

Vacuum simulations of the β -NMR end station at the VITO beamline

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Introduction

The goal of the "Versatile Ion-polarized Techniques Online" (VITO) project is to provide laser polarized ions to three different end stations. These polarized ions will serve as a femtometer sized probe which will be used for a wide range of experiments coming from biophysics to surface science.

One of these end stations will be the β -NMR station which will be focused on biophysics. One of these is β -NMR studies of proteins containing Ca^{2+} , Cu^{+} and Zn^{2+} which is not possible with the conventional NMR method. However in order to study the proteins in surroundings similar to the human body they must necessarily be in a liquid environment.

This presents a challenge as water will only remain liquid if the pressure is higher than 10 mbar. The ISOLDE beam line is at the order of 10^{-6} mbar. Furthermore since water is highly polar this introduces difficulties in vacuum systems. The aim of the project is to carry out simulations in order to determine the amount of water that travels upstream.

Preparation

The simulations were carried out with Molflow+¹ which is a "Test-particle Monte-Carlo simulator". The input to Molflow is a file describing the geometry of the vacuum system in the STL format. In my case there already existed 3D drawings of the chamber. These were however in the 3DXML format which is not readily converted to STL.

The procedure which I established for the conversion was to open these in "Simlab Composer" where I could also remove features which were unimportant for the simulation. After editing the geometry was saved in an intermediary which could be opened by Rhino 5. With Rhino it was then possible to export to STL.

¹<http://test-molflow.web.cern.ch>

It should also be noted that Molflow is not well suited for our pressure region of interest. We however believe that it will serve as a nice guide for further studies.

Simulation

When the file is imported into Molflow the rest is straight forward. One click on the facets (surfaces) where the pumps would be and just enter the pumping speed. In order to simulate the droplet of water in the system a little sphere was drawn in Autodesk Inventor and imported into Molflow. A picture of it marked in red is shown below.

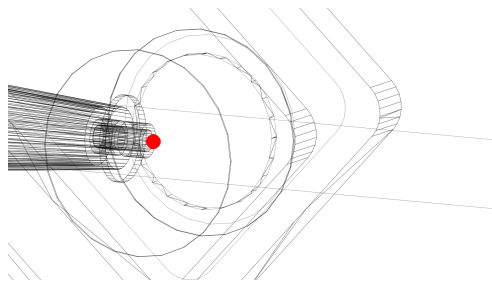


Figure 1: A picture of the water source in the chamber.

All there was left was to define that it emitted water and then press go! A screen shot after running the simulation a few minutes is show in fig. 2.

First of all it is clear qualitatively that the differential pumping system is doing a very good job of keeping the water in the experimental chamber since the green lines are concentrated there.

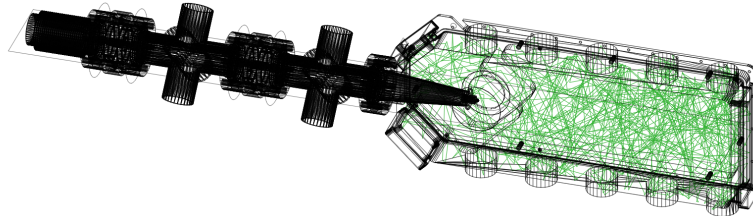


Figure 2: Screen shot of Molflow after it has been running a few minutes. The green lines are particles trajectories. The black is the geometry.

Molflow also have a nice data collection tool which basically allows you to measure the pressure at a given position. The data is shown in fig. 3. From this it is quite clear that the pressure in the experimental chamber is uniform except for just in front and inside the first pinhole where there is a high pressure zone. The effect of this is that almost 15% of the emitted water flows past the red transmission line. It should also be noted that effect of the differential pumping is a pressure drop between one and two orders of magnitude for each.

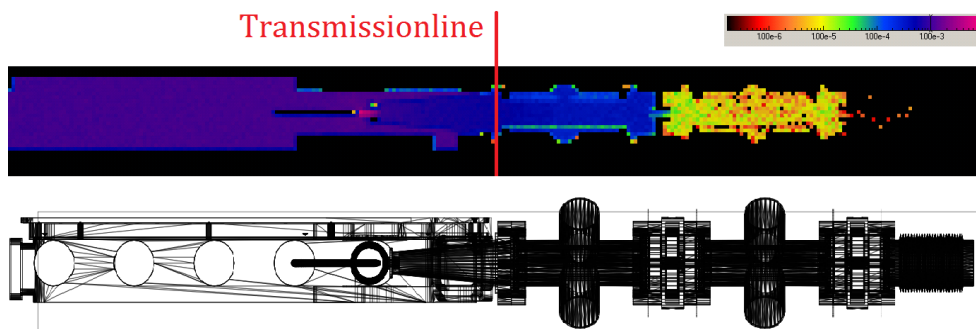


Figure 3: The pressure map of the chamber.

The solution to this was quite simple. The amount of water that enters the pinhole is related to the solid angle of the pinhole as seen from the droplet. Hence moving the droplet just a few centimeters made the water transmission droplet below 5%.

Conclusion

In this paper it is found that with the β -NMR line in its present shape 15% of the water would flow upstream. This results are found with Molflow. It is however also found that it is possible to get this lower than 5% by just moving the droplet a few centimeters back. However it is necessary to perform simulation on the beam transmission in order to determine if the is feasible.