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Simulation of helium flow through ion guide with COMSOL Multiphysics

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Abstract

Simulation of helium flow through ion guide with COMSOL Multiphysics

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The program COMSOL Multiphysics was used to simulate a flow of helium gas transporting ionized fission products out of an ion guide. Two important parameters to study from the simulation was the evacuation time and velocity of the ions. The mean evacuation time was shown to be 0.1173s, and the velocity of a single particle peaked at 2500m/s, 1000-1500m/s being more common.

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1 Populärvetenskaplig sammanfattning

När en fission (kärnklyvning) sker uppstår fragment av atomer som kallas fissionsprodukter. Ett sätt att ta vara på produkterna är att låta en gas flöda genom utrymmet där fissionen sker, för att bromsa upp och föra med sig produkterna. I det experiment vi har studerat var utrymmet en ca 1dm lång cylinder, med en konformad utgång. Gasen sprids via en diffuser, en platta vid ingången med mindre hål placerade på ett sådant sätt att spridningen ska bli optimal. Helium är en lämplig gas för detta då det är en ädelgas och därför inte reagerar med de ämnen som den ska transportera ut. I detta projekt har en simulering av gasflödet utförts, för att se hur lång tid det tar att transportera ut produkterna. Det visade sig att genomsnittstiden var 0.1173s. Programmet som användes var COMSOL Multiphysics.

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2 Introduction

2.1 Background

Fission has been studied extensively since it was discovered in Berlin in 1938 [1]. The discovery led to almost fifty years of work on radioactivity and development of modern nuclear physics to describe the components of atoms. However, today there is still no theory that describes all aspects of nuclear fission.

The atomic fragments (two light nuclei) that spawn after a heavy nucleus undergoes fission are called fission products. Some of these products are very useful. A common product, Cs-137 [2], is used in medicine and industry as a radioactive source. Besides useful applications, it is also interesting to study fission products, especially since not everything that spawns after a nuclear fission is known. Studying these closely can be hard though, since many of them have a very short half-life, which makes them radioactive.

In Finland, at the University of Jyväskylä the Ion Guide Isotope Separator On-Line, or IGISOL, have been producing fission-products for research for 3 decades [3]. Lately they have been working together with the applied nuclear physics department at Uppsala University. The researchers in Uppsala are primarily interested in the yield of fission products from different nuclei. This can be used to optimize current nuclear power plants and will help in the designs of future nuclear power plants.[4]

2.2 Objective

Figure 1 shows the layout of IGISOL. At section 1 is the ion guide in which the fission actually happens. Through the ion guide flows helium which slows down the fission products after the reaction and leads them out of the ion guide. The objective is to simulate this helium flow through the ion guide to determine how long it takes for the fission products to leave the ion guide, this is called evacuation time. If possible, it is of great interest to compare two different fission products to see if the evacuation time differs between them. Since Iodine-135 and Zirconium-100 are two common fission products, they were compared to each other.

Another aspect of the simulation is to determine if there are any pockets in the ion guide with a very long evacuation time or pockets where the fission products can get stuck. The simulation was done in a program called COMSOL multiphysics. COMSOL uses the finite element method to simulate and model different kinds of physical phenomena, it can even solve coupled physical problems, hence the name multiphysics. Some parameters were received from Finland in order to make a reasonable simulation, they are visible in table 1.

Table 1: Values of the inlet pressure with the corresponding outlet pressure in the ion guide

Inlet pressure	Outlet pressure
50 mbar	0.0094 mbar
82 mbar	0.018 mbar
101 mbar	0.021 mbar
154 mbar	0.03 mbar
200 mbar	0.038 mbar
252 mbar	0.05 mbar
306 mbar	0.065 mbar
347 mbar	0.078 mbar
400 mbar	0.098 mbar

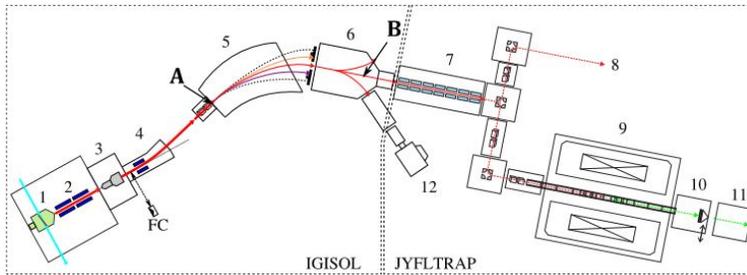


Figure 1: The layout of the IGISOL groundfloor. The green area marked "1" is the ion guide. Components 2-6 are electrodes and magnets for sorting of the fission products. Components 7-12 are detectors and setup for spectroscopy[3]

3 Method

Since neither of the participants in this project had any prior experience with COMSOL Multiphysics, it was necessary to start from the very beginning by looking at tutorials online and join webinars. It turned out that COMSOL had a very vast catalog of tutorials and lessons online, so it did not take too long to get comfortable with the program. In figure 2 you can see the model builder of COMSOL, you generally start from the top and work your way to the bottom to complete the simulation.

3.1 Creating geometry

The first thing you need to do is defining the dimensions you work in, and since the ion guide schematics are in 3D, a 3D model was created. There is a built-in feature that allows you to directly import CAD-files into COMSOL which was very useful. The schematics imported are visible in figure 3. To the left is the backframe and the outlet. In the middle there is the target, this is where the large nuclei gets hit by the proton ray. The circular disk is the gas diffuser and furthest to the right is the frontframe where the gas enters. The target of the CAD-schematics were removed since they did not impact the flow, and having them in the simulation only made the simulation take longer time and being more difficult to solve.

For COMSOL to be able to interact with a geometry, it has several built in functions. It works with domains, boundaries, edges and points. The words describe themselves to some degree, but there will be mentioning of them later on in the report and they are important to understand. The domains are the volumes, for example, the inside of the ion guide is a domain.

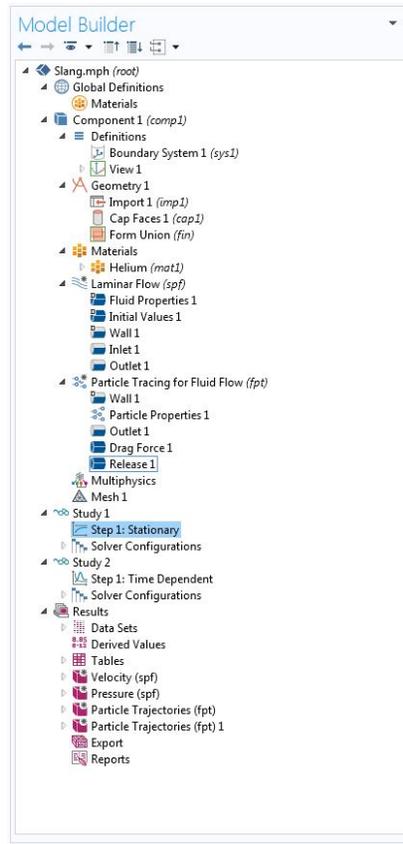


Figure 2: The model builder of COMSOL that shows the layout of how to work with the program

Boundaries are the faces of a domain, for example the inlet and outlet are boundaries. Edges encircle the boundaries and at the end of every edge there is one point.

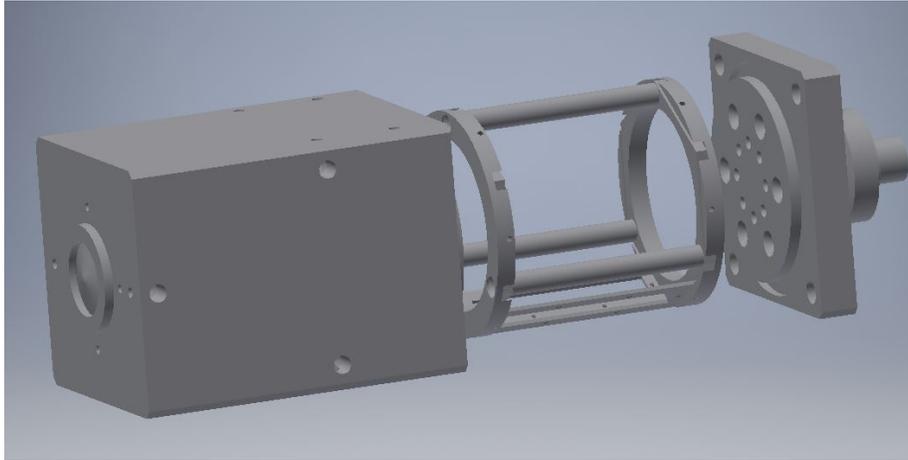


Figure 3: Exploded CAD-drawing of the ion guide

3.2 Materials

When the geometry was up and running, the next step was to set up the materials. Since it is a helium flow, helium was used as material. There was no need to define the box, because the material it is made of (aluminium) does not affect the flow.

3.3 Physical models

After the geometry it was time to decide what physical models to use. It was concluded that "laminar flow" would be the best approximation of the helium-flow. "Particle tracing for fluid flow" was also chosen so that the fission products can be traced as they were evacuated by the helium flow. An important part about the physical models was where it should be applied, the boundaries selected for this was the inlet and the outlet. The domains selected for this was the cylindrical middle of the ion guide and the narrowing cylinder leading to the outlet. COMSOL can decide what happens at the edge of the chosen model with the function "walls", because of this it is not necessary to apply the two models to the rest of the body, because it would only make it more difficult to compute.

As mentioned, COMSOL can combine multiple physical models to solve more complex problems. To combine the laminar flow and the particle tracing, a

function was used called "drag force", this simulates the drag force created by a stationary particle inside a fluid flow.

3.4 Tools in COMSOL Multiphysics

There were a couple of tools in COMSOL that turned out to be extremely important and well-fitted for tracing particles in a gas flow. The first and perhaps most important of them was "Cap Faces". With Cap Faces, the user selects two edges of the geometry, the edges must form a, preferably circular, loop. COMSOL then defines a domain based on what these two edges encloses. This was very helpful, to be able to define the inside of the geometry as a domain where the helium flowed. Before that, the inside was just considered void and could not be defined.

A second tool that really helped during the later stages of the task was "Release", which was a tool that followed with the physical model "particle tracing in fluid flow". It randomly places a specified amount of particles in the domains you select. It places them in such a way that they are not in contact with each other or the walls. The user can assign properties to the particles, and the properties of Iodine-135 and Zirconium-100 were chosen. It is not possible to run one simulation with more than one kind of particle, so two simulations had to be done in order to compare the two. The combination of the physical models and this tool allowed us to simulate the scattering of fission products over the geometry, and the helium transporting it.

3.5 Mesh

The next step was the mesh. Meshing is the method of expressing your geometry in many small elements, usually triangles. COMSOL calculates the boundary conditions of each small triangle to form the larger picture. There are options to customize the mesh or let COMSOL build one based on your geometry. If COMSOL builds the mesh there are 9 different orders of accuracy. The orders range from extremely fine to extremely coarse (a total of 9 degrees). The difference between the orders is the amount of elements, the larger the amount, the better the approximation.

3.6 Study

Once the mesh was in place you select a study that matches the physical models chosen. The study used for the laminar flow was stationary since it was not time dependent. For the particle tracing a time dependant study was used for it to be possible to track the particles as they moved through the geometry. The next thing was to compute the simulation. The time it takes for the solver to compute the simulation depends mostly on the meshing. After a simulation is complete there are options to plot the results for analysis or export the data for other uses.

4 Results

Figure 4 shows the first simulation. Figure 5 shows the evacuation paths of 100 particles, and figure 6 shows the evacuation time of 1000 particles. The reason why there are fewer particles in figure 5 than in figure 6 is because 1000 paths made it hard to distinguish both patterns and single paths.

Figure 7 shows a simulation where the particles get stuck if they hit a wall inside the ion guide. An average evacuation time was calculated in MATLAB with the data from figure 8. Figure 8 shows the evacuation time for Iodine-135 and Zirconium-100. The average evacuation time was 0.1176 seconds for Iodine and 0.1170 seconds for Zirconium. The median time was 0.0803s.

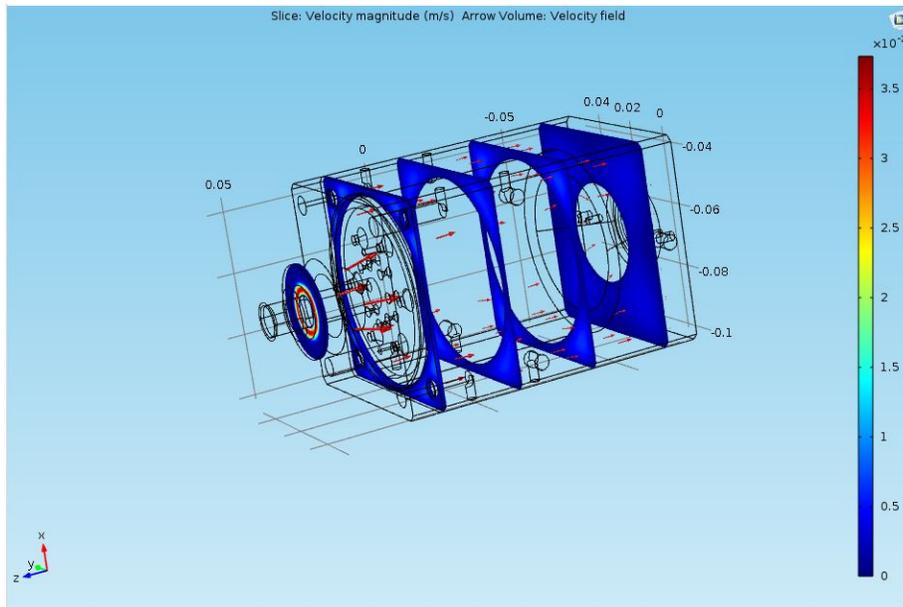


Figure 4: The first simulation, the flow runs in the walls of the ion guide instead of through it. The arrows shows the direction of the velocity field and the bar to the right shows the velocity in m/s

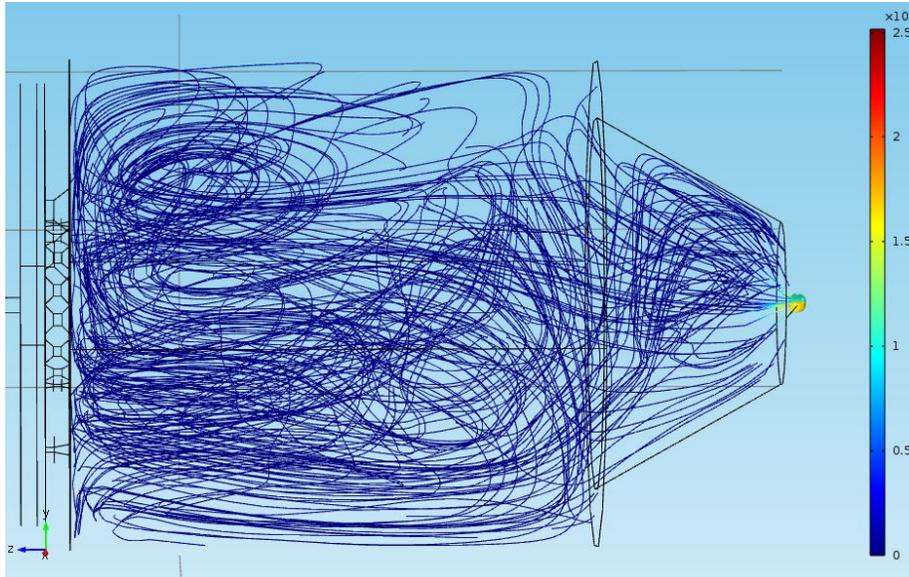


Figure 5: The paths for the Iodine-135 when they are affected by the flow seen at $t=1$. The bar to the right shows the velocity for the particles at the outlet in m/s.

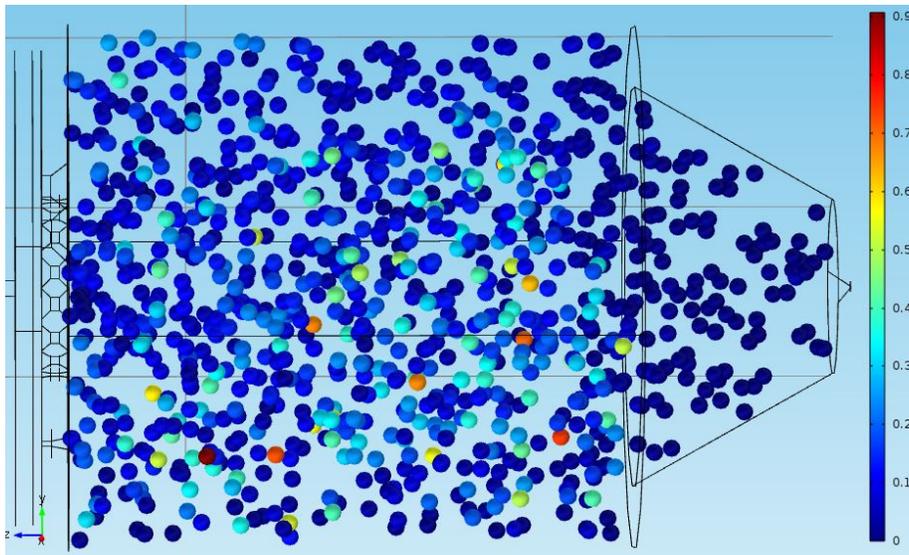


Figure 6: Evacuation time for 1000 randomly placed Iodine-135 particles seen at $t=0s$. A blue particle has a lower evacuation time and a red has a higher evacuation time. The bar to the right shows the evacuation time in seconds

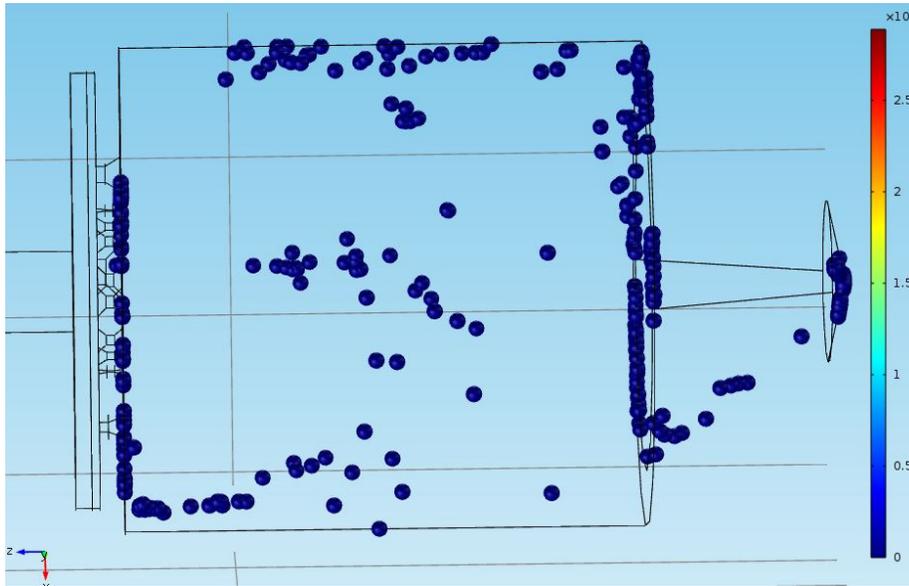


Figure 7: Shows where 1000 Iodine-135 particles get stuck in the geometry

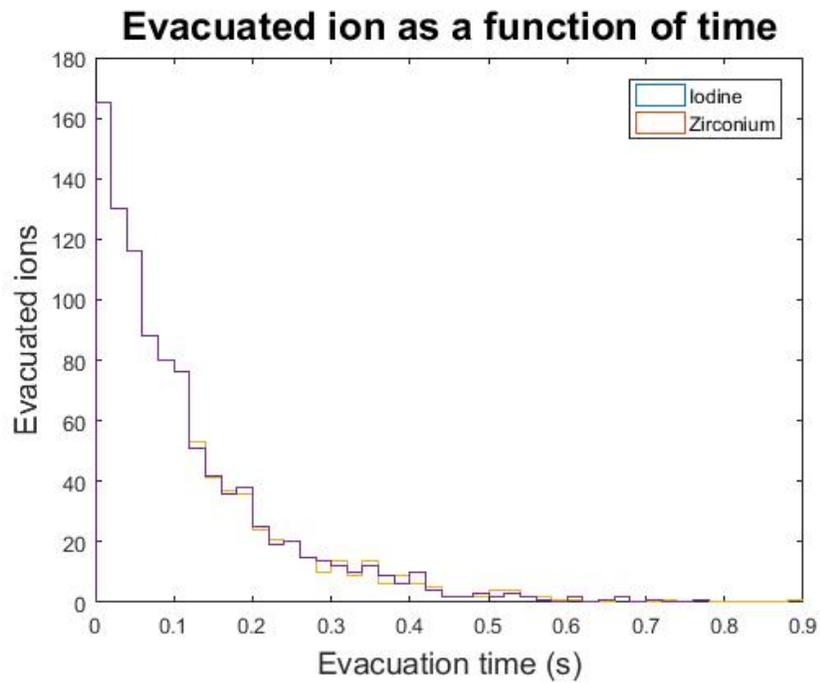


Figure 8: A histogram which compares the evacuation time of the Iodine-135 and Zirconium-100 isotopes.

5 Discussion

5.1 CAD schematics

There were a few problems at first when working with COMSOL. The first one was experienced when trying to implement the geometry from Autodesk Inventor. Apparently the latest COMSOL release was not installed on the university computers so it was not compatible with the latest Inventor release. This was quite easily resolved by saving the Inventor schematics into .stp files which are a common CAD-type file.

The next challenge was probably the most difficult one. Since COMSOL uses domains to apply physics, the geometries need to be solid for it to create a domain. So if there is a chamber filled with air for instance you make the whole chamber solid and then specify the inside of the chamber as air. This seems obvious in hindsight but was far from it with only a couple of days practice. The COMSOL videos was not really helpful here either, since they were very thorough they always built their own geometry. Because of that they already made it a solid and never really cared to explain why it was necessary. An attempt was made to solve this by adding two disks in Autodesk Inventor to close the inlet and outlet. A simulation was made with this attempt, and that result can be seen in figure 4.

5.2 The physical models

Laminar flow was chosen as model of the flow. Another option would have been to go with some form of turbulent flow. Inside of the ion guide arguments can be made that a turbulent flow is a more appropriate candidate. However the path to the inlet is a long straight tube, and having turbulent motion here would make the velocity just before the gas diffuser inaccurate. This will however remain as an unanswered question, that it is possible to get a more accurate approximation with the use of another fluid flow. It was also considered using "structural mechanics" to get proper interaction between the gas and the ion guide, which was made out of aluminium. It turned out that "structural mechanics" was used to study stress on geometries rather than interaction such as flow around objects or bouncing particles, so it was not used. Particle tracing was used because it was the only model which allowed us to trace particles in a fluid flow.

5.3 First simulation

Figure 4 shows how the gas flows through the walls of the geometry and finally to the outlet. With the result from this simulation it became clear that one needed to fill the entire geometry to run a correct simulation. Since the schematics are built with walls as solids and the holes as hollow(as one would expect), theoretically an inverted model could be used in COMSOL. The size of the walls does not matter in the simulation as long as the helium flow stay inside

of them. This would have worked in this case but it seemed like a complicated solution to change the entire schematic. Later on, the tool "cap faces" was found. Cap-faces closes holes and defines the volume inside as a domain. The geometry was now solid with the original schematics. But now a problem with the original schematic arose, apparently the inlet goes straight into the gas diffuser, but there was not any room for the gas to spread out when it hit the diffuser, it just hit a wall and got stuck. To solve this, a disk was placed so that it filled the 3mm void between the end of the inlet and the diffuser. This allowed the gas to spread and enter the diffuser. The reason cap faces did not work here was because there were no holes to close, there were simply no holes at all.

5.4 Meshing

One of the biggest problems during the work was to get the mesh right in COMSOL. Just getting the program to mesh the whole geometry could be problematic since the CAD-files contained some really narrow edges and boundaries and symmetrical difficulties. However a coarse mesh smoothed out the edges and allowed for a quick simulation. A finer mesh would of course lead to a better solution, but far longer simulation times. Since the only access to COMSOL was on the university computers there was not an option for over-night simulations. Another issue was that the solver converged for coarser meshes, but not for finer. No good explanation was found for this phenomenon, a forum post on COMSOL showed that the problem exist, but no clear answer was given.[5] Due to the fact that the solver converged and a good result was given, the problem was left unresolved and the project moved forward.

5.5 Results discussion

Every run in the results are done with the particle properties of I-135. Except for the run when the comparison in figure 8 was made.

Figure 4 shows the first simulation that COMSOL managed to solve. However, the flow only runs through the walls of the ion guide, and not through it. This is because the insides of it were not defined as a domain. A bad simulation, but it made us realise more about how the program works and especially that the insides of the ion guide had to be defined.

In figure 5 the paths of the particles as well as the velocities are shown. The paths are almost constantly blue due to the high outlet velocity. At the outlet the velocity reaches 2500 m/s but has an average velocity of approximately 1500 m/s. The big difference between the velocity inside of the ion guide and the velocity by the outlet is reasonable due to the pressure differences and the very small outlet diameter.

Figure 6 shows each particle's evacuation time before they started to move ($t=0$). This way it is possible to spot any areas with higher/lower evacuation

time. Near the outlet it is quite clear that the particles has a lower evacuation time then the rest of the geometry. For the middle of the ion guide the evacuation time is spread evenly and nothing clear can be said of different pockets with higher/lower evacuation time. Figure 8 was plotted with data extracted from figure 6. With this data an average evacuation time was calculated, and it was 0.1173s. A measurement inside the IGISOL facility suggest an evacuation time of 0.250s[3]. An average evacuation time of 0.1173s is reasonable because the evacuation time of 0.250s is from the inlet to the outlet, while the particles in the simulation are evenly distributed through the geometry.

In reality, the particle's are charged, and when they touch the aluminium walls they get stuck. So, in figure 7 a simulation was made to see how many particles out of 1000 get stuck in the geometry. 152 out of the 1000 particles exited the ion guide, the rest got stuck. This simulation gives a more realistic model, but since there are millions of particles from the fission, a simulation in which less than 1000 particles evacuate is very unlikely. It is difficult to make any conclusions about the comparison of different isotopes in figure 8, the difference was very small. So small that other forces that was neglected in the simulation would create a margin of error bigger than the noticed 0.006 seconds.

6 Conclusions

COMSOL Multiphysics was easy to learn and understand, learning an entire new program in just a couple of weeks seemed like quite a task, but thanks to the great help from their vast collection of tutorials it was not long until some basic simulations was done. The particle tracing was not planned from the start, because it was not considered possible. The idea came later on, and the results were really good.

No clear pockets of higher or lower evacuation time were found in the ion guide, this means that the gas diffuser spread out the gas evenly.

The difference between the two isotopes evacuation time were too low to make any conclusions about their size and weight having any effect on the evacuation time.

If someone were to continue this project some questions are left unanswered in this report. One could change the flow from laminar to turbulent flow, for a better fluid flow approximation. Or maybe molecular flow which would bring in electromagnetism amongst the particles. This could lead to a better particle tracing approximation. If one would have more time or a better computer, simulations with 100 000 and more particles could also be an option, as well as creating finer meshes for the simulation.

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