

TMP study meeting Vacuum simulations (MolFlow) tutorial

KEK, 31st May 2024 Marton Ady

Molflow version: 2.9.24

1) Vacuum equations



Gas input Pumping speed Pressure $\rightarrow p = Q/S$ Gas throughput $\rightarrow Q = C * dp$ Conductance Pressure difference

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 SA 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



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:

Facets details]
Impingrate 4.84493e+22 1.16664e+23	Density [1/m3] 4.13957e+20 9.89511e+20	Density [kg/m3] 19318e-05 4.61772e-05	Pressure [mbar] 0.0166479 0.0401661	\v.mol.speed[m/ 468.158 471603	s Hits 335211 162078	
Show colum Sticking Sticking 2 Sided Mesh sample Density[1/m3] Abs. Check All	nn v Opacity vertex nb v Count mode v Density[kg/m Uncheck A	Structure Area Memory F Pressure Updal	Link Temperature Planarity Mol.speed te	 ✓ Desorption ✓ 2D Box ✓ Profile ✓ Hits 	 ✓ Reflection ✓ Texture UV ✓ Impingrate ✓ Des. 	

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:

Fo	rmula Editor			_ 🗆 X
г F	ormula list ———			
	Expression	Name (optional)	Value	
	QCONST/P436	External pumping speed	24.863	\square
	QCONST/P9	Internal pumping speed	59.865	
				T
E	Recalculate now		Move Up Move	Down
Ē) Format			

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

Recalculate no	ow M	love Up Move Down
Pn (Pressure (r	n (Absorption on facet n), Dn (Desorption on facet n), Hn (Hit o (mbar) on facet n), DENn (Density [1/m3] on facet n)	on facet n)

• *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:

9	Molflow+ 2.6.40 64-bit (F	eb 23 201	7) [neg_cartdridge_pump.stl]	
File	e Selection Tools Face	t Vertex	View Test Time	
2	Load Load recent	Ctrl+O ▶		
	Insert geometry	•	To current structure	
	Save Save as	Ctrl+S	Io new structure	
	Export selected facets Export selected profiles			
	Export selected textures	1		
	Egit			

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

Sides:	2 Sided
Opacity:	q
- ·	(4)()

 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**:

Profile:	None	
	None	h
	Pressure, density (ជី) 👘	Ľ
r	Pressure, density (∛)	ŀ
	Incident angle	ŀ
🕞 🖂 Simulati	Speed distribution	ŀ
ZZ Sim	Orthogonal velocity	
((Onn		1

• 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:

Advanced facet parameters
C Texture properties
Enable texture
Resolution: 10 cells/cm 0.1 cm/cell
Count desorption
Count absorption Count transparent pass
Angular coefficient Record direction vectors
Texture cell / memory
Memory: 10.25MB Cells: 86691
Additional parameters
Reflection: Diffuse
Accomodation coefficient: 1
Teleport to facet: 0
Structure: 1 Link to
Moving part
Wall sojourn time
Attempt freq: 1e+13 Hz; Binding E: 100 J/mole
View settings
Draw Texture Traw Volume Quick Apply
C Dynamic desorption
Use file: No map loaded Avg.yield: mol/ph
Avg.flux: ph/s/cm2 Avg.dose: ph/cm2

- 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**):

			Texture Scaling
_			Current Current
Toe	ols Facet Vertex View	Test Tim	Min 0.000E+00 Autoscale Use colors Min: 1745E-03
\sqrt{x}	Add formula		Max 1.000E+00 🔽 Include constant flow 🗌 Logarithmic scale
	Update formulas now!	Alt+F	Set to current Apply Swap 913KB Max: 7.218E-02
:	Texture Plotter	Alt+T	c Gradient
	Profile Plotter	Alt+P	
d.	Texture scaling	Ctrl+D	
۲	Global Settings		
	Moving parts		Show: Pressure [mbar]

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:

	Ŧ	E								
	P									
	Text	ure plotter	[Facet #24	H I					_ 🗆 X	
	 √d 0 1 2 3 4 5 6 7 8 	0 0.0202228 0.0182977 0.0174749 0.0171831 0.0211007 0.0148332 0.0169713 0.0163354 0.0175373	1 0.0157825 0.0163815 0.0224298 0.0183288 0.0175813 0.018519 0.0181711 0.0181711 0.0171598 0.0174506	2 0.0154987 0.0175156 0.0162897 0.0158781 0.0150755 0.0150755 0.0161178 0.0183551 0.0188017	3 0.0191653 0.0174399 0.0204605 0.0170948 0.0136042 0.0177968 0.0175731 0.0137271 0.0157503	4 0.0172336 0.0170112 0.0165911 0.0206991 0.0153895 0.0184217 0.0160751 0.0160751 0.0177103 0.0150606	5 0.0209262 0.018731 0.0168021 0.0147844 0.0193926 0.0166374 0.0160434 0.0133624	6 0.0181991 0.0185911 0.0186339 0.0164671 0.0156785 0.0165523 0.0150148 0.0190298 0.0148107	0.016 0.016 0.016 0.02 0.011 0.011 0.011 0.011 0.011 0.011	
N		Save utosize	Find Max. Autosize	on every up	date (disable	V for smooth	iew: Pressu scrolling)	re (mbar) Dis	Timiss	

• 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:

No such	file X
8	D∖\ă→ ▼ă√-ă→ ¥ă→ jă→ ³ă→ ∄ \æl¥æl-èªlăŭ®ă→ lă⊽jă∛¤ă→ «zip Doesn't exist. Remove from the Recent files menu?
	Yes No

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...

Velcome screen and	new user accounts
View and copy your accounts and new u	international settings to the welcome screen, system user accounts.
	Copy settings
anguage for non-Ur	nicode programs
This setting (system text in programs the	locale) controls the language used when displaying at do not support Unicode.
Current language fo	or non-Unicode programs:
can an gauge re	
English (United	Kingdom)

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

🔗 Region Settings	×					
Select which language (system locale) to use when displaying text in programs that do not support Unicode. This setting affects all user accounts on the computer.						
Current system locale:						
English (United Kingdom)	\sim					
Beta: Use Unicode UTF-8 for worldwide language support OK Cancel						

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



Result

Now MolFlow can load UTF-8 filenames:

Molflow+ 2.9.23 beta (May 15 2024) 日本語のファイル.zip] File Selection Tools Facet Vertex View Test Time About

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

👰 Molflow+ 2.9.23 beta (May 15 2024) [日本語のファイル.zip]							
File	e Selection Tools Facet Vertex	View	Test	Time	About		
New, empty geometry							
	Load C	rl+0					
	Load recent	•	D:A	ã→ ▼ ã⊽	'ā→ ¥ā→ jā→ ³ǎ→ \æl¥æl~èªlãữ®à→ lã⊽jã⊽¤ã→ «.zip)		

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

Molflow website: cern.ch/molflow

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