Molflow+ tutorial

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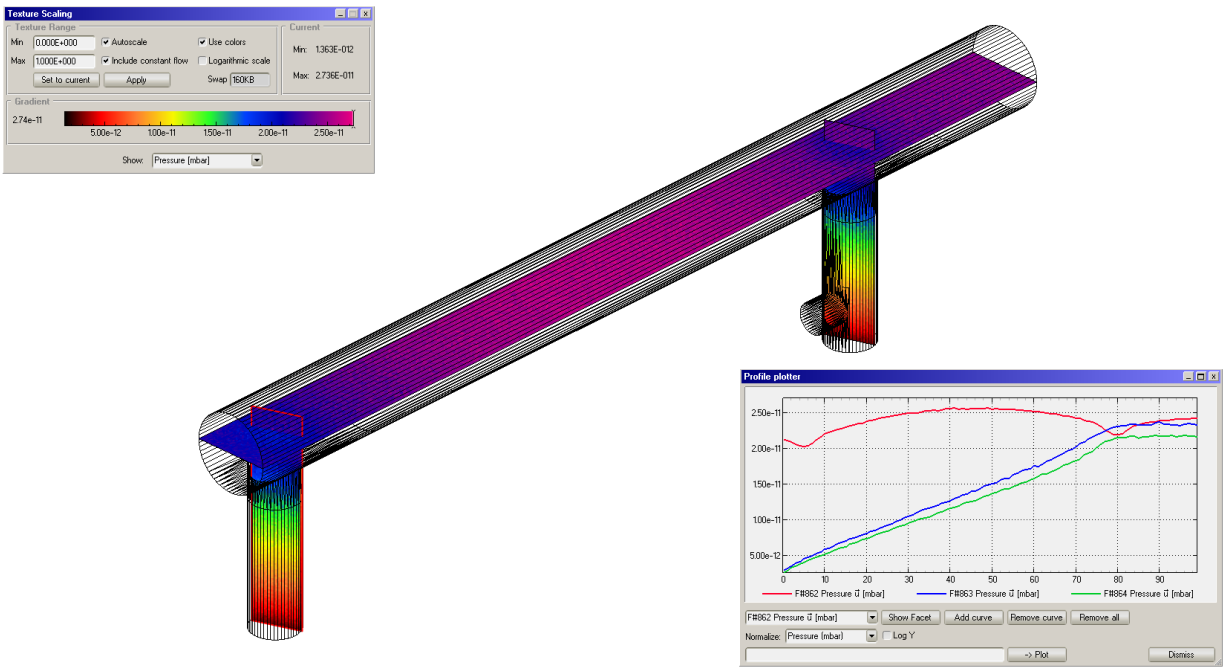
(more on http://test-molflow.web.cern.ch/ → Molflow documentation→AVS-61)

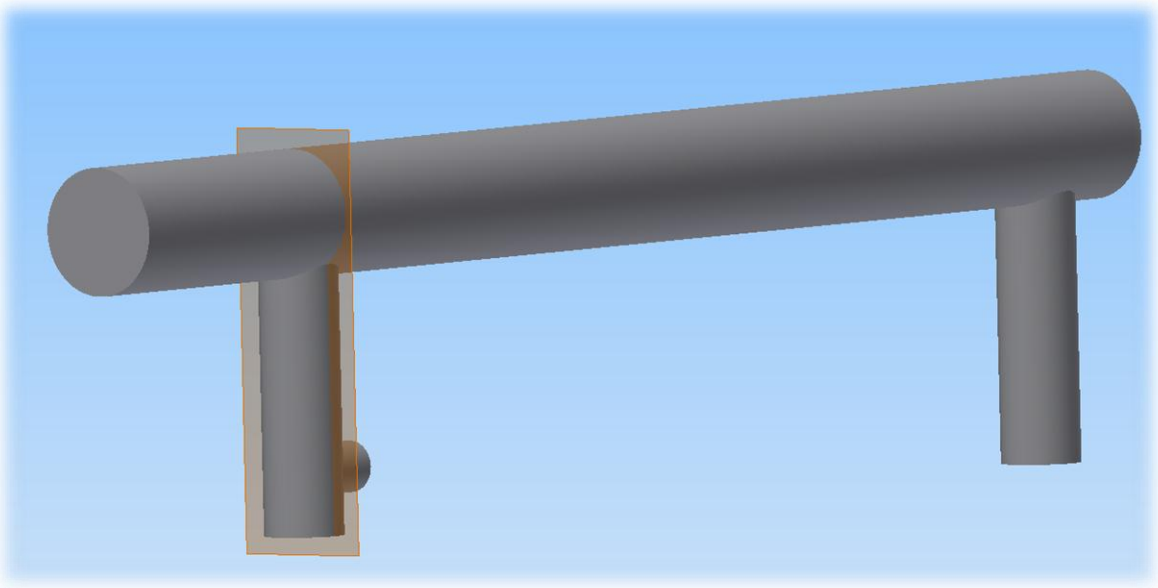


A simple accelerator part with a pumping port

Creating the geometry

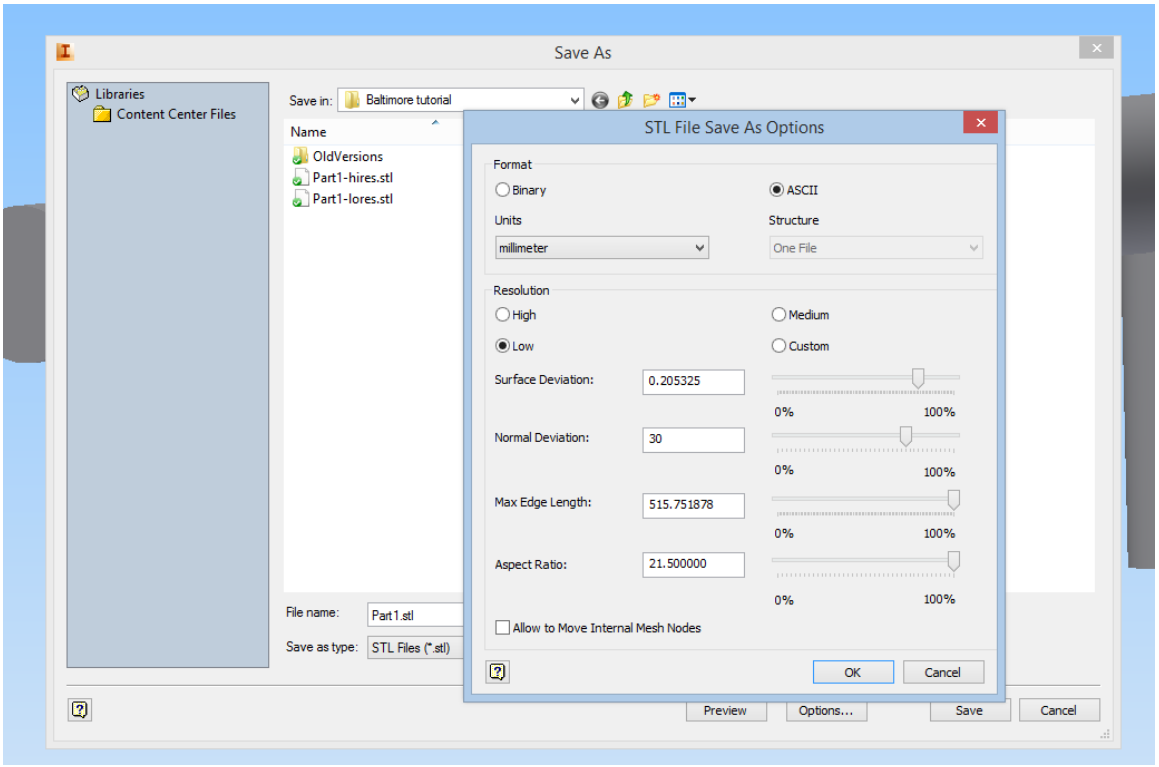
The workflow with Molflow begins with this step, however this will not be part of this tutorial, since many different CAD modeling programs exist.

Below is a model that we have created with Autodesk Inventor 2014 using sketch and extrusion commands.



To use it in Molflow, we need to export it to the STL format. Usually we have several options:

- One important aspect is the resolution (in this tutorial we begin with a high resolution setting)
- The file must me ASCII (as opposed to binary)
- We can choose any length units to create it, but we'll have to remember what we used



Importing the geometry

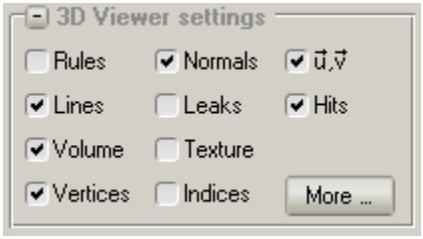
The STL file that we have created can be opened directly in Molflow. The only question asked will be the length units we have used (an STL file contains only numbers, without units).

In this tutorial, we begin with the "high resolution" STL file, then later we'll see if it makes any difference.

- Launch Molflow
- Choose File / Load
- Open Part1-hires.stl
- Molflow asks you the length units, which in our case are **millimeters**

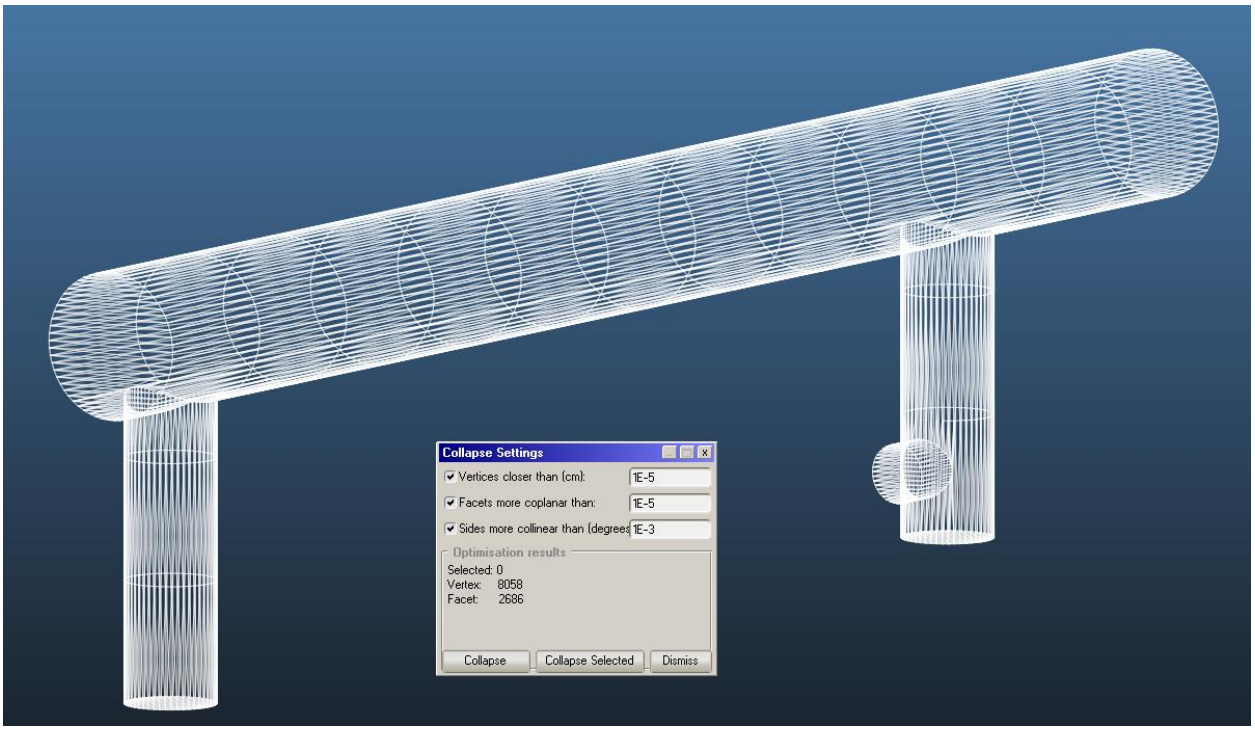
Molflow then opens the file, and pops up the Collapse dialog.

- You can rotate the geometry by holding down the right mouse button
- You can change between wireframe and volume view on the top right "3D Viewer Settings" Panel:



- You can turn on autoscale at the bottom right:

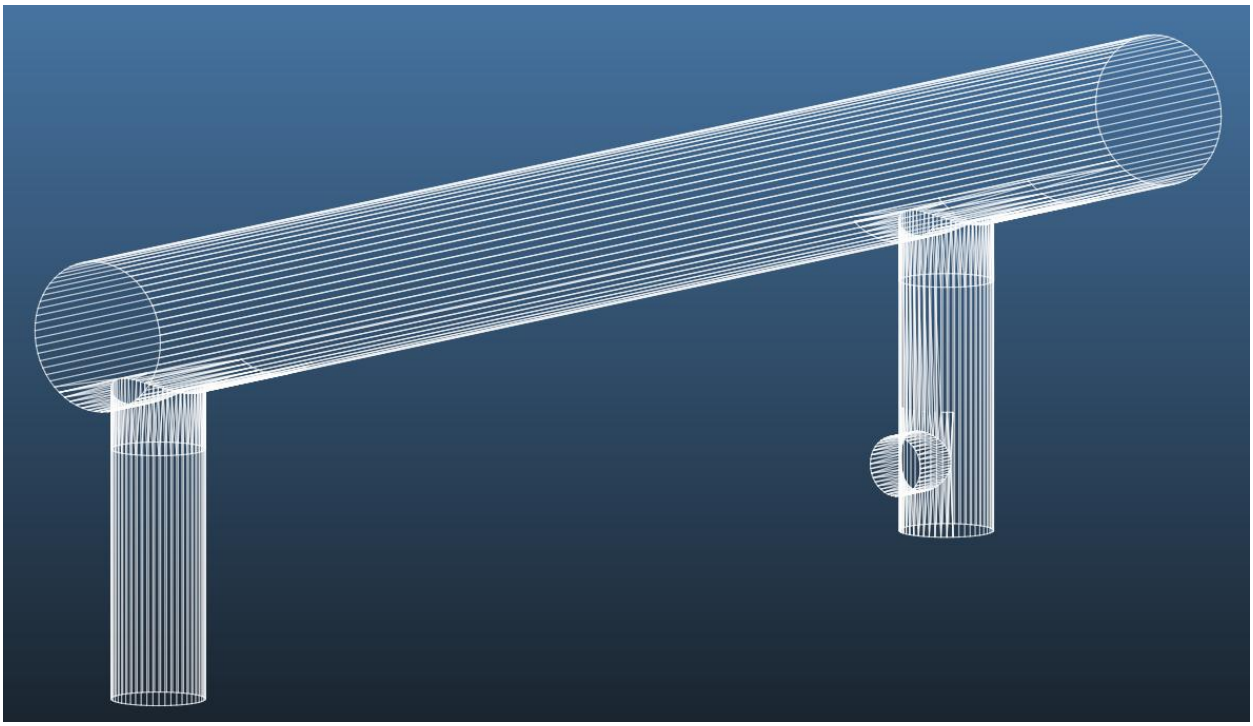
 (leftmost button)



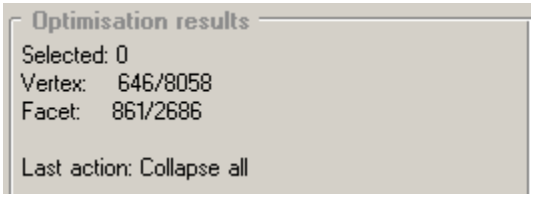
Collapsing

STL files consist of N triangles and 3xN vertices. We could have a cleaner geometry with less facets by merging coplanar triangles. This saves computation time and eases handling.

- Click the Collapse button without changing the parameters in the dialog
- Molflow asks is you want to remove isolated vertices – click OK



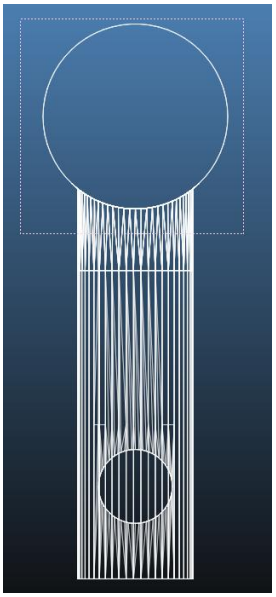
Now you have a collapsed geometry, where Molflow has reduced the number of vertices from 8058 to 646, and the number of facets from 2686 to 861.



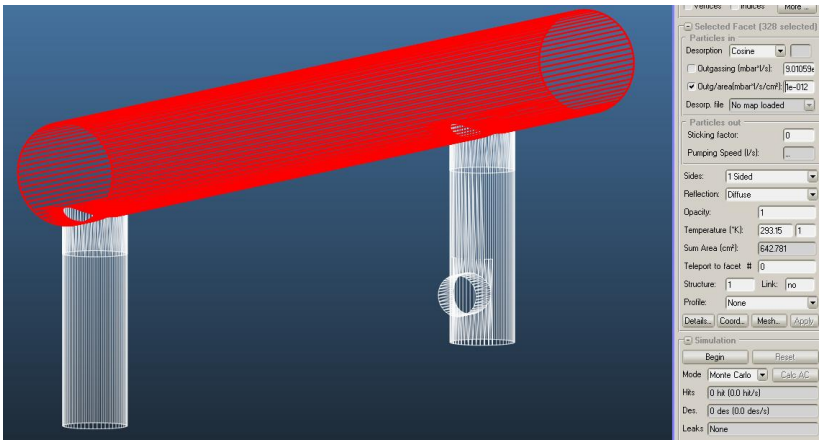
Add gas source

We'll select the wall of the tube and set it as outgassing source:

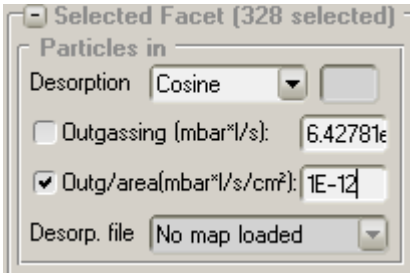
- On the bottom left of the Molflow window, click **front** to go to front view
- Draw a selection rectangle around the tube part like this:



- You should have selected exactly 328 facets. We'll set up outgassing on them:



- On the right hand panel, in the "Selected Facet" box, set the following for the "Particles in" panel:

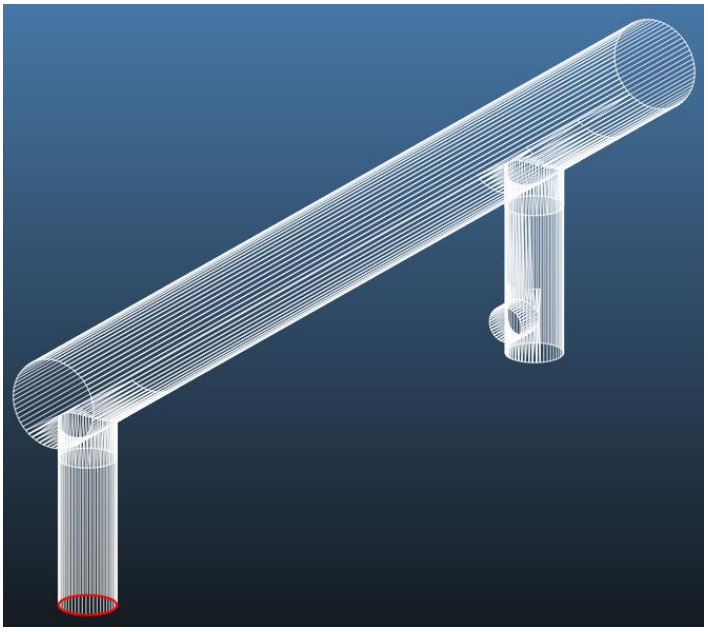


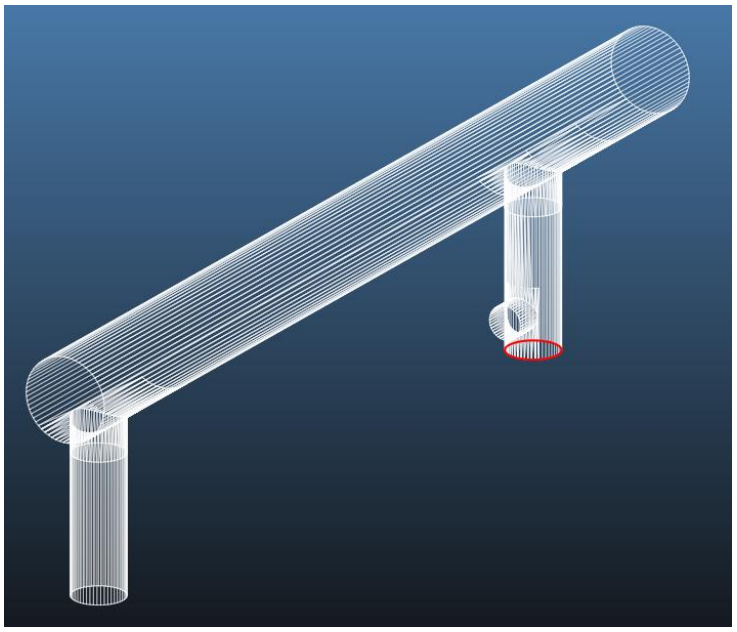
  - Desorption: **cosine**
  - Select second checkbox (Outgassing/area (mbar*l/s/cm2)
  - To the second checkbox, enter 1E-12
  - Click Apply or press Enter

With this, you have defined a uniform outgassing of 10^{-12} mbar.l/s/cm^2 on the surface, typical for stainless steel.

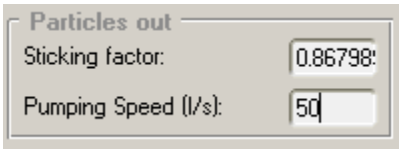
Add pumps

- Select one by one the two facets corresponding to pump locations (Facets 163 and 533)





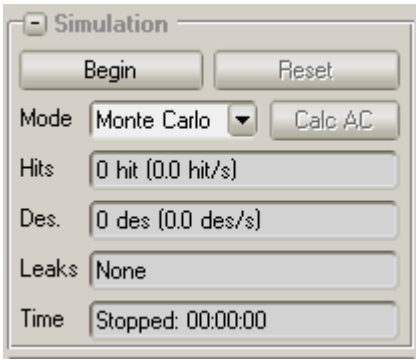
- When selected, in the “particles out” panel, enter 50 l/s as pumping speed:



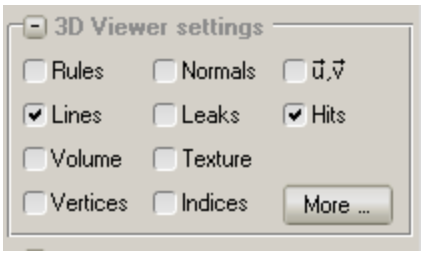
- Click apply or press Enter, then repeat it for the second pump facet

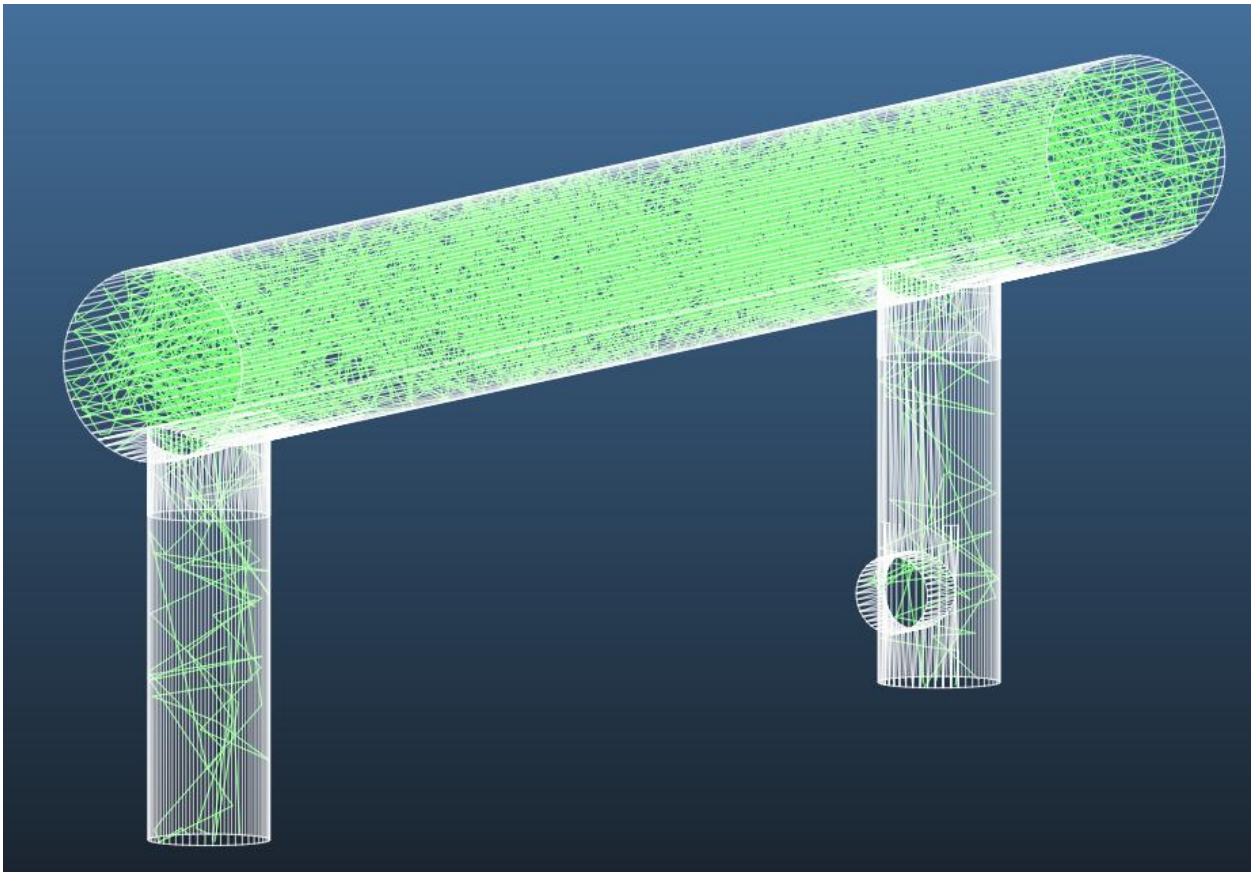
Launch the simulation

That was everything we needed to set up the simulation. We have the gas sources and the pumps: click on the **Begin** button on the Simulation panel:



- You can visualize particle trajectories by selecting the **Lines** view option:





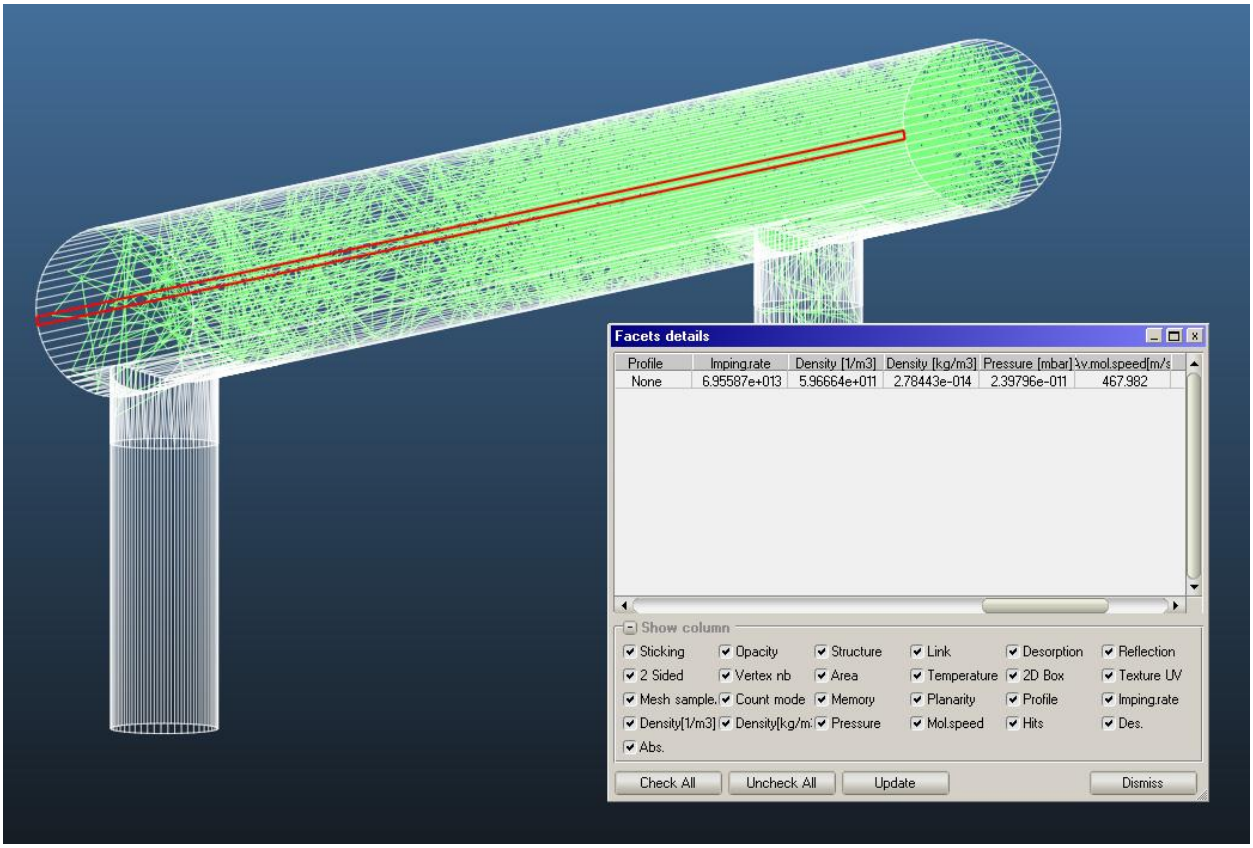
Reading results

Now that the simulation has been set up, we'll go through different ways of reading pressure data in our system.

First method: facet details

Advantage: No preliminary setup required, simple
Disadvantage: Shows only the average for the whole facet

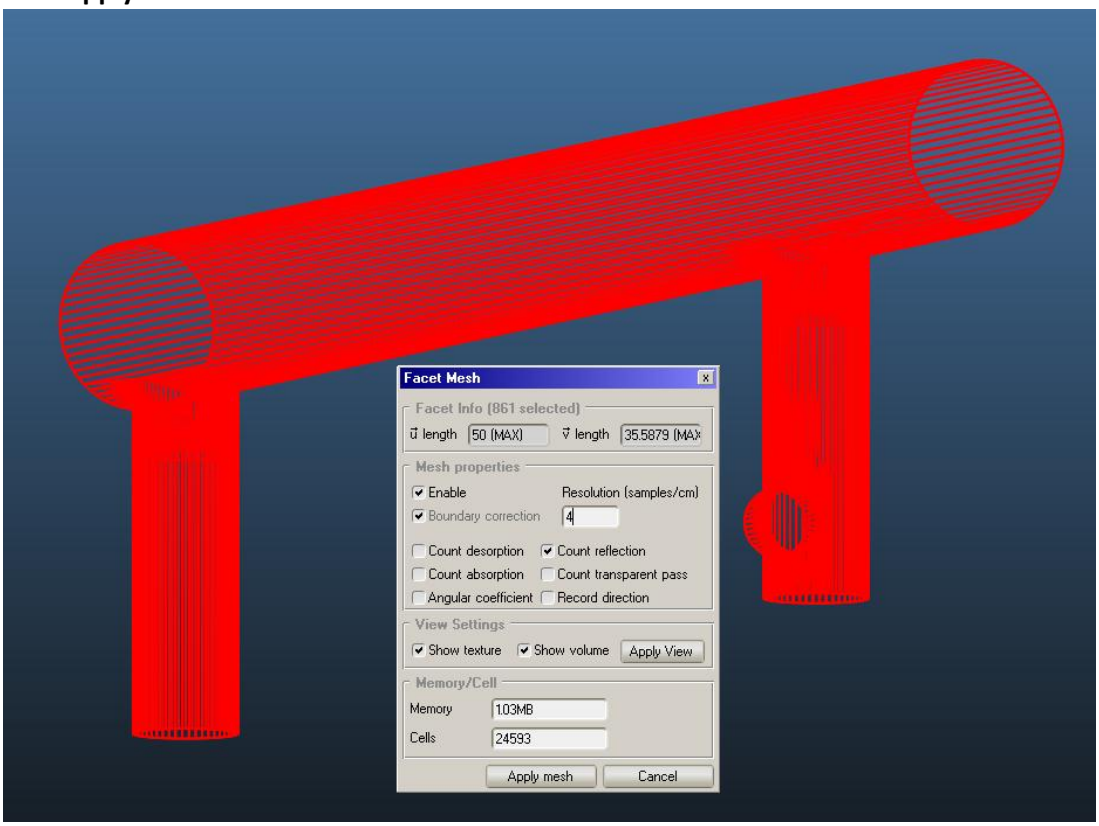
- Select any facet(s) on the wall
- Click the **Details…** button
- In the Facet Details window, you can see the average pressure (in mbar) on the selected facet(s)



Second method: textures on all facets

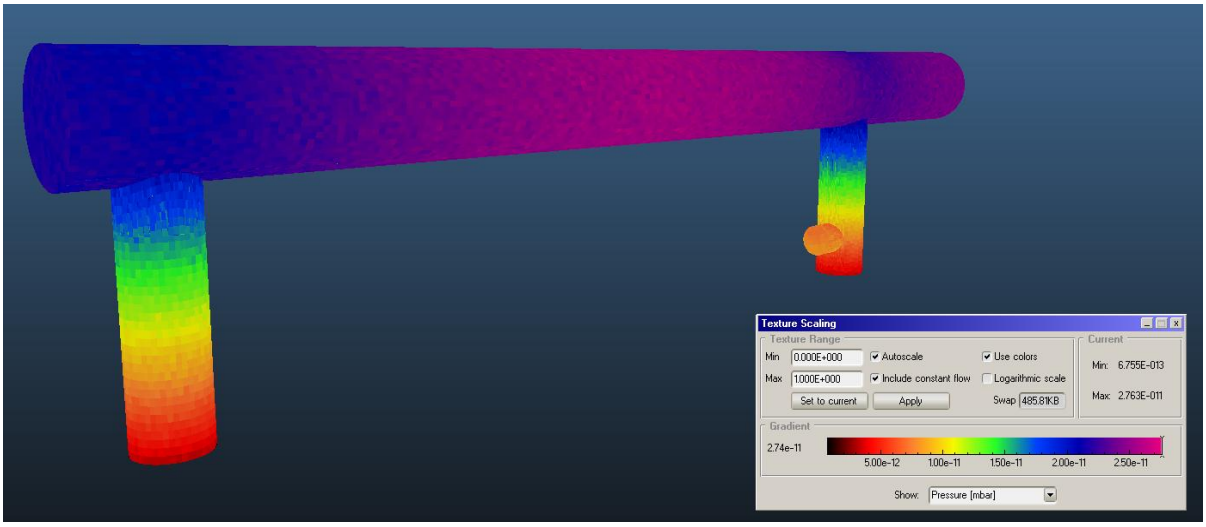
Advantage: can be set up with a few clicks, colorful, covers whole geometry
Disadvantage: for big geometries, memory requirement can grow very fast with level of detail

- Select all facets (CTRL+A or by drawing a big selection box)
- Click the **Mesh…** button on the right, it brings up the mesh dialog box
- Check the box near "Enable" – therefore facets will have a texture
- Check the box near "Count reflection" – molecule bounces on the wall will be recorded
- Set resolution to 4 sample / cm (one texture cell will be 0.25x0.25 cm)
- In the memory textbox, you can see that this setting will result in 24593 cells, with a light memory footprint of 1MB
- Click **Apply Mesh**

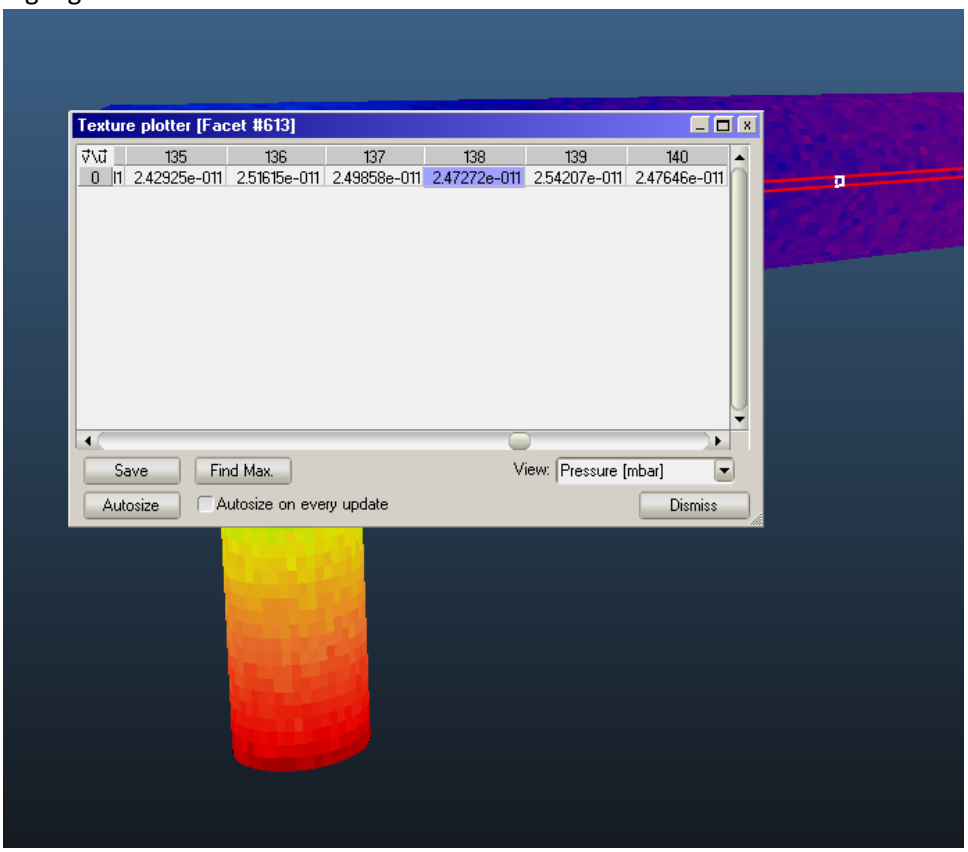


- Now launch the simulation with the **Begin** button
- Now, as the simulation runs, walls of the system are color-coded based on their pressure.

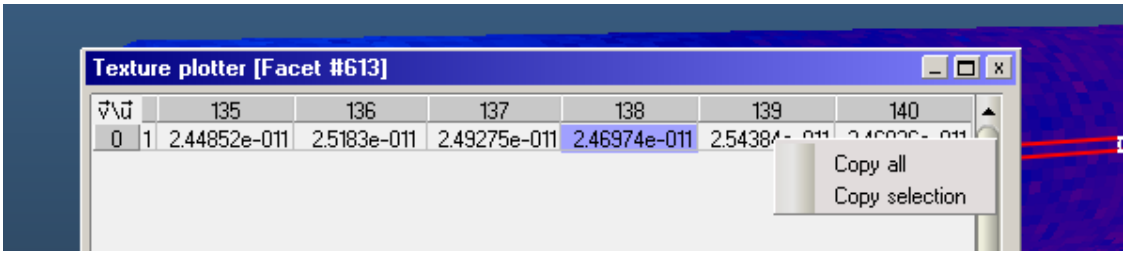
- To see or adjust the scale, select Tools/Texture scaling or press the shortcut (CTRL+D)



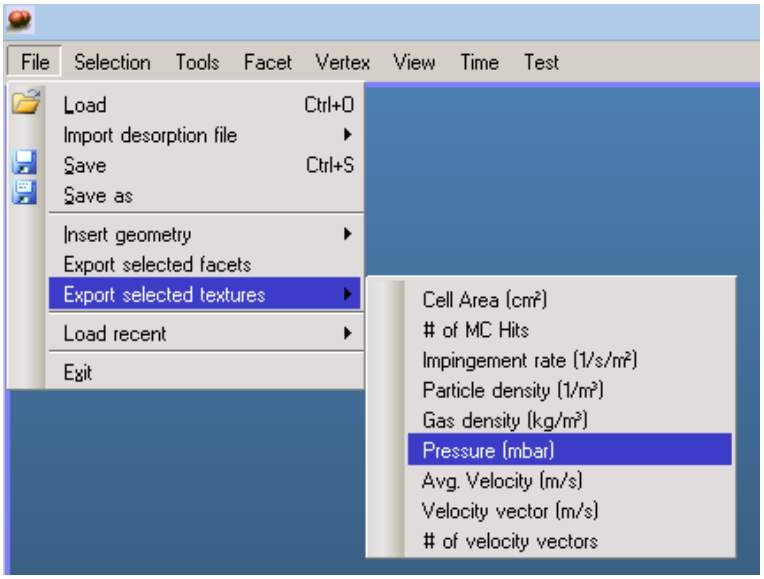
- To read the values of individual cells, you can use Tools / Texture Plotter. This opens a dialog.
- Then selecting any facet will fill the dialog with the cell values. Clicking on a cell in the plotter window will highlight the cell on the facet with a white frame:



- To export textures, you can right-click in the plotter window and use the copy command (will put the table on the clipboard)



- To export multiple or all textures, you can select the facets in question and use the corresponding menu item:

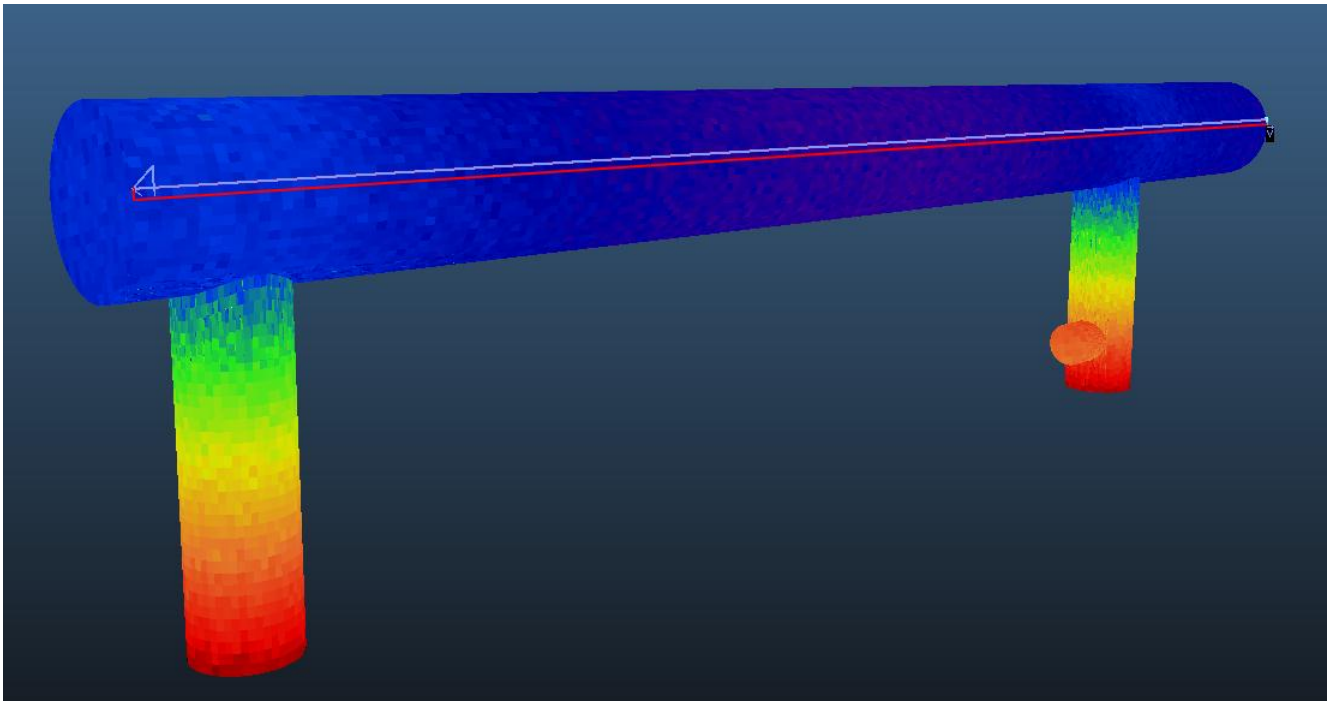


Third method: profiles

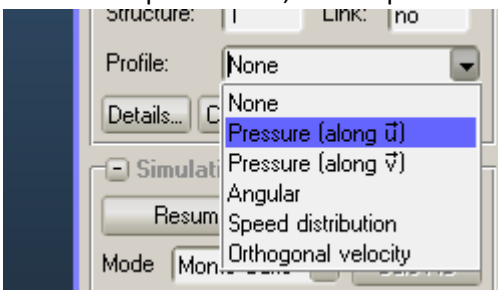
Advantage: Visualization within Molflow, good for comparing pressure on different facets
Disadvantage: works on rectangular facets only, only 100 slices

Profiles divide a facet into 100 equal slices, and plot a graph of the values on each slice. You must add a profile manually to each facet, then view the results in the profile plotter.

- Select any facet
- Check its orientation by ticking the "u,v" checkbox in the top right corner. Usually the longest side is the U vetor, while the V vector is prependicular to it

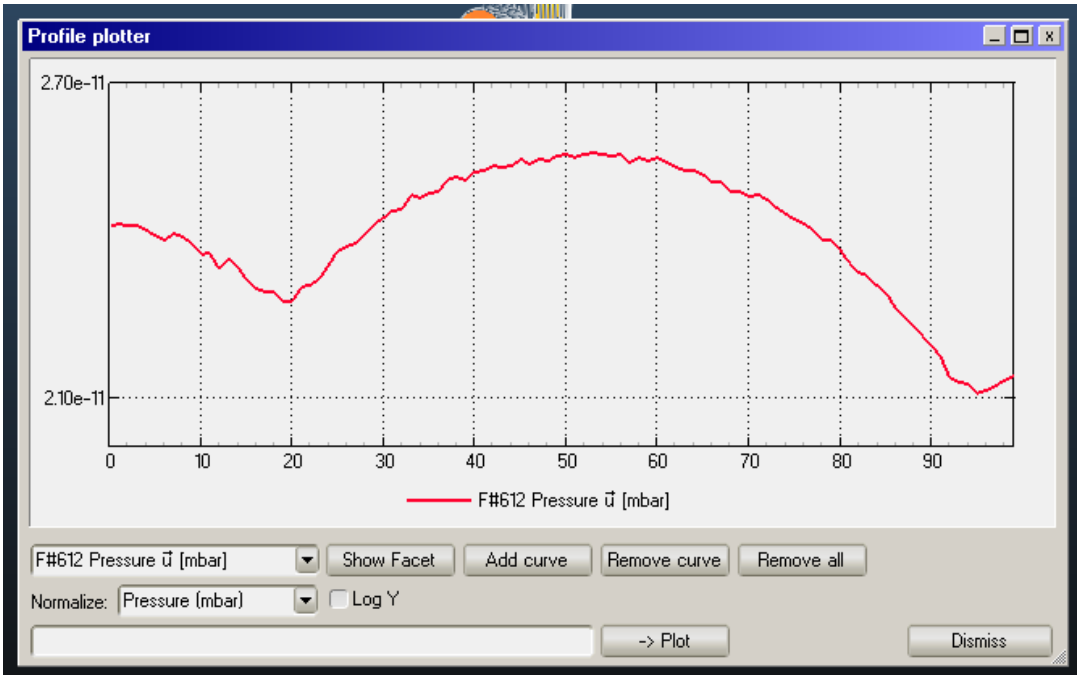


- In the facet parameters, set the profile to Pressure along u and click Apply



- Open the profile plotter (Tools / Profile Plotter)

- Select the facet to plot from the dropdown list and press “Add curve”



- Clicking on part of a curve displays the local value.

By adding more curves, you can view several facet profiles on the same plot.

Fourth method: counter facets

Advantages: shows pressure in the volume, large surface collects a lot of statistics
Disadvantage: you have to manually add them to the geometry

Counter facets are transparent facets whose sole purpose is to show a profile or a texture in the middle of the volume. While requiring some practice to set up, they are very useful to show pressure properties in characteristic locations of the vacuum system.

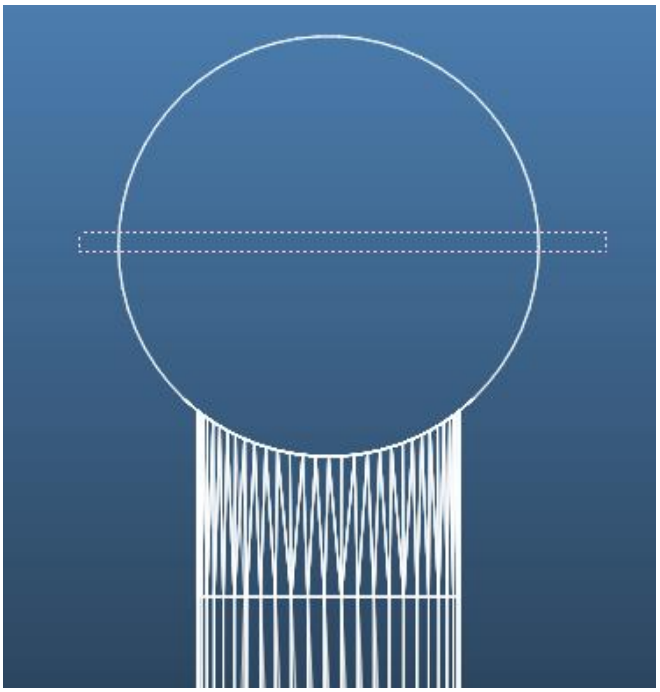
Before we proceed, we'll remove all textures and profiles created in the previous points:

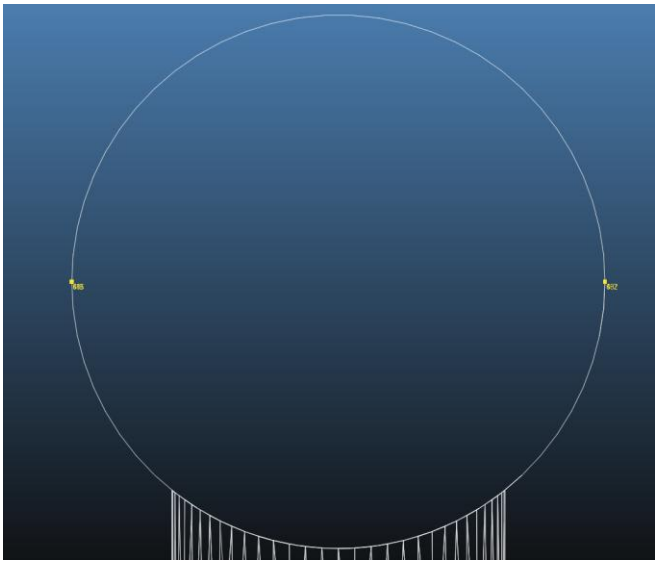
- Select all facets
- In the facet parameters panel, select Profile: None and click apply
- Click the Mesh… button. In the dialog, uncheck "Enabled" and click Apply Mesh – this will remove textures from all facets.

Now we can proceed.

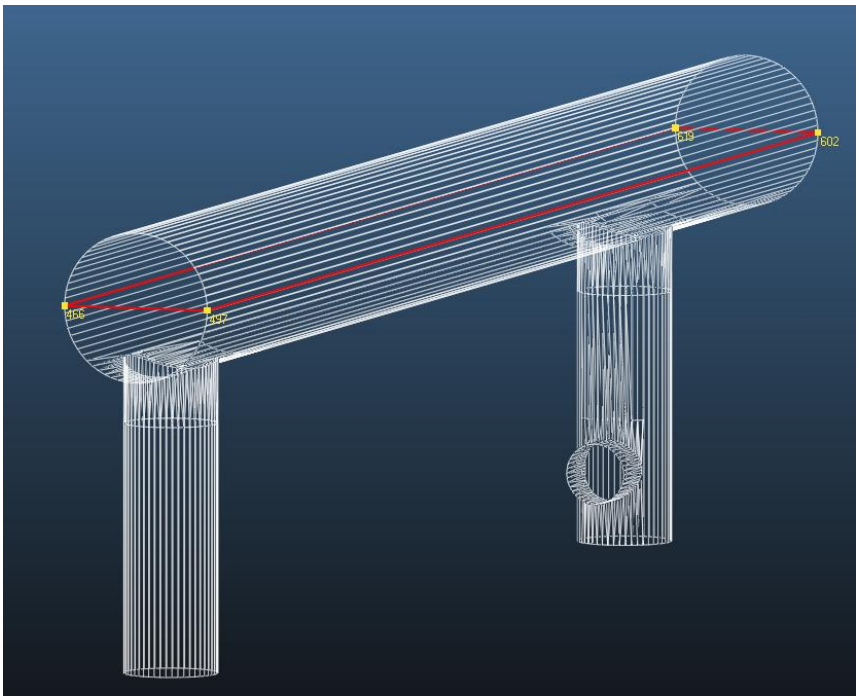
To create a new facet in Molflow, we have to select (or even create) some vertices, then construct a plane from them.

- Select the **vertex tool** in the selector mode (bottom right):
   (the vertex tool is the third from left)
- Choose front view
- Draw a selection box across the center, when successful it selects four vertices:

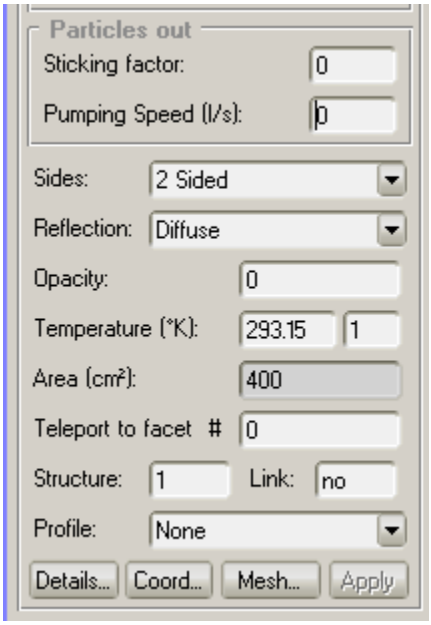




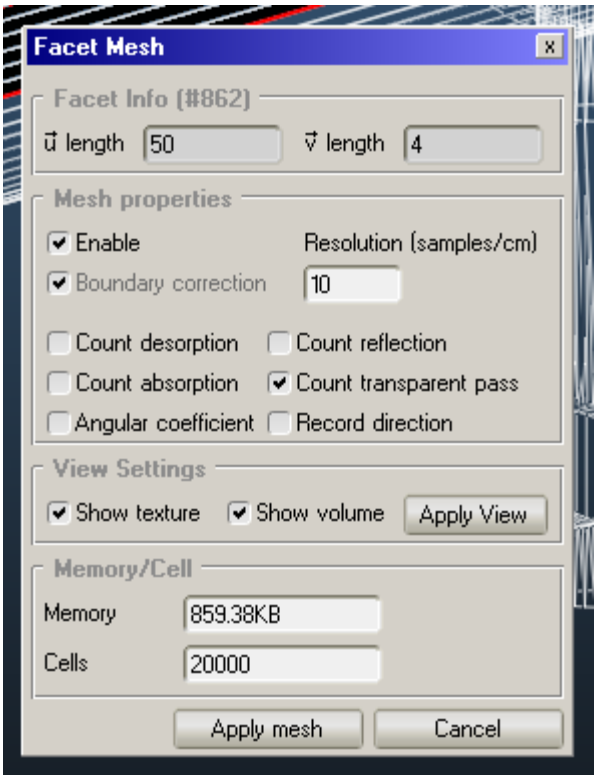
- From the menu, choose Vertex / Create Facet from Selected / Convex Hull to construct a new rectangular facet in the middle:



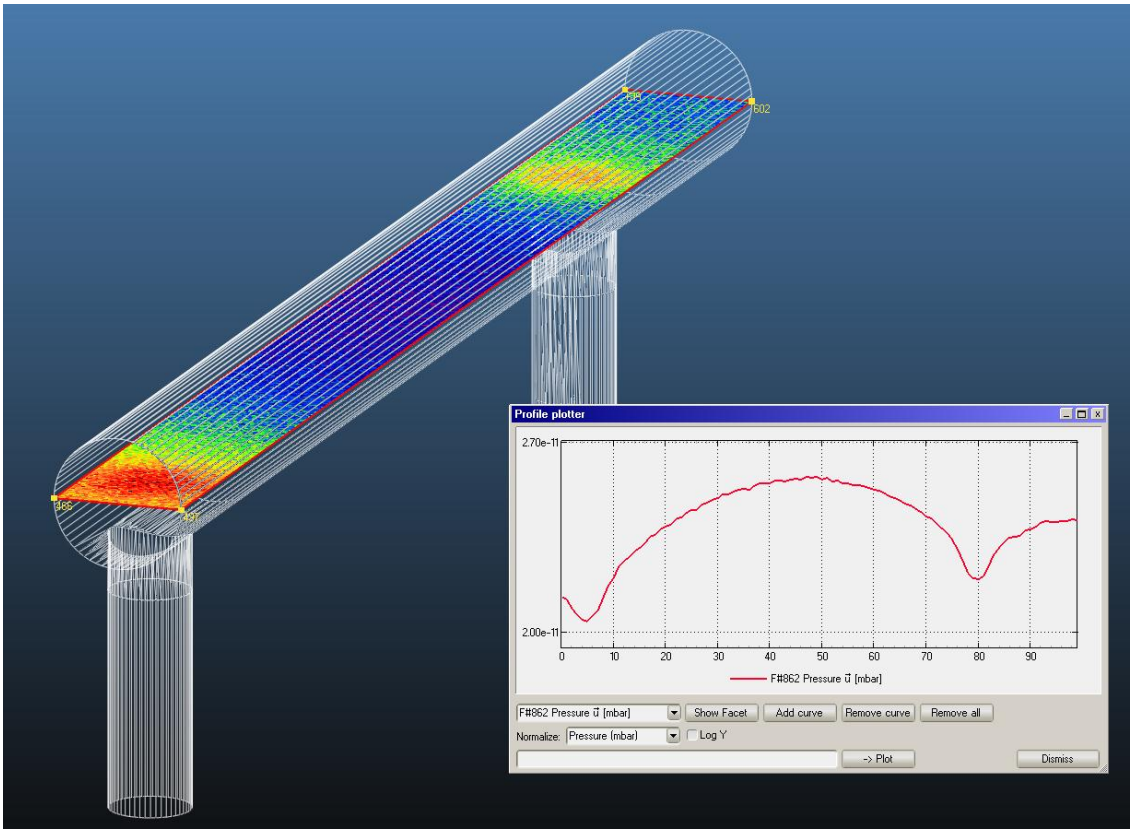
- Make it two-sided and transparent: on the facet parameters panel, set opacity=0 and 2-sided:



- At this point you can also add a profile: set profile to Pressure along u
- Add textures. The process is the same, but this time you have only one facet, so set a higher resolution (10 samples/cm) and select **Count transparent pass** (since the facet is transparent, instead of bounces, we have transparent passes through it):

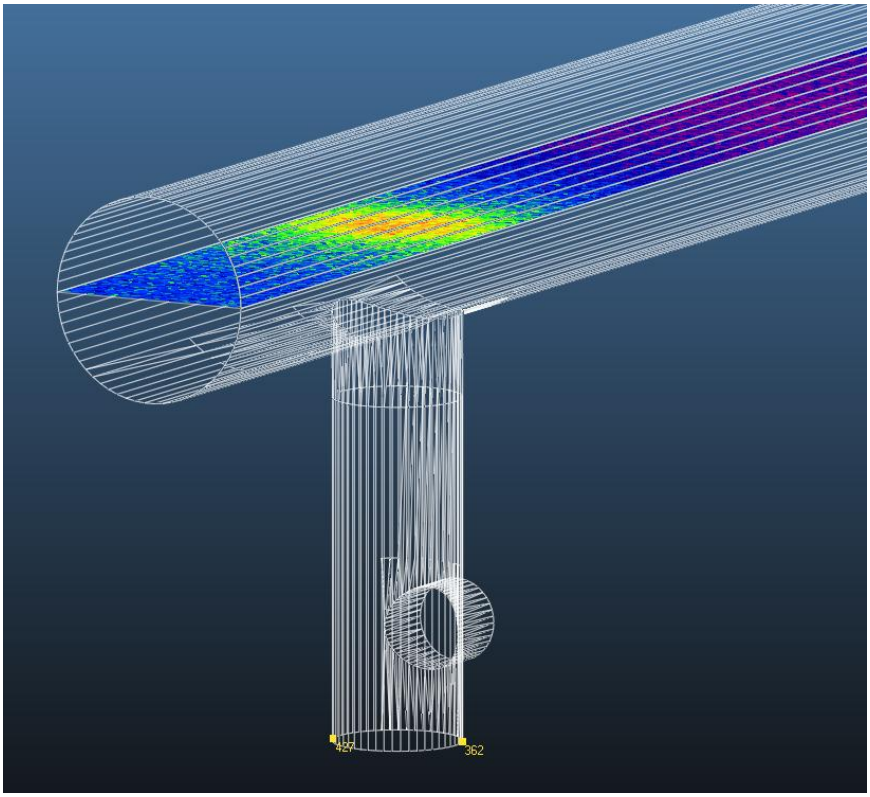


- Launch the simulation: it will show you the pressure in the middle of the pipe:

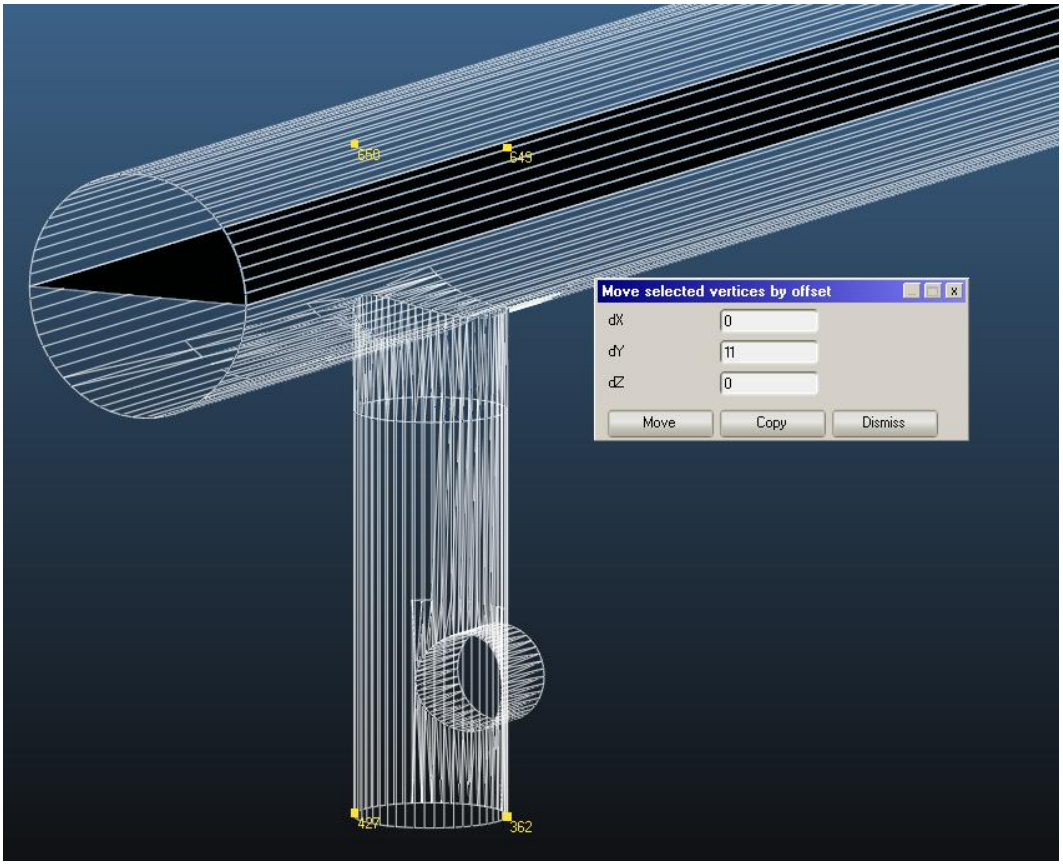


In the following, we'll add two vertical counter facets. This step will teach you how to copy vertices and facets.

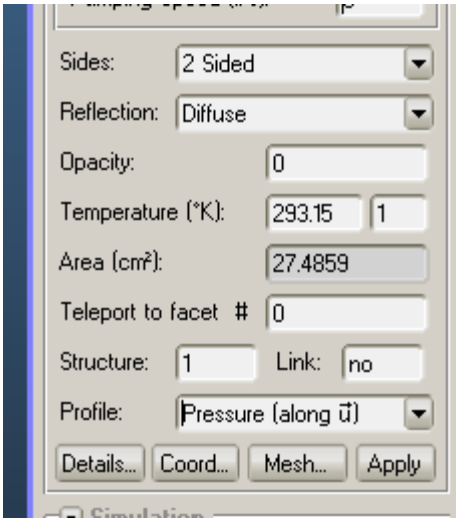
- Select two arbitrary vertices on the bottom pumping port. Ideally they are two opposite vertices, but this is not strict:



- With the Vertex / Move selected command, bring up a new dialog
- Turn on the "Rules" view option on the top right. This shows you the coordinate system: the Y axis points "up"
- Enter 11 into the dY field and press Copy. This will create a copy of the two selected vertices 11cm above the originals:



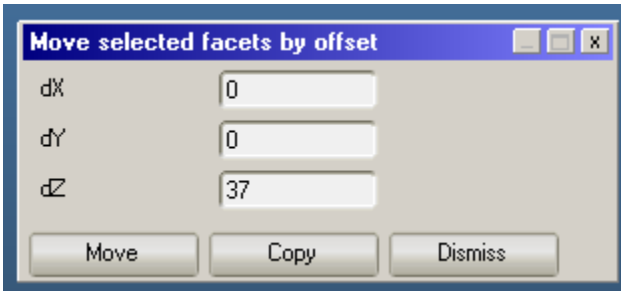
- With Vertex / Create facet from selected / Convex Hull (shortcut: CTRL + D), construct a new counter facet
- Finally, make it transparent, two-sided and add a profile, all this with the facet parameters:



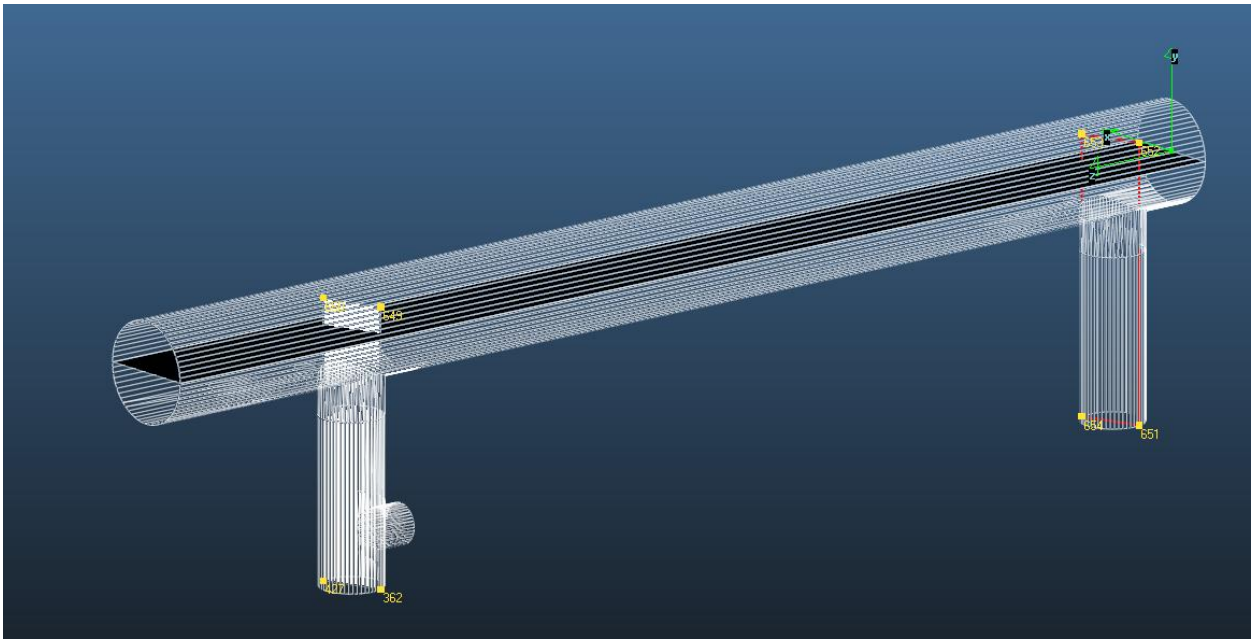
Instead of repeating the process for the other vertical pipe, it is more elegant to simply copy the facet we just created:

- With the facet that we created selected, open the Facet / Move… dialog.

- Enter 37 as dZ offset: this will create a copy in the other pipe:

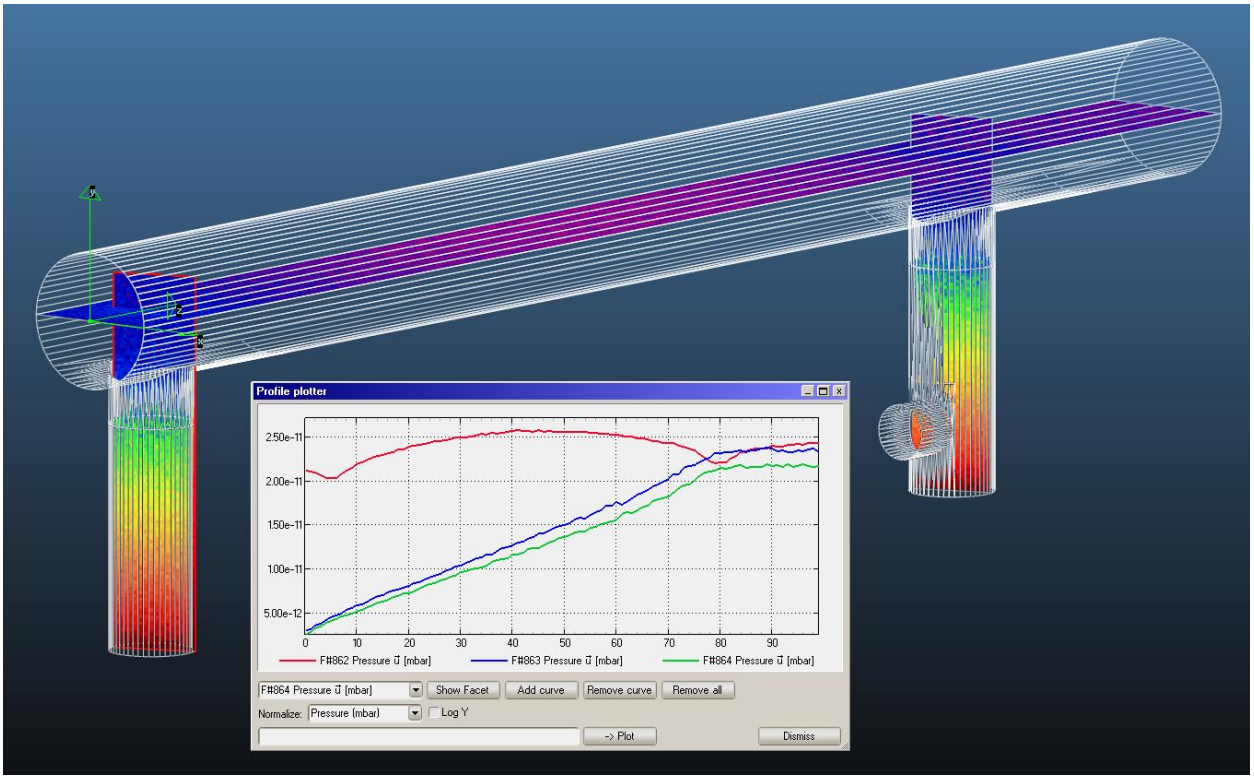


- Press Copy, which creates a counter facet in the other pipe, which will be already 2-sided and transparent.



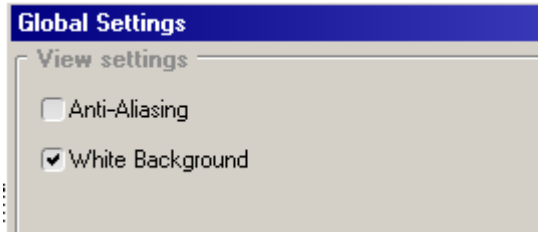
- Add a “Pressure along U” profile to the new facet
- Select both facets and add a texture (resolution: 10/cm, with **count transparent pass** option)

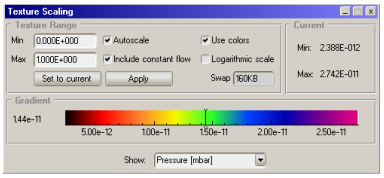
- Launch the simulation. You might notice that textures / plots converge faster this time.

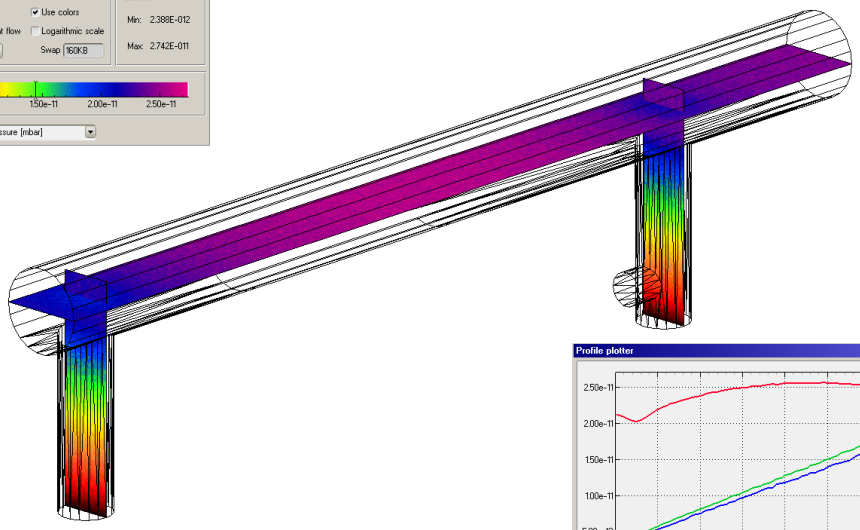


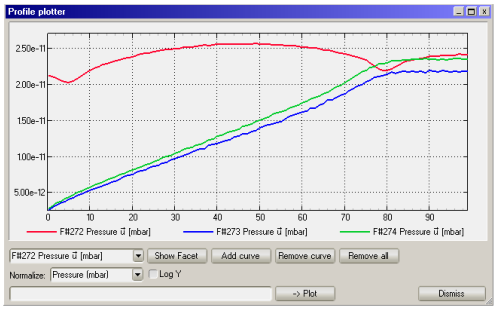
Hint: sometimes you might want to include your results in a paper or on a slide. You can remove the blue gradient background:

- Open Tools / Global Settings
- Deselect Anti-Aliasing and enable White Background:







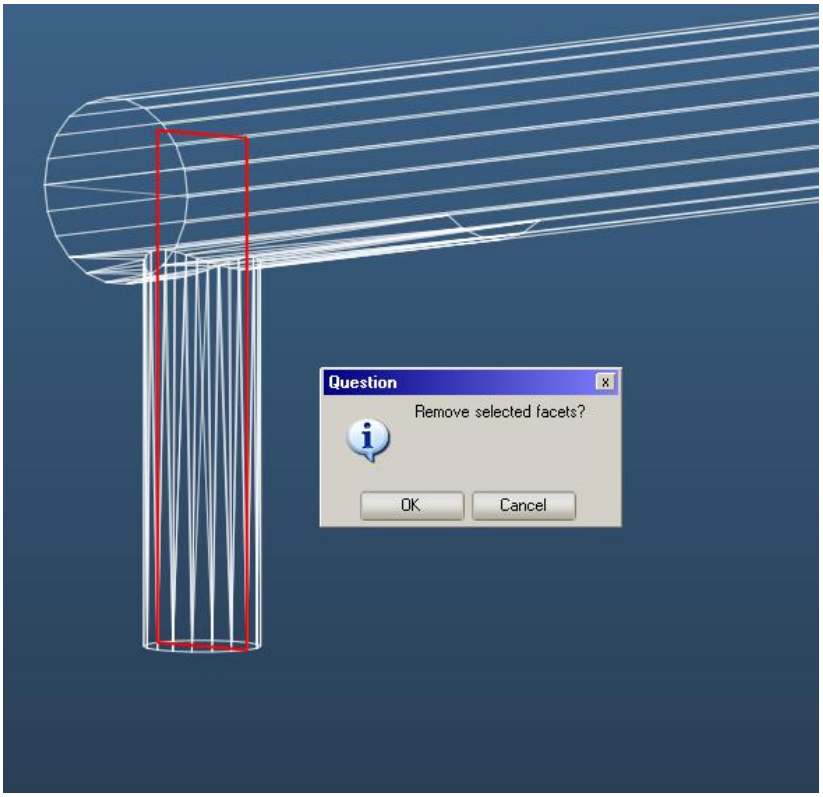


A simple optimization problem

Now that we have set up a simple system with gas source and pumping, let's see a practical use of Molflow. We'd like to see how the pressure is affected by putting the pump closer to the port.

We'll prepare the geometry by removing the vertical facet in the pumping port that has no stub. This will ease us to change its length.

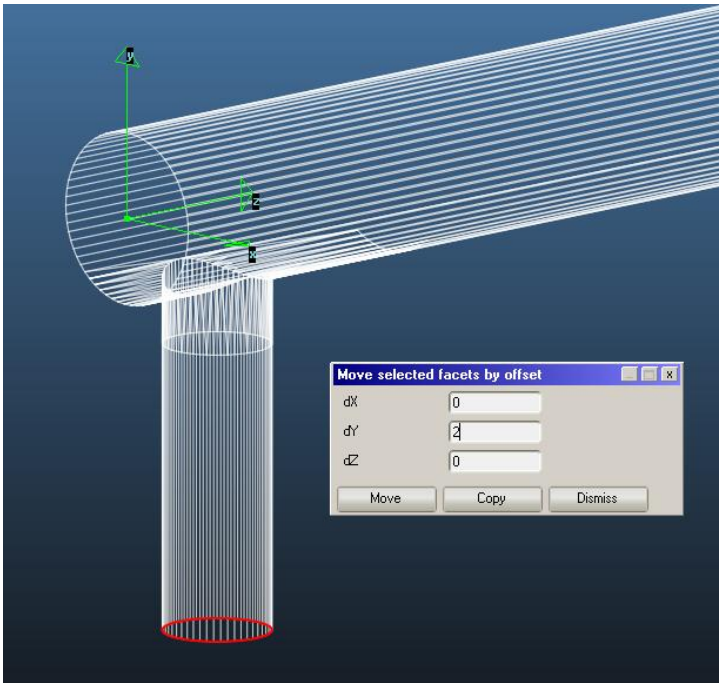
- Select the vertical counter facet
- Delete it by selecting Facet / Remove Selected (shortcut: CTRL+del)



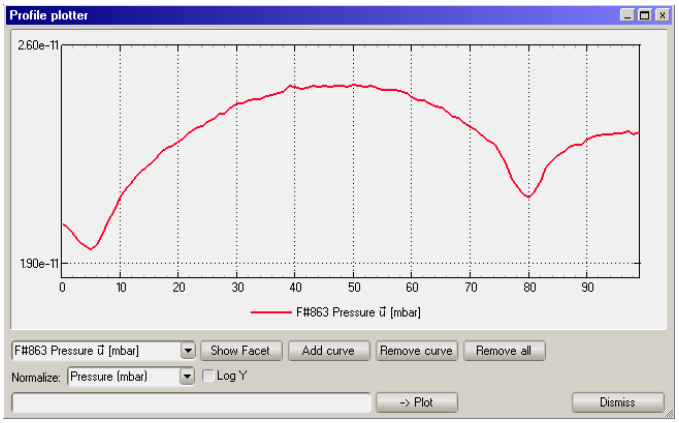
Now we will move the pump closer.

- Select the facet representing the pump

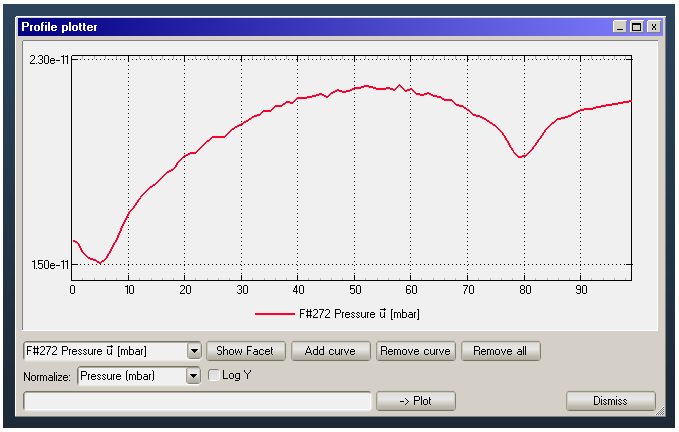
- Open the Facet / Move dialog



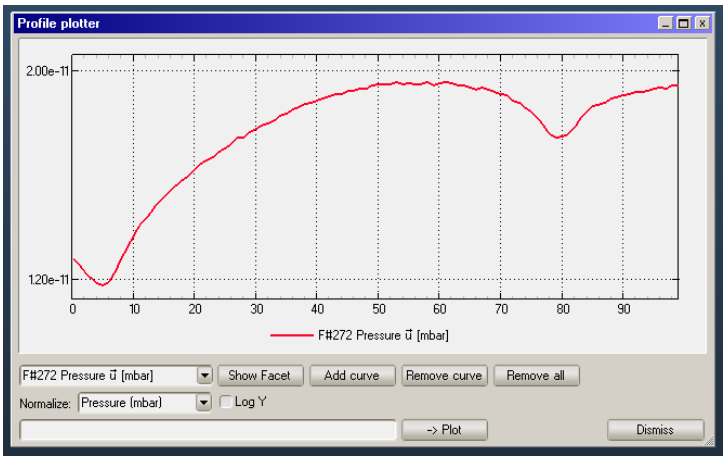
- Set dY offset to 2cm and press Move.
- Your pump is now closer. Let's see if it's more efficient.
- Start the simulation and plot the pressure profile on the horizontal counter facet



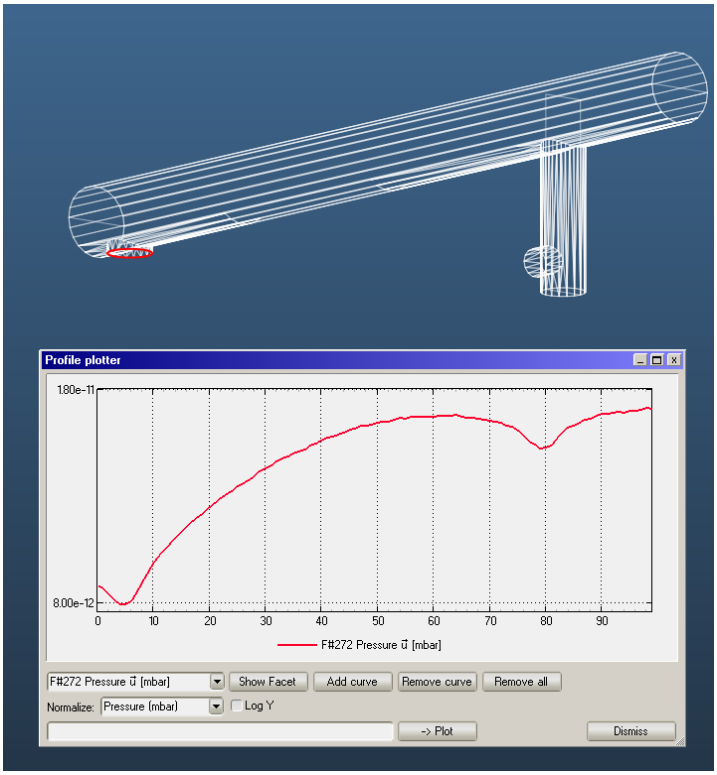
Profile for original geometry. Lowest pressure: 1.95E-11 mbar



Profile for pump that is 2 cm closer. Lowest pressure: 1.7E-11 mbar



Profile for pump 4cm closer. Lowest pressure: 1.45E-11 mbar



Profile for pump as close as possible. Lowest pressure: 8E-12 mbar

This small example gives an idea about the engineering applications possible with Molflow.

Periodic boundary conditions (teleport)

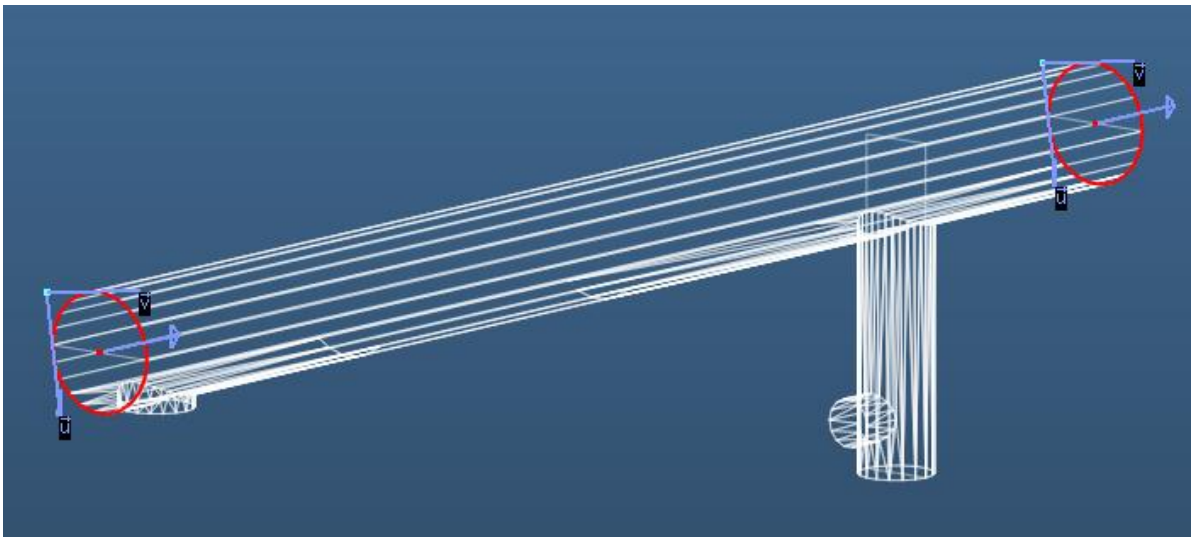
This final example shows how we can convert our accelerator section to a continuous, periodic machine. What we need is simply to connect the end sections, therefore "teleport" molecules back to the beginning when they are about to leave.

To set up a teleport between two facets, the following six conditions must be met:

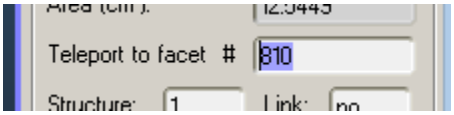
1. Both facets have the same shape
2. Both normal vectors point in the same direction
3. U, V vectors of facets are oriented the same way
4. Optional: in most of the cases, one of the two facets will receive molecules from its back (side opposite to its normal). In order to detect hits from its back, it has to be **2-sided.**
5. Facet A must teleport to facet B
6. Facet B must teleport to facet A

We will fulfill these conditions step by step:

- Select both facets
- Check the orientation of the normal and the U, V vectors (you might need to enable their display in the viewer settings in the top right corner)
- Very likely you have to reorient one of the two facets.
  - Use Facet / Swap normal (CTRL+N) to change the orientation of the normal vector
  - Use Facet / Shift Vertex (CTRL+H) to change U,V vector orientation
- If you have done everything correctly, you would see an identical orientation when you select both facets:

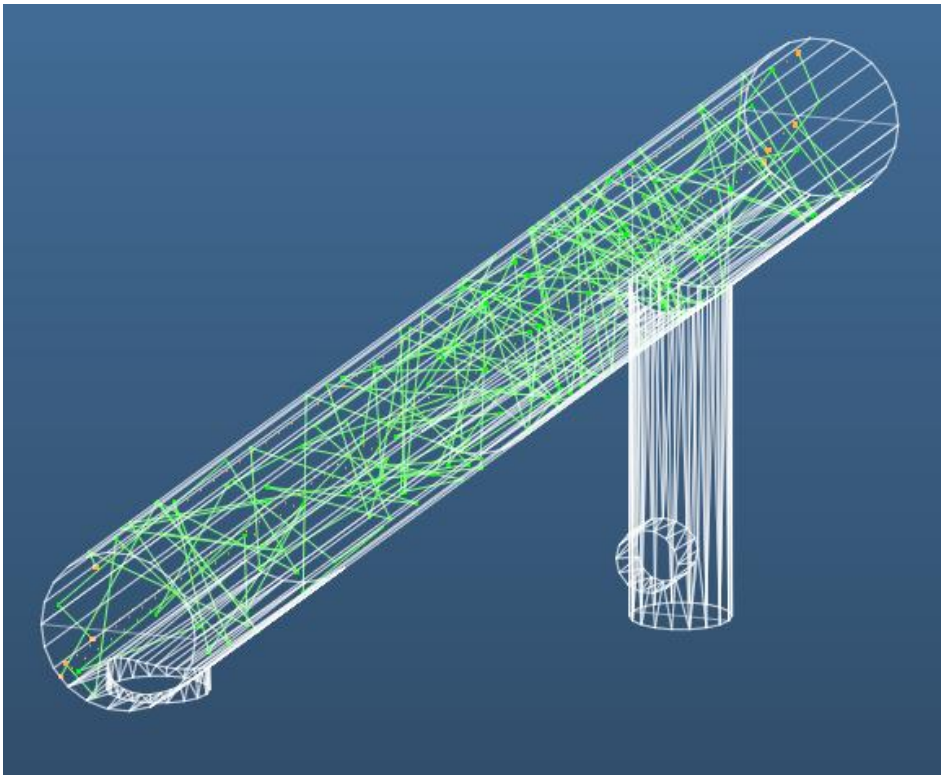


- Change the facet whose normal points outwards of the system (or simply both facets) to 2-sided
- Select one of the facets, and in the facet parameters panel, enter the **other** facet's number as teleport destination, and click Apply:

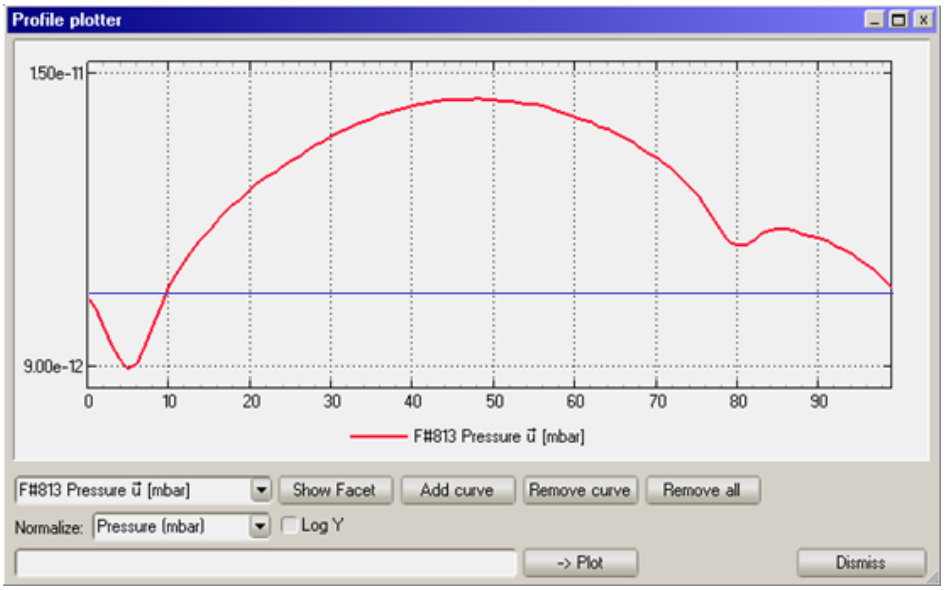


- Select the other facet, and enter the previous facet's number as teleport destination.

- That's it. You can begin the simulation. Teleports are displayed as orange dashed lines:



- And you can see that the pressure of the machine is now the same at the ends, which are the same logical point:



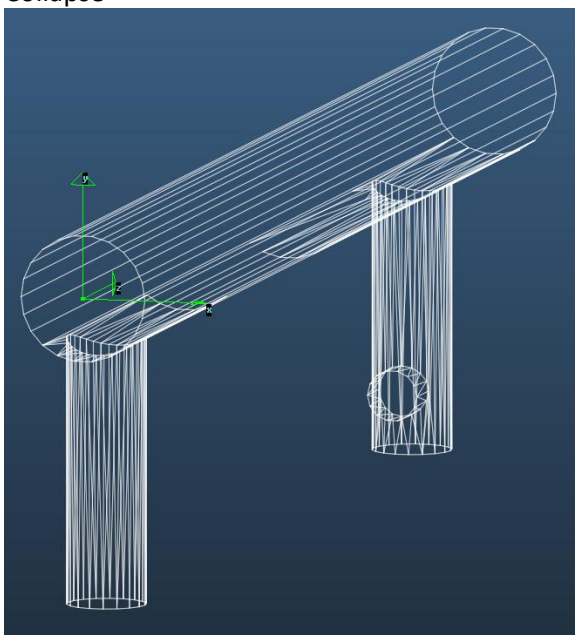
You can find the solution at this point as **hires-solution-teleport.geo7z**

Comparison of high and low resolution geometries

This extra step is to demonstrate that for vacuum simulation, it is usually the best practice to go for simple geometries. We will compare two models, each originating from the same geometry created in Autodesk Inventor, but exported with different resolutions.

Low resolution model

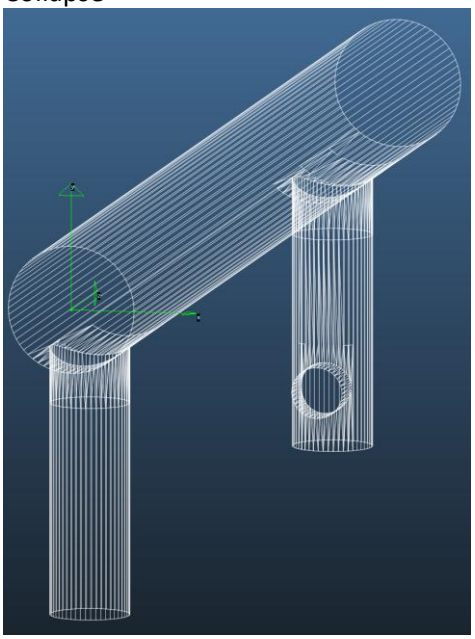
- Open **Part1-lores.stl**
- Choose millimeters as units
- Collapse



- You have 271 facets

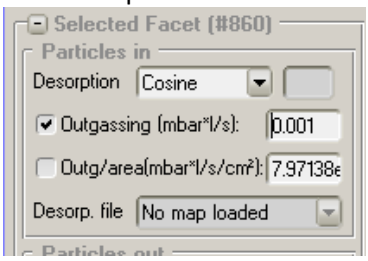
High resolution model

- Open **Part1-hires.stl**
- Choose millimeters as units
- Collapse

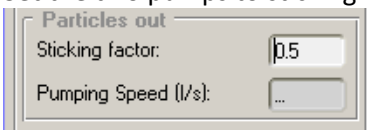


- You have 861 facets

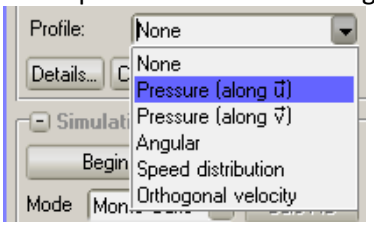
- Add desorption to the end facet (circular facet at the origin): 10^{-3} mbar.l/s



- Set the two pumps to sticking=0.5

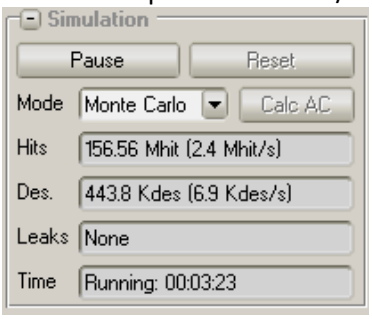


- Add a profile to one of the longitudinal facets on the wall

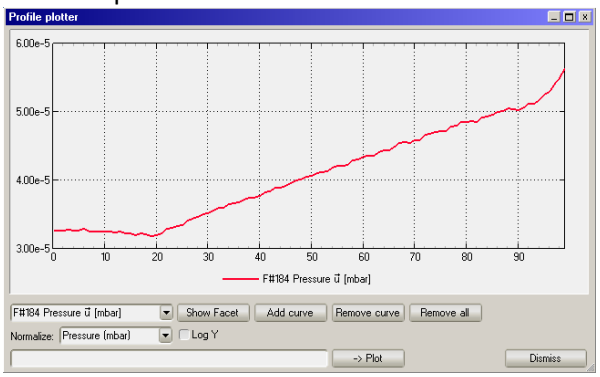


- Plot the profiles in the texture plotter

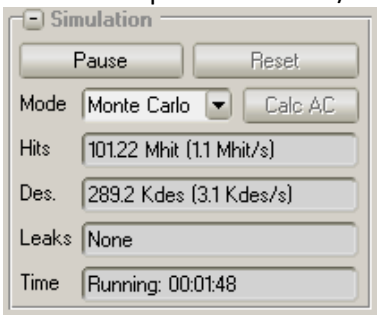
- Simulation speed is 2.4MHit/s



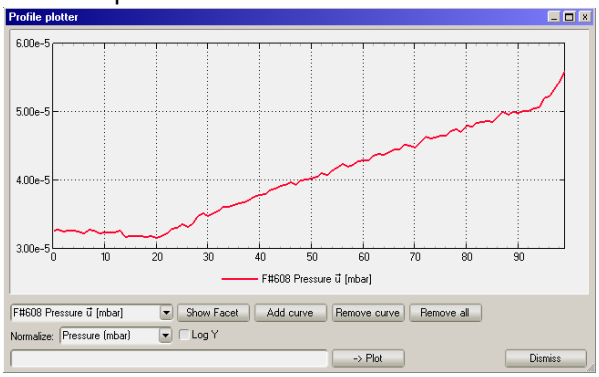
- Pressure profile:



- Simulation speed is 1.1MHit/s



- Pressure profile:



Conclusion: by choosing a lower resolution, we have doubled the simulation speed

Suggested reading:

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