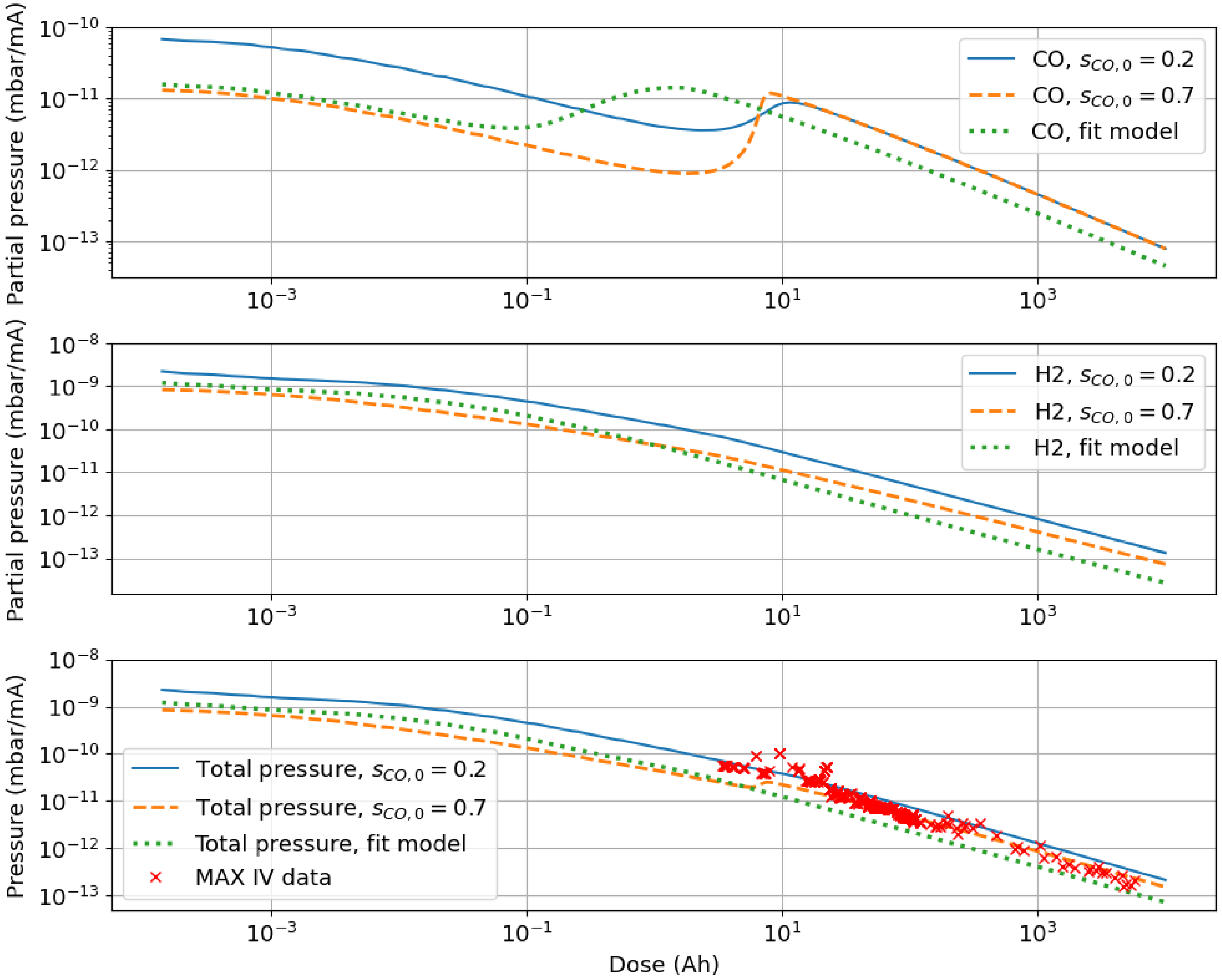


Code validation: MAX IV crotch absorber simulation





Code validation: MAX IV crotch absorber simulation



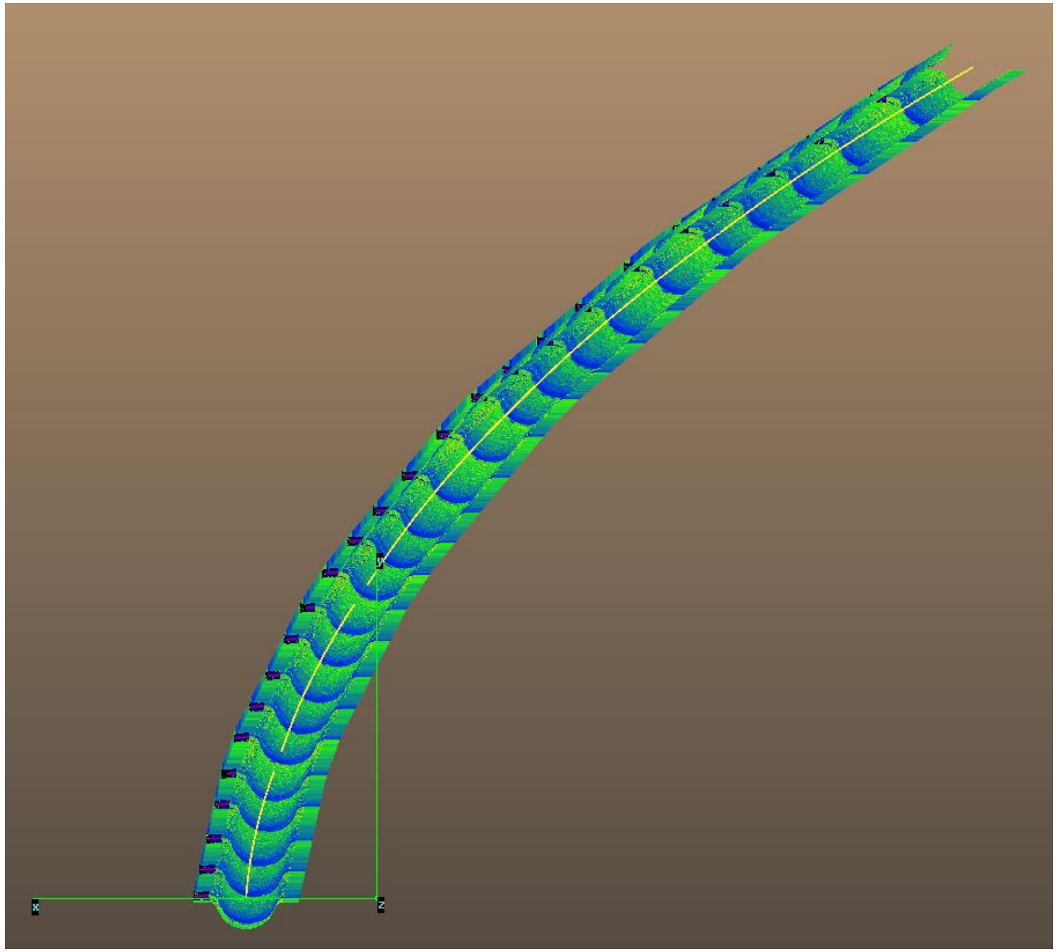
Other usage example: Simulating a leak in FCC-ee

Geometry with photon absorbers every ~5.6 m
Beam pipe fully NEG-coated
(design maybe not up to date...).

1. **Get photon flux density from SynRad (pictured).**

2. **Simulate using MolFlow/VacuumCOST.**

   - Introduce a 1e-5 mbar*l/s leak occurring after 100 Ah of conditioning.



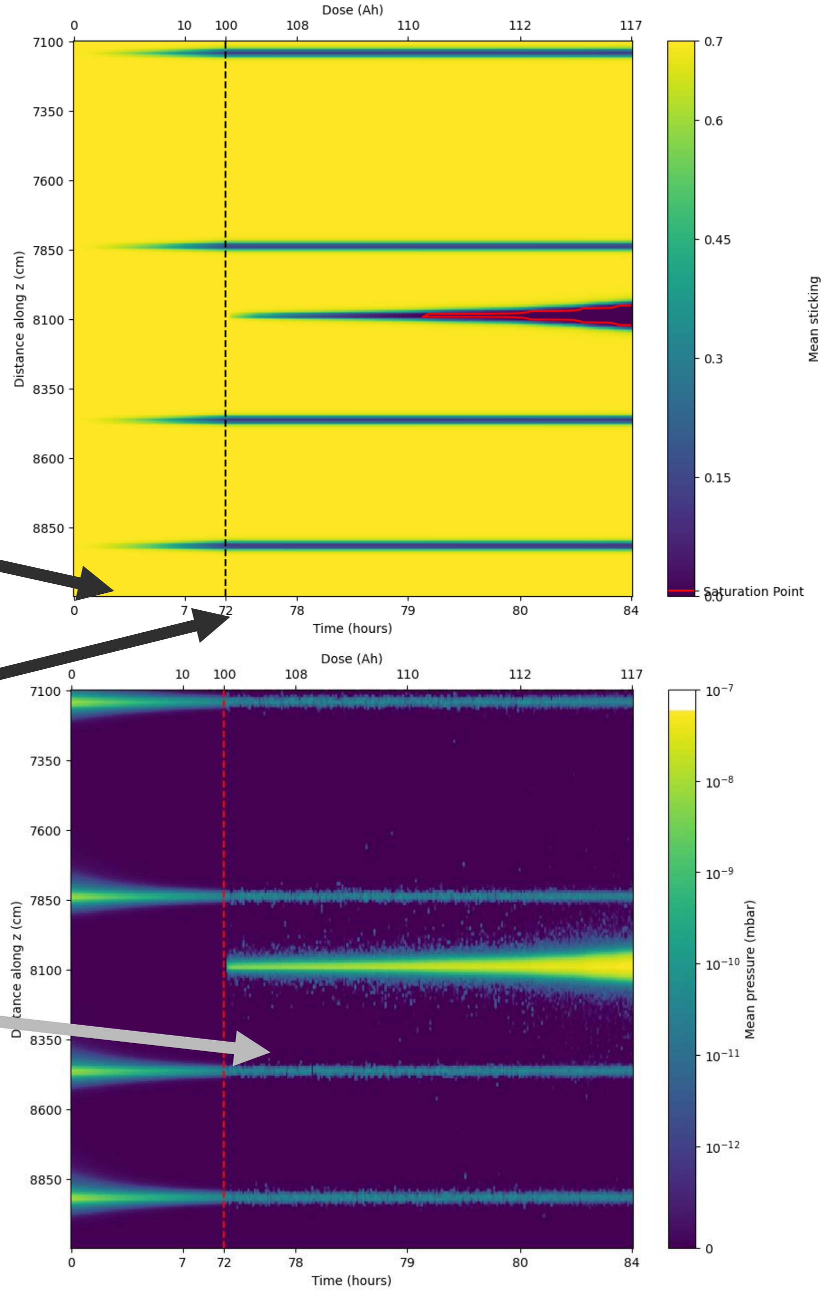
Simulating a leak in FCC-ee

Zoomed in on region with 4 absorbers.

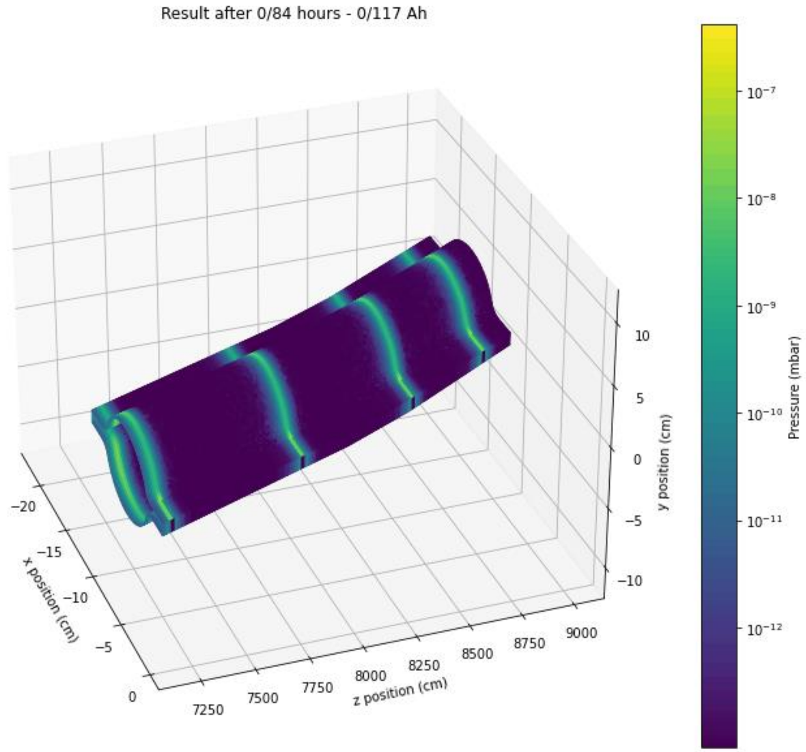
Temporal resolution decreases with conditioning.

Temporal resolution increases when leak occurs.

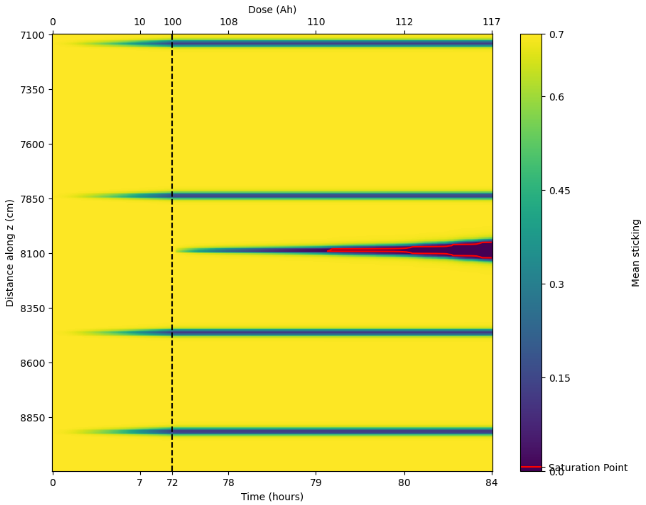
Insufficient statistics!

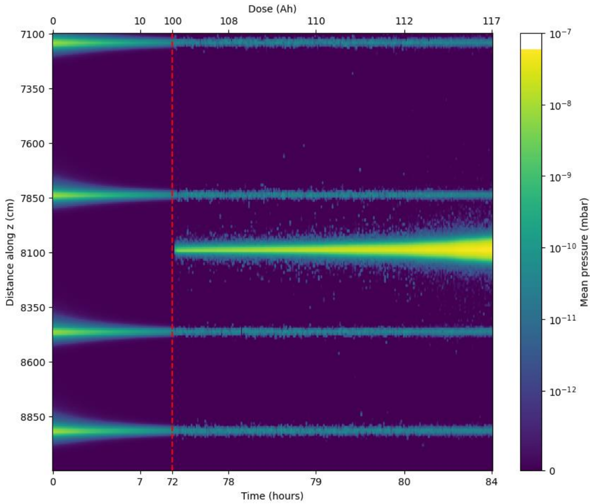


Leak in FCC-ee (improved statistics)

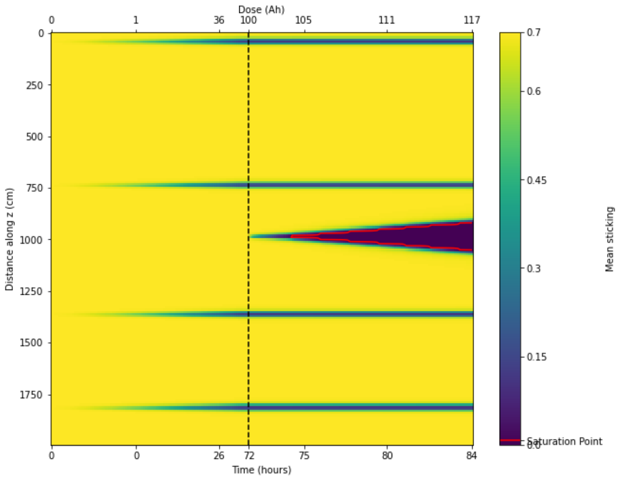


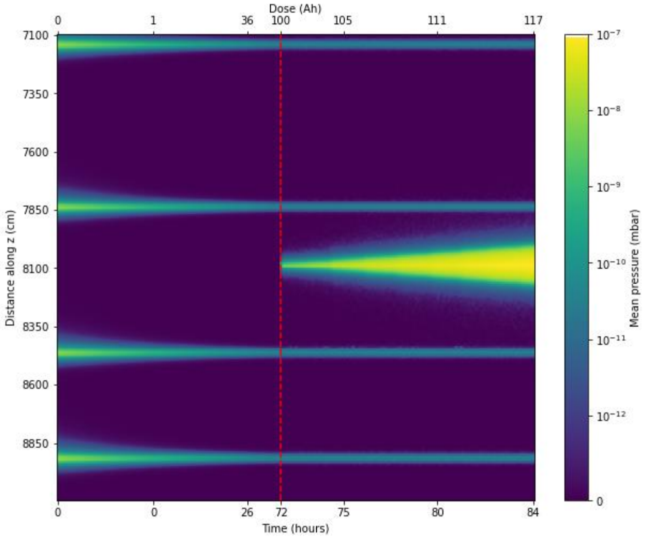
Before (36 hrs CPU time)



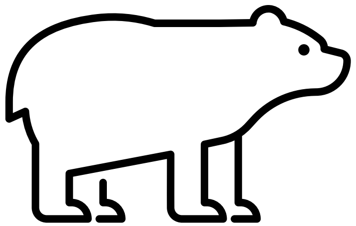


After (75 hrs CPU time)





Things to bear in mind



- **Each iteration will create a new file.**
  - Can use a lot of disk space for simulations with large geometries and many iterations (and high spatial resolution requires many facets!).

- **Only one gas species can be simulated at a time.**

- **No GUI → A little bit of programming knowledge is required (but not much!).**

- **Finding the right trade-off between simulation time and statistics + resolution takes a bit of trial and error..**
  1. Start by simulating a short time rather than simulating the full physical time desired.
  2. Decide from there the CPU time per iteration and temporal+spatial resolution required.

Summary and outlook

VacuumCOST can simulate NEG saturation front, pressure evolution, leaks, etc. but:

- **Beware of sticking model sensitivity.**
- **Spatial/temporal resolution highly affects accuracy of results!**

This feature will hopefully be implemented directly in MolFlow at some point in the future...

Code available at: https://gitlab.cern.ch/phenriks/vacuumcost

Paper: https://doi.org/10.1016/j.vacuum.2023.111992

References

[1] Yasunori Tanimoto: Presentation at JSAP 2016.

[2] Paolo Chiggiato & Pedro Costa Pinto (Oct 2006): Ti-Zr-V non-evaporable getter films: From development to large scale production for the Large Hadron Collider**. Thin Solid Films, 515(2), 382-388. DOI: 101016/jtsf200512218**

P.L. Henriksen, M. Ady, R. Kersevan: Vacuum chamber conditioning and saturation simulation tool (VacuumCOST): Enabling time-dependent simulations of pressure and NEG sticking in UHV chambers. **Vacuum Volume 212, June 2023, 111992. DOI: 10.1016/j.vacuum.2023.111992**

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Backup slides

Choosing NEG sticking models

Standard models in VacuumCOST:

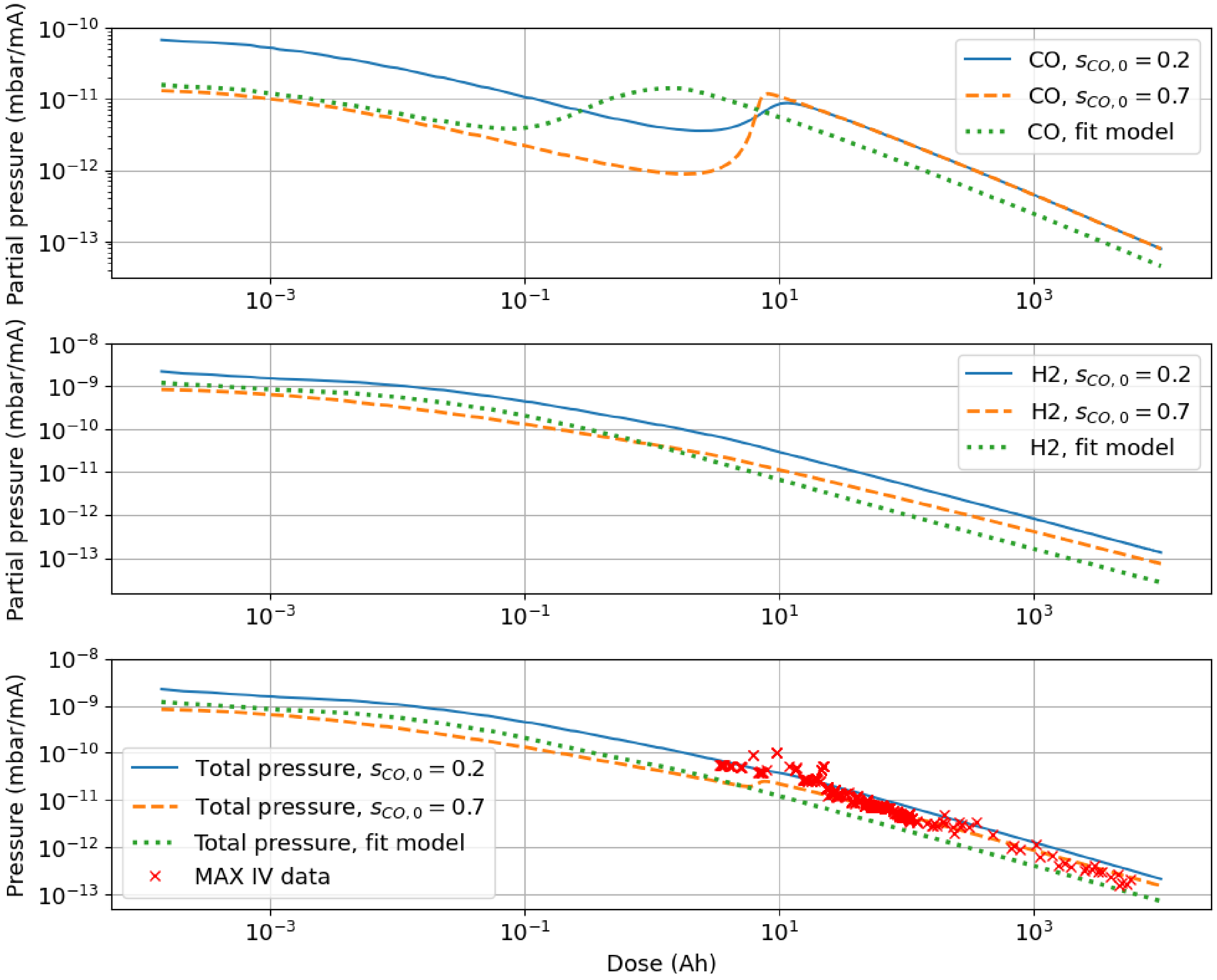
$$s_{CO} = s_{CO,0}\left(1 - \frac{Q_{CO}}{Q_{CO,ml}}\right)$$

$$s_{H_2} = s_{H_2,0}\left(1 - \frac{Q_{CO}}{Q_{CO,ml}}\right)^2$$

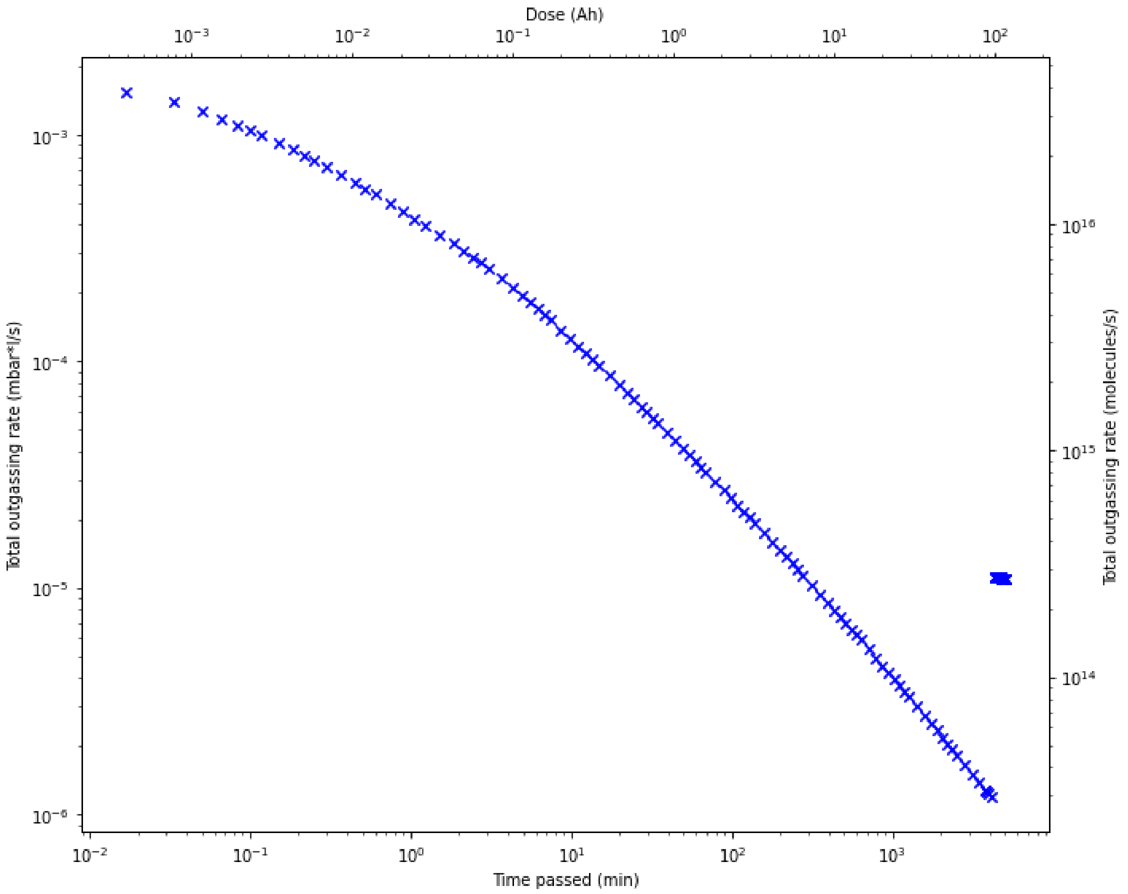
$$Q_{CO,ml} = 2 \times 10^{15} \text{ molecules/cm}^2$$

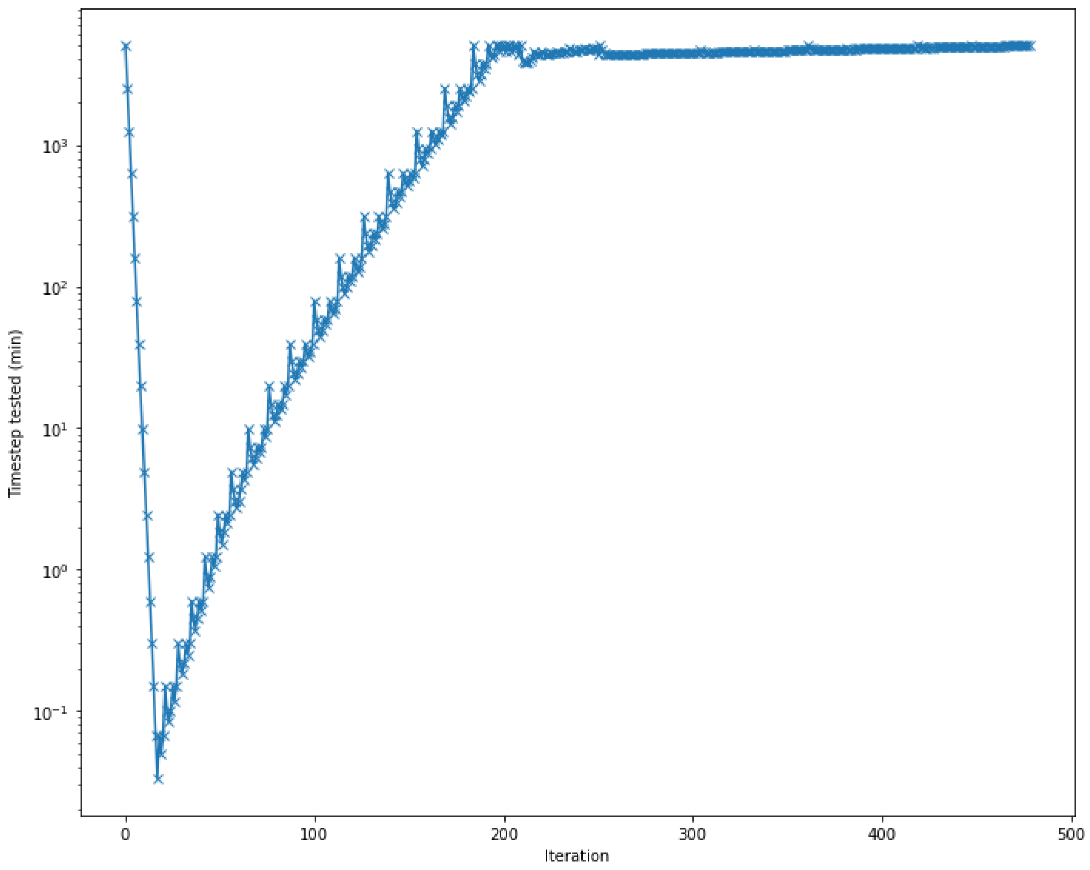
$$s_{CO,0} = 0.7 \text{ and } s_{H_2,0} = 8 \times 10^{-3}$$

Ref. [2]



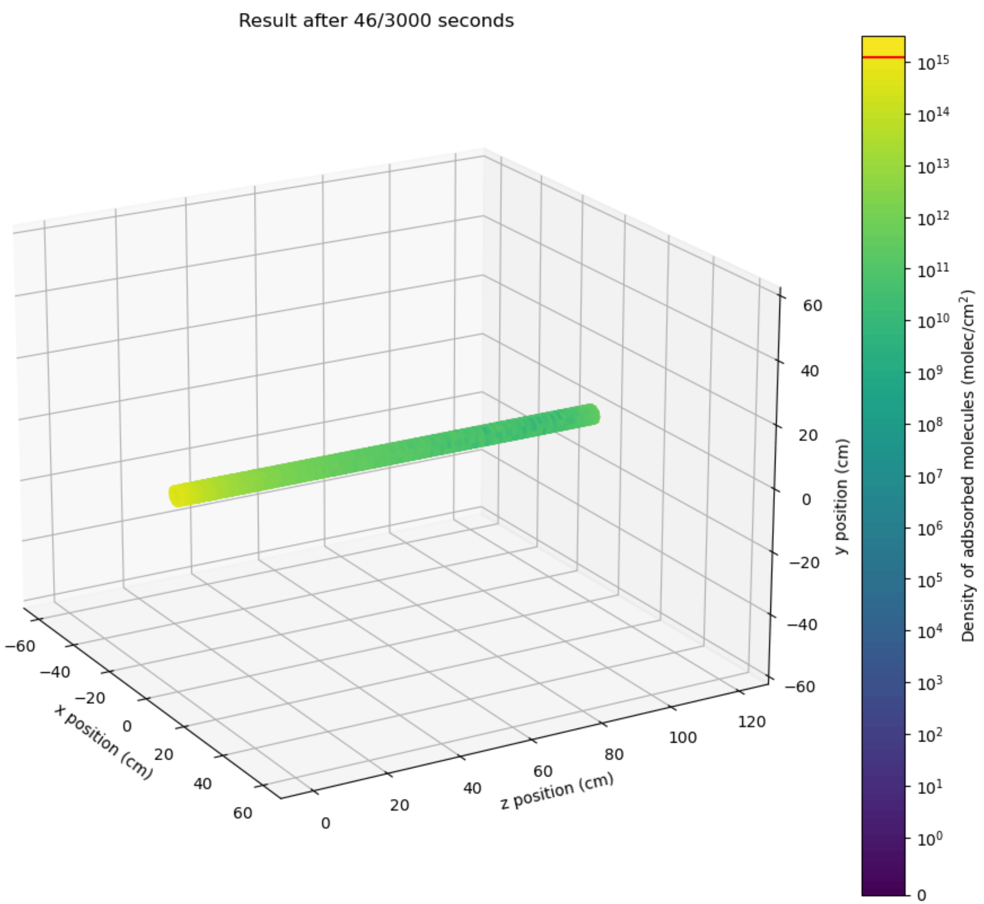
Simulating a leak in FCC-ee



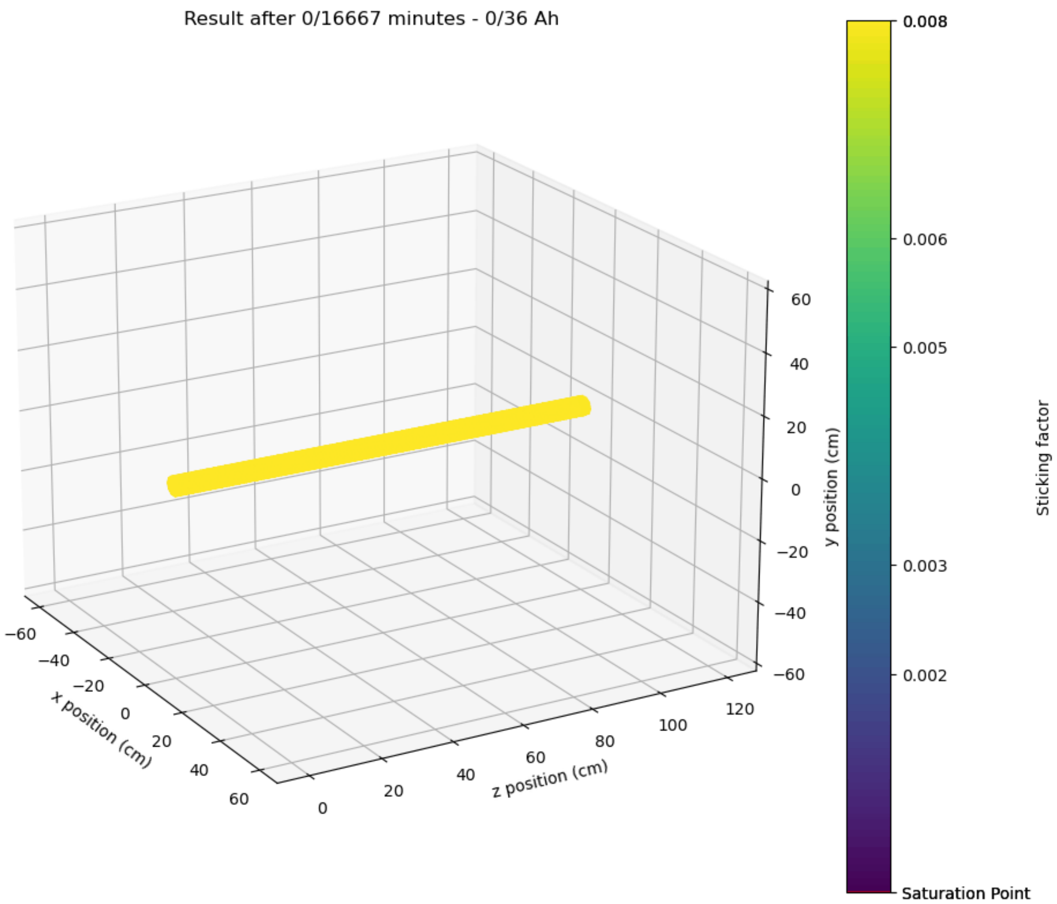


Two example of simulation results

Constant CO injection from left side of pipe



PSD of H_2 in closed tube



Recommended user-modifications to code

Things that should always be modified:

- Model-dependent parameters: Surface material, gas species, pumping speeds, “active facets”, selection group names, texture data from SynRad, etc.
- Scripts for post-processing of data.

Settings users should consider modifying:

- Sticking models.
- Criteria for injecting time steps.
  - Relative + min change in sticking.
  - Disregarding microfacets.