Molflow+ tutorial

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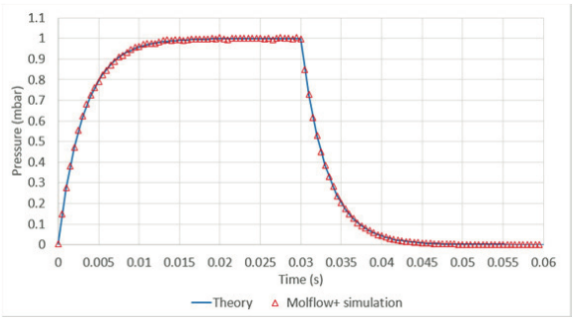
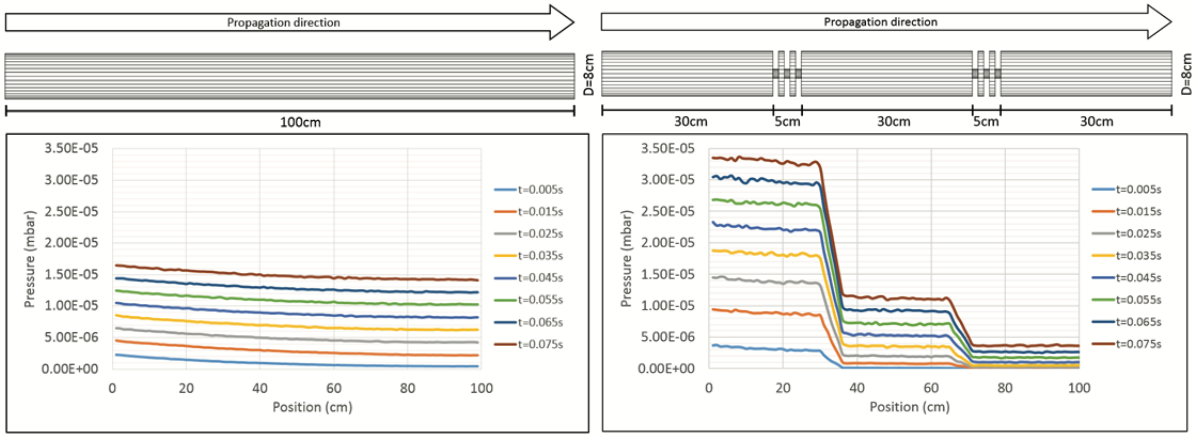
(more on http://test-molflow.web.cern.ch/ → Molflow documentation→AVS-61)





Time-dependent examples

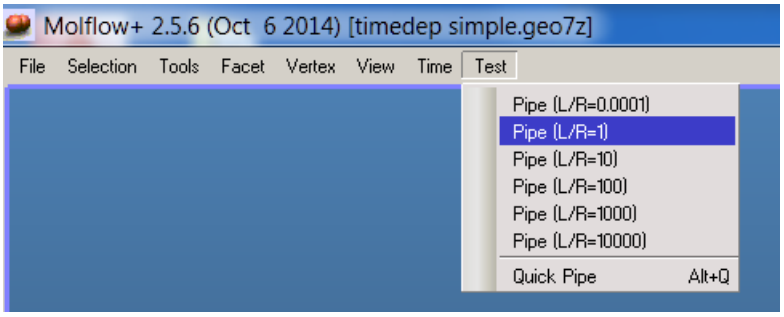
In this tutorial we will see a simple example that familiarizes you with the time-dependent mode of Molflow, then we'll see a real usage example. This tutorial shouhld be done after the first one, which introduces you the basics of Molflow.

A simple time-dependent example

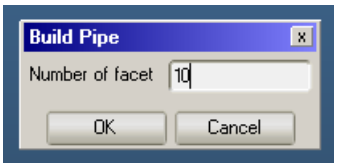
The purpose of this example is to show you the basic idea behind time-dependent simulations, and get you familiar with the controls. We will simulate a gas injection then a pump-down process.

For this, we will use the simplest geometry possible: a short cylinder. The reason is it is a simple volume which isn't conductance-limited.

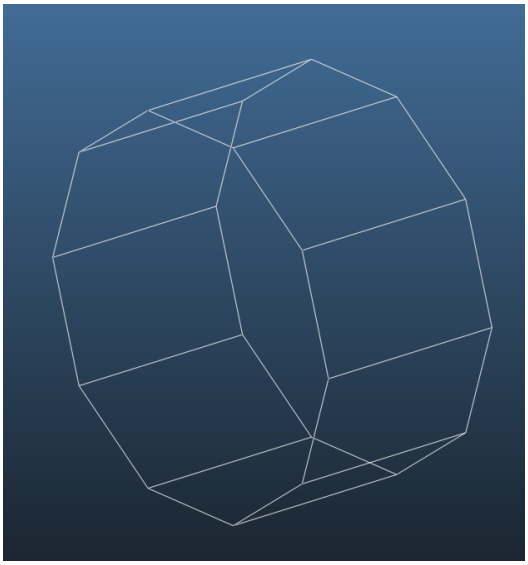
- Open Molflow
- From the Test menu, choose Pipe (L/R=1)



- Choose a small number of side facets, for example 10:

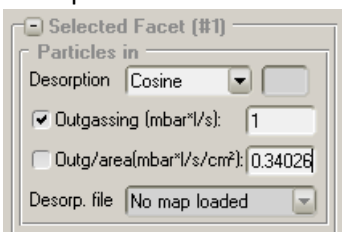


- There you go, you just created your simple cylinder:



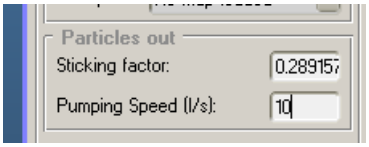
Reminder: You can zoom in/out with the mouse wheel, rotate the geometry with the right mouse button pressed, pan (move) with the middle mouse button pressed, and enable/disable volume view in the top right corner

- Add outgassing. For this, select one of the circular facets. In the Particles In section, choose “Cosine” as desorption and set it to 1E-4 mbar*l/s. When it’s ready, you should see this on the right side:



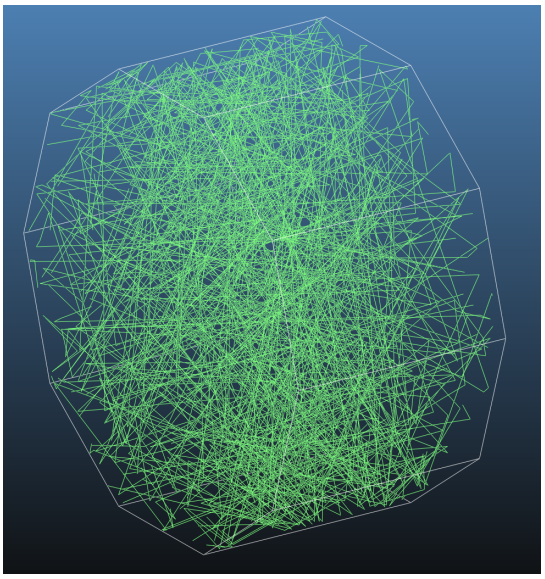
- Click Apply

  Note: When you use the Test menu to create a cylinder, an outgassing of 10mbar*l/s is set by default. Feel free to modify it to 1E-4 mbar*l/s.
- Set up pumps: select both circular facets **one by one**, and set a pumping speed of 1 l/s in the Particles Out section:

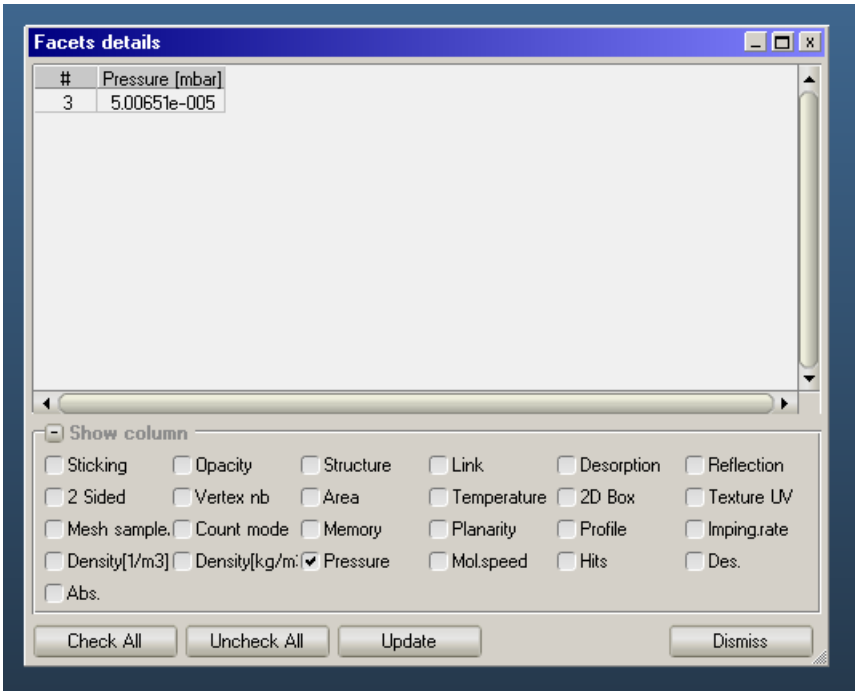


  As you type into the Pumping Speed field, the sticking factor updates automatically, based on the gas type and the temperature.
- Click Apply.

Now you have a working simulation: you can test it by pressing the Begin button, just like in the previous tutorial. By enabling the “Lines” view option, you’ll see the particle trajectories:



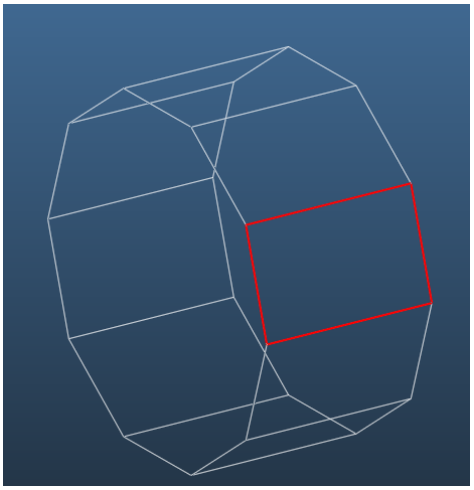
And by clicking on any facet and selecting the “Details…” button, we can see the pressure in the system:



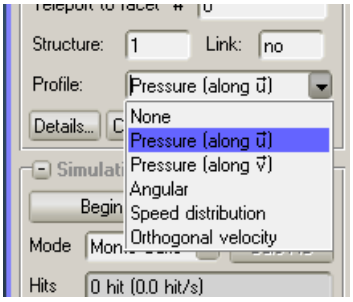
If you used the values suggested in the tutorial, you should get 5E-5 mbar steady-state pressure.

At this point, our simulation isn't particularly useful, nor time-dependent. So let's progress step by step! First, we'll add a profile to one of the longitudinal facets, that will serve as as a pressure indicator:

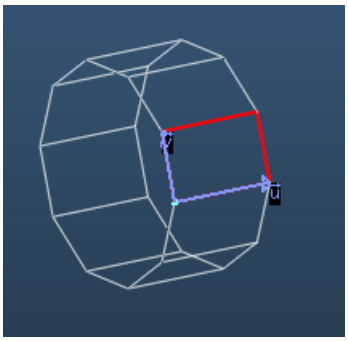
- Select one of the longitudinal facets:



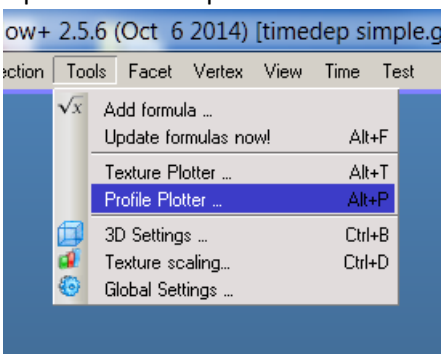
- In the facet parameters panel, set its Profile field to Pressure along u and click Apply:



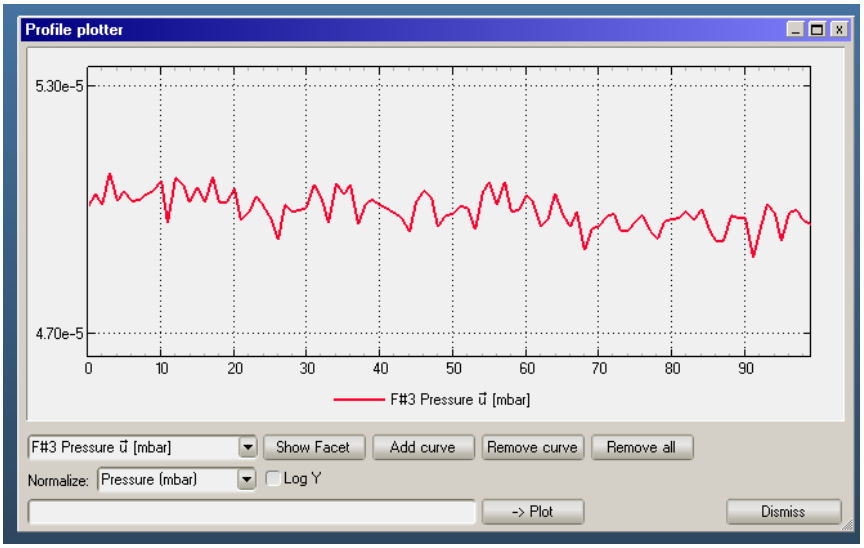
- Note: in this context the “along U” means that the facet is divided into 100 segments pointing towards the U vector. You can visualize the U vector by enabling “u,v” in the upper right corner:



- Begin the simulation
- Open the Profile plotter:

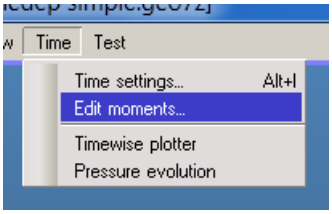


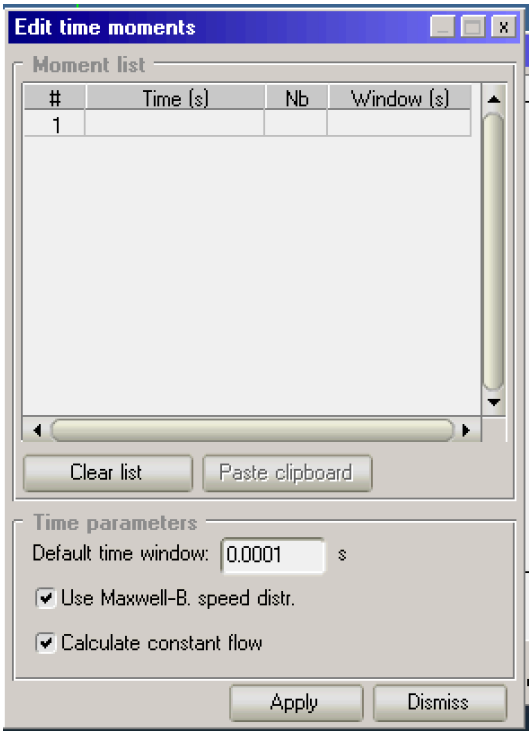
- The profile plotter doesn’t contain any curves by default, so click the “Add curve” button. Then you should see the pressure in the form of a nearly uniform plot:



For the moment, this is enough – let’s make the simulation time-dependent!

Everything begins in the Time / Edit moments… menu:



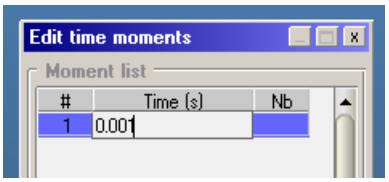


Now let's go through the parameters!

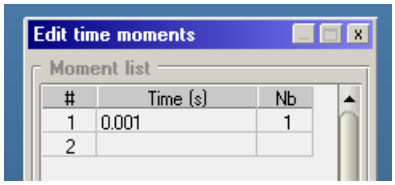
The user can define which moments he/she is interested in – and at those moments Molflow will calculate the pressure in the system. Note that the simulation is not chronologic, i.e. all moments are calculated at the same time.

- Each line has a field for the moment(s), the number of moments and the time window.
- The Time window length is a very important parameter. It can be regarded as an averaging length. In fact, Molflow performs time-dependent simulations by counting at what time the hits happen on the walls. Let's say we're interested in the pressure at t=1s. Obviously, no hit will happen at *exactly* 1.00000 seconds, therefore we have to define a tolerance. Setting the time window for 0.2s, for example, will catch every hit between t=0.9s and t=1.1s
    - Setting a small time window will reveal fast changes of the pressure, but statistical scattering will be high as the pressure needs to be calculated from fewer Monte Carlo hits
    - Setting a long time window will hide fast changes of pressure but will provide less scattering
    - As a thumb rule, the time window length should be a few orders smaller than the length of the process we're trying to simulate
- The "default time window" is a helper field: every line will have this value copied by default
- The Use Maxwell-B. speed distribution should be left on in most cases. If turned off, all molecules will have the same speed, which provides about 5-10% simulation speed increase, but the density calculation will be incorrect, and you'll hide effects where some preliminary fast gas molecules propagate quickly
- The Calculate constant flow option is on by default: in that case molecules are traced until pumped. If turned off, moelcules are traced until the last moment defined by the user, see below. If we're not interested in the steady-state results, we can turn this off, therefore a new molecule will be traced as soon as the flight time of the previous one reaches the last interesting moment.
- Back to the Moments list: this is where you can define the moments when you're interested in the pressure. For each moment, all textures and profiles have different values, therefore the memory requirement is realtively

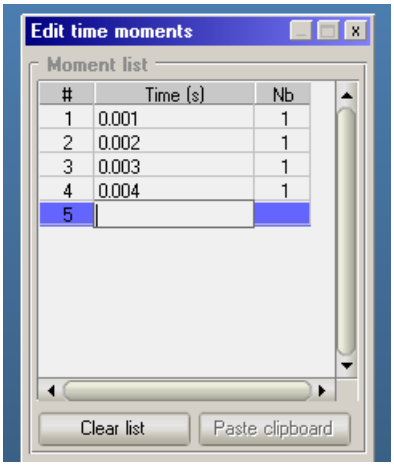
high. Simply enter a moment (in seconds), then **click out of the text field**, so your enetered value is parsed:



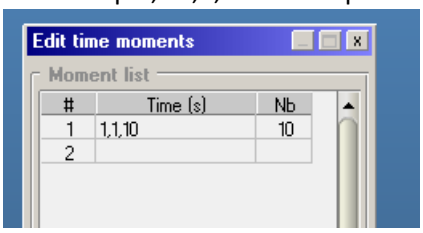
-> clicking out ->



- We can enter one value per line:

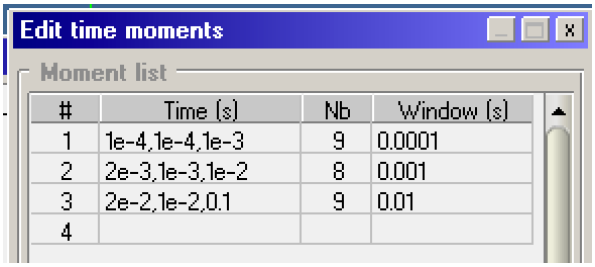


- …but by doing so, we would spend a lot of time to define a series of moments. Therefore, you can define a serie in the floowing format: **first_moment,increment,last_moment**
- For example, "1,1,10" corresponds to 1,2,3,4,5,6,7,8,9,10 seconds. You can try it out:

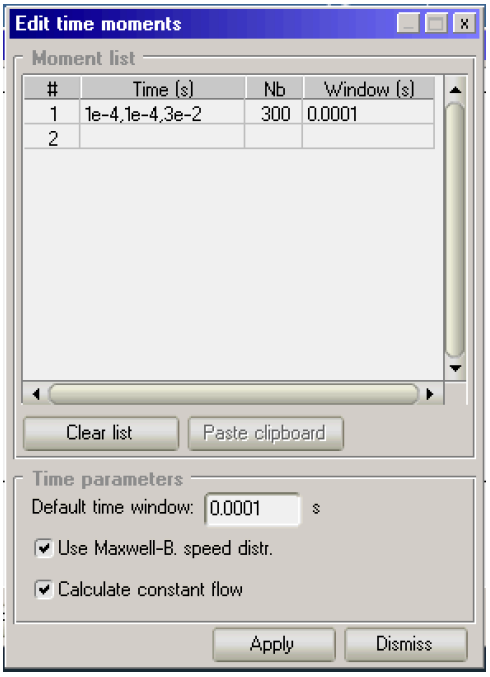


Note that the "Nb" column shows 10, since in this range there are ten moments.

- Finally, you can also set a different time window for each line, typically for logarithmically increasing moments:



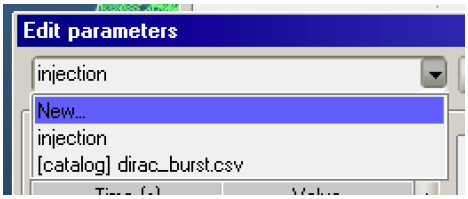
- And now let's set up the parameters the following way, suitable for our example:



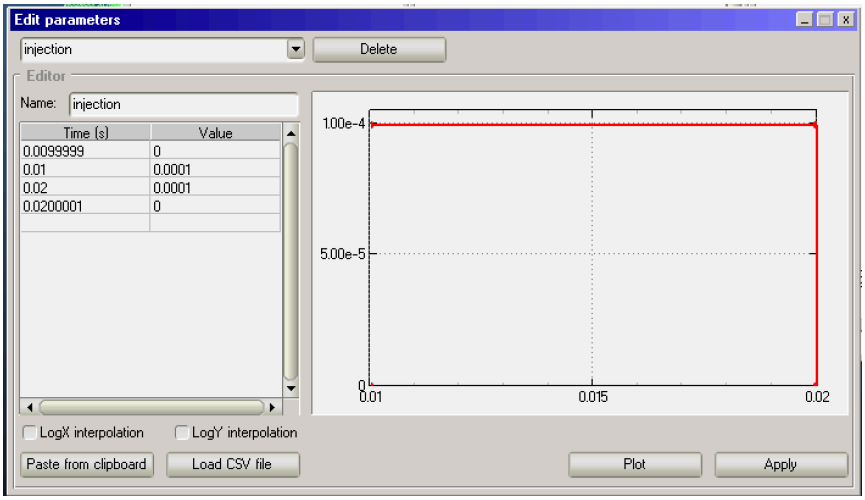
- The above parameters mean that we will calculate the pressure at 300 different moments: t=0.1ms, 0.2ms, 0.3ms, … , 30ms
- Click apply, and you can close the "Edit time moments" window.

- Now you have to change the constant outgassing (set to 1E-4mbar.l/s previously) to a time-dependent outgassing pulse. For this, you have to define an outgassing **parameter**. Click Time/Edit Parameters:

- In the Edit Parameters window, you will either see an empty window or a catalog of default time-dependent parameters. Choose New… in the dropdown list:

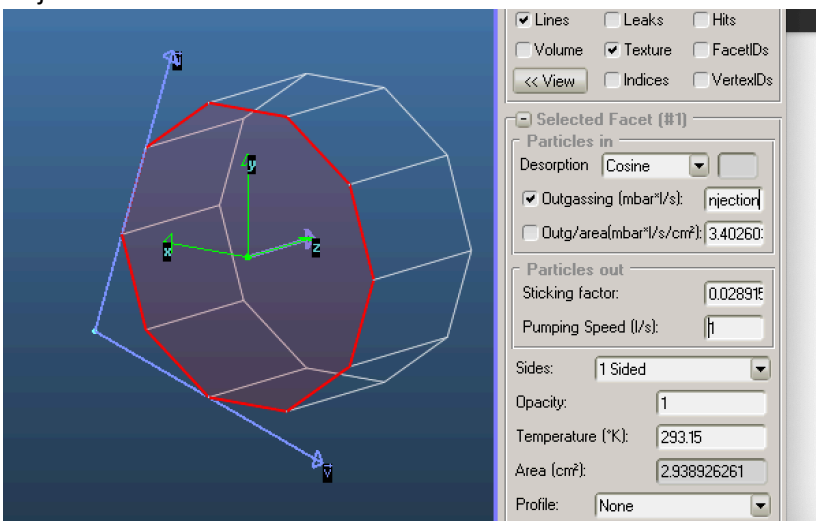


- Define the parameter like this and click Apply:



It means the following:

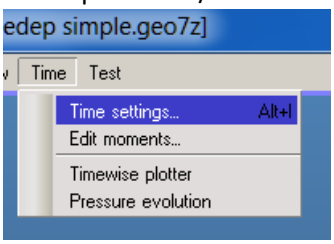
- From 0 to 0.01, there is no outgassing (0). Note that we entered 0.0099999 to avoid an overlap at t=0.01s
- There is a constant pulse from 0.01 to 0.02s of 1E-4mbar.l/s
- At 0.02, the gas pulse is drawn down to 0
- Note that Molflow always assumes the first and last values of a parameter from the beginning to the simulation, and to the end. Concretely, between 0.0099999, the first defined value (0) will be kept, and also from 0.020001 to the end
- The actual end of the simulation is the last recorded moment: it's the last defined moment plus half of the time window (in our case 30ms + 0.05ms = 30.05ms).
- Finally, the name of the parameter is arbitrary, you'll use it to reference to it (in our case, we call it "injection").
- Now you have to **assign the parameter** you defined to the outgassing facet: click on facet1, and write "injection":



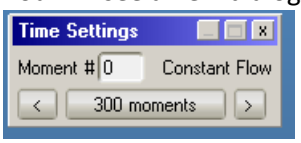
- Note: you can assign time-dependent parameters not only to outgassing, but also to sticking and opacity. Sticking allows to create time-dependent pumping, while time-dependent opacity allows to model opening a valve, for example.
- You are all set: **launch the simulation** (Begin button)

- Open the profile plotter again. You will see the same plot once again, corresponding to the steady-state pressure:

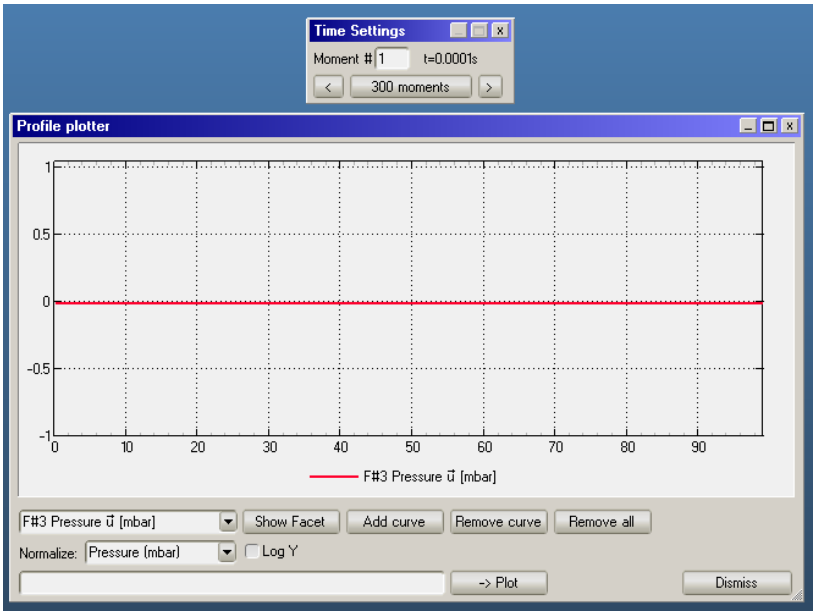
- Now open Time / Time Settings:



- You will see a new dialog appear in the top left corner:

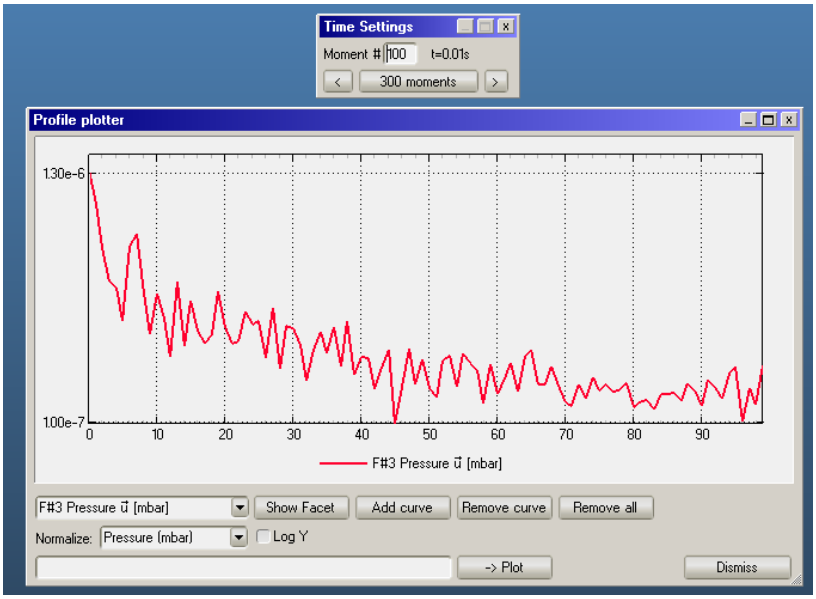


- Now click on the right arrow, and both the dialog box and the profile plotter will change:



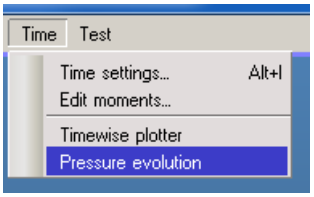
- What happened? Simply, now Molflow shows the first moment, at t=0.0001s, which is before the gas injection.

- Now, enter 100 in the text field and click enter to jump to moment 100 at t=0.01s:

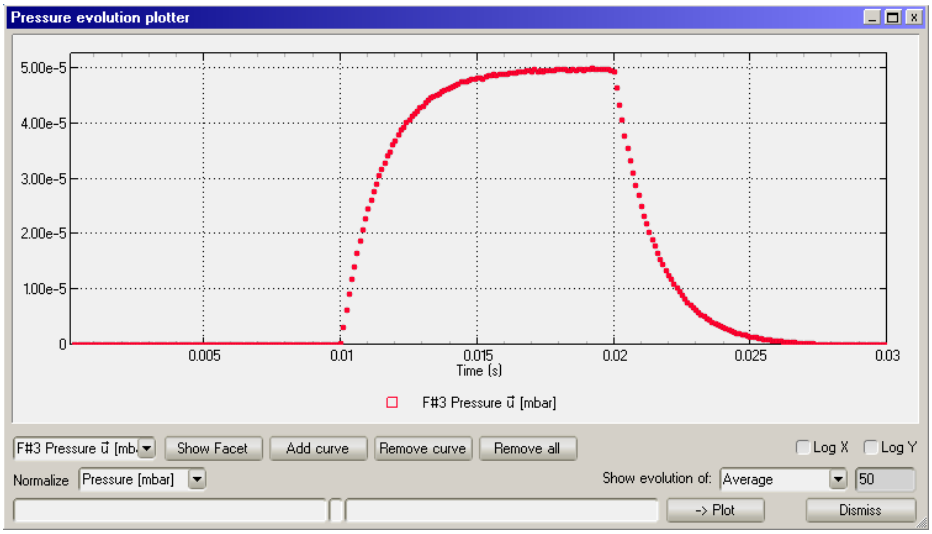


This is the beginning of the injection. You can see a small pressure appearing.

- Keep clicking the right button, and you'll see as the pressure evolves.
- There is a way to show the pressure evolution vs. the time. Open the Time / Pressure evolution plotter:



- Here is the evolution of the *average* pressure on the facet, as time progresses (select any facet and click Add):



- Let's explain the curve above. Until t=0.01 seconds, the pressure is zero.
- Between t=0.01s and t=0.02s, the gas converges to its "steady state" or "Constant flow" value of 5E-5 mbar. The rise is exponentials, governed by equation

$$p(t)_{injection} = \frac{Q}{S}\left(1 - exp\left(-\frac{S}{V}t\right)\right)$$

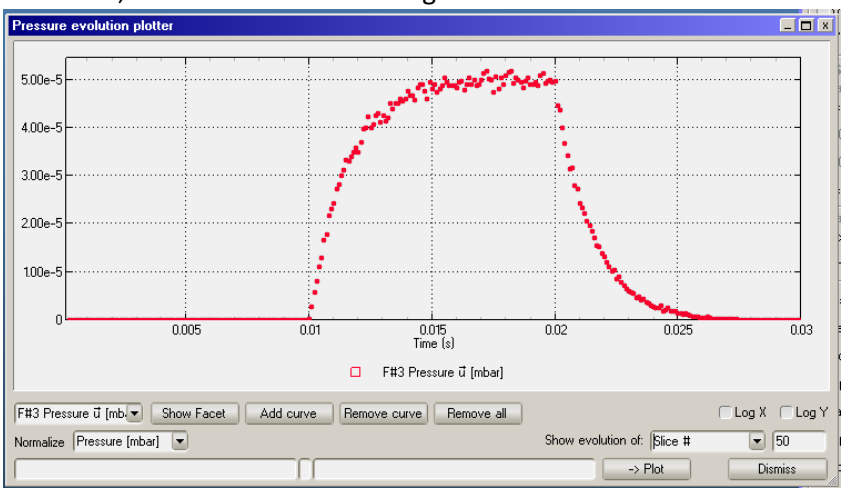
, where S is the pumping speed, Q is the outgassing and V is the colume of the cylinder.

- At t=0.2s we close the injection, but pumps still work – they pump down the residual gas, described by equation

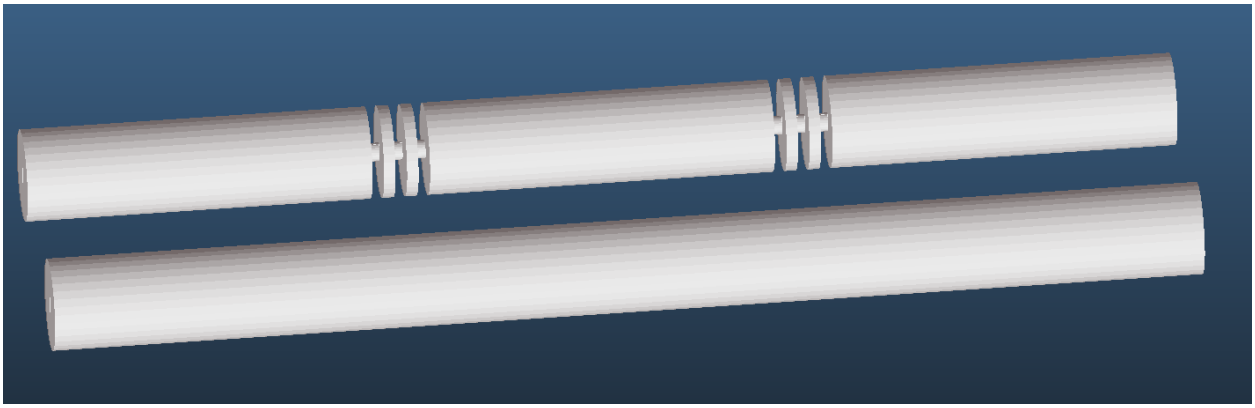
$$p(t)_{pumpdown} = \frac{Q}{S} exp\left(-\frac{S}{V}(t - t_{stop})\right)$$

- One last remark: each data point shows the *average* pressure an the facet at a given moment. If the pressure is not uniform on the facet, you can change this behaviour, and show instead a given slice (a profile consists of 100 slices):

- Of course, a slice contains on average 100 times less data than the full facet, so the scattering will be higher.

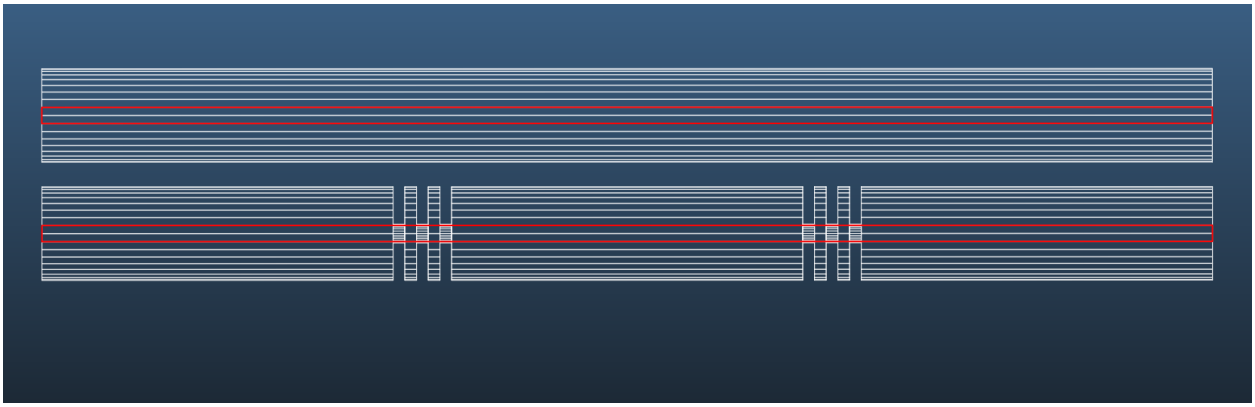


Practical example: effect of an ADL device

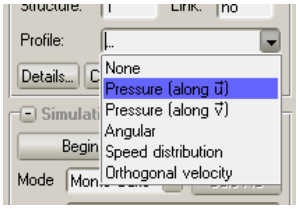


In this example we will inspect the propagation speed of H2 coming from one side of a tube. Then we'll see how much the pressure rise on the opposite end can be mitigated by inserting a simple ADL device.

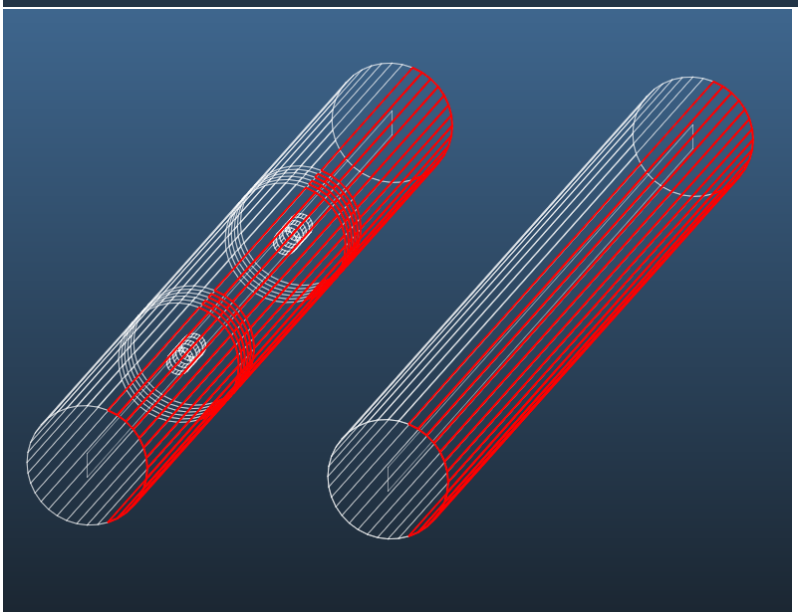
- The geometry is supplied. Open **adl_example.geo7z**



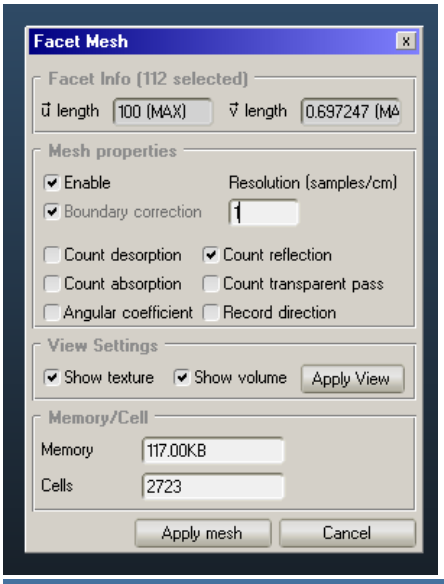
- You will see two versions of a 8cm long tube: one with and one without ADL. We will be comparing them.
- For your convenience, two transparent, two-sided facets are inserted in the middle of the tubes. They will show us the pressure. Select them and add profiles to them:

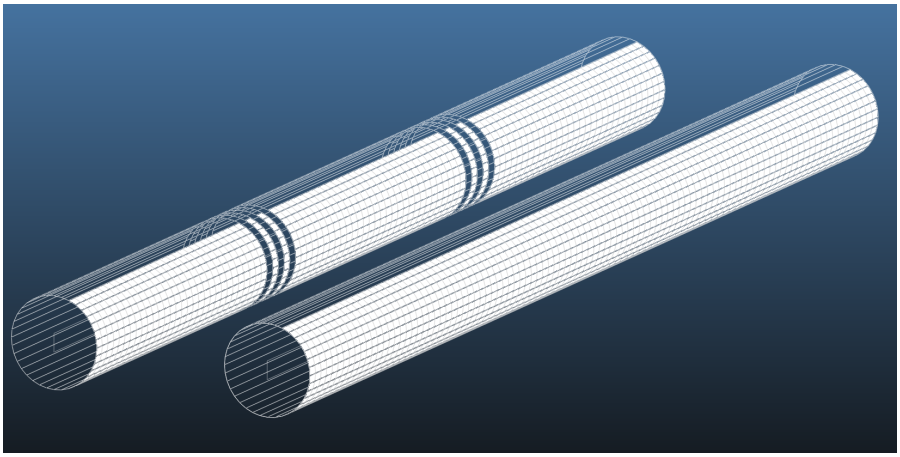


- Select a few longitudinal facets to add textures. The best way to select is the Front view:

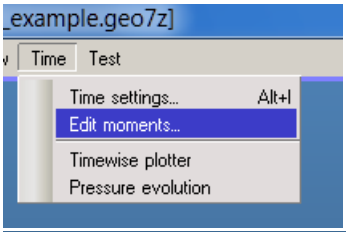


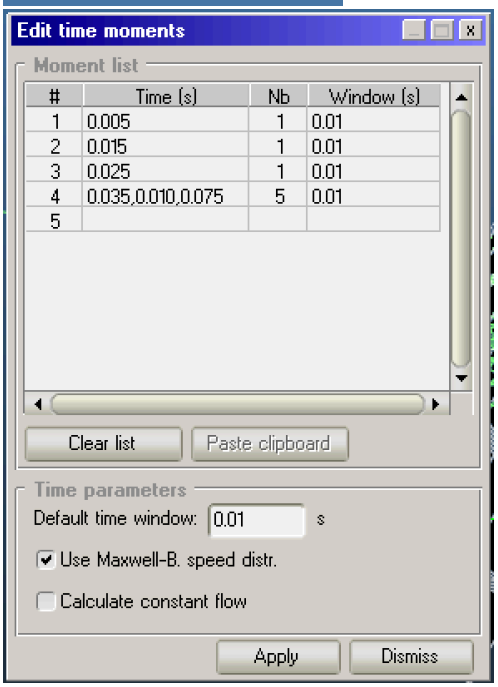
- Click the Mesh… button and add reflection textures:


Facet Mesh
Facet Info (112 selected)
u length
100 (MAX)
v length
0.697247 (MA
Mesh properties
Enable
Resolution (samples/cm)
Boundary correction
1
Count desorption
Count reflection
Count absorption
Count transparent pass
Angular coefficient
Record direction
View Settings
Show texture
Show volume
Apply View
Memory/Cell
Memory
117.00KB
Cells
2723
Apply mesh
Cancel

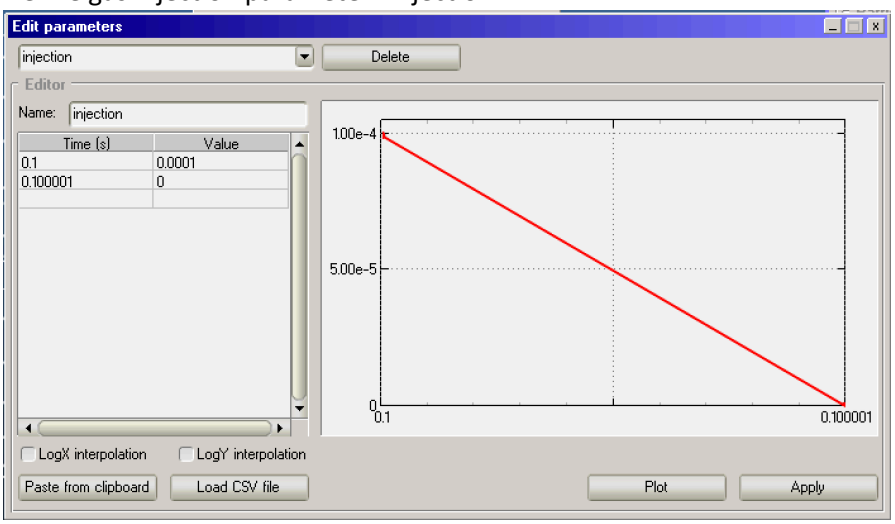


- Now define the time moments, as recommended below (Time / Edit moments):



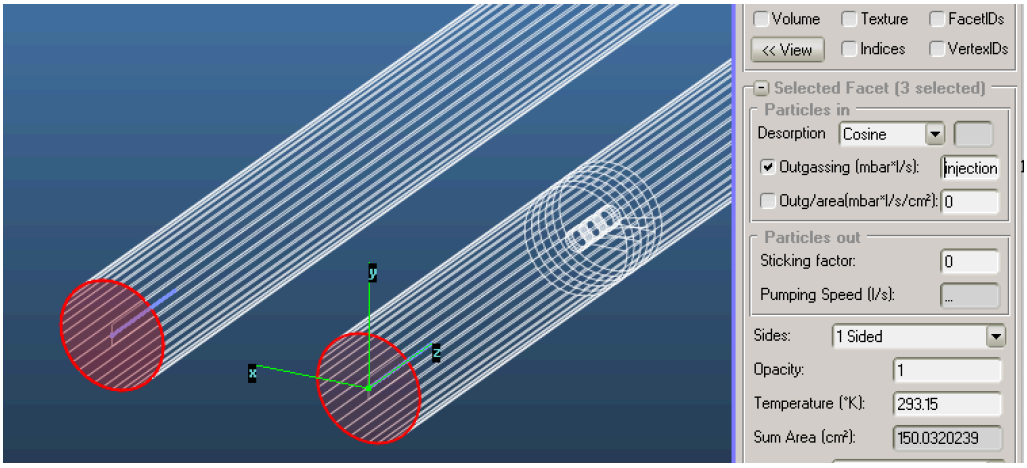


- What the above means: We will calculate the pressure at 8 different moments, at 5ms, 15ms, 25ms … 75ms. Note the range used in the fourth field, this is optional.
- The time window is 10ms
- Define gas injection parameter “injection”:

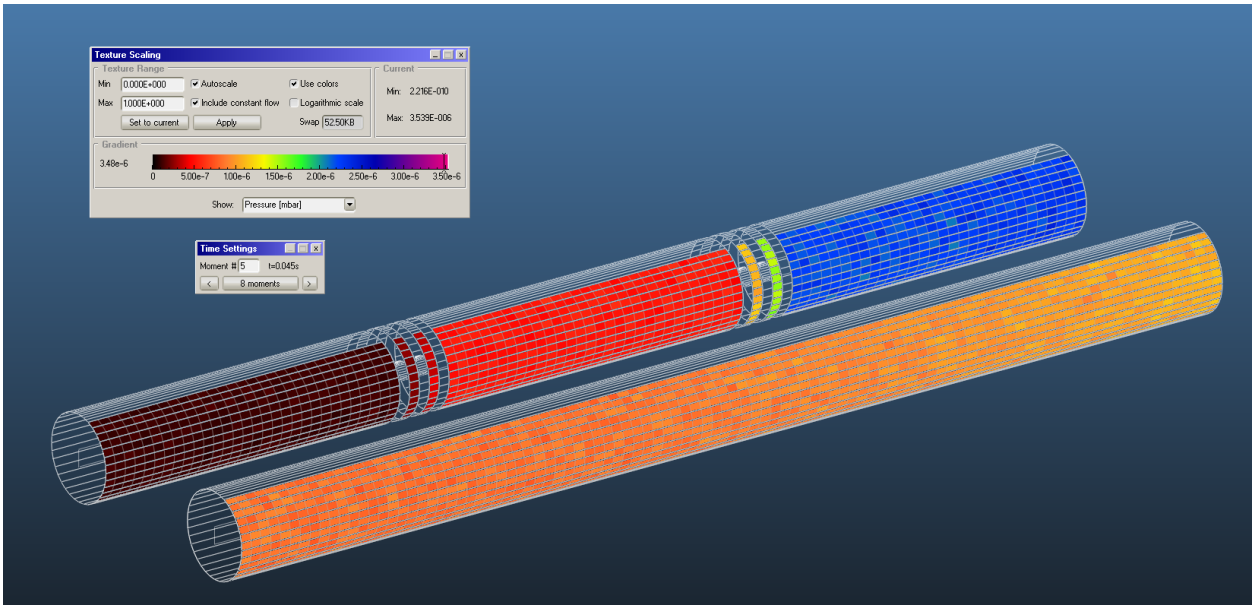


the above means that gas will be injected between 0 and 100ms with 1E-4mbar.l/s.

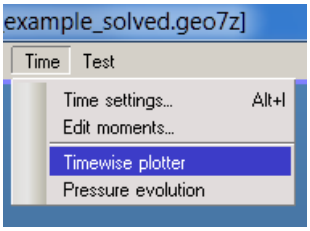
- Assign it to one side's end facets:

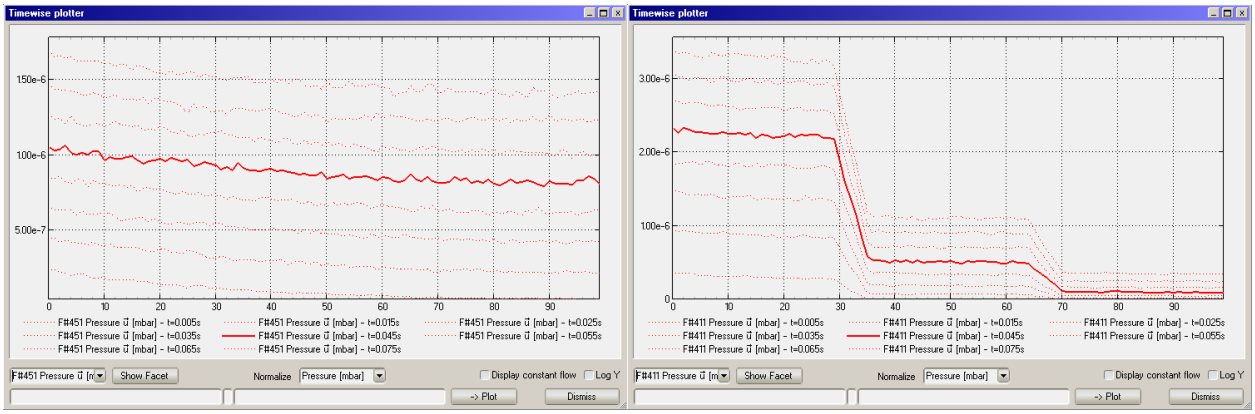


- **Important!** We didn't define pumps. Disable the *calculate constant flow* option, so molecules will only be traced until t=75ms
- Launch simulation, and using the textures and the Time Settings dialog, you can check the pressure buildup difference at any time moment:



- Or to visualize it in an elegant way, open Time / Timewise plotter, select the profile to plot, and see how the pressure builds up:



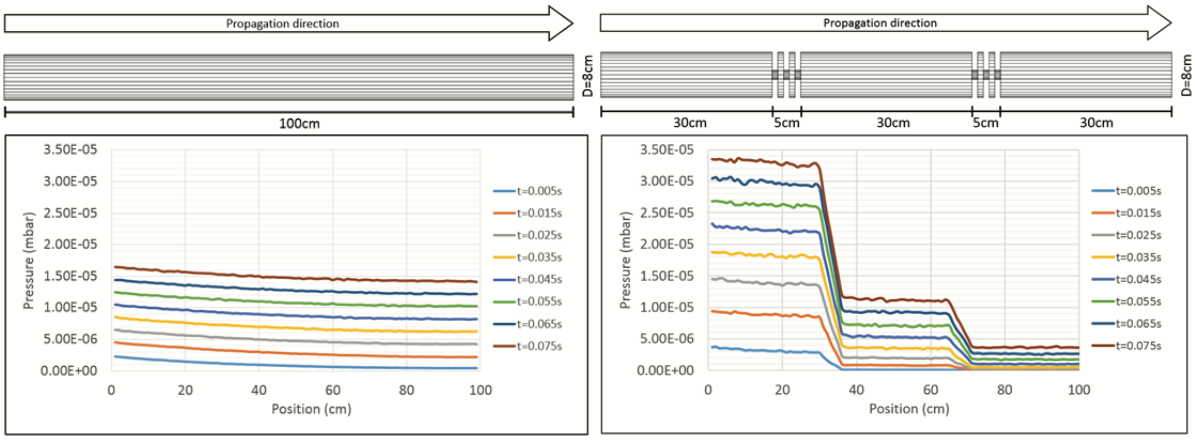


Left: pressure buildup on tube without ADL

Right: pressure buildup on tube with ADL

Note that the solid line is the one that you select in Time Settings

- This example shows how an ADL reduces the gas propagation. In a real world example, you would be free to vary the ADL shape and see its effect. After some post-processing, the final curves look like this:



Suggested reading:

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