course website

TMP study meeting

Vacuum simulations (MolFlow) tutorial

KEK, 31st May 2024

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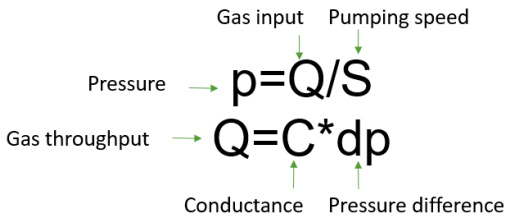
Molflow version: 2.9.24

1) Vacuum equations

Two fundamental equations of Ultra High Vacuum:



Units (most used at CERN):

P (pressure): mbar (1 mbar = 100 Pa)
Q (gas flow): mbar*l/s (1 mbar*l/s = 0.1 Pa*m3/s)
C (conductance): l/s
S (pumping speed): l/s

Conductance of a hole of area A:

C_{hole}=1/4 * <v> * A where <v> is the average molecule speed

<v> [m/s] = $\sqrt{\frac{8RT}{\pi M}}$ (M: gas molar mass in kg, T: gas temperature in K)

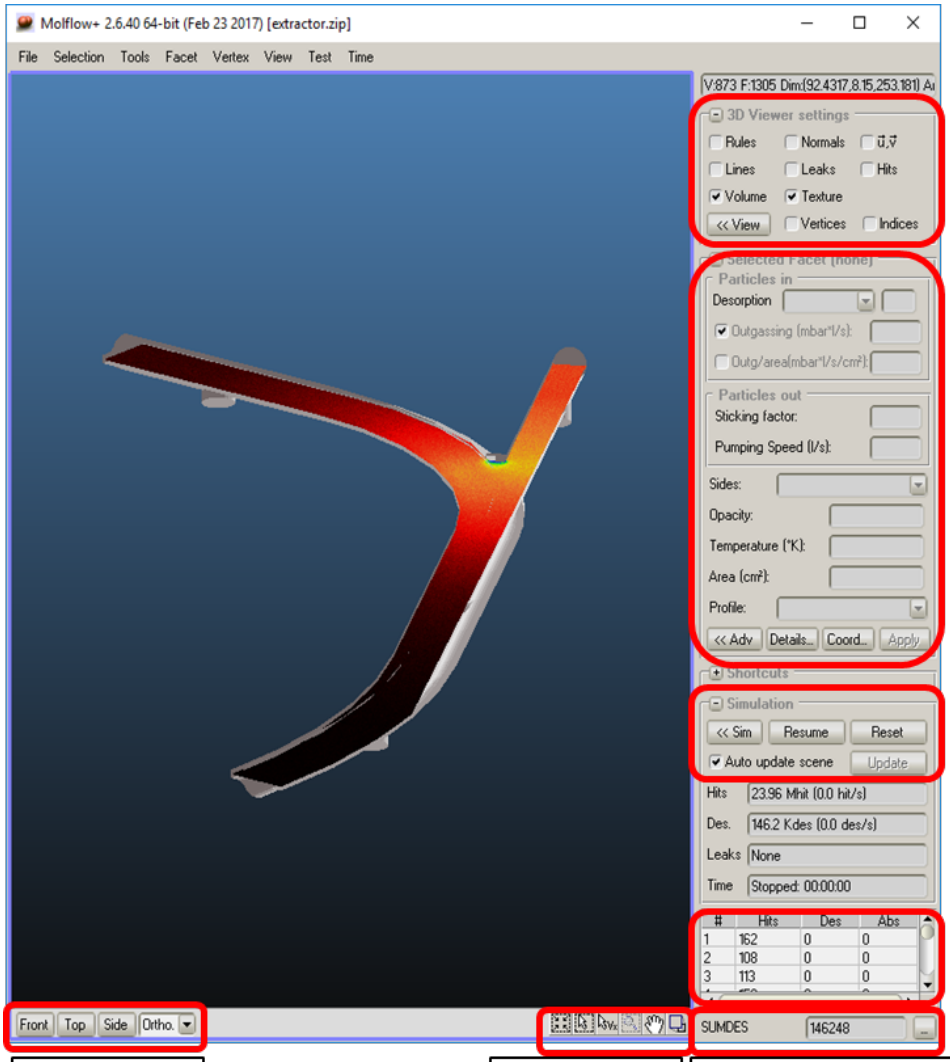
Pumping speed of an area with sticking factor ‘s’:

S = s * C_{hole} = s * ¼ * A * <v>

Local (effective) pumping speed at point B of a pump of speed S_A installed at point A:

$1/S_{eff,B}=1/S_A + 1/C_{A->B}$ where $C_{A->B}$ is the conductance between the two locations

2) Molflow cheatsheet



View controls
Here you can toggle what's on the screen, i.e. enable/disable the display of textures, particle trajectories, etc

Facet parameters
For the selected facets, you can set here:

- **Outgassing:** how many particles the facet is emitting
- **Sticking:** the pumping of the facet
- **Opacity:** how transparent the facet is
- **Profile and textures:** some of these are available in the expanding dialog when clicking on <<Adv

Simulation control
Start, stop and reset the simulation here

Facet list
You can select facets from here, and also check the number of Monte Carlo hits on each of them, which can serve as a diagnostic tool

Camera tools
You can return to the default Front / Top / Side view here

Selector tools
You can choose between vertex and facet selection, and also access the autoscale button

Formulas
You can define mathematical expressions that are evaluated here. You can refer to the pressure, number of hits, etc. of facets, and also global parameters like the gas mass.

Mouse controls:

Selection: left button

Rectangle selection: hold left button

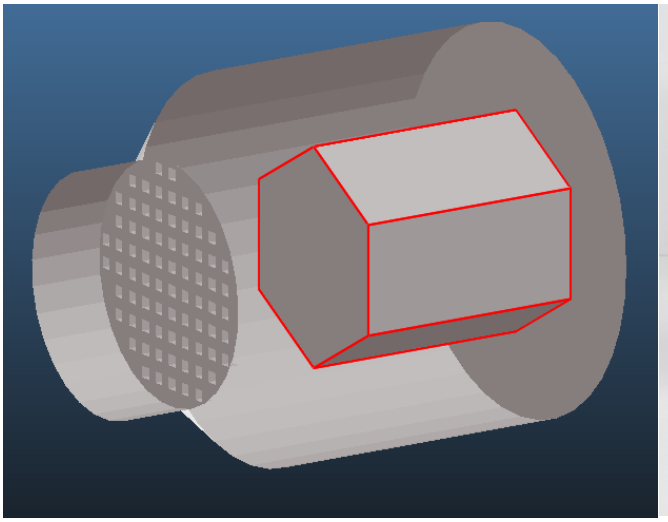
Add/Remove from selection: hold SHIFT to add, CTRL to remove

Rotation: right button (slow rotation: hold SHIFT)

Pan: hold middle button (or D on keyboard)

Zoom: mouse wheel (slow / fast zoom: hold SHIFT / CTRL). Alternatively, hold Z on the keyboard and the left mouse button, and drag up/down

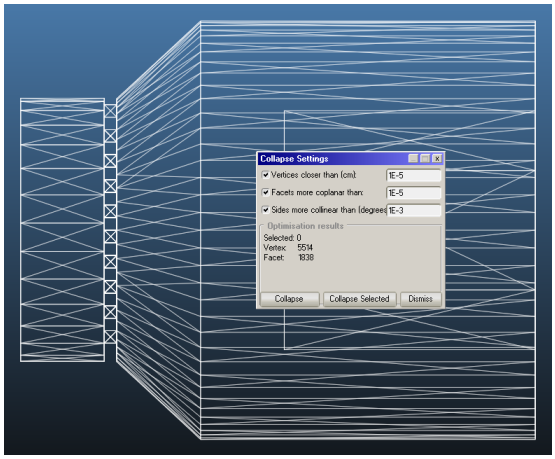
3) Guided work: Effective pumping speed calculation

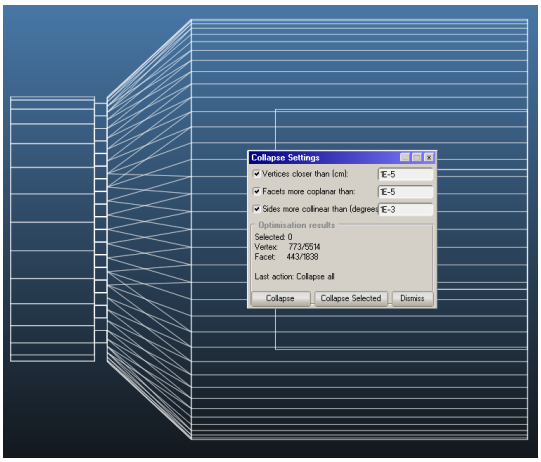


In this, first part we will approximate the effective (local) pumping speed of a NEG cartridge pump's pumping port. The goal is to use this result in the second part, when we'll be simulating a part of an accelerator.

Opening and collapsing the file

- Load **neg_cartridge_pump.stl**, a file originating from the CAD program, and choose **centimeters** as units.
  Hint: STL files are also used by 3D printers, and as such, most CAD programs can export to it.
- Since this file – at its opened form – contains only triangles, we need to **collapse** it: leave the default parameters as they are and click collapse:

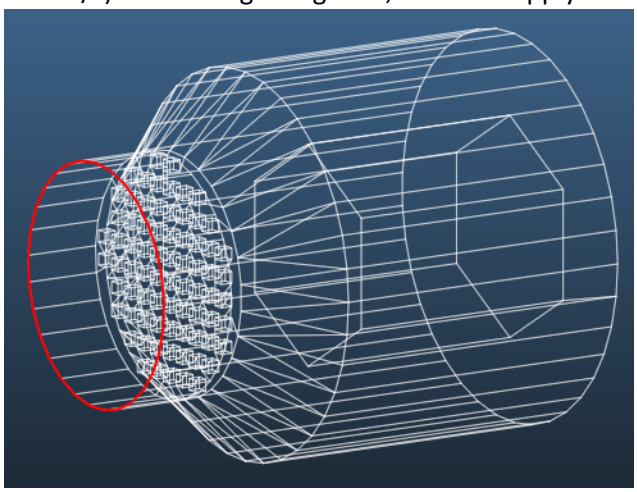


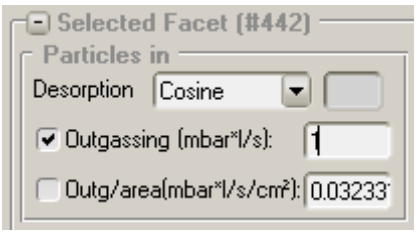


- You can now save the collapsed file in Molflow format, so during the tutorial you can save it with one click. Choose File/Save, give the file a name, and press enter – Molflow will append the default .zip extension.

Setting up desorption

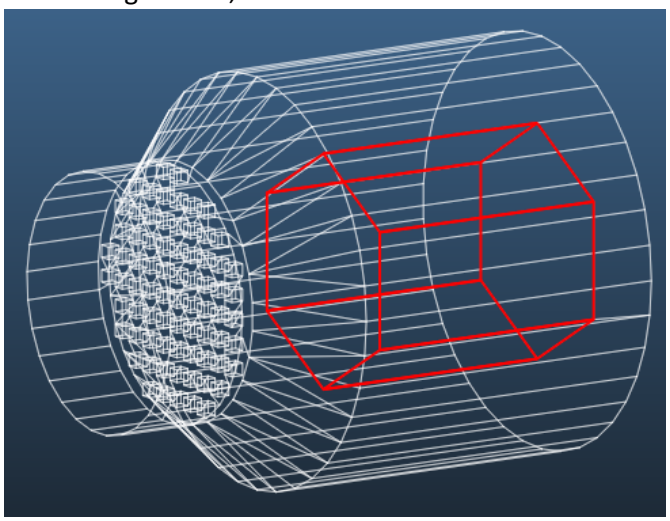
- Select the pump entrance facet. On the right side, choose **Cosine** outgassing, then enter **"1"** (equals to 1 mbar.l/s) in the Outgassing field, and click Apply:

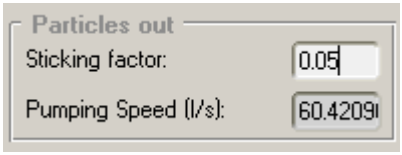




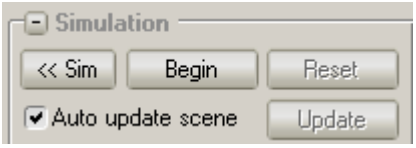
Setting up pumping

- In this model, the pumping surfaces are those representing the NEG coating: they are the sides of the hexagonal volume.
- Select the six facets. *Hint:* you can select the hexagonal volume (7 facets) by a rectangle selection then deselect the end cap by a second rectangular selection holding CTRL
- Set sticking to 0.05, a conservative value for NEG. Don't forget to press ENTER or click Apply.

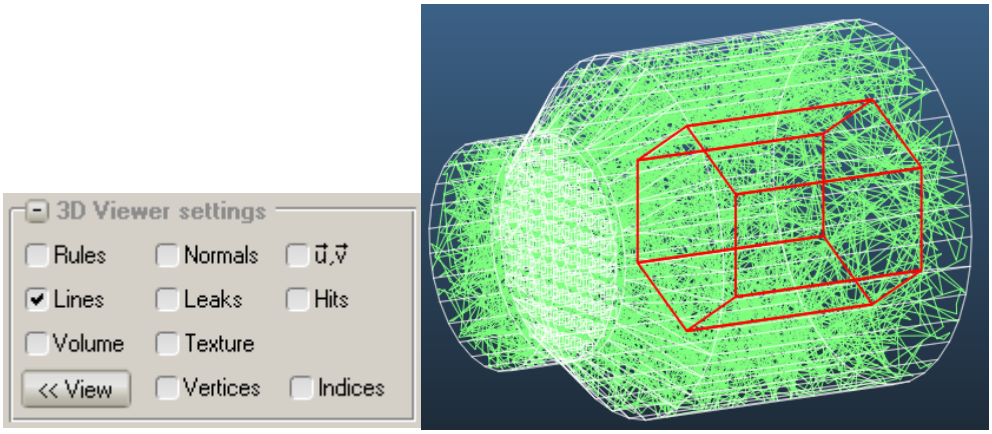




Launching the simulation

- That's it! You have successfully set up outgassing and sticking, therefore allis ready to calculate.
  - Click the Begin button: 

- Turn on molecule trajectory display (**Lines** option, upper right) to check if everything is as intended:



Extracting results

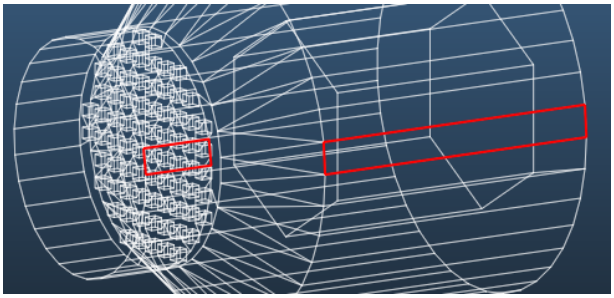
The simulation can be stopped after a few seconds. It's a good time to save results.

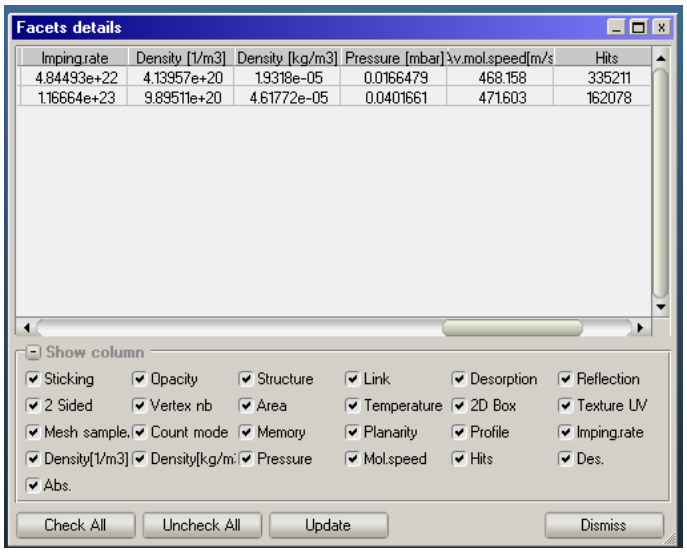
We will see four different ways of getting the effective pumping speed:

- By reading the pressure on facets
- By using formulas
- By using profiles
- By using textures

Reading pressure on facets

Select a facet near the entrance and one on the inside of the cartridge volume, the click Details. In the **Facet Details** window, you can read the pressures on the facets:





Staying at the values of the above screenshot, using the first equation of this note:

$$P_{local} = Q / S_{eff}$$

At the entrance: 0.04 mbar = 1 mbar.l/s / S_{eff} -> S_{eff} = 1/0.04 = **25 l/s**

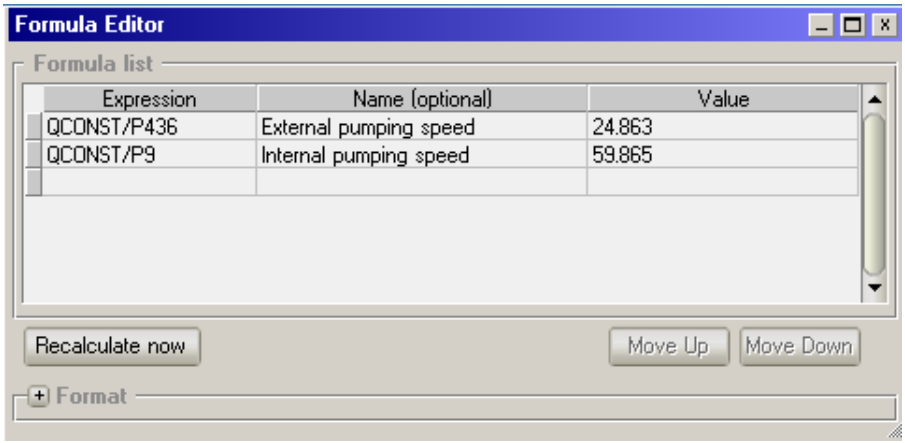
At the pump volume: 0.016648 mbar = 1 mbar.l/s / S_{eff} -> S_{eff} = 1/0.016648 = **60 l/s**

Small note: you can verify that these values are correct. Select any of the NEG facets. You will see that the pumping speed (corresponding to our sticking factor of 0.05) is 10 l/s. As we have six of these facets, the local pumping speed is indeed 60 l/s.

Using formulas

We can let Molflow evaluate the above equations for convenience. The calculated pumping speeds will be updated every second as the simulation is running, giving us an idea when the calculation has converged.

- In the Tools/Formula Editor menu option, we create new formulas, as in the screenshot:



  Explanation: QCONST is the outgassing, P436 is the pressure on facet #436 (in red)
- We add a second formula. Expression: QCONST/P9 (facet 9 is inside)
- *Hint1:* you can access a cheat sheet of available formulas by expanding the Format panel

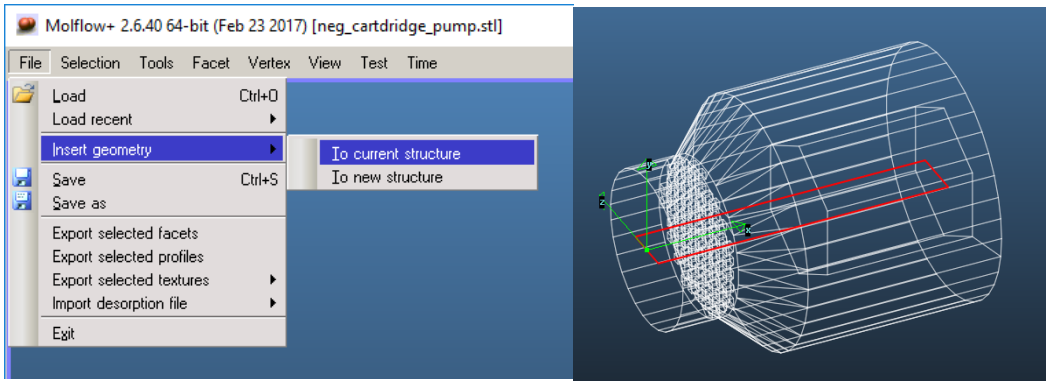
- *Hint2:* if the values in the formulas don't appear or don't update, open the **Global Settings** dialog (Tools / Global Settings), check **Auto-update formulas** and click **Apply above settings**

Using profiles

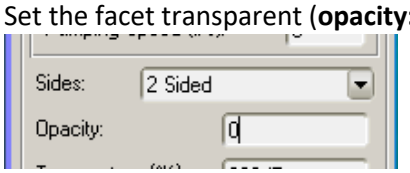
On **rectangular** facets, you can enable profiles which allow quick plotting of the pressure in a direction. Profiles can be set up on existing facets (on the walls), but for our purposes we will use **a transparent facet** that goes through the volume.

Although Molflow has geometry editing options, for simplicity we'll import an extra facet.

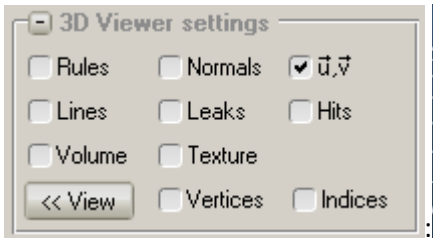
- Choose File / Insert geometry / To current structure and open **pump_profile.zip**:

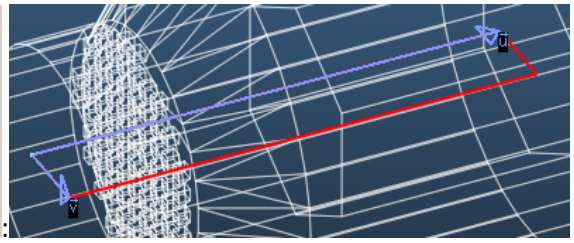


- Set the facet transparent (**opacity: 0**) and **2-sided:**

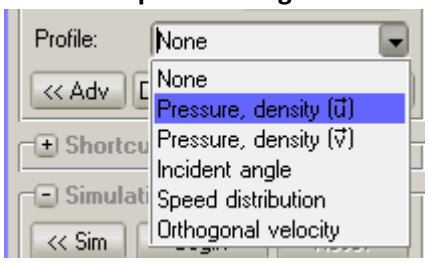


- Enable the **U,V vector** display (upper right), and check that the U vector is oriented along the facet's longer side:

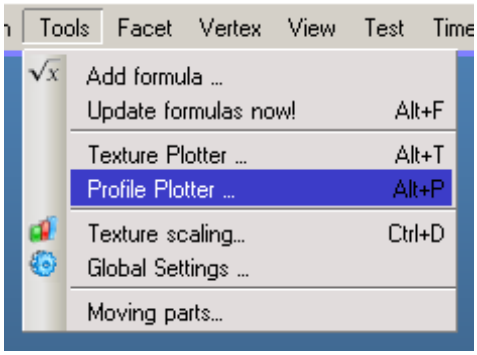


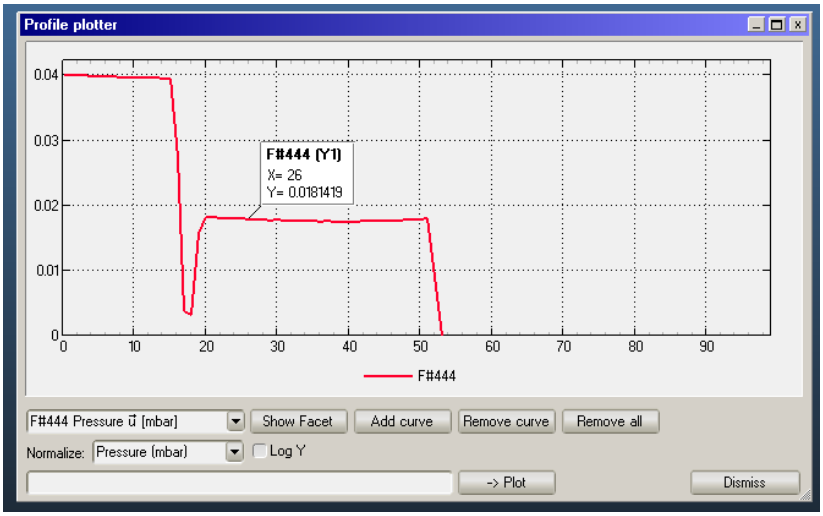


- Enable the **profile along the U vector:**



- Open the profile plotter, chooses the profile you just added and click **Add curve**, then run the simulation:





- When the simulation is stopped, clicking on the graph reveals the value. You can verify two things:
  - The pressure only drops at the grill (limited conductance)
  - Within volumes, it's almost constant (large conductance)
- Reading the pressure values (0.04 and 0.018 mbar) we can calculate the same pumping speeds

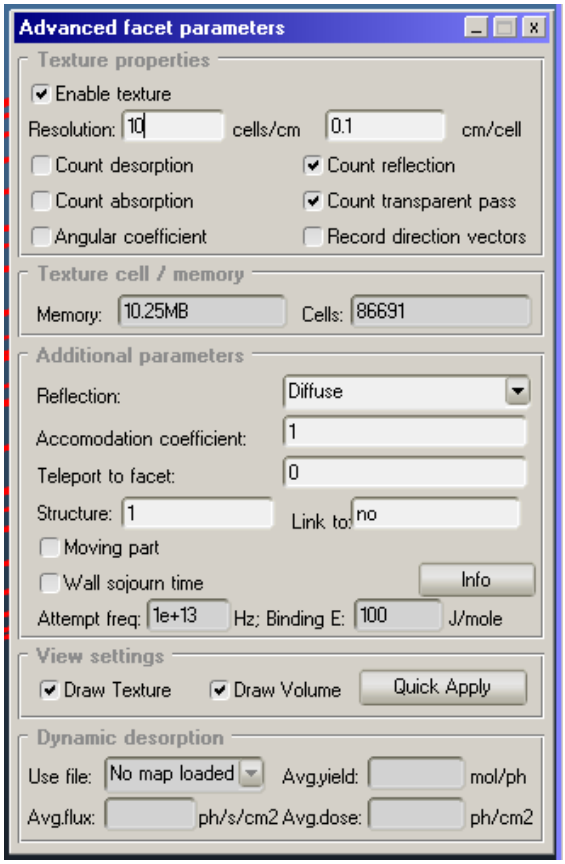
Using textures

Textures are color-coded pressure values displayed directly on the facets.

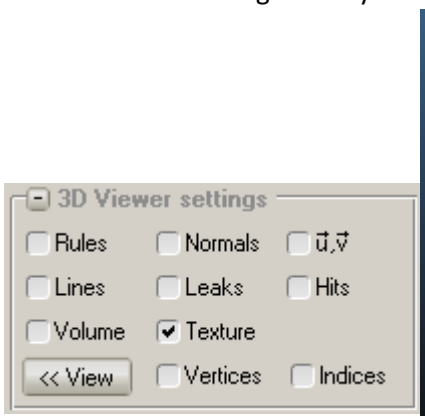
For simplicity, we'll enable textures on all facets.

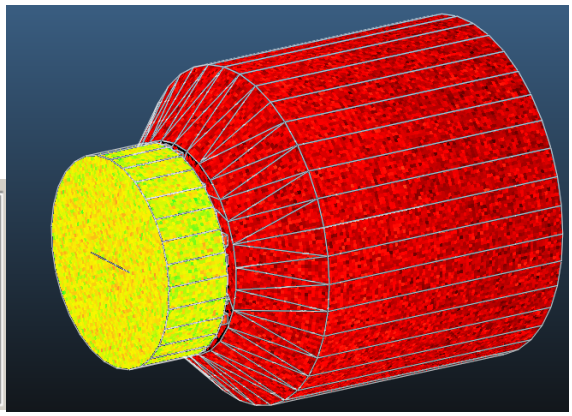
- Select all facets (by a rectangle or with the shortcut **CTRL+A**)

- On the facet parameters menu, open the advanced options by clicking on the << Adv button:

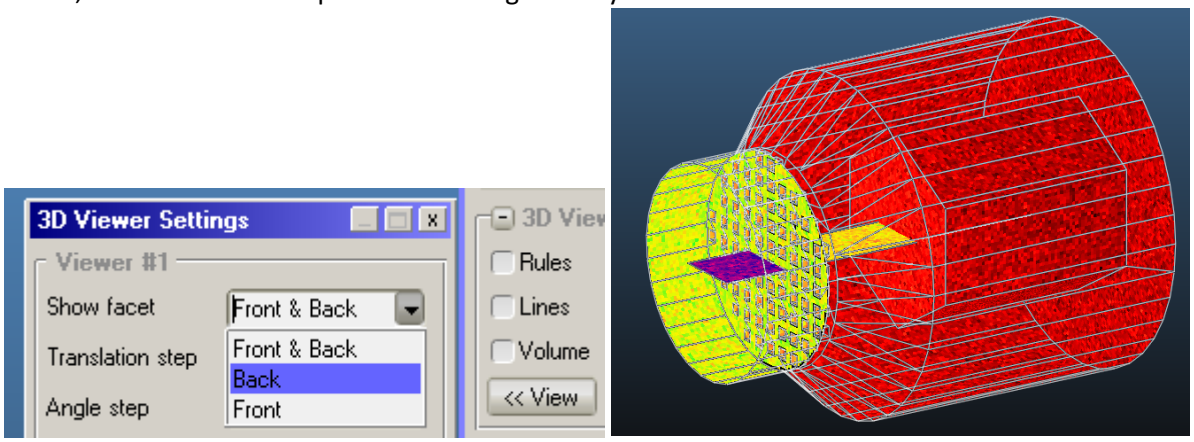


- Click **Enable texture**
- Set the resolution to **10 cells/cm**, a good compromise between details and speed
- Choose **Count reflection** and **Count transparent pass** as options. The former will count pressure on the walls, the latter on the transparent facet we've added for the profile
- Run the simulation. If you turn on the **Texture** option in the upper right corner, you should see the pressure distribution over the geometry:

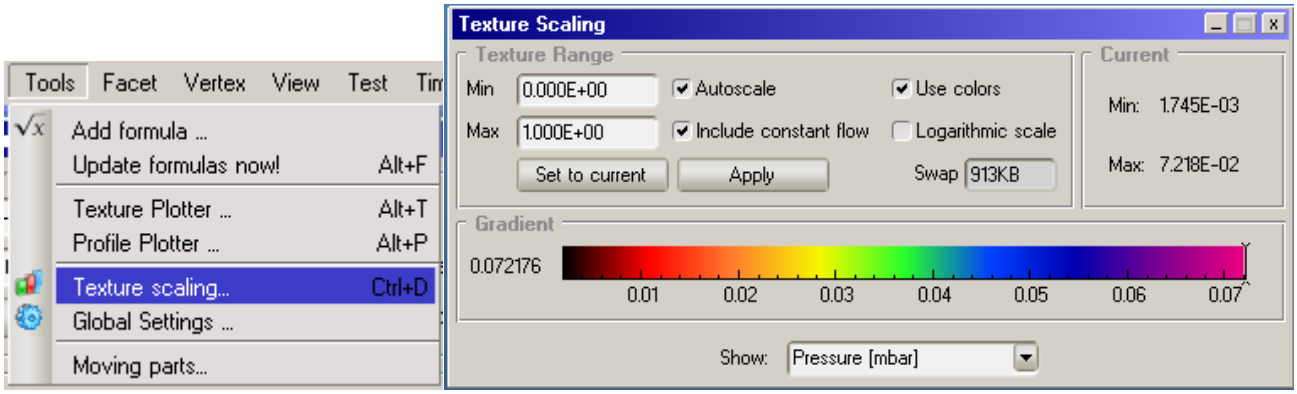




- In the advanced viewer options (click the **<<View** button), you can choose to render only the back side of facets, which will allow to peek inside the geometry:

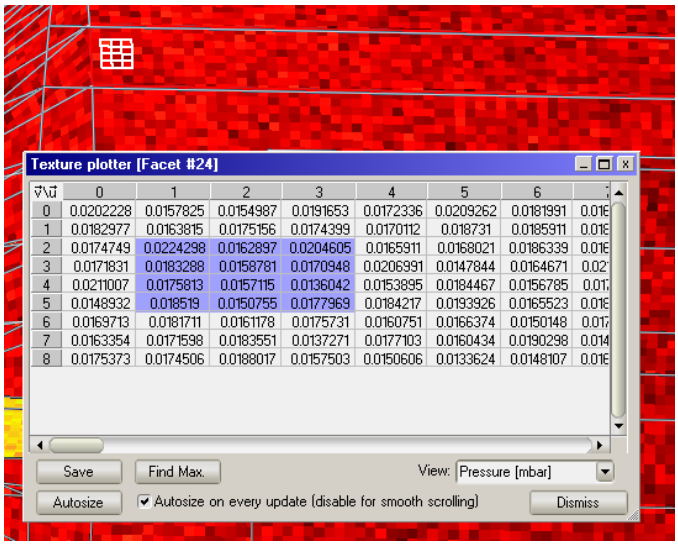


- Finally, to interpret the colors, open the **Texture Scaling** window (**CTRL+D**):



Here, among others, you can switch on logarithmic view, which is more suitable for plotting large pressure differences.

- Finally, you can extract pressure values from a texture by **selecting a textured facet** and opening the **Texture Plotter** window:



- As seen above, clicking on a cell (or a range of cells) highlights the position on the texture.

It's a good idea to save the simulation now.

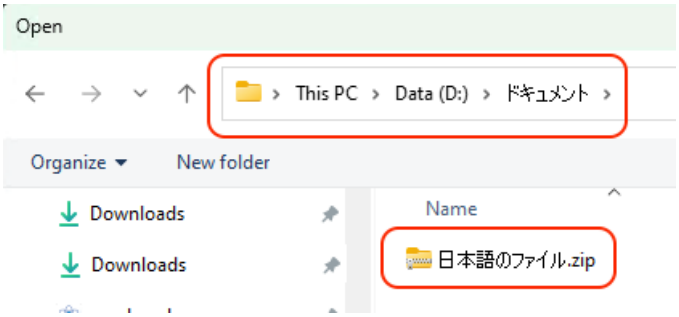
You can find the solution in the file **cartridge_pump_solved.zip**

3) Appendix (Windows only): make MolFlow recognize UTF-8 filenames

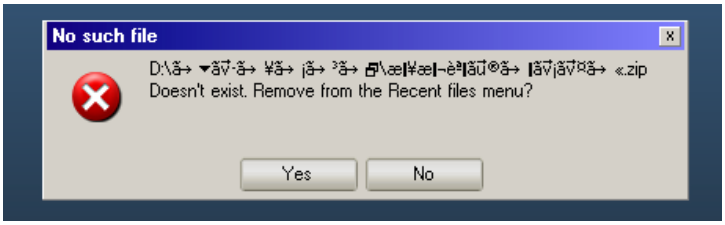
The problem

If the path (or the name) of the file contains 2-byte (UTF-8) characters, Molflow throws a "not found" error:

Trying to open `D:\ドキュメント\日本語のファイル.zip`:



We get the following error:

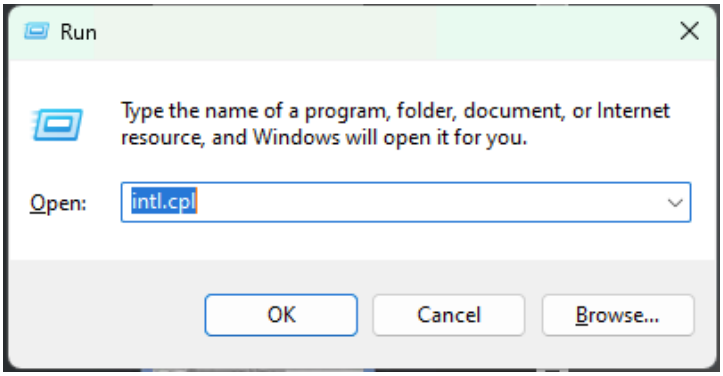


Fix: enable UTF-8 support in Windows

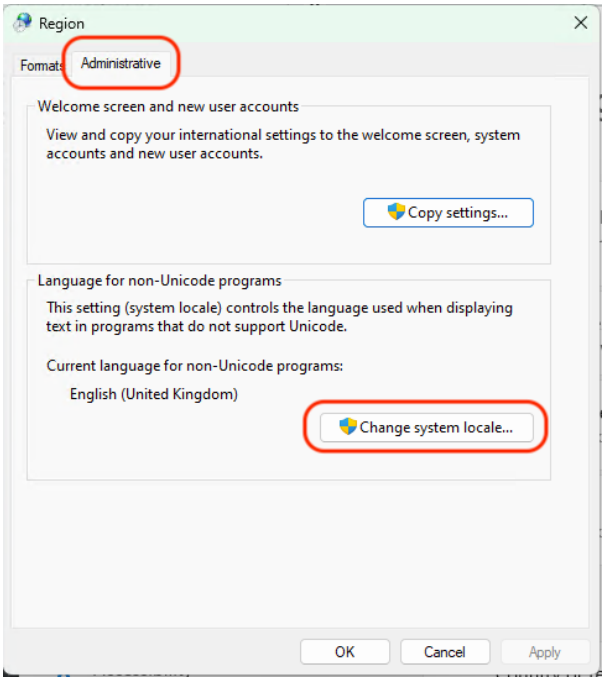
This only works for recent Windows versions:

- Windows 10 May 2019 update or later
- Windows Server 2019 version 1809 or later
- Windows 11

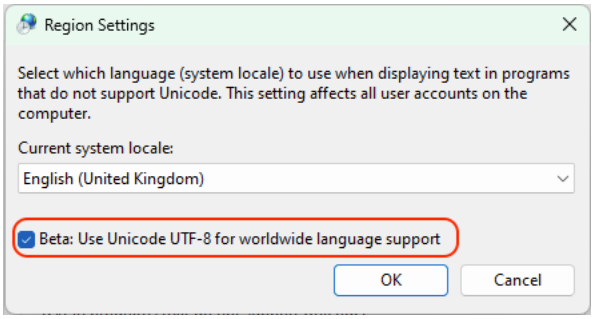
Go to Run... (Windows key + R) and type `intl.cpl`:



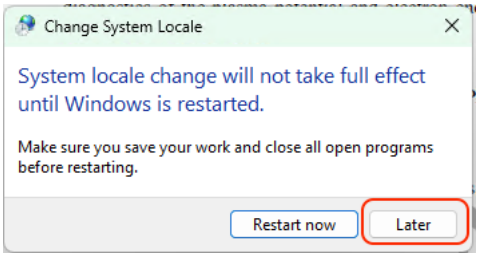
In the window that appears, switch to Administrative tab and click Change system locale...



Enable UTF-8 (available in up to date Windows versions only)



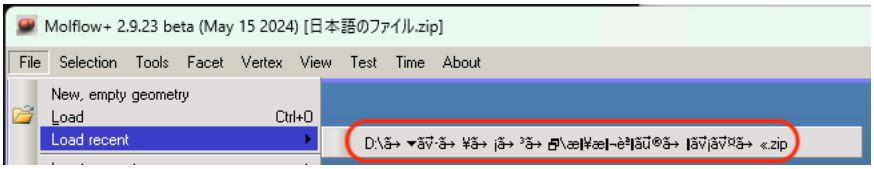
You don't need to restart Windows, but you have to restart MolFlow.



Result

Now MolFlow can load UTF-8 filenames:

Please note that MolFlow's UI still won't display UTF-8 characters correctly:



After working with MolFlow, you can disable UTF-8 again if it causes problems in other applications.

Molflow website: cern.ch/molflow

Tutors' contact: marton.ady@cern.ch