# TE-VSC-SCC training

## Using Molflow for sputtering simulations

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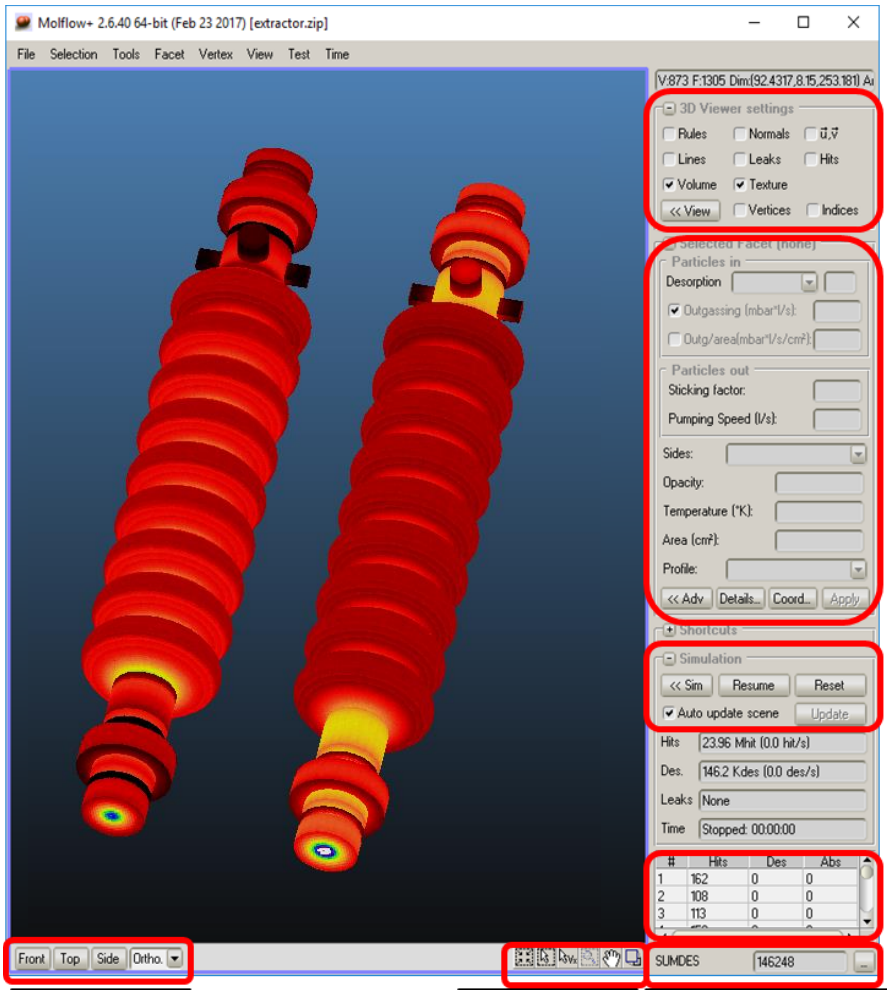
## 1. Molflow cheatsheet




**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

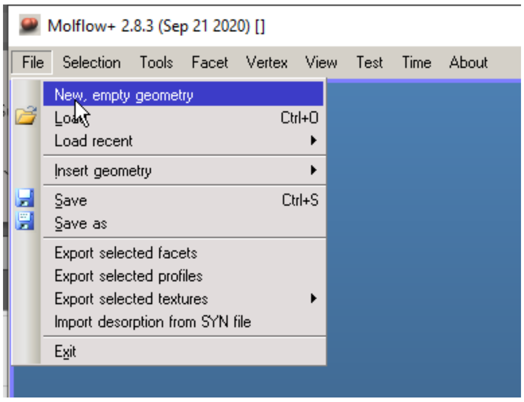
**Zoom:** mouse wheel (slow / fast zoom: hold SHIFT / CTRL)

# 2. Guided work: Sputtering in an ellipse-shaped chamber

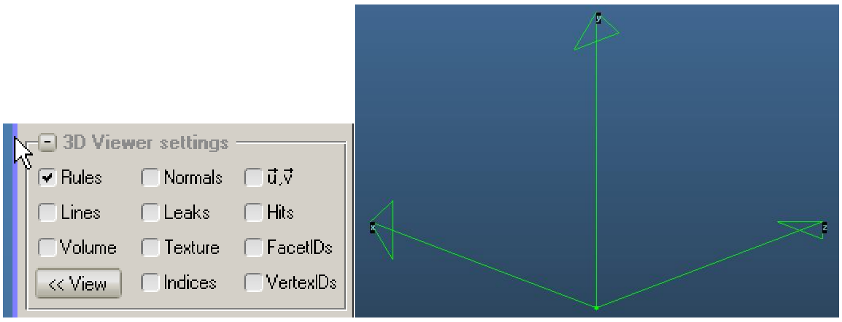
- We'll use Molflow's built-in tools to draw ellipse chambers
- We'll add cathodes
- We'll sputter and see which configuration is the best

## a) Clear the field

You can start a new geometry from scratch with the File/New command:



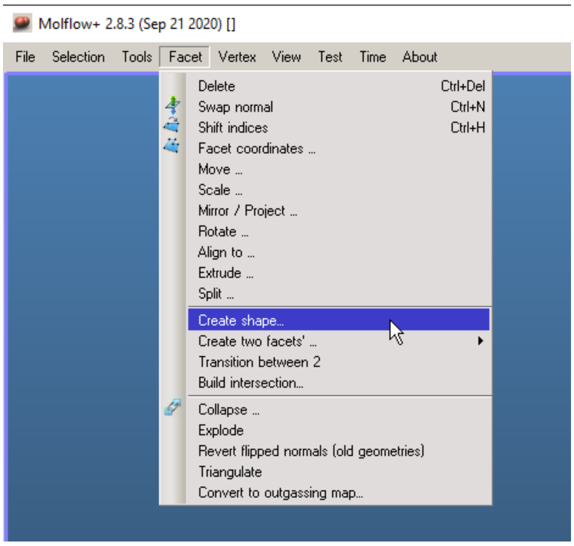

You can turn on the "Rules" view option (upper right) to display the coordinate system:




## b) Draw an ellipse

We'll first create the end cap of our chamber.

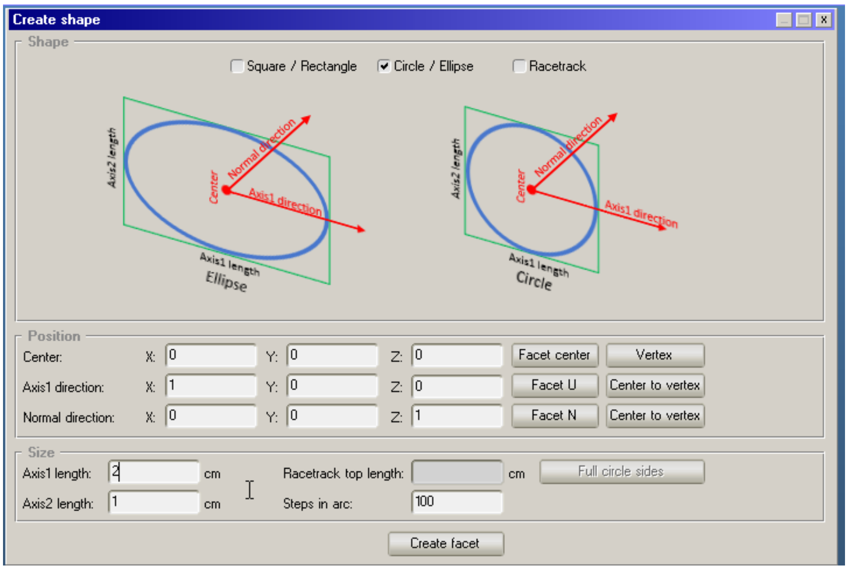
Select Facet/Create shape:

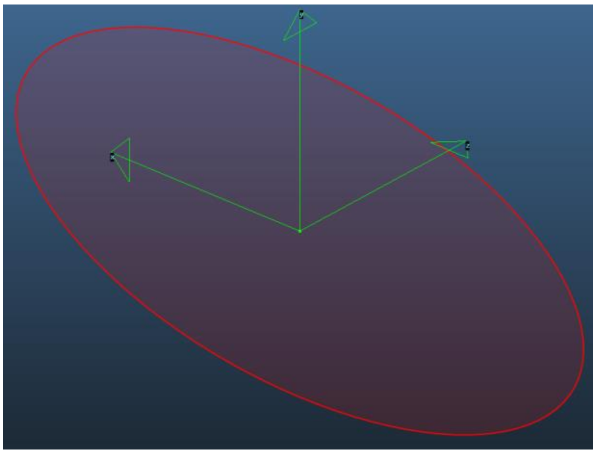



Then we'll draw an ellipse with the following parameters (see image below):

**Type:** circle/ellipse
**Center:** 0,0,0 (default) **Axis1 direction :** 1,0,0 (default) **Normal direction :** 0,0,1 (default)

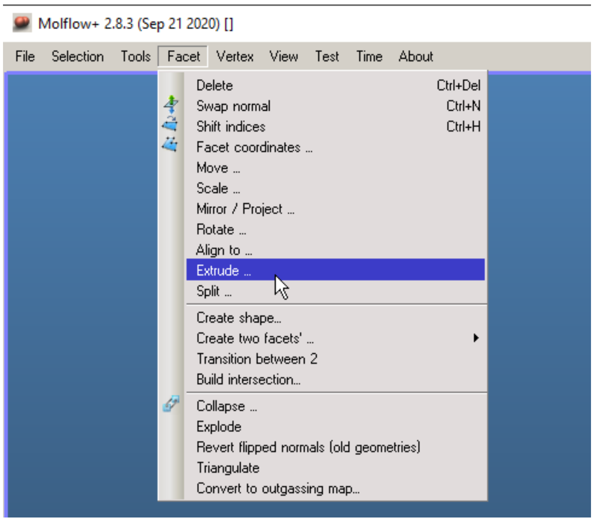
**Axis 1 length :** 2 cm **Axis 2 length :** 1 cm
**Steps in arc:** 100



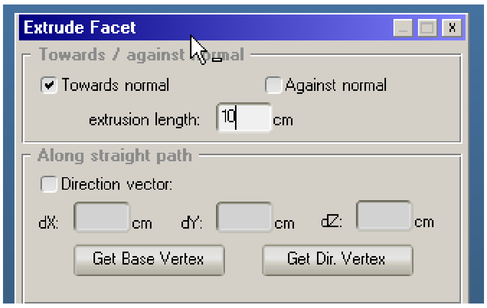



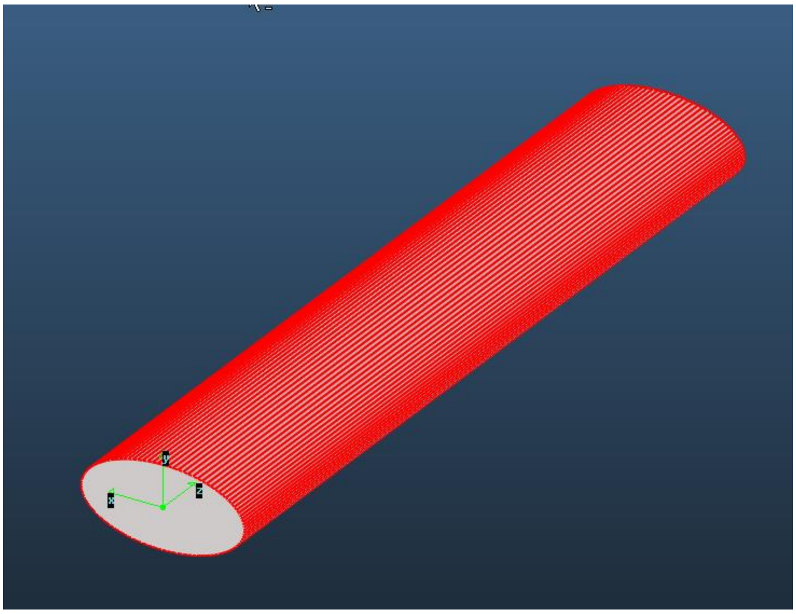
## c) Extrude to a chamber

Choose Facet/Extrude:




Then extrude 10cm towards the facet's normal:



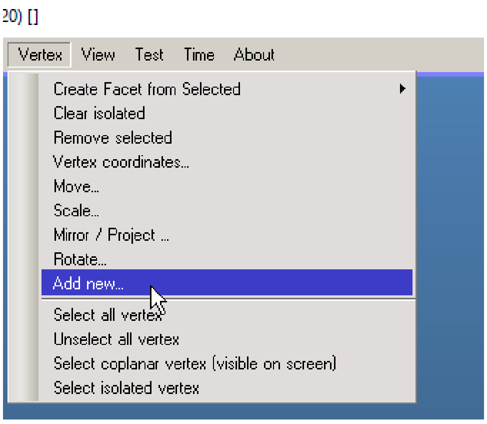
And the chamber is ready.

## d) Add the cathode

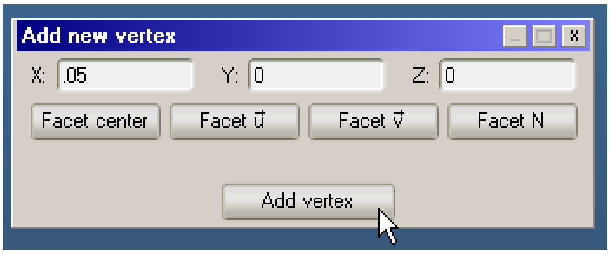
Our cathode will be represented by a long, thin rectangle.

There are several ways to create such a long, narrow facet, we could use the “create shape” again. We’ll create the shape by coordinates.

Select Vertex/Add new…

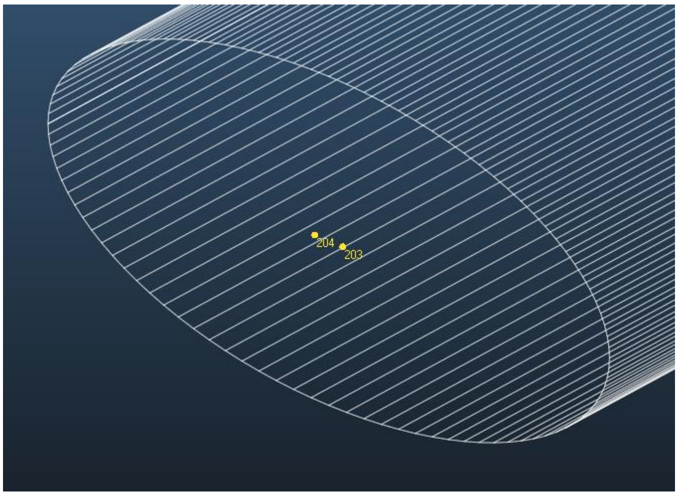



Type **-.05** (units are cm) to the X coordinate and click “Add vertex”:

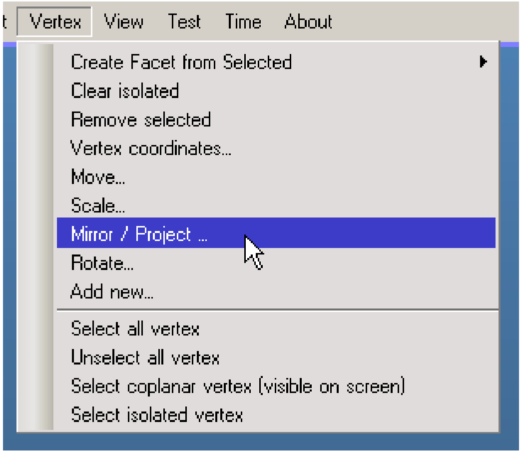


Repeat the same with **-.05:**

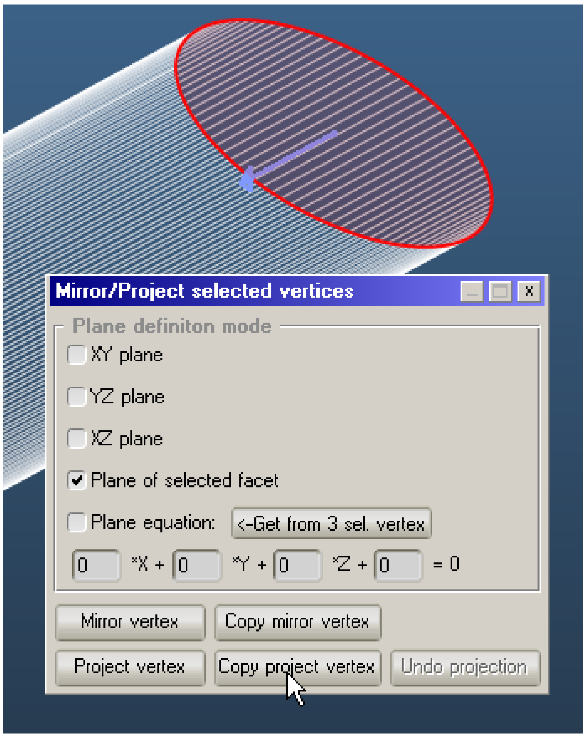

Now we have two vertices at one cap, we would like to copy them to the other:



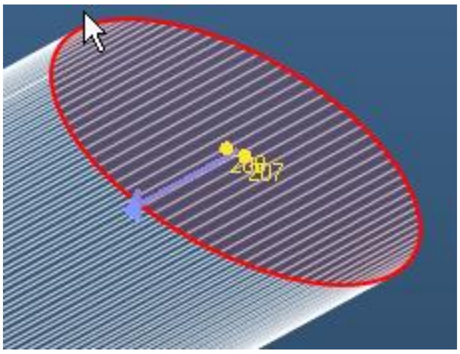

Choose Vertex/Mirror-Project:




Select the opposite end cap and in the dialog choose “Plane of selected facet”:

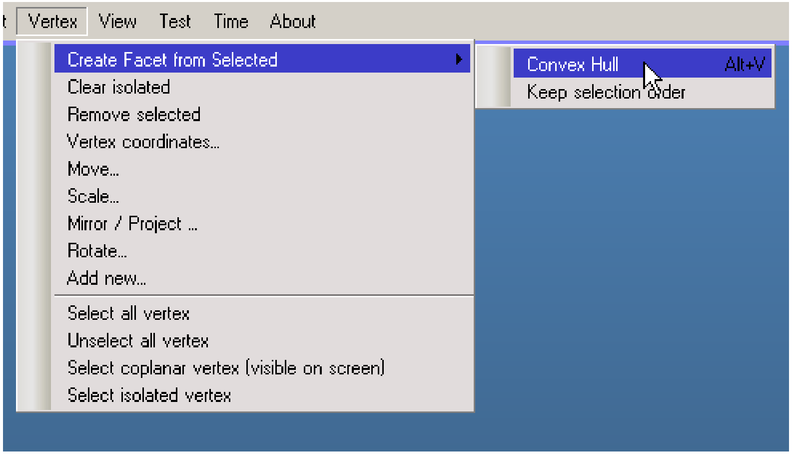



Then click **Copy project vertex**. That will make a copy of the two vertices to the opposite cap:

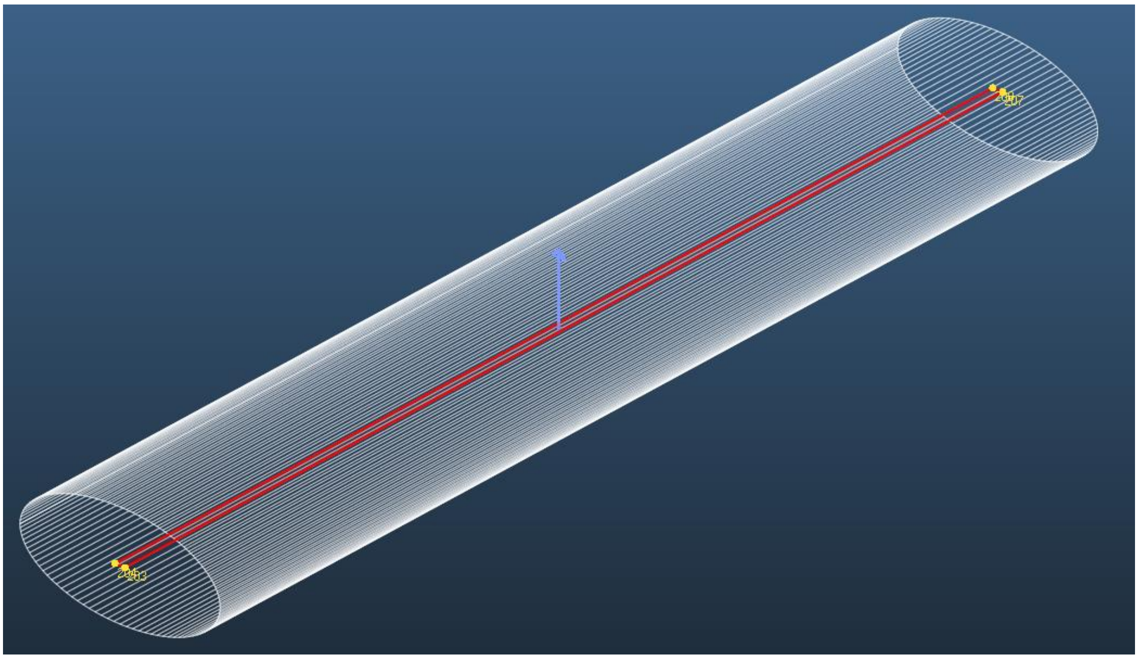


Now we are ready to create the cathode from the four corners.

Choose Vertex / Create facet from selected / Convex Hull:




This will create the actual cathode facet:



(TAB-click anywhere to deselect the yellow vertices)

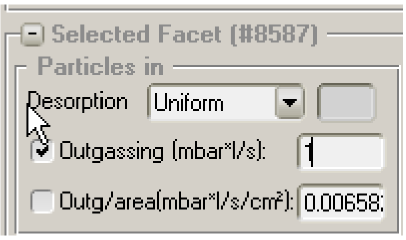
It is recommended that you save the file now.

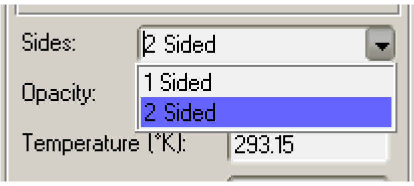
### e) Setting up the simulation

For any Molflow simulation, we need a gas source and a sink (usually a pump). We will set them up now.

With the cathode facet selected, give it a “uniform” outgassing on the right side.
Uniform refers to the directional distribution -> we will have the same sputtering flux in every direction around the cathode.

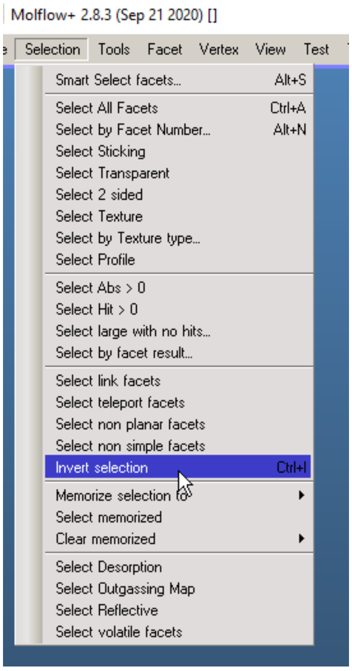
Also, set the facet to 2-sided, so it sends particles both upwards and downwards:



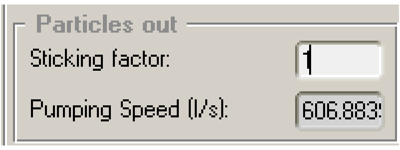




Now you must select the side walls and set them **sticking**.

The easiest way to select side walls is to select the cathode (if not already selected), then invert the selection (Selection / Invert or CTRL+I):




Now, with the walls selected, set the sticking factor to 1 (100% absorption probability):

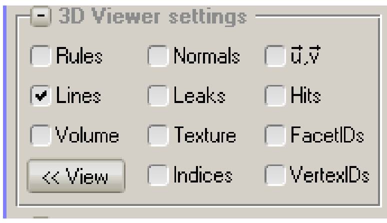


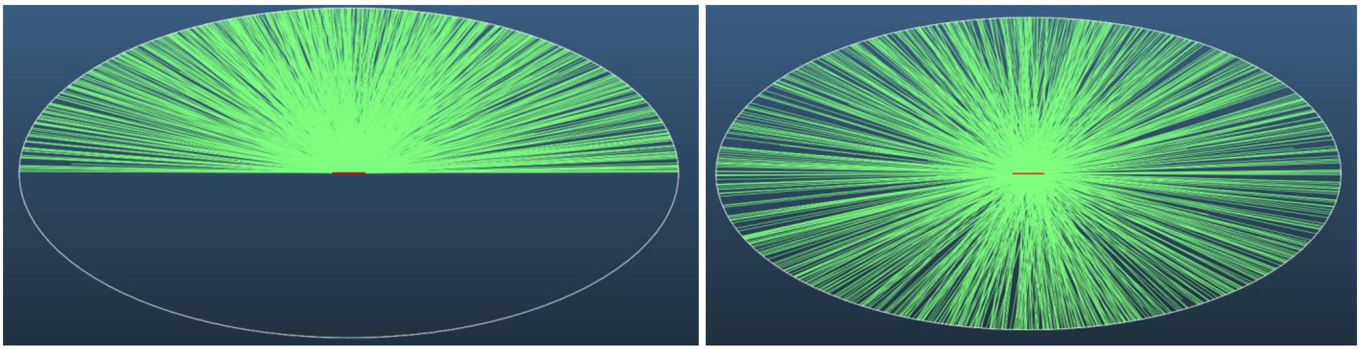

## f) Launch the simulation

That's it! Click the Begin button to start simulating:


Your simulation is now running.

If you click the Front view (lower left) and turn on "Line" display, you can see the particle trajectories:

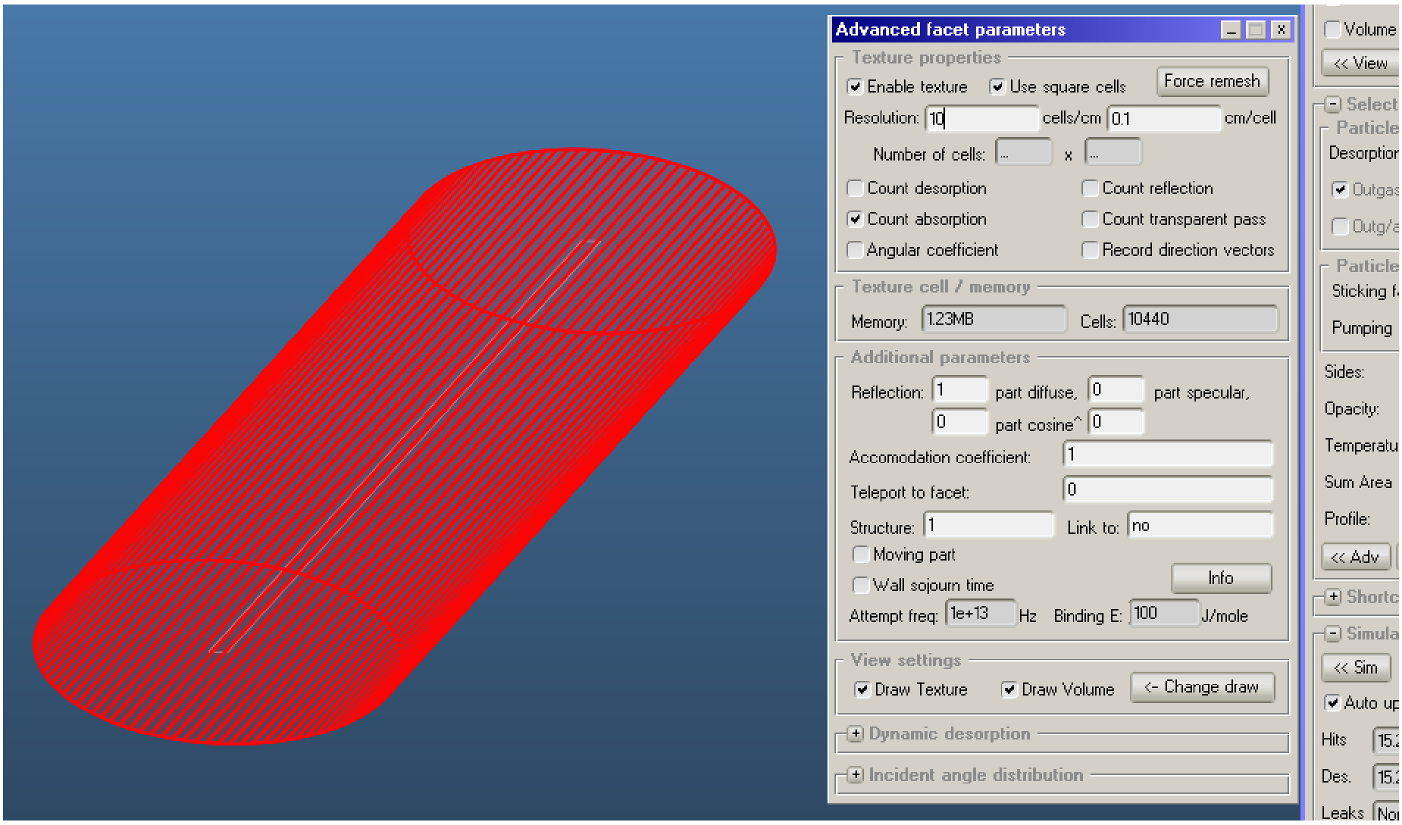



Note: if your particles are only flying in one direction (left), you have to set the desorbing cathode to 2-sided (right).

## g) Post-processing: Setting up textures

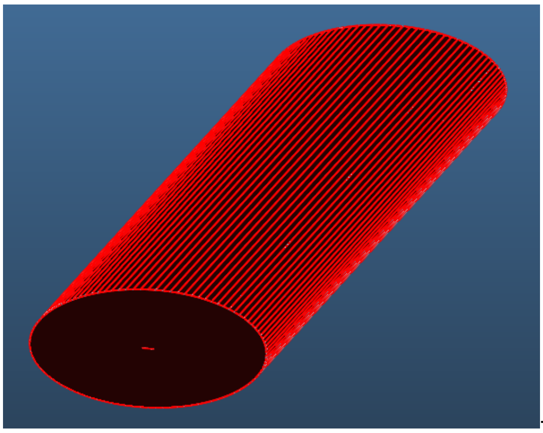
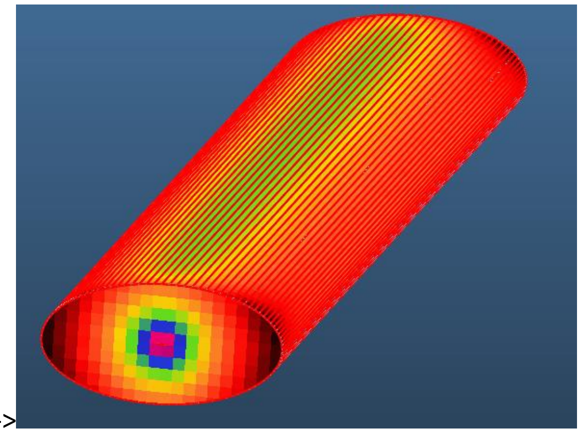
Our goal is to set up color maps that show us the sputtering thickness. In Molflow, it is achieved through measuring the impingement rate (particle flux).

First, select the wall facets, including the end caps. (For example, by selecting the cathode and inverting selection), then open the **Advanced facet parameters** panel (<<Adv button):

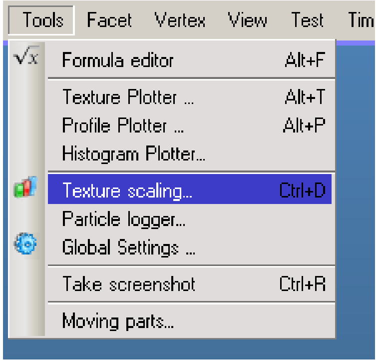


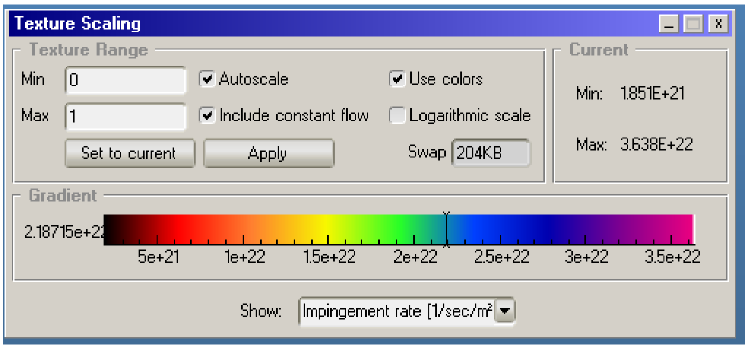

Since we are recording textures on sticking walls, we must choose the **count absorption** option.

The texture resolution should be 10 cells/cm (see above). Click apply on the right side to mesh the facets. Then, launching the simulation again, you will see the first colors:

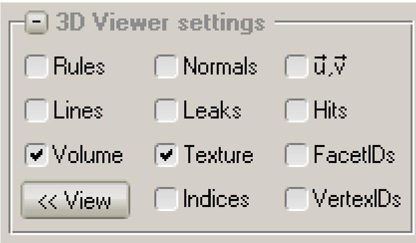

->


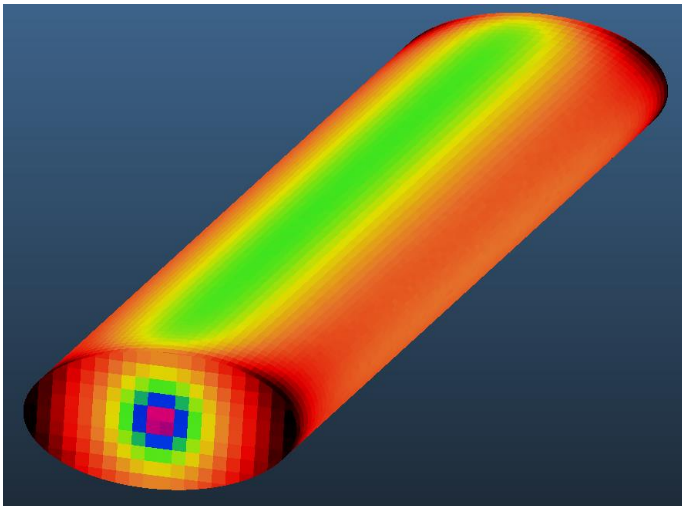
Finally, to show the impingement rate, open Tools/Texture scaling and set the textures to Impingement Rate display:




The **Volume** view option, combined with Texture, shows the clearest image:



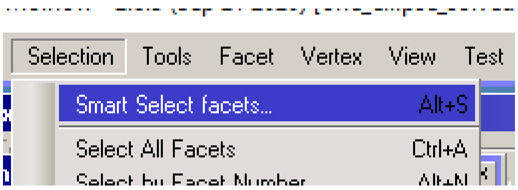



### h) Post-processing: plotting thickness profile

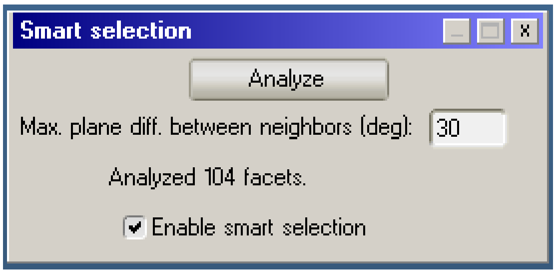
While color codes are useful for qualitative analysis, plotting the profile along the wall allows to compare different configurations.

We will simply select all wall facets and export the hit count.

Use Selection / Smart Select:



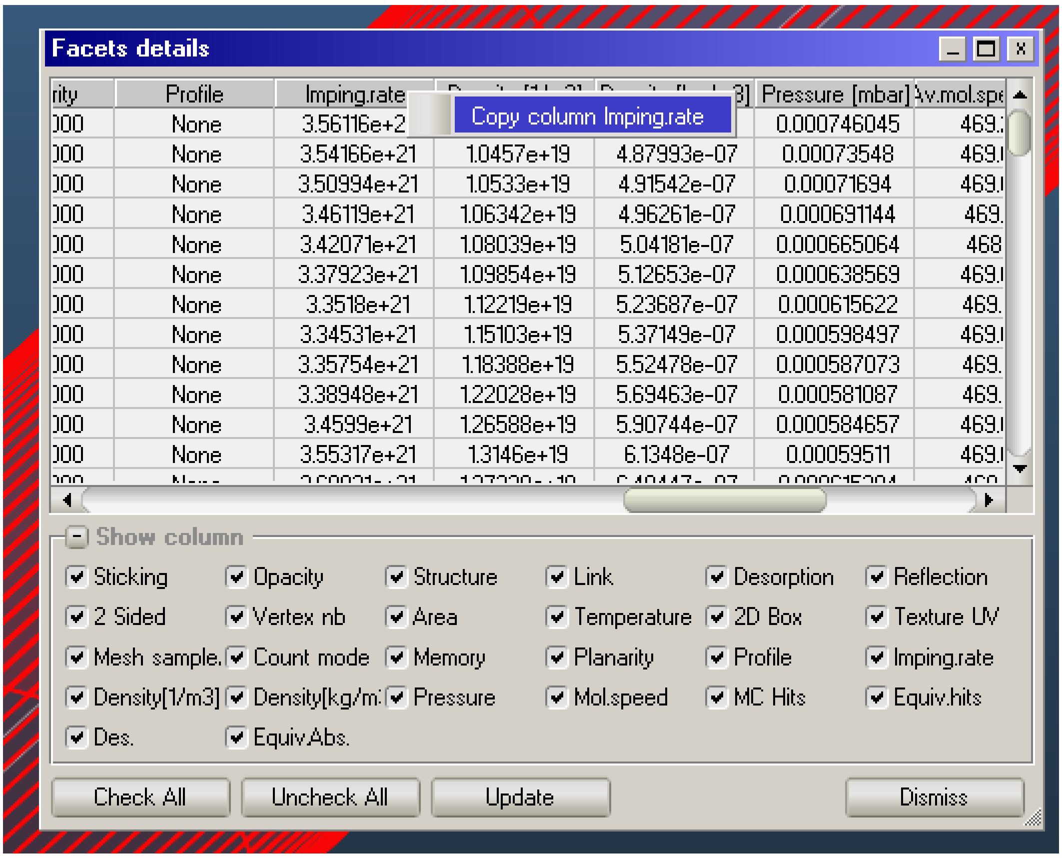

Click analyze – it will check which facet is the neighbor of others (only to do once):




Then with this window open, you can select the wall of the ellipse with one click (you should have 101 facets selected):

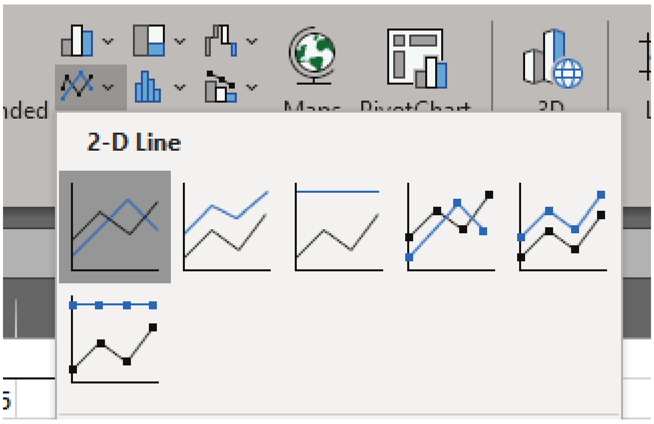

Click facet Details button:

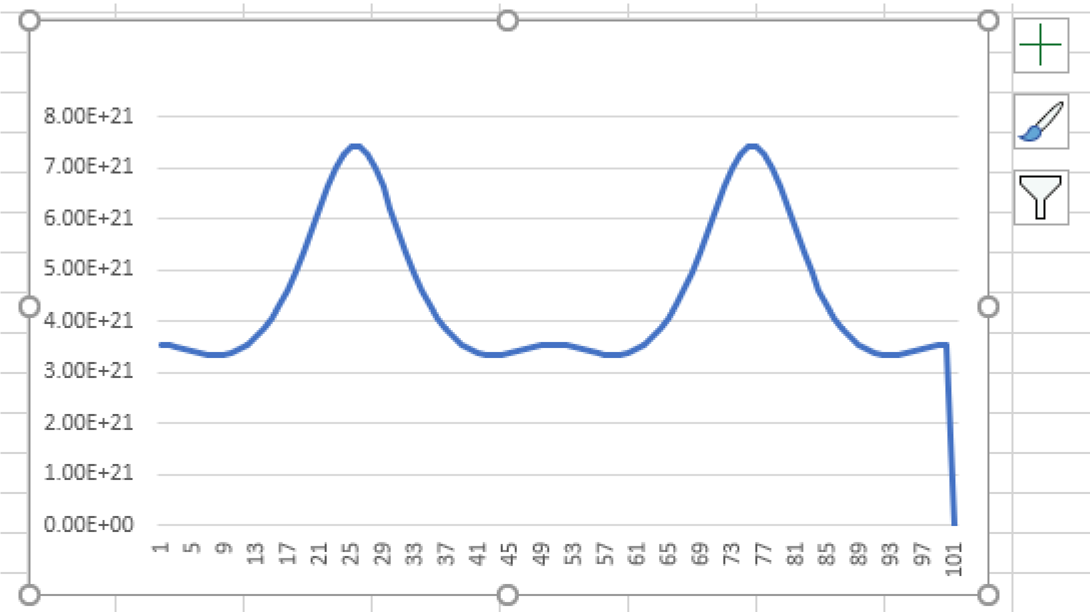

Scroll to the Impingement rate column and right-click it, select Copy:




Paste the copied column in an empty Excel sheet, select the pasted Hit column and plot it by Insert/Line plot:

| | A | B | C | D | E |
|---|---|---|---|---|---|
| 1 | | | Case1 | | |
| 2 | 2 | 4016719 | 0 | 4.02E+06 | |
| 3 | 3 | 4041478 | 0 | 4.04E+06 | |
| 4 | 4 | 4095649 | 0 | 4.10E+06 | |
| 5 | 5 | 4167176 | 0 | 4.17E+06 | |
| 6 | 6 | 4278839 | 0 | 4.28E+06 | |
| 7 | 7 | 4412585 | 0 | 4.41E+06 | |
| 8 | 8 | 4581887 | 0 | 4.58E+06 | |
| 9 | 9 | 4792995 | 0 | 4.79E+06 | |
| 10 | 10 | 5041372 | 0 | 5.04E+06 | |
| 11 | 11 | 5327763 | 0 | 5.33E+06 | |
| 12 | 12 | 5683065 | 0 | 5.68E+06 | |



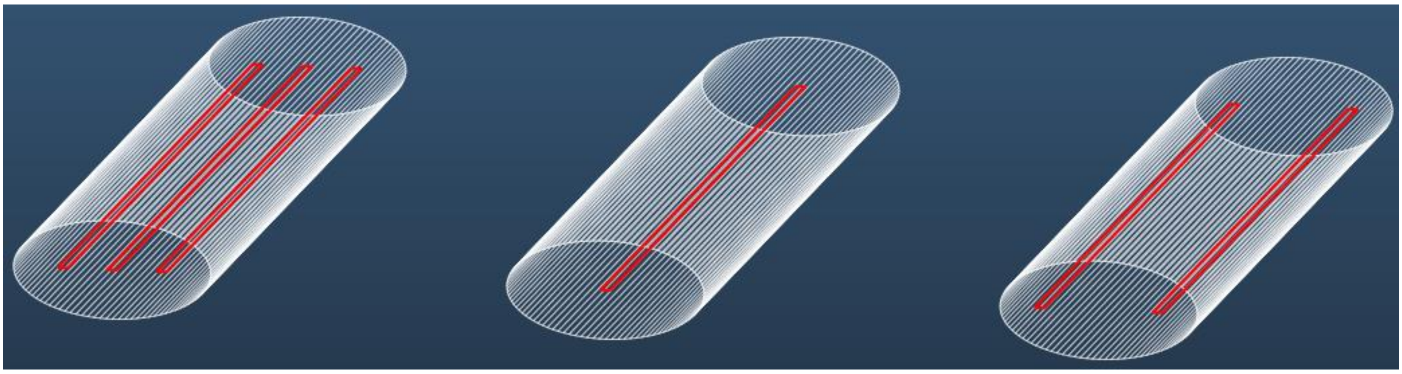




This is your baseline, single-cathode thickness profile, which will be compared with optimized configuration.

In the next steps we will optimize the cathode configuration to compare results.

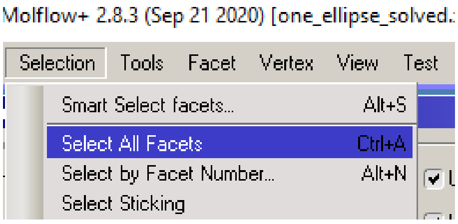
### i) Optimizing configuration

We can simulate several configurations at the same time, so one way to optimize the cathode configuration is to make copies of the geometry to be coated, and run the simulation with different setups, at the same time:

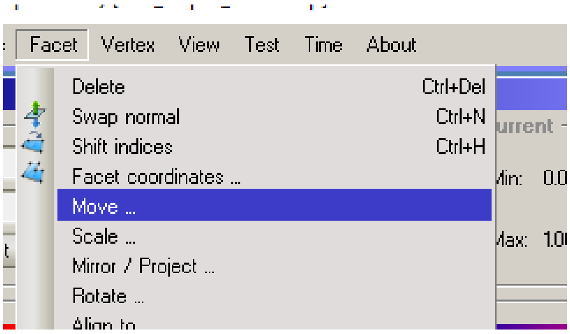


In this exercise, we'll try 3 different cathode setups, and compare the thickness.

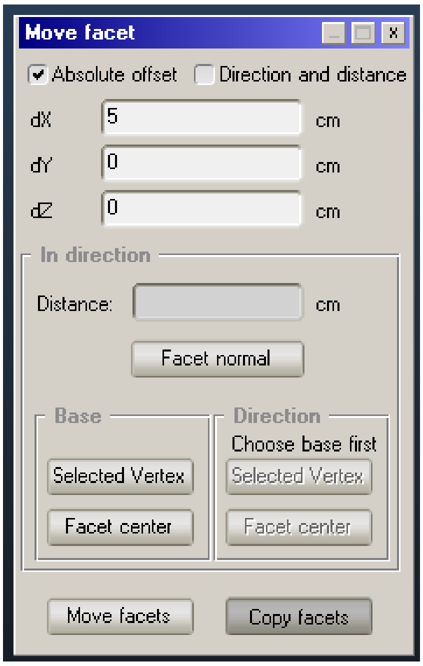
Select all facets to make a copy:



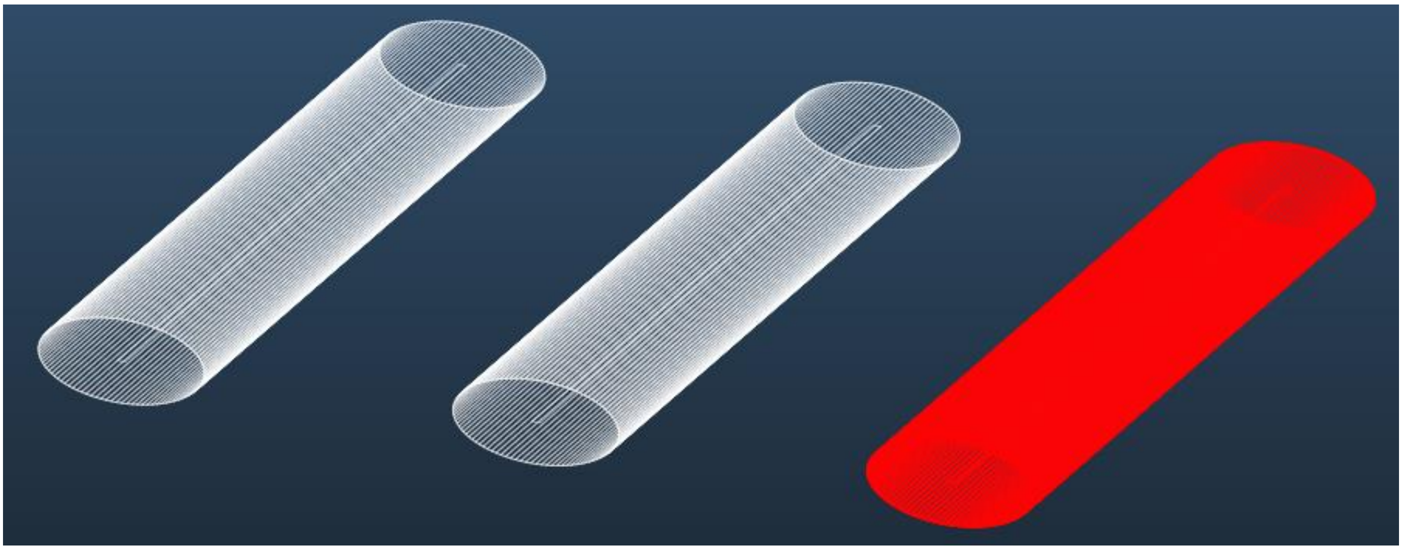

Select Facet / Move:




Move the facets to the right, then to the left by +5 and -5 cm X offsets, clicking **Copy facets**:

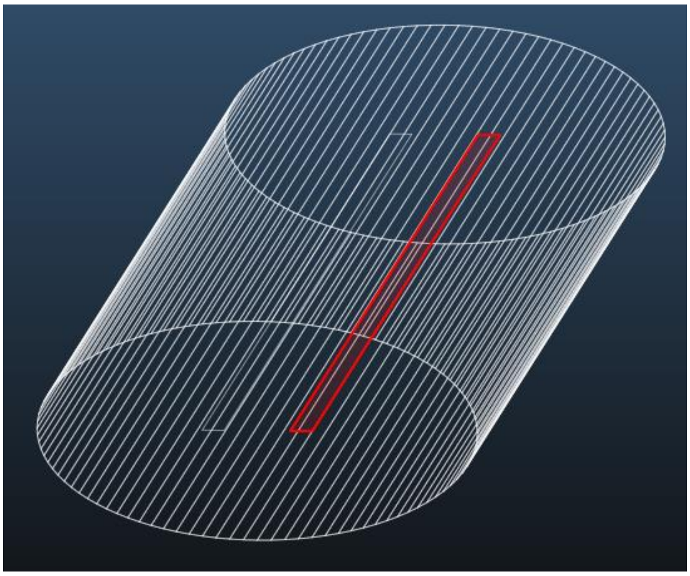



Between the two copies, you'll have to select the middle structure again (as copy source):



After the copy, the target is selected by default, so in case of error, you can delete it (CTRL+DEL).

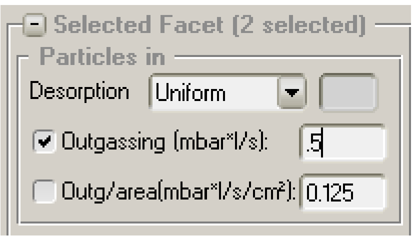
Now you can select the cathodes on the left and right, and using the Move / Copy commands, you can achieve custom configurations (up to you):



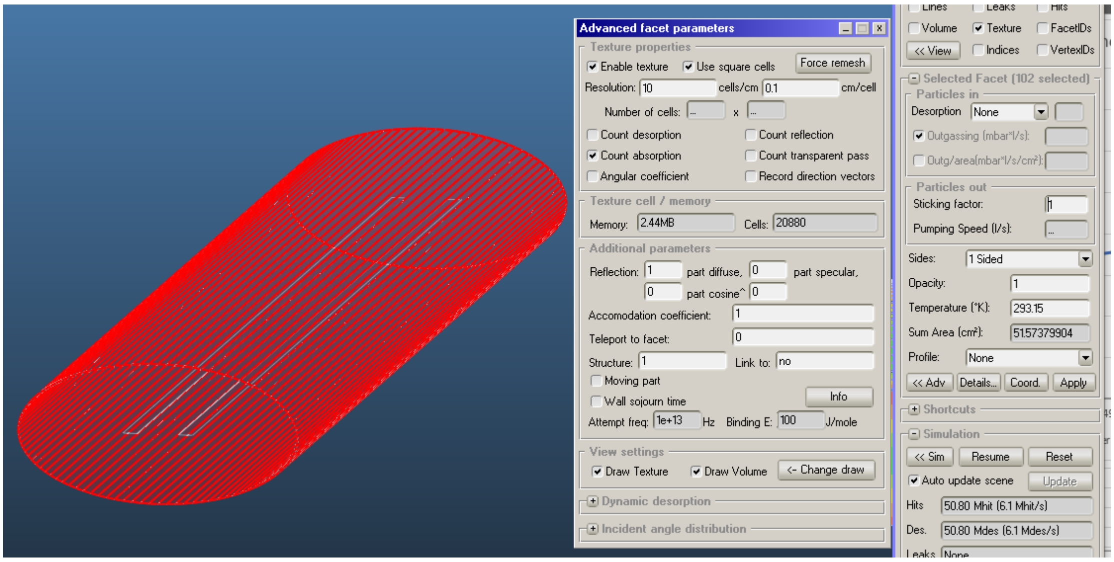
Example cathode configuration with +0.2 and -0.2cm offsets from center position.

**Important:** set the outgassing to be the same in total for all configuration, so that results are comparable.

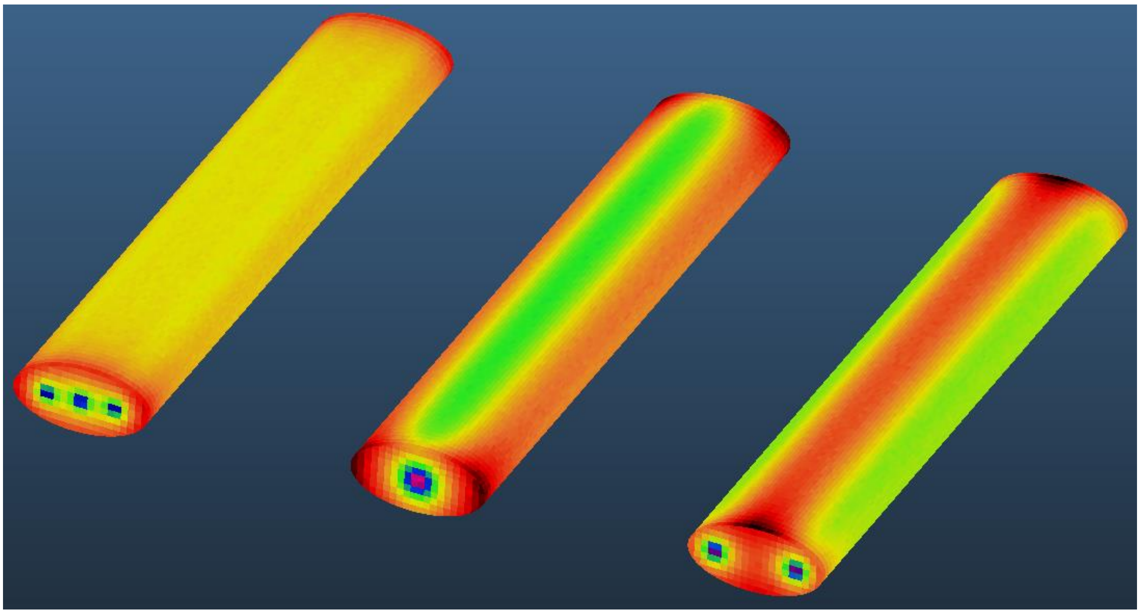
For example, a 2-cathode configuration should outgas 0.5mbar*l/s each, so the total outgassing is 2*0.5=1, comparable with the original single-cathode setup:

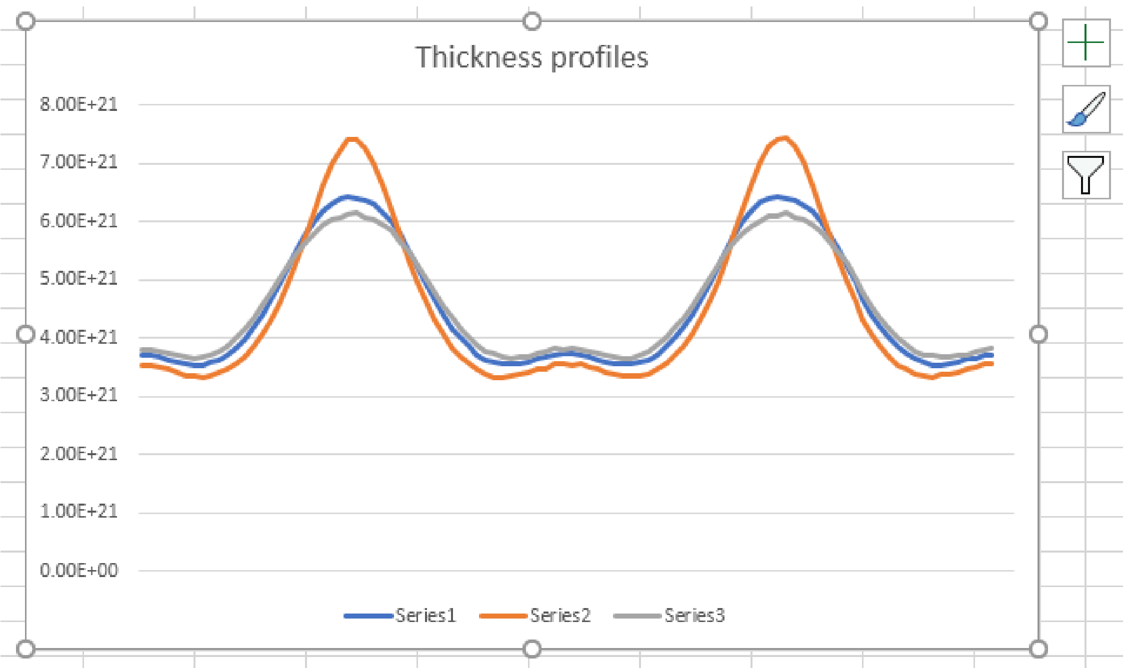



**Add textures** to the copied structures (textures are not copied for performance reasons):




Launch the simulation to compare, and extract the plots to finish, repeating the column copy steps:





# 3. Individual work

In this second exercise you'll work with a real-life geometry, which is harder because facets are randomly oriented.

## a) Input files

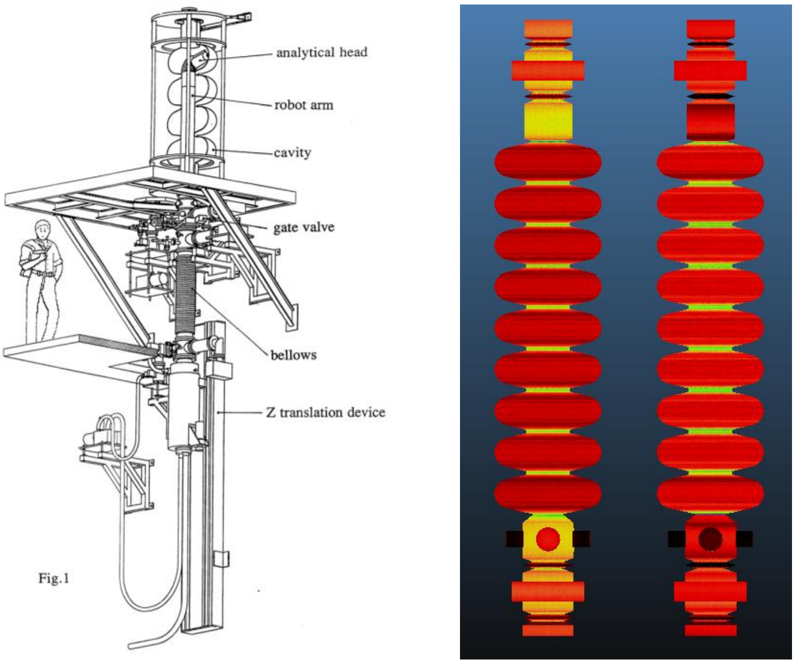
You'll have the…

- CAD model (rfcavity.stl)
- The Excel sheet for post-processing (impingement_template.xlsx)

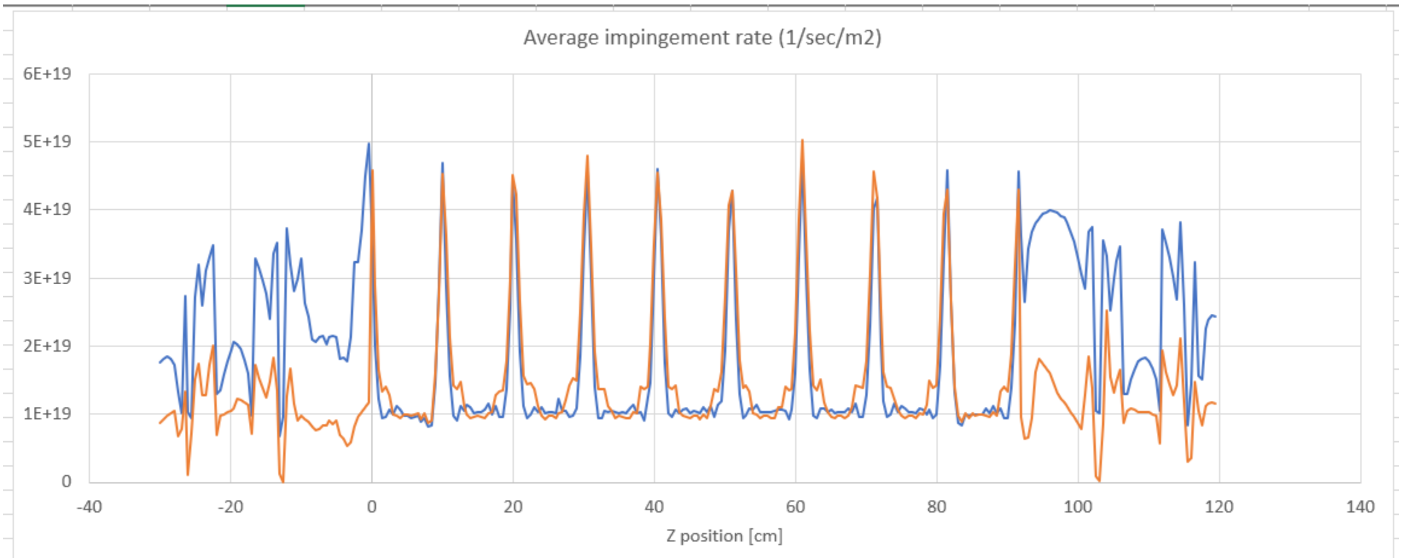
## b) Exercise

You have to build a simulation to show thickness along the RF cavity, from a cathode in the center.

Once you solve the uniform case, you'll optimize the sputtering to achieve a more uniform thickness by a "moving cathode" sputtering: you'll desorb different gas quantities along the length – trying to achieve a more uniform thickness.




Moving sputtering/diagnostics instrument.
Source: [http://cds.cern.ch/record/256049/](http://cds.cern.ch/record/256049/)
("An instrument for internal surface analysis of LEP 200 superconducting radiofrequency cavities")




Possible solution with original (blue) and optimized (orange) thickness.

## c) Steps

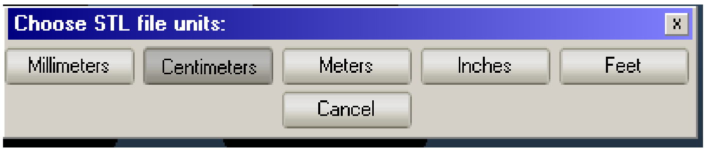
One way to solve the exercise is by the following steps, like the previous case:

1. Import geometry by opening STL file and collapsing
2. Create cathode facet
3. Add outgassing to cathode
4. Add sticking to walls
5. Launch the simulation for a quick test
6. Add textures to walls
7. Export textures and paste them in Excel template to plot thickness profile
8. Make a copy of the geometry (second, optimized version)
9. Break up the cathode to smaller parts
10. Vary outgassing on smaller parts to achieve more uniform thickness
11. Compare two (uniform vs non-uniform) thickness profiles

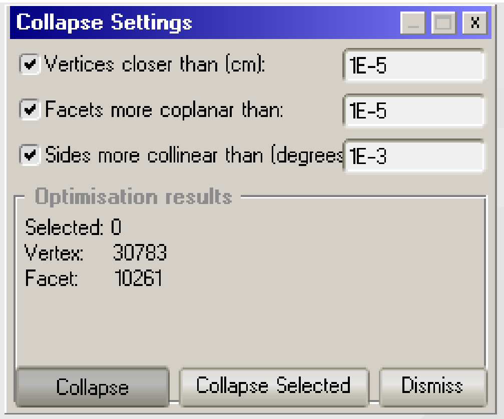
## d) Hints / instructions for each step

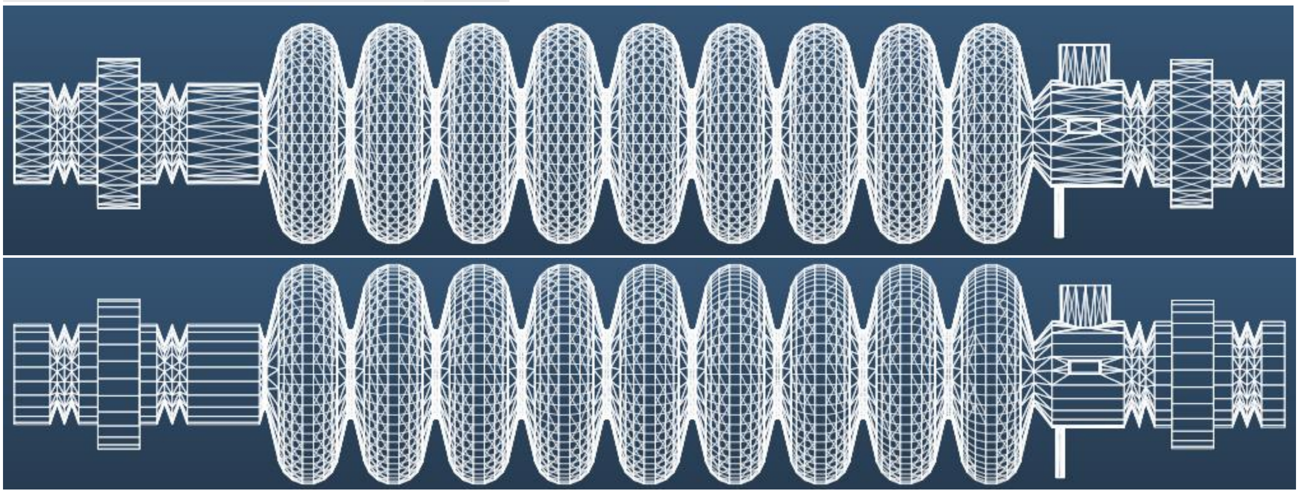
### 1. Opening and collapsing file

- When you open rfcavity.stl, Molflow will ask the units of the file: they are **centimeters**:




- A “Collapse” window pops up, leave the default values and click Collapse (to merge triangles into facets):



*triangulated vs collapsed geometry, main differences on the sides*

### 2. Creating cathode

There is an easy and an “elegant” way to create the long, rectangular cathode facet.

**Easy way by manually entering the coordinates:** Choose Vertex/Add New, and create four vertices at these XYZ coordinates:

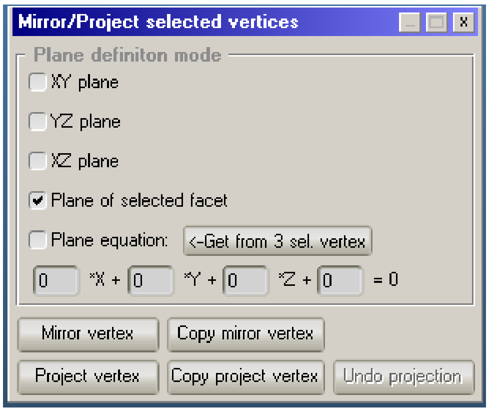
- 0.25, 0, 121.9
- -0.25, 0, 121.9
- 0.25, 0, 30
- -0.25, 0, 30

Then select Vertex / Create Facet from Selected / Convex Hull to create the rectangle

**Elegant way:** you don't need to know the end cap coordinates, since Molflow can automatically project the vertices on the facets.

Create two vertices at (0.25,0,0) and (-0.25,0,0).

Use the Vertex / Mirror-Project command to project these vertices to the end caps (with the plane of selected facet option):




### 3. Add outgassing to cathode

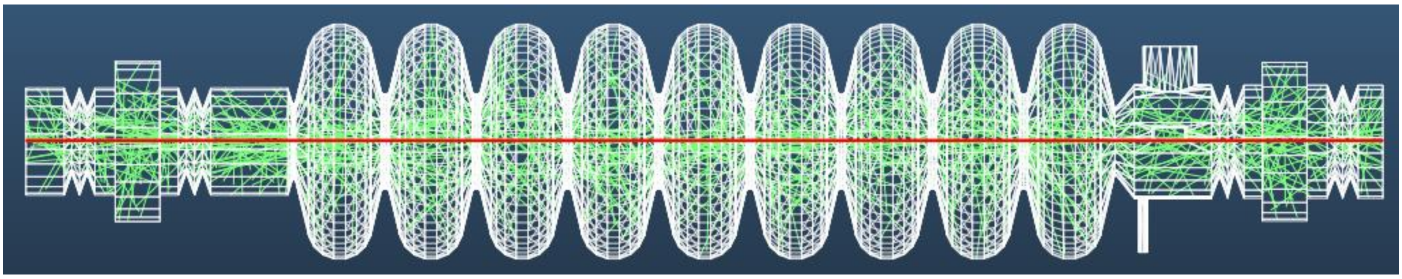
Set it to two-sided, and add an arbitrary value of "Uniform" outgassing

### 4. Add sticking to walls

To select walls, either select the cathode and invert selection, or use Selection / Smart select and click on the wall. Don't forget the end caps. Set sticking to 1.

### 5. Launch simulation

Just click the Begin button on the right. Turn on "Lines" and "Leaks" display, you should have lines but no leaks:

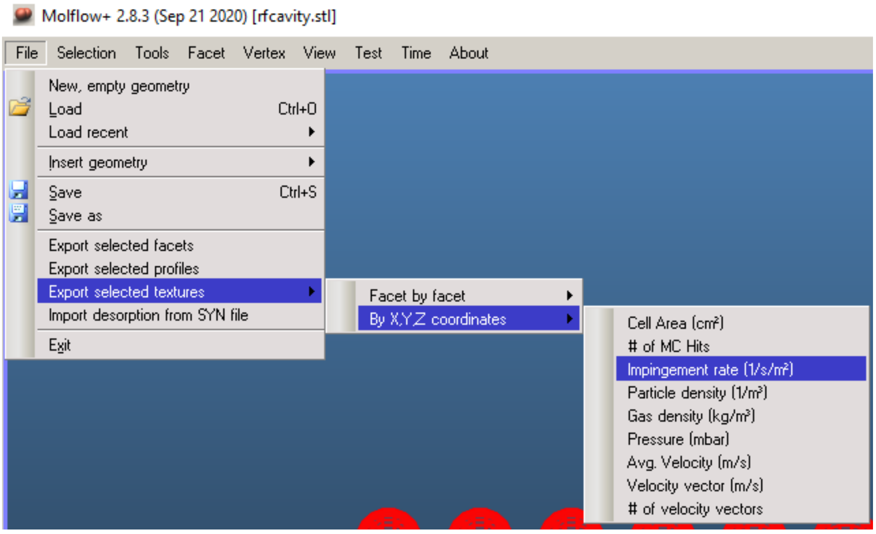


### 6. Add textures to walls

Select the walls (as in point 4), open the advanced parameters panel (<<Adv) button on right, use the "Count absorption" option with 1cm/cell resolution and click Apply.

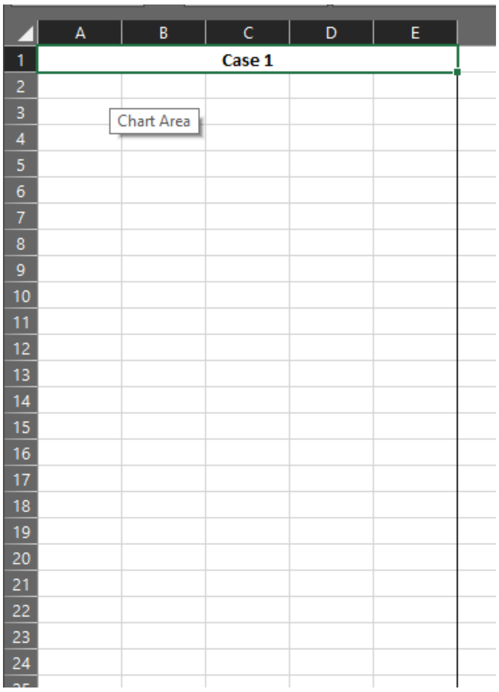
### 7. Export textures to Excel and plot them

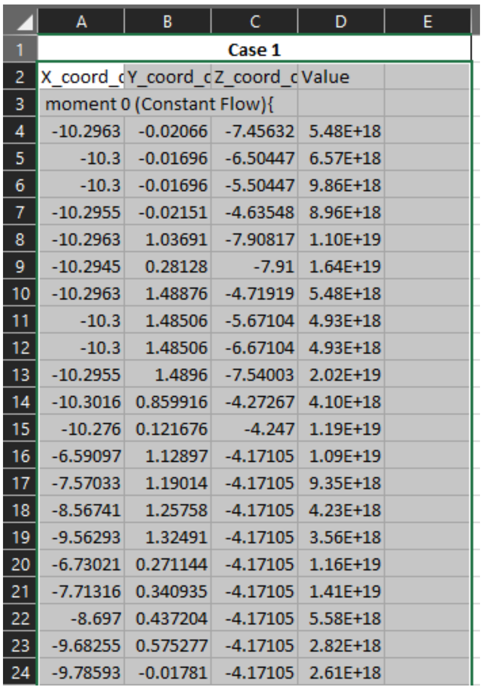
Select textures (Selection / Select Textured), the choose File/Export selected textures/By X,Y,Z coordinates/Impingement rate




Save it to a text file (for example export.txt), open the file, select all the data in it and copy to clipboard.

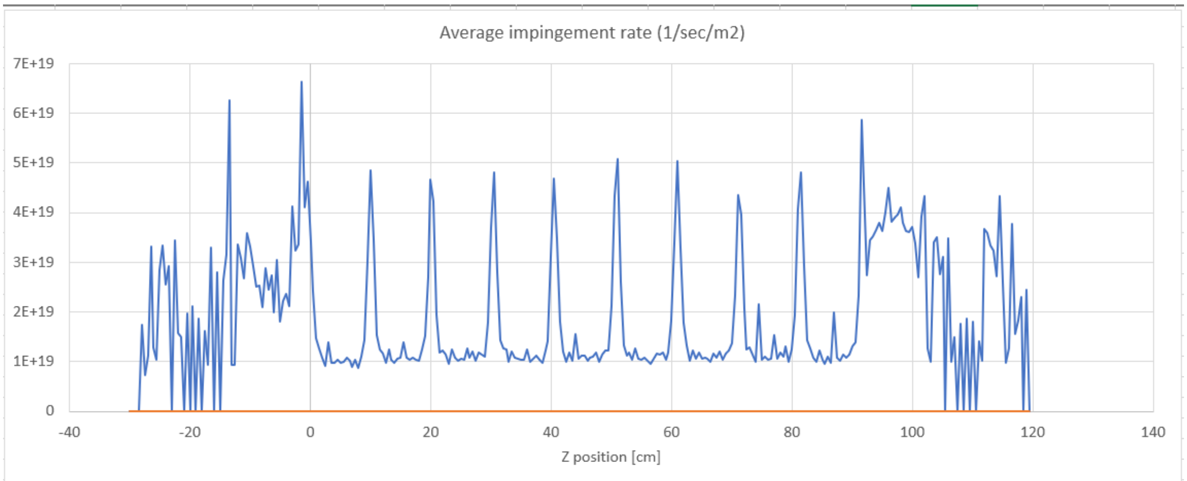
Then open **impingement_template.xlsx**, and paste the (four) columns into the A2 cell (case 1):



| | A | B | C | D | E |
|---|---|---|---|---|---|
| 1 | Case 1 | | | | |
| 2 | X_coord_c | Y_coord_c | Z_coord_c | Value | |
| 3 | moment 0 (Constant Flow){ | | | | |
| 4 | -10.2963 | -0.02066 | -7.45632 | 5.48E+18 | |
| 5 | -10.3 | -0.01696 | -6.50447 | 6.57E+18 | |
| 6 | -10.3 | -0.01696 | -5.50447 | 9.86E+18 | |
| 7 | -10.2955 | -0.02151 | -4.63548 | 8.96E+18 | |
| 8 | -10.2963 | 1.03691 | -7.90817 | 1.10E+19 | |
| 9 | -10.2945 | 0.28128 | -7.91 | 1.64E+19 | |
| 10 | -10.2963 | 1.48876 | -4.71919 | 5.48E+18 | |
| 11 | -10.3 | 1.48506 | -5.67104 | 4.93E+18 | |
| 12 | -10.3 | 1.48506 | -6.67104 | 4.93E+18 | |
| 13 | -10.2955 | 1.4896 | -7.54003 | 2.02E+19 | |
| 14 | -10.3016 | 0.859916 | -4.27267 | 4.10E+18 | |
| 15 | -10.276 | 0.121676 | -4.247 | 1.19E+19 | |
| 16 | -6.59097 | 1.12897 | -4.17105 | 1.09E+19 | |
| 17 | -7.57033 | 1.19014 | -4.17105 | 9.35E+18 | |
| 18 | -8.56741 | 1.25758 | -4.17105 | 4.23E+18 | |
| 19 | -9.56293 | 1.32491 | -4.17105 | 3.56E+18 | |
| 20 | -6.73021 | 0.271144 | -4.17105 | 1.16E+19 | |
| 21 | -7.71316 | 0.340935 | -4.17105 | 1.41E+19 | |
| 22 | -8.697 | 0.437204 | -4.17105 | 5.58E+18 | |
| 23 | -9.68255 | 0.575277 | -4.17105 | 2.82E+18 | |
| 24 | -9.78593 | -0.01781 | -4.17105 | 2.61E+18 | |

This will automatically plot the thickness along axis Z:



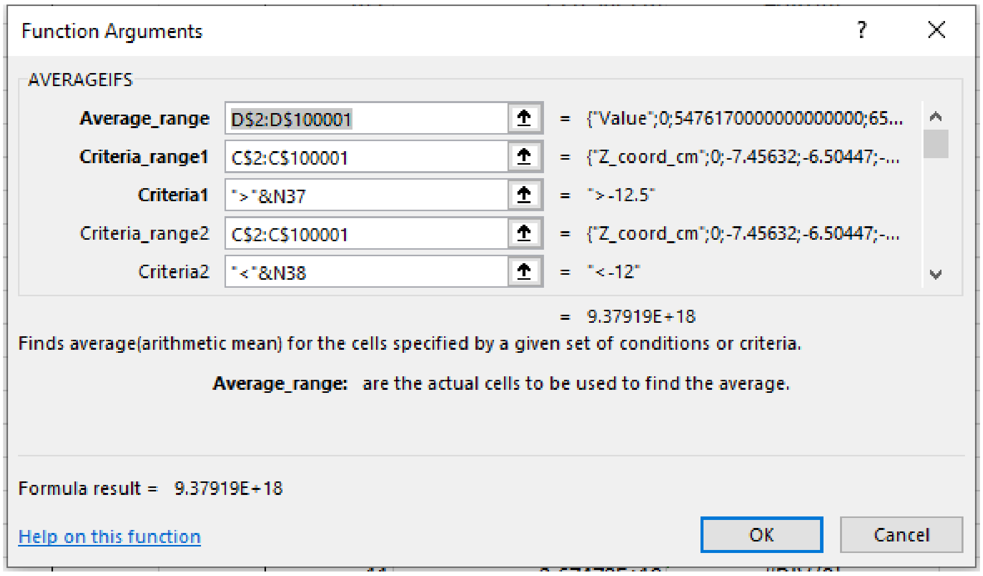

**Explanation:**

The texture cells are exported as (X,Y,Z,impingement_rate) value quartets.

Excel averages all cells that lie within a select range of Z coordinates:

| | |
|---|---|
| -13.5 | 6.26906E+19 |
| -13 | 9.30367E+18 |
| -12.5 | 9.37919E+18 |
| -12 | 3.35686E+19 |
| -11.5 | 3.08035E+19 |
| -11 | 2.67478E+19 |
| -10.5 | 3.59753E+19 |

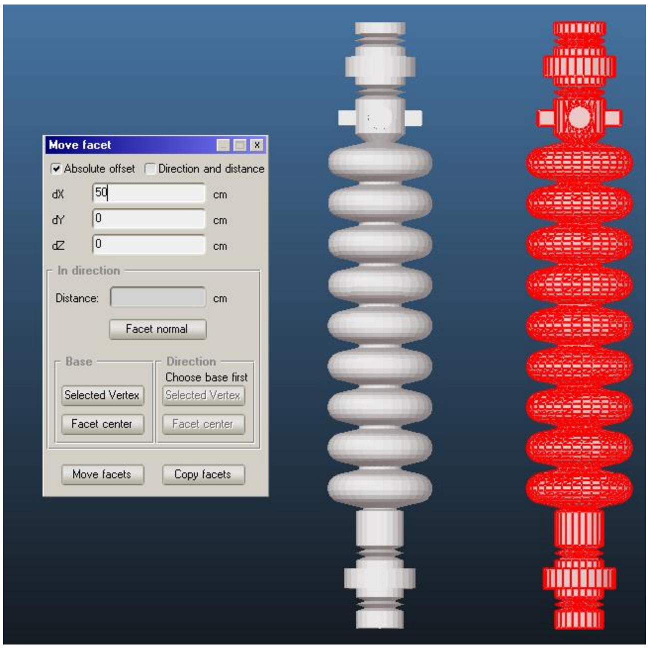
```
=AVERAGEIFS(D$2:D$100001,C$2:C$100001,">"&N37,C$2:C$100001,"<"&N38)
```




This is called conditional averaging (AVERAGEIFS function): if the Z coordinate in the C column is within two values (defined in the N column), then the cell will count towards the average.

## 8. Make a copy of the geometry

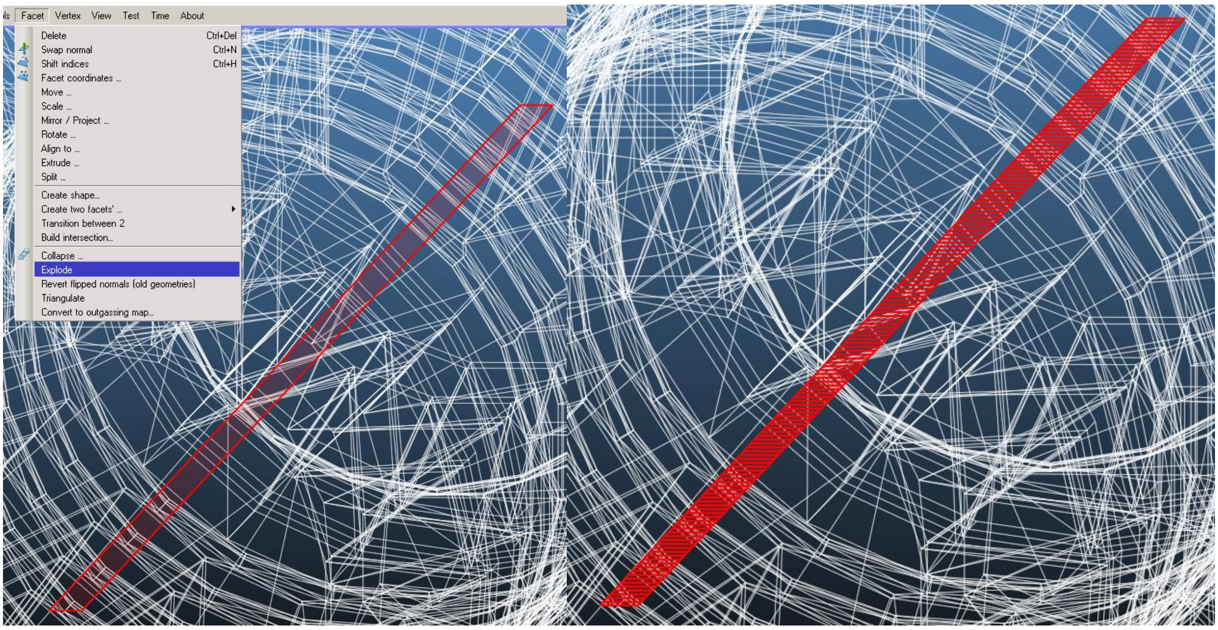
Select all facets, and using the Facet/Move command make a copy by applying an 50cm X or Y offset.




Finally, add textures to the copied RF cavity (textures are not copied).

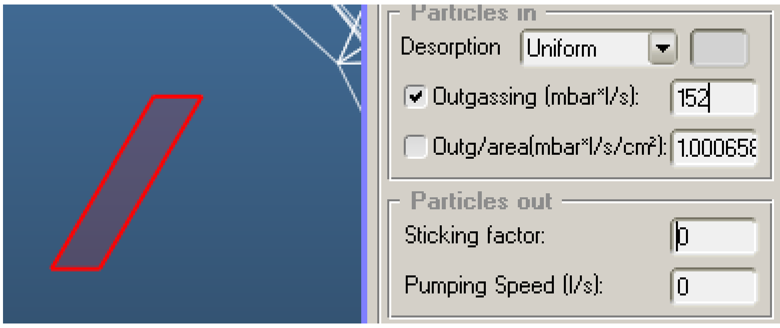
## 9. Break up the cathode to smaller parts

- On one of the two cathodes, add a texture (any option, for example “count absorption”) with 1cm/cell resolution
- Choose Facet / Explode

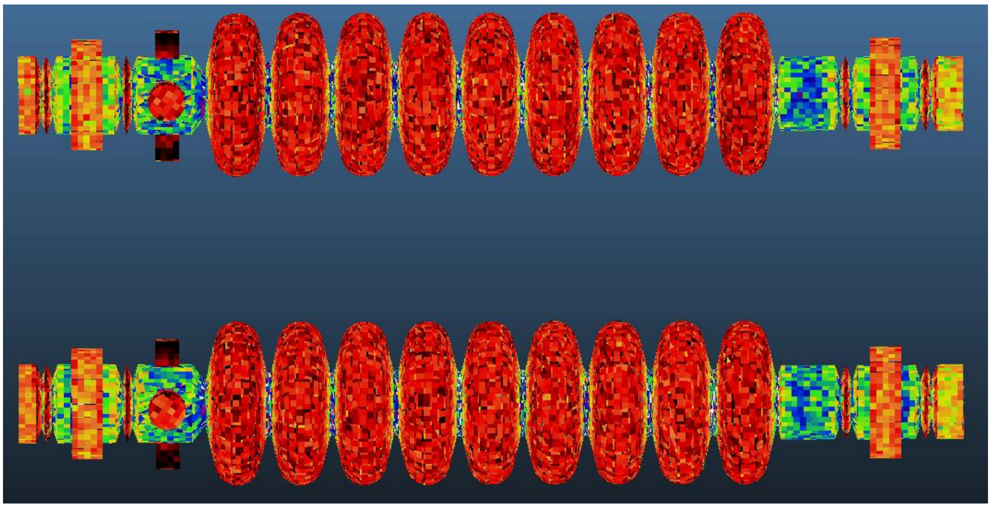



- Set the same outgassing (for example 1) on all 152 small cells:


- Select the other (not exploded) cathode and set 152 as outgassing, so that total outgassing is the same

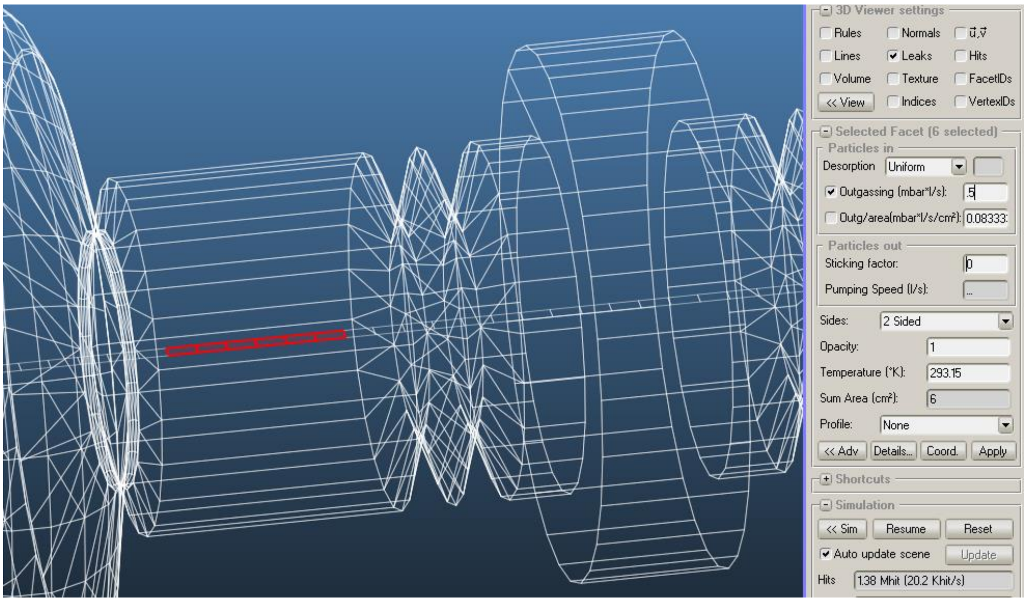



- Test the simulation and the resulting textures, the colors should be the same:

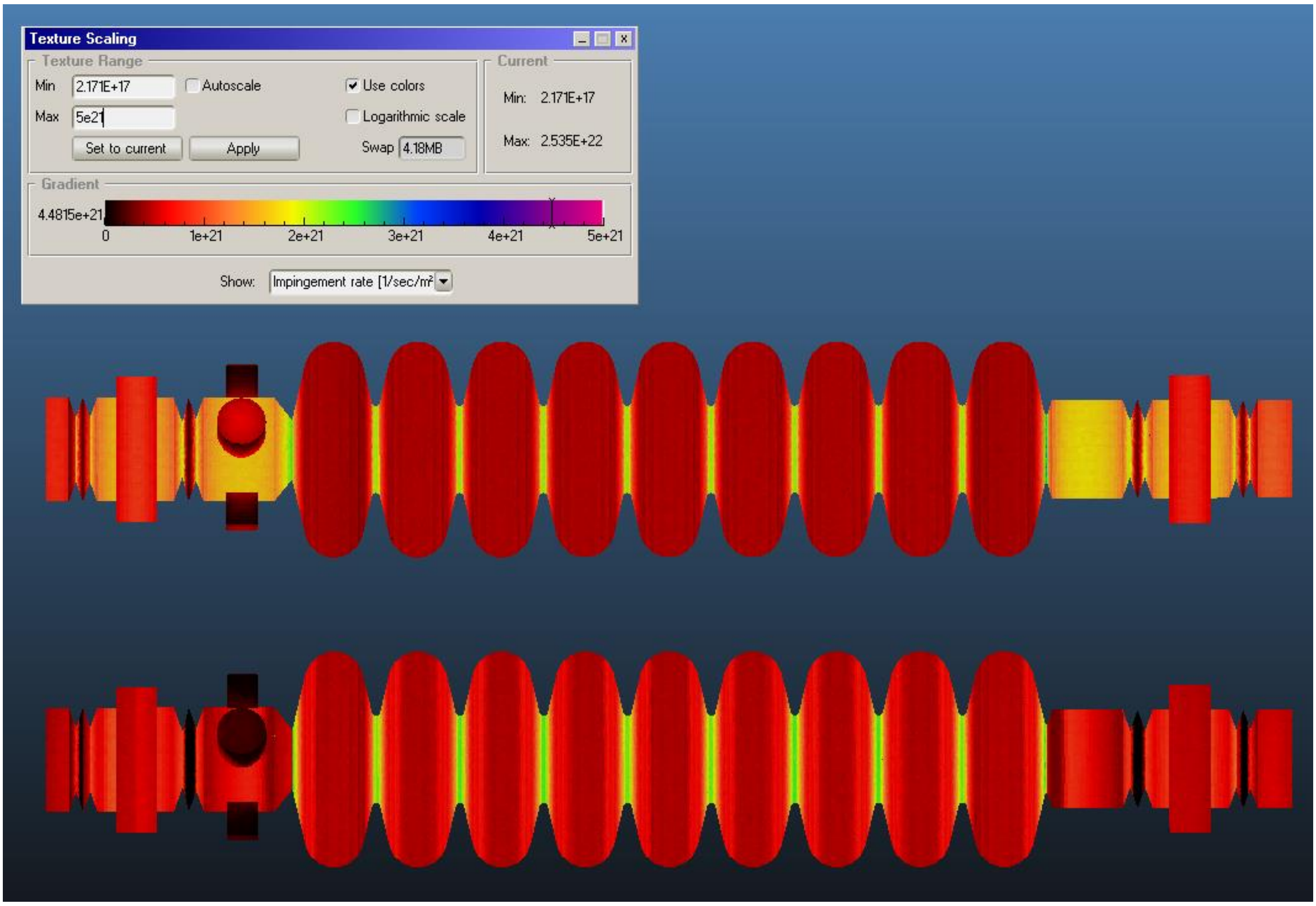


## 10. Vary outgassing to achieve uniform thickness

Where the impingement is too high or too low (for example, ends), adjust the outgassing by selecting smaller parts of the cathode. This corresponds to the sputtering time at that position in real life. After every change, rerun the simulation and check the result:




When you have a good (enough) uniformity, adjust the total outgassing on the other cathode for comparison.



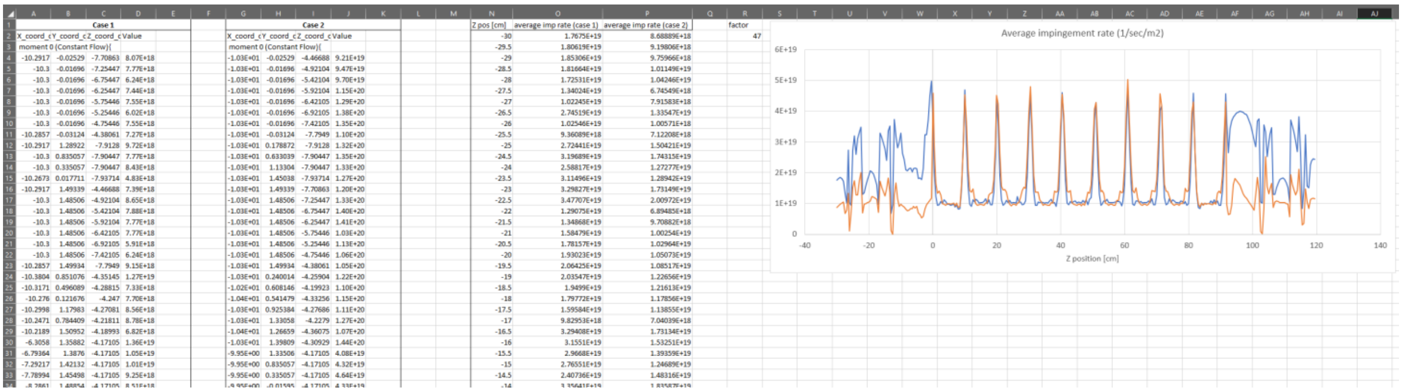

*Original, uniform outgassing (TOP) and equalized outgassing (BOTTOM). Note the differences on the edges.*

## 11. Compare thickness profiles

Select one of the RF bodies, and repeat point 7: export textures to a file and paste to Excel. If you use the template, it will be plotted.

Repeat the process for the other RF cavity and paste the values in “Case 2” in the template sheet.

This will plot the two thickness profiles against each other:




*Solution: Pasted data from Case 1 and Case 2, plotted against each other.*

**Well done!**

# 4. More info and tutorials

On the website (Molflow documentation, mainly for vacuum simulations):