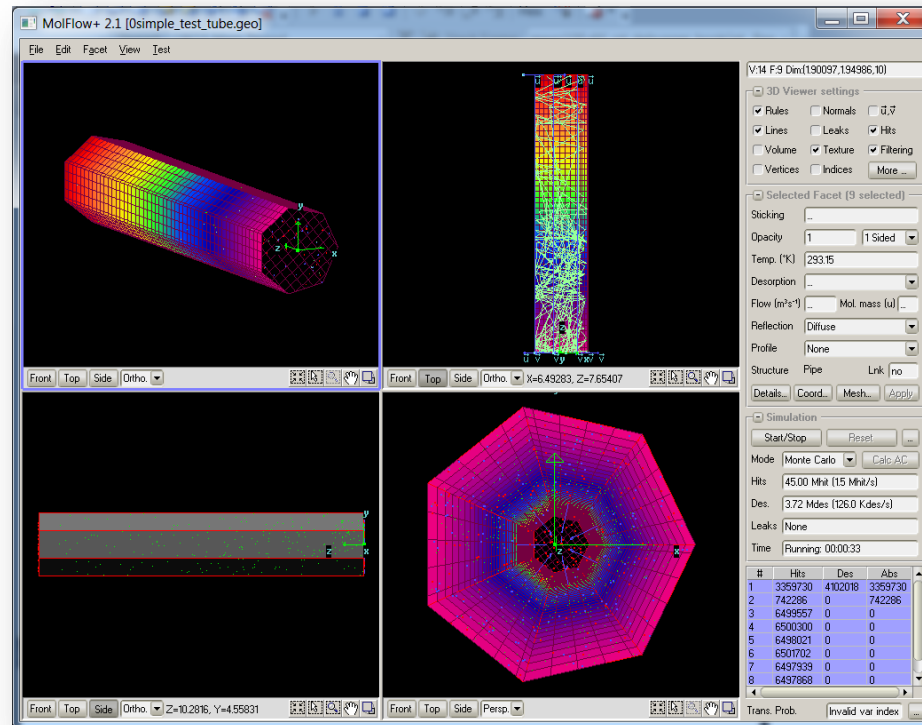


A 10-minute introduction to

# Molfow+

A test-particle Monte Carlo simulator for UHV systems

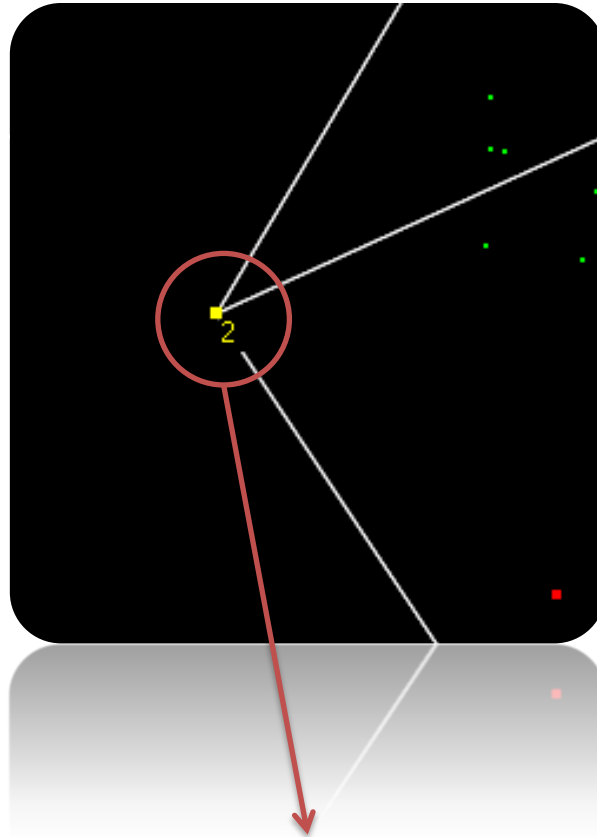


# The basics

First, let's learn the Molflow terminology and the interface in a few slides.

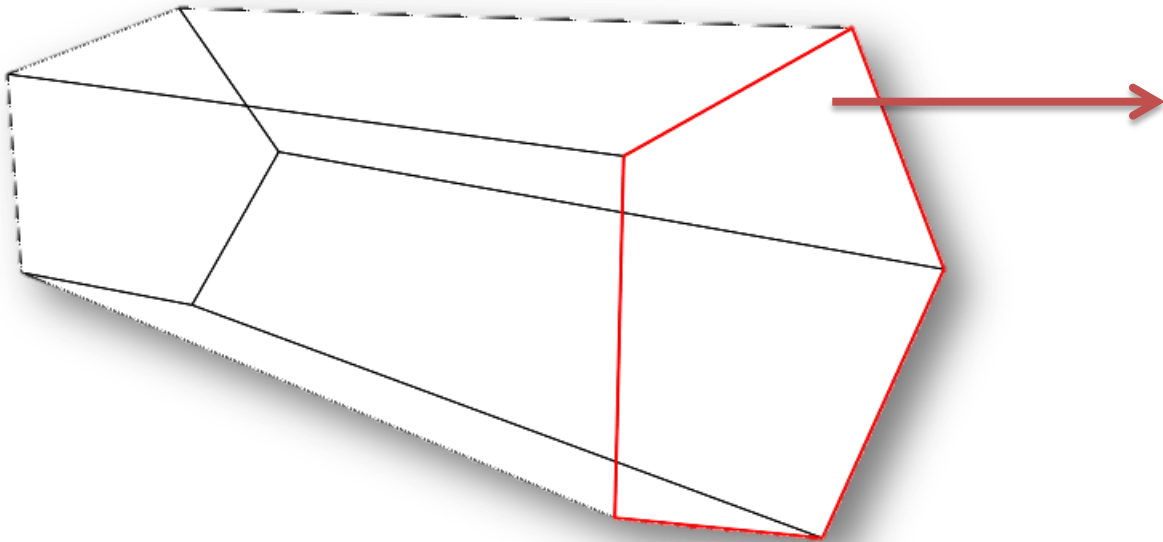
Or, if you prefer learning by doing it,  
[skip to the tutorial part.](#)

# Vertex



A vertex is a point in the 3D space.

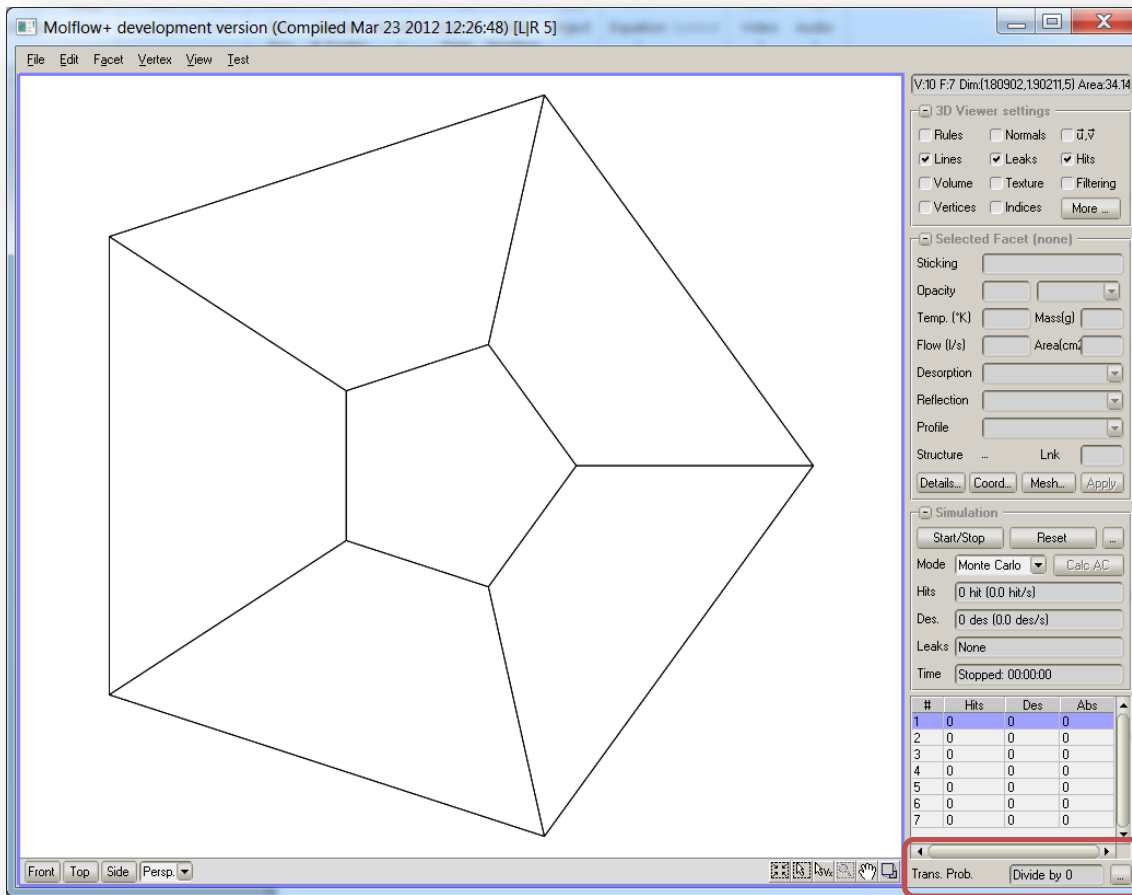
# Facet



A facet, also called polygon is a side of our 3D object. It is an outline that connects vertices.

It is an important term in Molflow, as many properties (temperature, outgassing, pumping speed, etc..) are *facet parameters*, which means that they can be adjusted individually for each facet.

# The interface



## Geometry properties

- Shows information about the geometry size, number of vertices and facets

## View settings

- Change view settings for the current *viewer* (see next slide)

## Facet parameters

- Change facet properties
- Access further features (mesh, coordinates,...)

## Simulation control

- Start/stop/reset simulation
- View simulation statistics

## Facet list

- See the number of hits on each facet
- Select facets (multiple: hold CTRL)

## Formulas

- A list of formulas that get calculated as the simulation runs (transmission probability for example)
- Use Edit / Formulas menu to add / remove

## View Selector

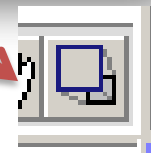
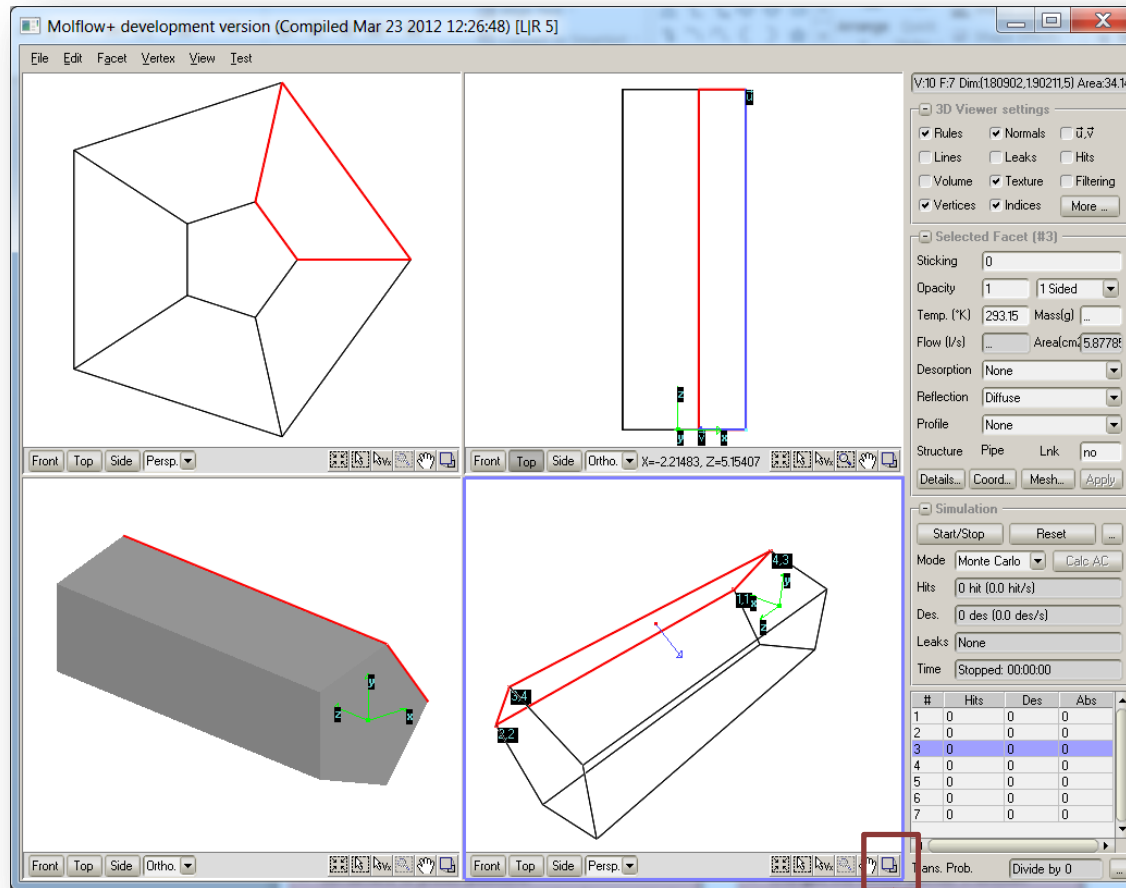
- Set camera to preset positions
- Change projection type (orthographic / perspective)

## Tool Selector

- Changes the mouse pointer's function
- Will be explained later in this guide

# The viewers

Molflow allows you to use four different *viewers*, each of them can have different settings and different camera angles. The active viewer is marked by the thick violet outline



**Expand button**  
Use this to maximize the current viewer

# Camera control

**Left click**  
To select a facet / a vertex, depending on the tool used (next slide)  
*Holding ALT and dragging with the left mouse button also moves the camera*

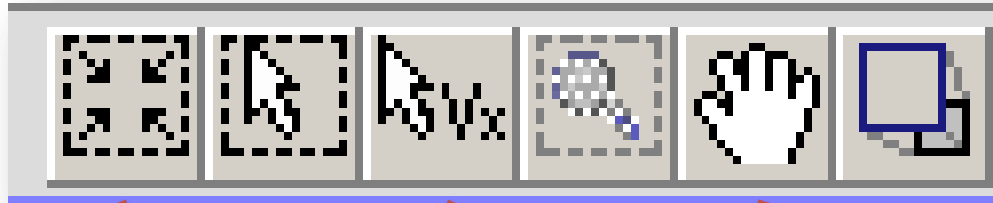
**Press and hold**  
the mousewheel to drag the camera  
**Scroll**  
The mousewheel to zoom in/out  
*Holding CTRL scrolls slower, holding SHIFT scrolls faster*

**Hold and drag**  
the right mouse button to rotate the camera  
*Holding CTRL and dragging with the right button also zooms in/out*



# Viewer Tools

To select things



## Autoscale

Click to fit the whole geometry on in the viewer

## Facet selector

Default setting. If you click several times on the screen, facets under your mouse pointer get selected in a cycle.

You can also **draw a selection box** by holding the left button to select facets inside the box.

**CTRL-click:** subtract from selection

**SHIFT-click:** add to selection

## Vertex selector

Click near a vertex on the screen: the vertex closest to your pointer gets selected.

You can also **draw a selection box** by holding the left button to select vertices inside the box.

**CTRL-click:** subtract from selection

**SHIFT-click:** add to selection

## Hand tool

Now deprecated by middle mouse button drag.

If selected, you can move the camera by dragging with the left mouse button.



# Facet parameters

So these are parameters can be set facet-by-facet:

## Opacity

Probability that a molecule going through the facet will actually interact with it

## Volumetric pumping speed

The pumping speed and the sticking factor are related. Update one of them and the other will be calculated

## Superstructure properties

These functions are for large structures linking several geometries, their implementation is to be improved.

The image shows a software dialog box titled "Selected Facet (#47)". It contains several input fields and dropdown menus. The parameters are: Sticking (0), Teleport (0), Opacity (1), 1 Sided (dropdown), Temp. (\*K) (293.15), Mass(g) (28), Flow (l/s) (-0), Area(cm<sup>2</sup>) (0.6282), Desorption (None), Reflection (Diffuse), Profile (None), Structure (Pipe), Lnk (no). At the bottom, there are buttons for "Details...", "Coord...", "Mesh...", and "Apply". Red arrows point from various text boxes to specific fields in the dialog.

## Sticking factor

Probability that a molecule hitting the facet will be absorbed

## Teleport destination

Particles hitting this facet will get transferred to the entered facet index (for periodic structures)

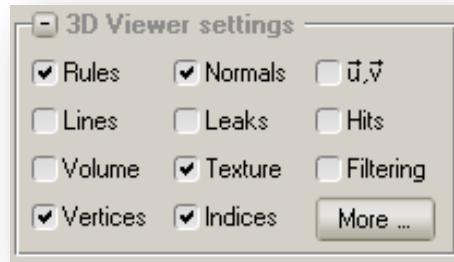
## One- or two-sidedness

A one-sided facet is opaque on the side where its normal vector is pointing, whereas a two-sided will catch particles from both sides. Also affects the pressure calculation and the desorption

## Desorption type

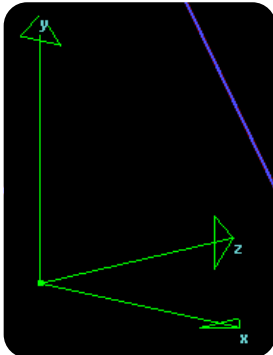
Probability distribution type. The outgassing rate is proportional to the facet area (as of ver.2.3)

# Viewer parameters



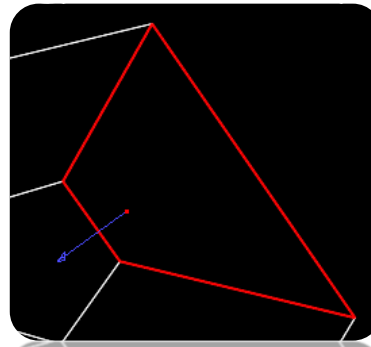
## Rules

Toggle the base vectors of the coordinate system



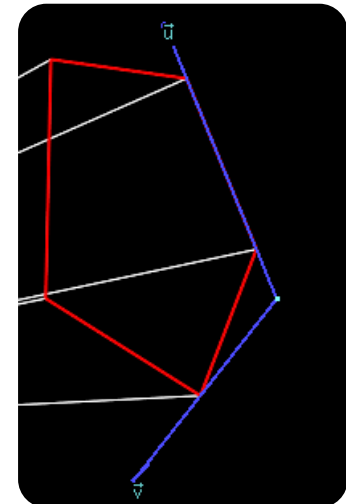
## Normals

Show the orientation of the facet (interesting in case of 1-sided facets)

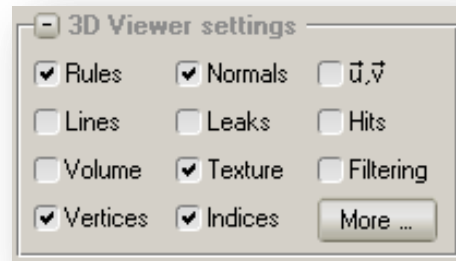


## U, V vectors

The own 2D coordinate system of the selected facet

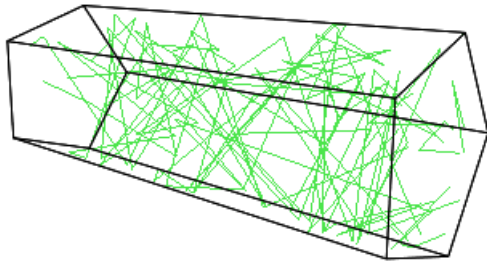


# Viewer parameters



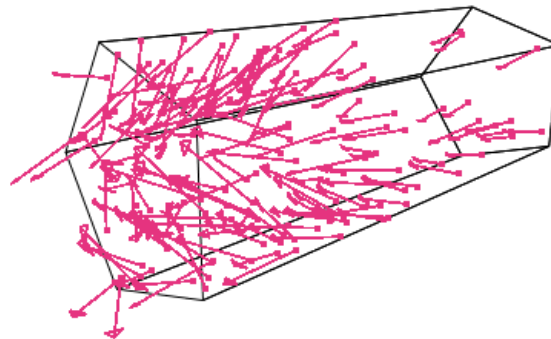
## Lines

Particle trajectories



## Leaks

If a molecule escapes from the system, show where the last hit occurred and in what direction the molecule rebounded before leaving



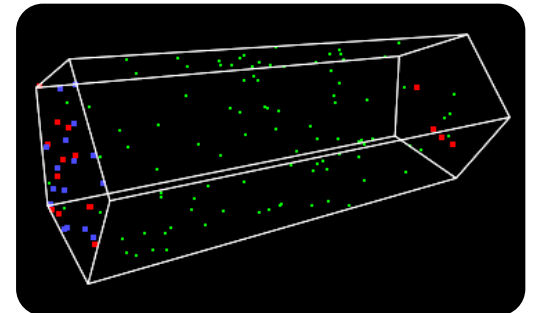
## Hits

Particle collisions with facets.

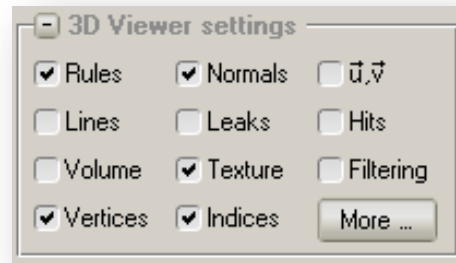
**Red:** Absorption

**Blue:** Desorption

**Green:** Reflection / Transparent pass

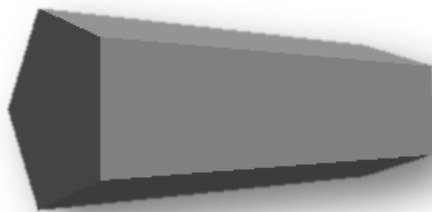
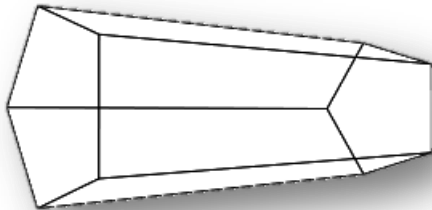


# Viewer parameters



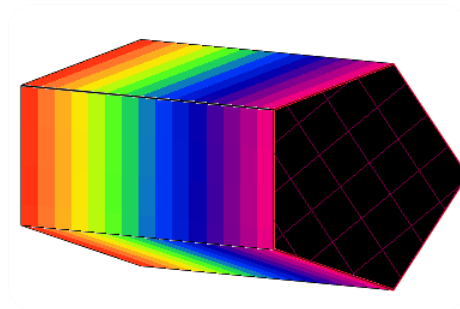
## Volume

Switch between volumetric or wireframe view mode



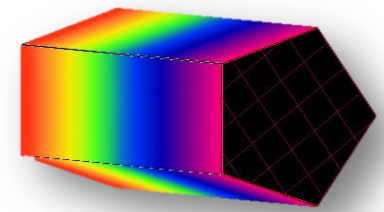
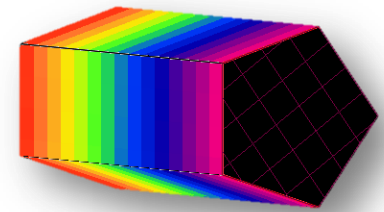
## Texture

Show or hide textures (see later)

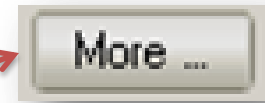
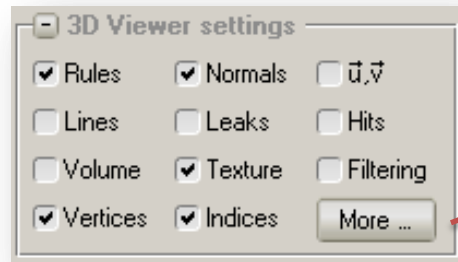


## Filtering

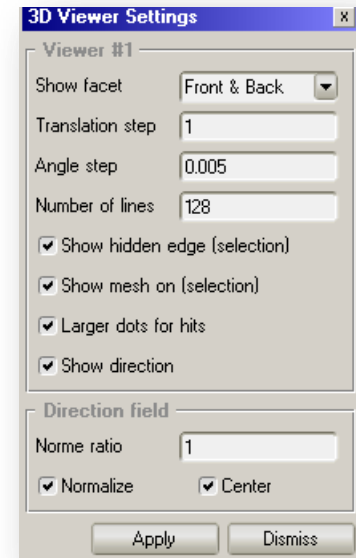
Apply a Gauss filter to textures



# Viewer parameters

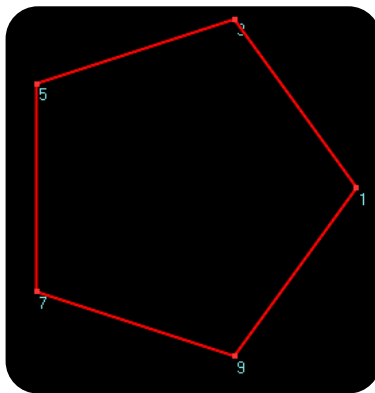


Further options...



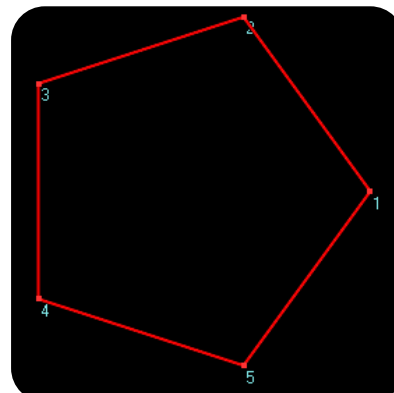
## Vertices

Shows the identifier of vertices on selected facets



## Indices

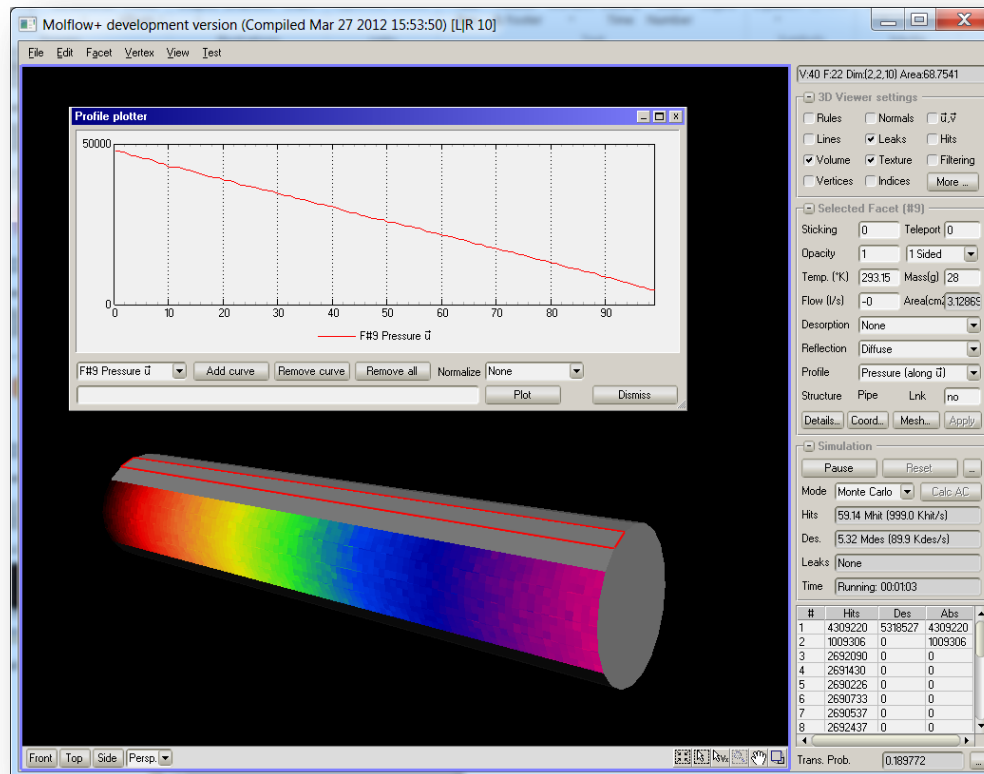
Shows the index of vertices on a given facets (starting from 1 for each facet)



Not part of this quick start guide.

# Tutorial: a simple pipe

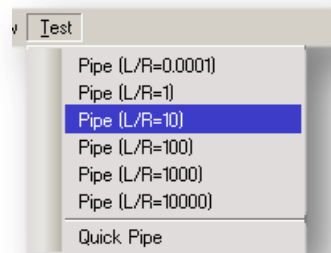
In this example, we'll calculate the transmission probability and the pressure distribution of a pipe.



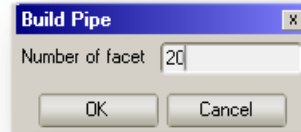
All steps of this tutorial are demonstrated in a video on the website.

# Create geometry

- From the Test menu, choose a test pipe with L/R ratio of 10



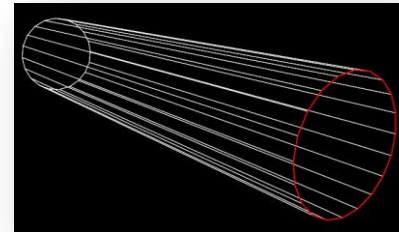
- Let its surface consist of 20 facets:



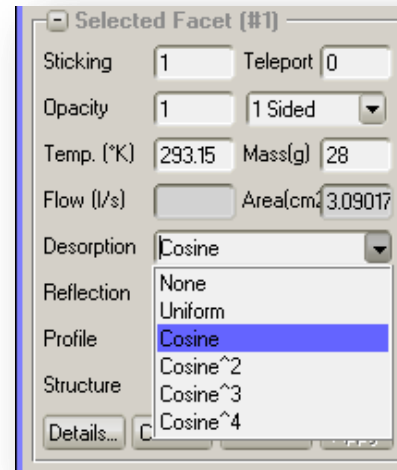
- Note that test pipes have some parameters set by default. Nevertheless, we'll set them again, for the sake of learning how to do it.

# Define gas inlet

- Click on one end of the pipe. Keep clicking without moving the mouse until the top facet is selected (red outline):



- On the right (facet parameters), change “Desorption” to cosine and sticking to 1:



- Click





# Define gas inlet

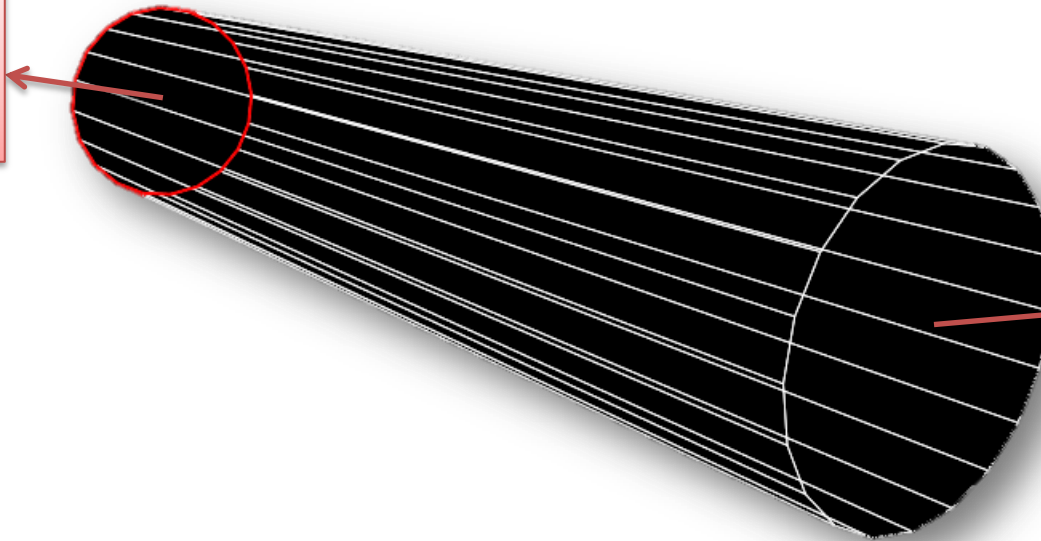
- What we just did:
  - Defined that particles will desorb from one end of the pipe
  - And by setting sticking to 1, if a particle gets back to the inlet, it will be “absorbed”: removed from the system

# Define pumping

- Now select the opposite side of the tube

**Opposite facet  
(pump)**

Now select it: our pump  
will be connected here



**First facet  
(desorption)**

We've defined  
desorption here

# Define pumping

- Now we can define the volumetric pumping speed in the facet parameters:

**Sticking factor and pumping speed**  
They will be converted to each other using the facet area, the temperature and the mol. mass

Sticking	0.54987	Teleport	0
Opacity	1	1 Sided	
Temp. (*K)	293.15	Mass(g)	28
Flow (l/s)	20	Area(cm <sup>2</sup> )	3.09017
Desorption	None		
Reflection	Diffuse		
Profile	None		
Structure	Pipe	Lnk	no

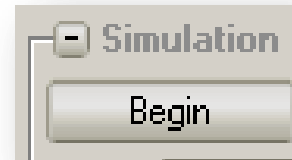
Details... Coord... Mesh... Apply

- Click

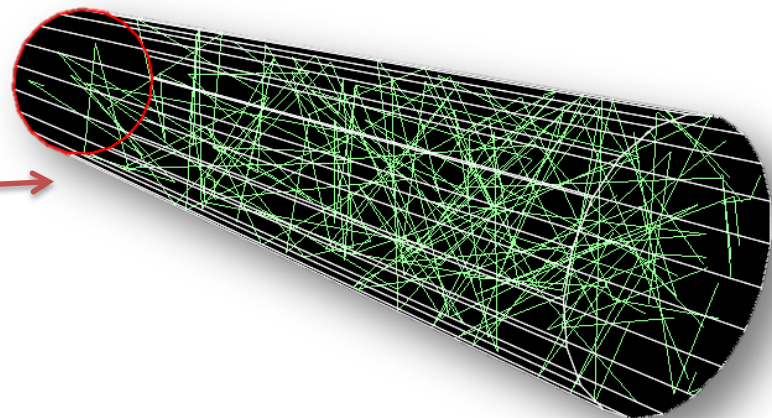
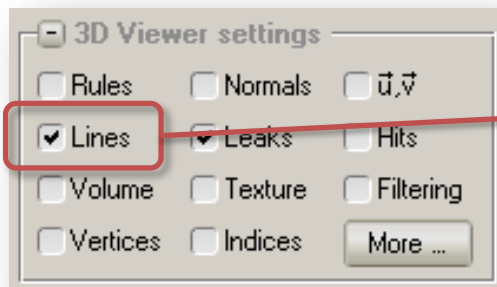


# Begin simulation

- Now our simple system is ready. Launch the simulation by clicking

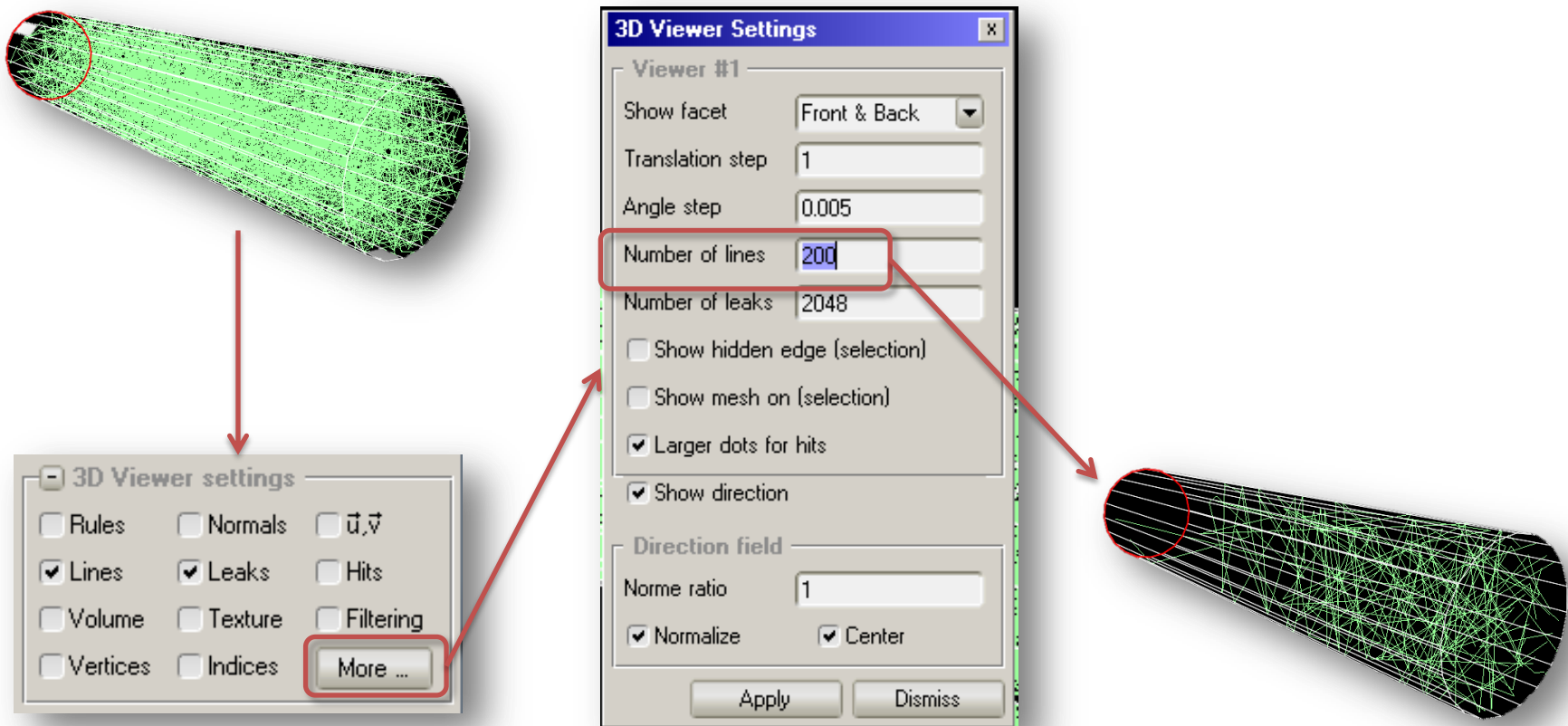


- The simulation is now running. If you enable “Lines” at the viewer parameters, you can visualize the trajectories of the particles:



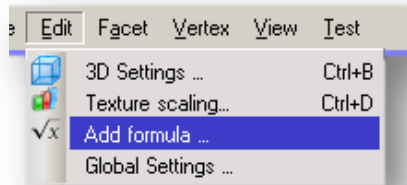
# Quick hint


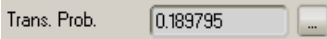
- If too many lines are displayed, reduce them at the viewer parameters:



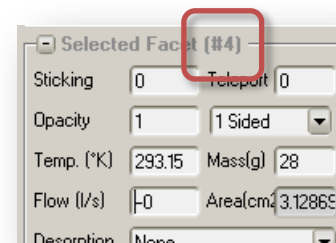
# Transmission probability

- Now that we have a running simulation, let's calculate some data. To do that, open the formula editor:



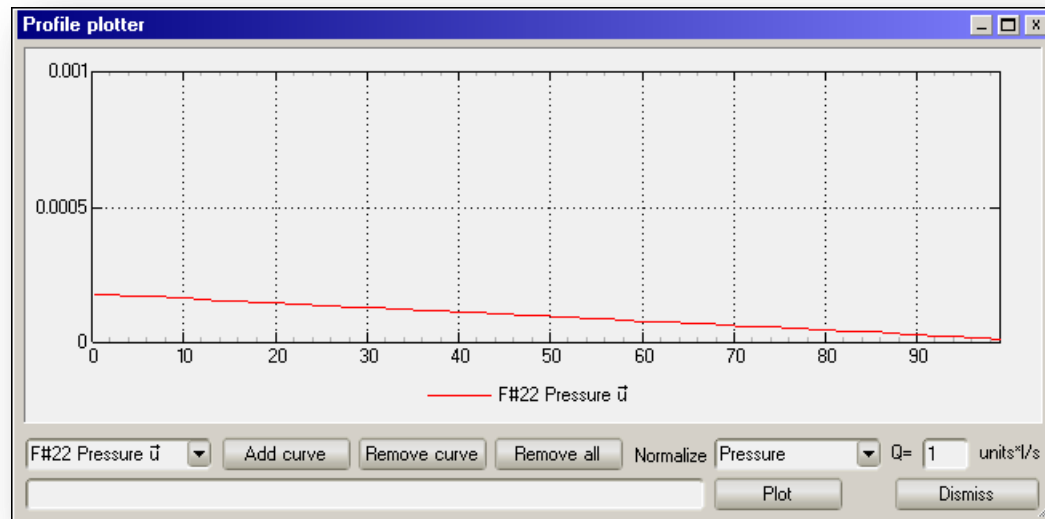
- Write "transmission ratio" as formula name, and " $A1/D2$ " as the formula. This means "*number of absorbed molecules on facet #1/number of desorbed molecules from facet #2*". Click . Now you will see the calculated formula on the lower right corner: 

- Hint: the above formula might be " $A2/D1$ ", depending on which facet you defined as for desorption. You can find out a facet's number by selecting it, and reading the title of the facet parameters editor:



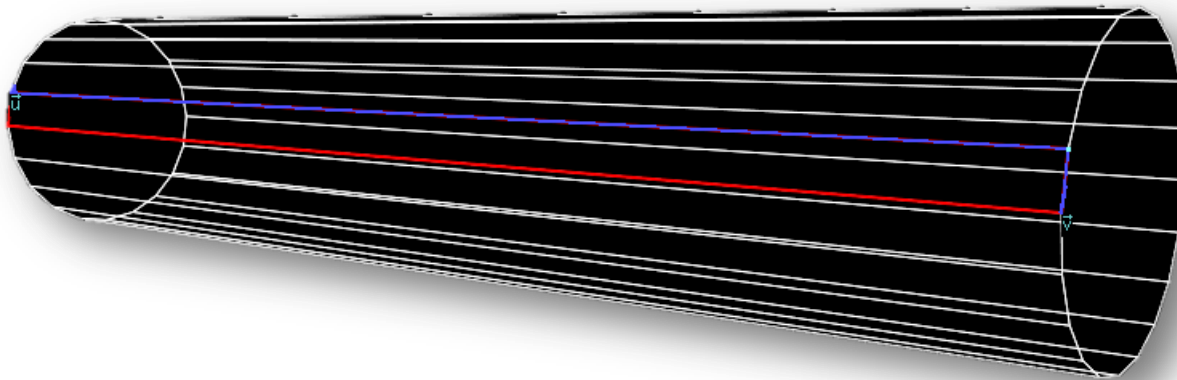
# Pressure profile

- Now we'll visualize the pressure along the side of the tube.



# Pressure profile

- Select a side facet, and turn on the “u,v” vector display in the viewer parameters:

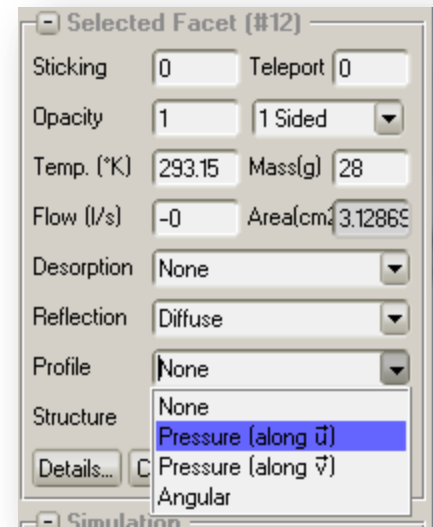


- As we can see, the  $u$  vector is directed along the length of the tube



# Pressure profile

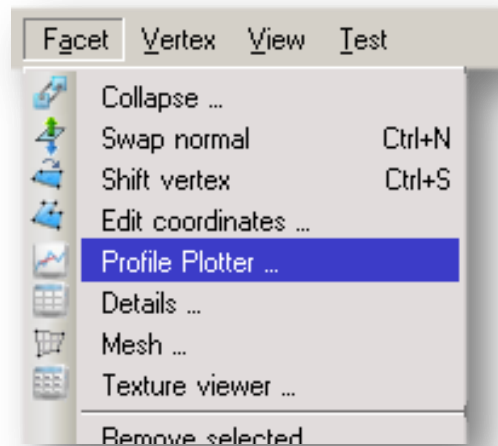
- On the facet parameters, choose “pressure along  $u$ ” in the profile settings:



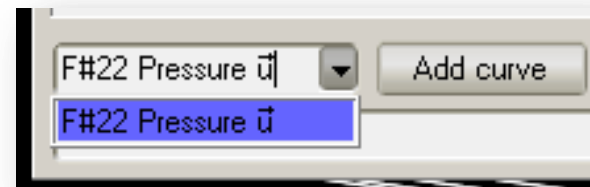
- This instructs Molflow to calculate the pressure along the axis  $u$

# Pressure profile

- To view the pressure, open profile plotter:

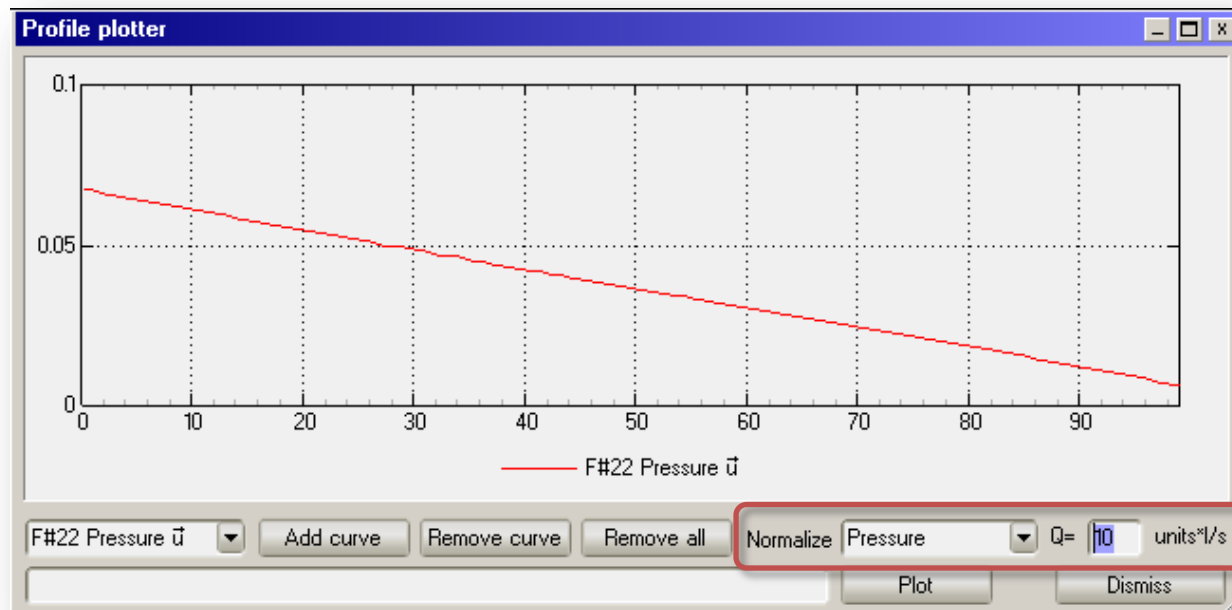


- Then choose the profile you just set (bottom left), and click Add Curve



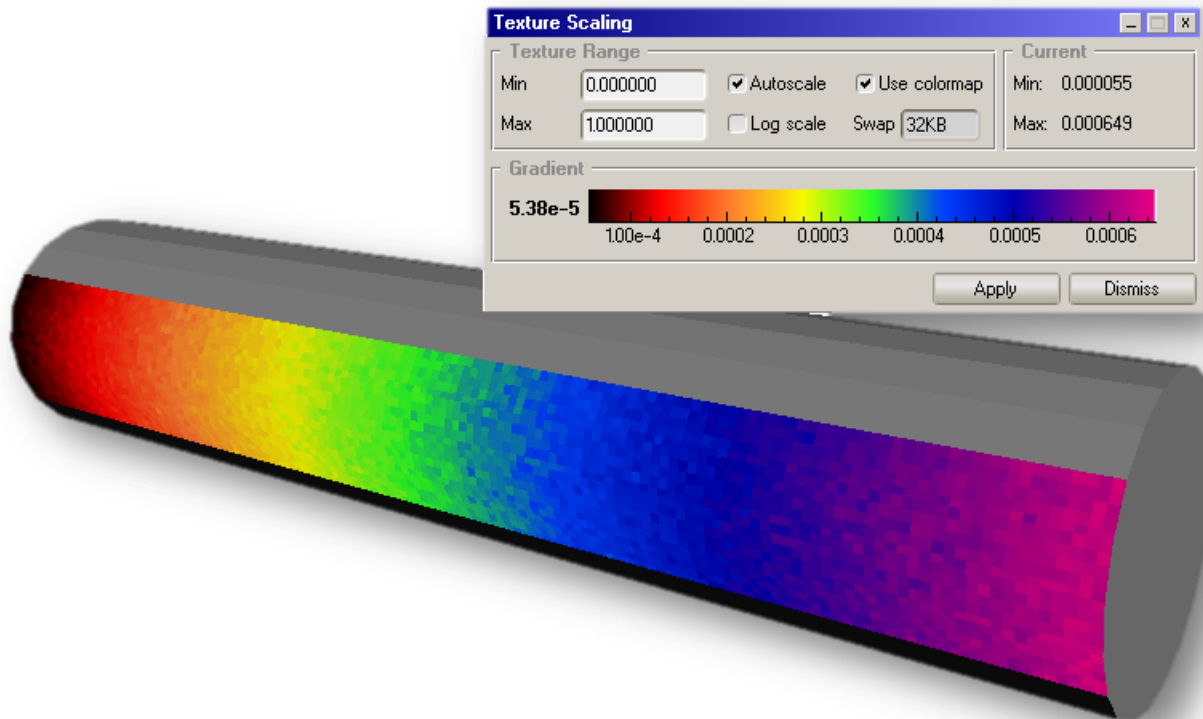
# Pressure profile

- To calculate the pressure in (for example) *mbars*, choose “pressure” under normalize options and enter the total outgassing in *mbar*\*liter/sec:



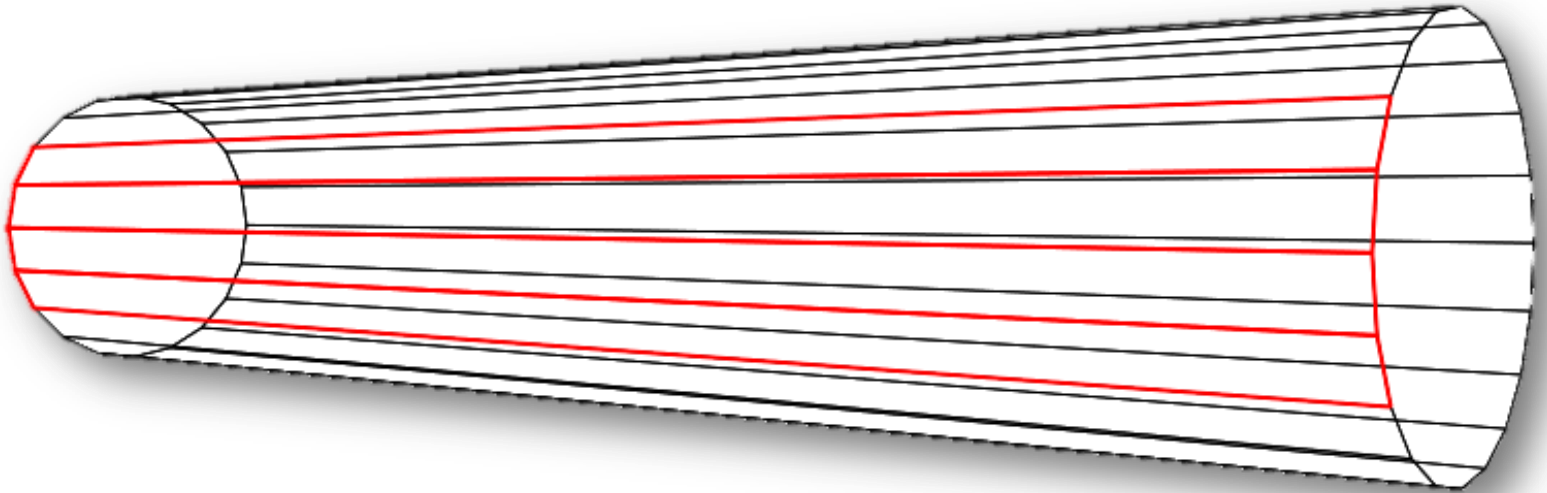
# Adding a Texture

- Textures are an other way to visualize local pressure information. We will add them now.



# Adding a Texture

- Select a few (or all) facets where you'd like to view the pressure. Select multiple facets by holding the SHIFT key, unselect by holding the CTRL key:



# Adding a Texture

- Add a MESH. A mesh splits the facet into little blocks where the pressure is individually calculated. Click **Mesh...** in Facet editor:

The image shows a software dialog box titled "Facet Mesh" with the following sections and settings:

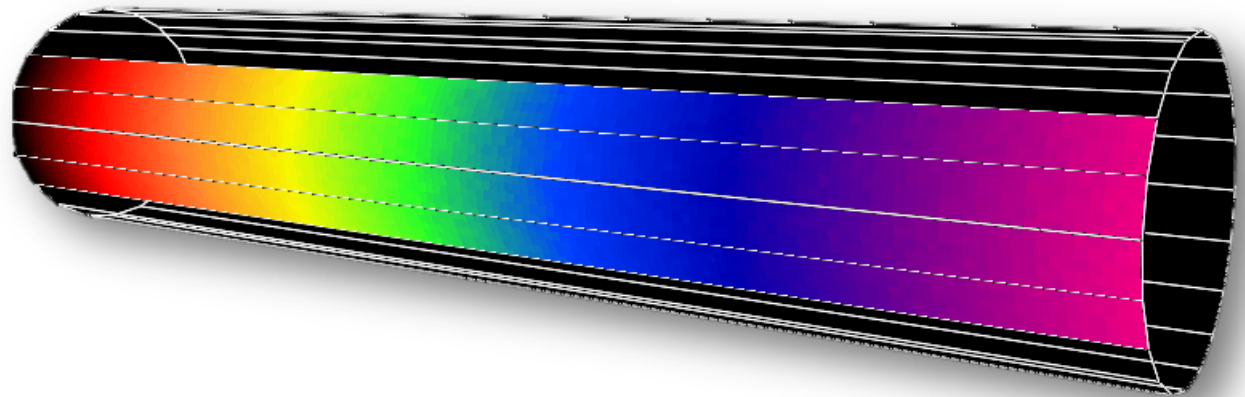
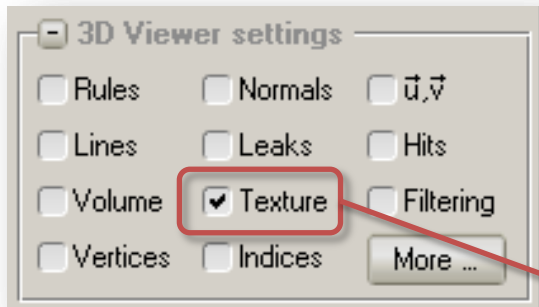
- Facet Info (4 selected):** U length: 10 (MAX), V length: 0.312869 (MA)
- Mesh properties:**
  - Enable
  - Boundary correction
  - Resolution (Sample/Unit): 15
  - Count desorption
  - Count reflection
  - Count absorption
  - Count transparent pass
  - Angular coefficient
  - Record direction
- View Settings:**
  - Show texture
  - Show volume
  - Apply View
- Memory/Cell:**
  - Memory: 70.31KB
  - Cells: 3000
  - Update
- Buttons: Apply mesh, Cancel

Five numbered callouts provide instructions:

- 1. Check ENABLE**  
So a mesh will be added
- 2. Boundary correction**  
As the mesh is rectangular, a facet's side might not entirely be in it. To correct for this area difference, check this option.
- 3. Set resolution**  
In this example, our facet's size is 10cm\*0.31cm, so we will add 15 mesh divisions / cm
- 4. Define what to count**  
In this example, we want to visualize the pressure, which is proportional to the number of molecule reflections
- 5. Apply mesh**

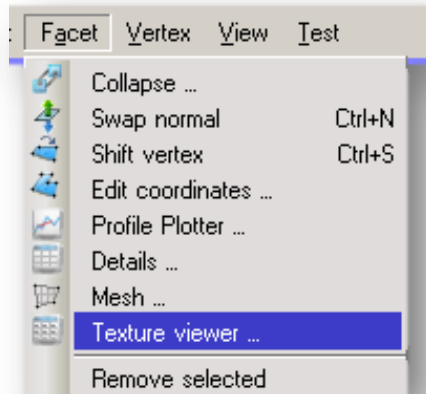
# Adding a Texture

- Turn on “Texture” in the viewer parameters to see the texture:

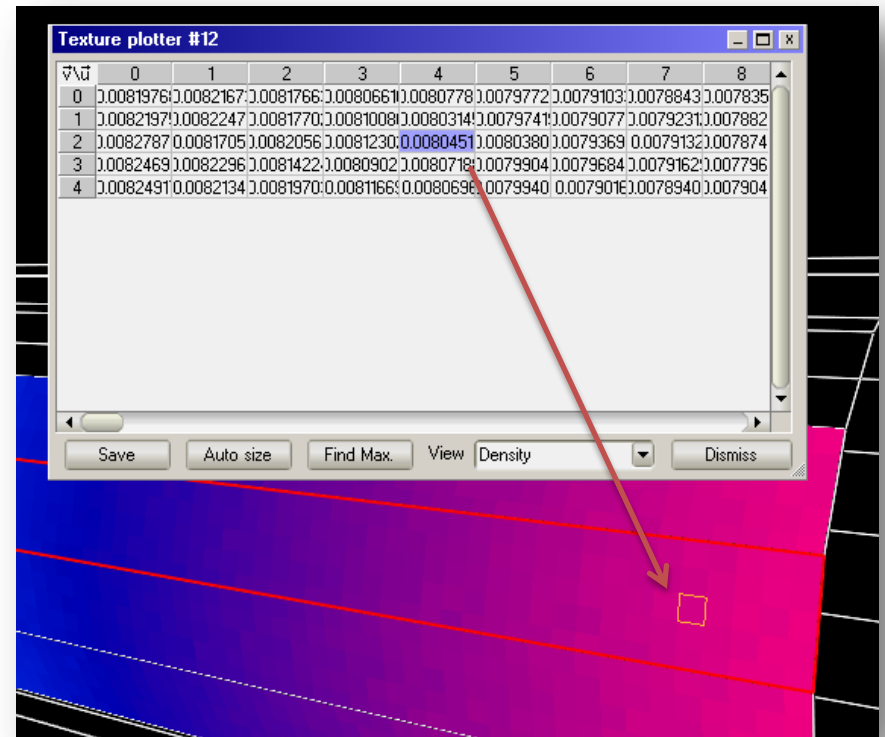


# Adding a Texture

View texture block values by selecting a facet with mesh and opening the Texture Viewer:



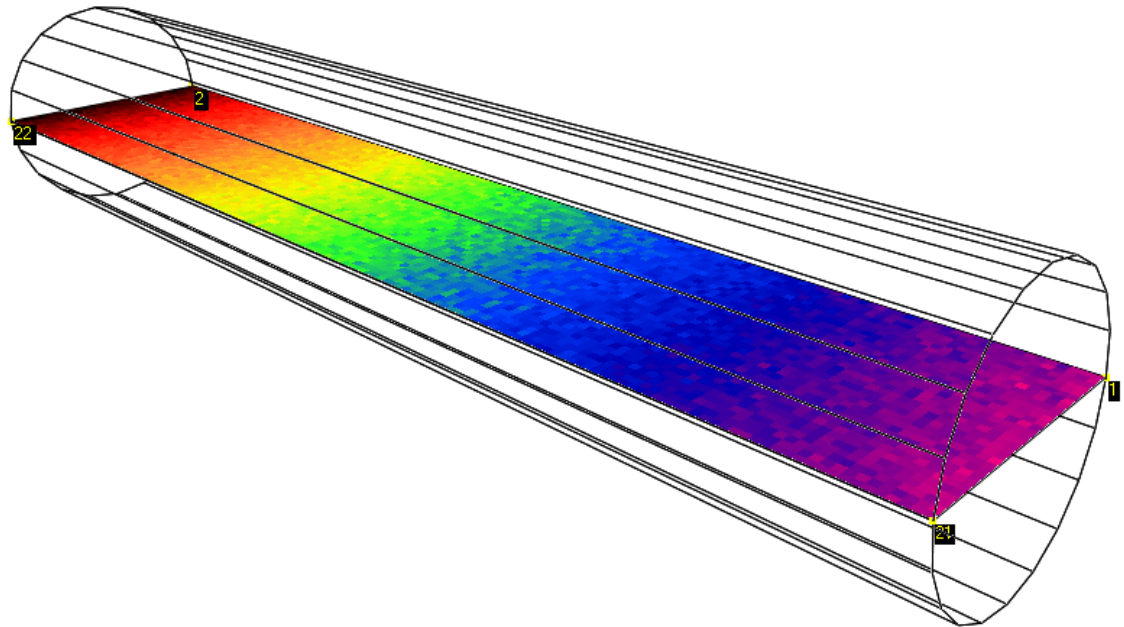
Selected cells' position will be outlined on the facet:





# Advanced: add a polygon

- Now that we've covered the basics, here's a useful feature. To visualize the pressure in the center of the tube, we will add a "dummy" polygon.

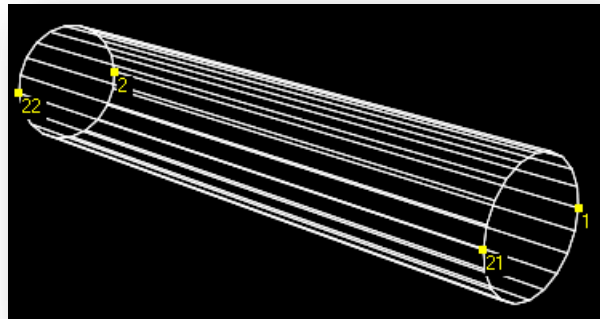


# Select vertices

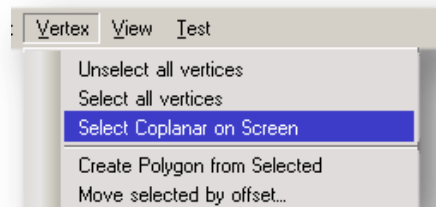
- Choose the vertex selector tool. Notice that the mouse cursor is now different.



- Select 4 vertices that will be the edges of the new polygon:

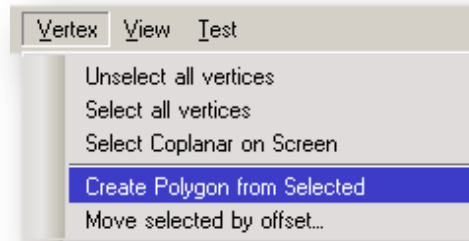


- Hint: after selecting 3 vertices (that define a plane), you can use the “Select coplanar” function to find the fourth:

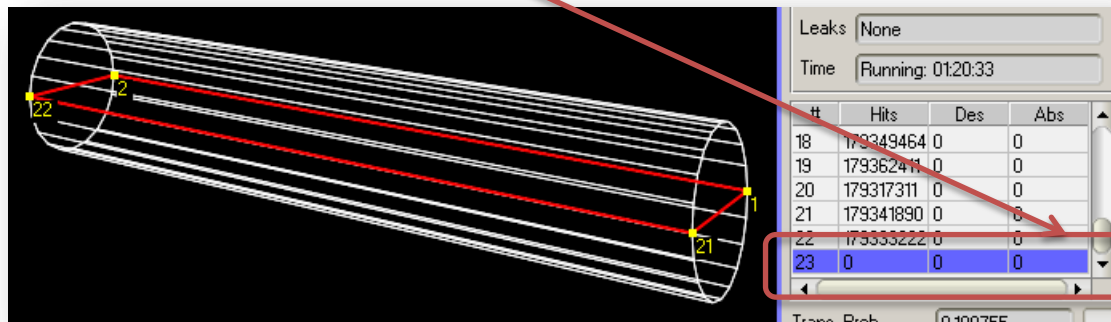


# Create the dummy polygon

- Now that we have the four edges selected, click “create polygon from selected”:



- Molflow creates a new facet. One way to easily select it is to click on the last entry in the facet list on the right:

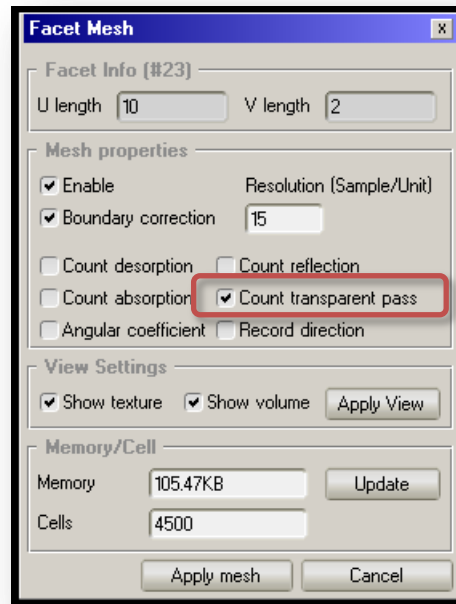


# Set facet parameters

- As this is a dummy facet, we want to tell Molflow that it shouldn't change our simulation. To do this, set the opacity to 0, and set the facet as 2-sided (to count particles from up and from down as well):

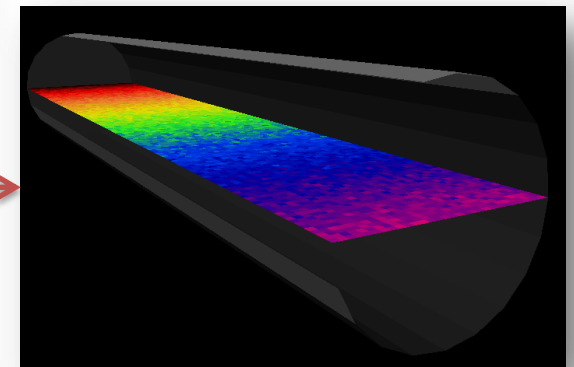
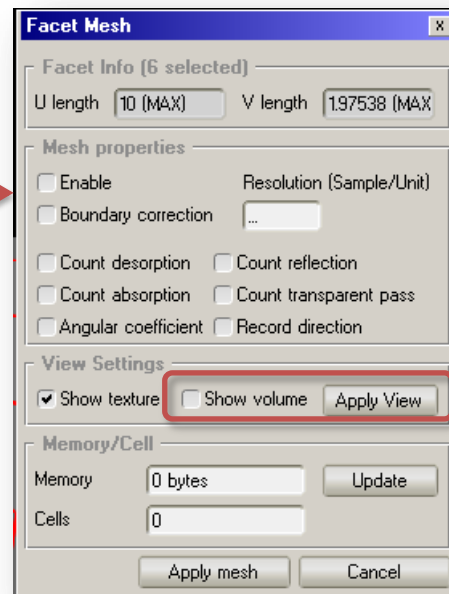
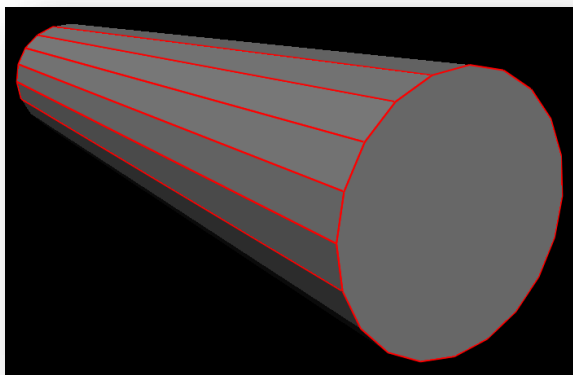


- And the last step is to add a mesh that counts transparent passes:



# Done!

- That's it! Start the simulation, and don't forget to enable the "Texture" option in the viewer parameters.
- One last trick: if you want to see the volume of a structure, while seeing the inside as well, turn off the "Volume visible" property of some facets, so they will become transparent:



# The end

- Stuck at one point?
- Found a bug?
- Have a suggestion?

Tell your ideas on the website, where you can also find a video tutorial.

(currently <http://cern.ch/test-molflow>)