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**Implementation of a flexible, open-source platform for ion mobility spectrometry**

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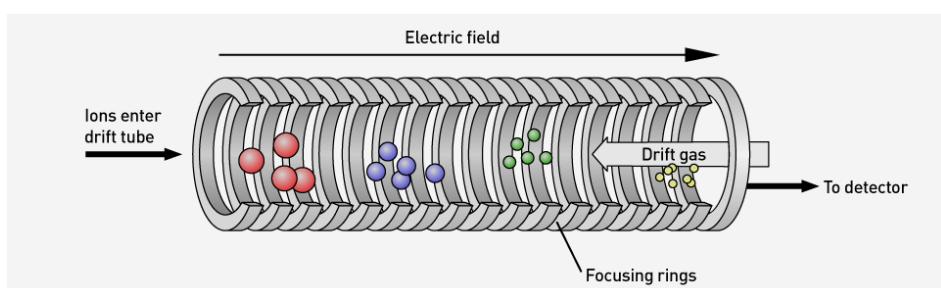
## 1 Introduction

The main objective of this project is to make an Ion Mobility Spectrometer. Ion Mobility Spectrometry (IMS) [1] is a method of conducting analytical research that separates and identifies ionized molecules present in the gas phase based on the mobility of the molecules in a carrier buffer gas. The IMS is a Time of Flight (ToF) sensor: it works by ionizing the sample and accelerating it through an electric field created by a series of strongly charged electrodes (11.5kV). The ToF of the ions is proportional to their mobility, which in turn is related to their size and shape. By comparing the mobility of the ions in the sample with those of known substances, the IMS can identify the presence of specific chemicals.

The goal would be to be able to analyze molecules that we would provide using a syringe at the front of the IMS.

The aim of this project is to prototype and test a low-cost IMS system that utilizes an easy-to-assemble IMS. Moreover, the open-source aspect is an important part of this project. Indeed, the built IMS will be part of a bigger project: it will be used to detect the chemicals present in an open-source bioreactor in Cali, Columbia, that has been built by the association Hackuarium (based in Renens). The bioreactor is currently in use, and one of its goals is to help local population to analyze wastewater. The research is based on a paper, “implementation of a flexible, open-source platform for ion mobility spectrometry” [2] published in 2018 by Tobias Reinecke and Brian H. Clowers.

There are numerous applications for IMS and it has the main advantage to work at atmospheric pressure (in contrast with mass spectrometry that requires most of the time 10<sup>-3</sup> torr) that would make it compact and affordable.



**Figure 1:** Schematic of the basic principle of an ion mobility spectrometer.[3]

## 2 Overview

Main parts of the IMS :

1. **Desolvation zone** : Insert and ionization of sample. Electrospray ionisation (ESI) [4]. Advantage: one can insert the liquid sample and ionize it through the same needle. Limitation : 5kV voltage source, 100uL/min flow rate through the needle.

Contains : Needle with sample to analyze; first part of the CAD casing (*Desolvation/28* or *Desolvation/29* and possibly *Extension*); first divider PCB; first half of the electrodes.

2. **Shutter** : Let the ions pass on command. Three grid shutter.

Contains : 3 very thin metal grids to put in between the middle electrodes (last desolvation electrode #29 and first drift electrode #30) of the IMS.



**Figure 2:** 1 of the 3 grids composing the ion shutter. The thickness of the grid is 0.1 mm and was produced in a photo chemical etching process in the referenced paper [2].

3. **Drift zone** : Acceleration of ions. Made by multiple electrodes connected to different voltages with the aid of a voltage divider. Limitation : 11.5kV voltage source.

Contains : Second part of the CAD casing (*Drift/28* or *Drift/29*); second divider PCB; second half of the electrodes.

4. **Detection** : Faraday plate. Transconductance amplifier converts the tiny ion current into a reasonable tension. Limitation : The current-to-tension AOP must be with very low bias current, and low noise (hence expensive).

Contains : Target CAD casing (*Cible*); target/Cible PCB; amplifier PCB.

5. **Monitoring** : A/D converter.

Contains : Microcontroller chip.

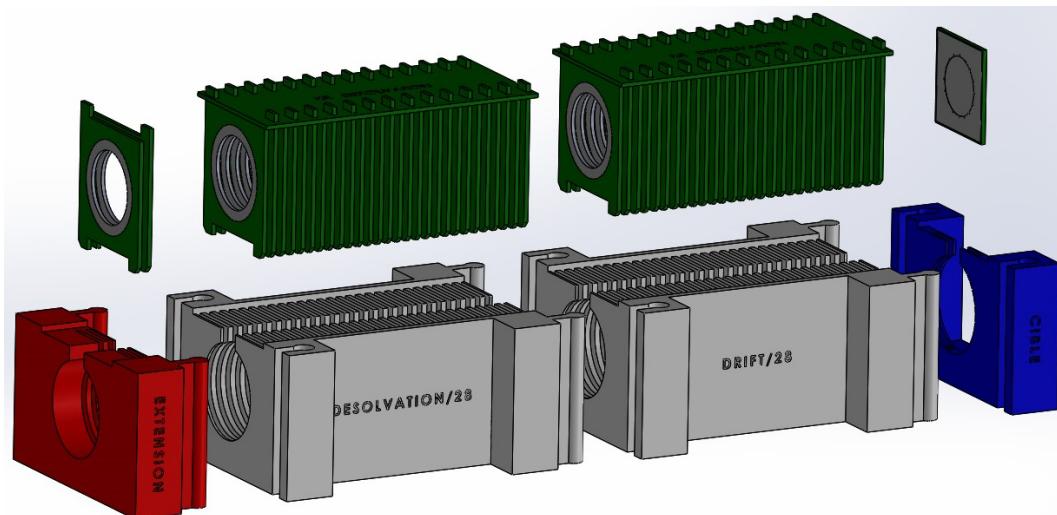
### 3 Current state

#### 3.1 CAD

The casing plays an important role in the reliability of the results. Inserting the electrodes in a box ensures that there is a regular space between them and that they are well aligned, producing the most uniform electric field possible. In addition, a modular casing has been designed so that parts can be tested separately and, in the future, other modules can be implemented according to the IMS needs, without having to change the entire design. Finally, it's important to optimize 3D printing and make electrode placement straightforward. Since the design is printed in PETG and the walls between the electrodes are only 0.8mm wide, the casing can easily break when the electrodes are handled. Also, because of the hole passing through the design, the print requires a lot of support that has to be removed. To overcome both these problems, a slit on the top has been created as shown on figure 4.

##### 3.1.1 CAD V2 (printed)

Here is shown the V2 version of the CAD, which is a simplified version to test for the target. It lacks a way to implement the grids (3-grid ion shutter and aperture grid) as well as a backside gas chamber for the target. It is currently printed and assembled, with 28 electrodes per zone (plus potentially 2 more in the extension if needed, to get 58 electrodes).

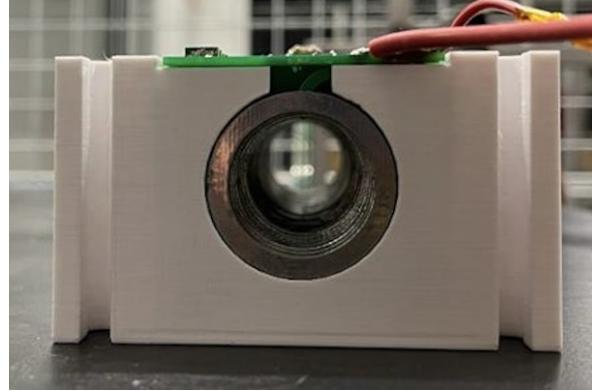


**Figure 3:** CAD of the current design of the IMS (V2). On the right, the 2-electrode extension section, followed by the desolvation section, then the drift and finally the target.

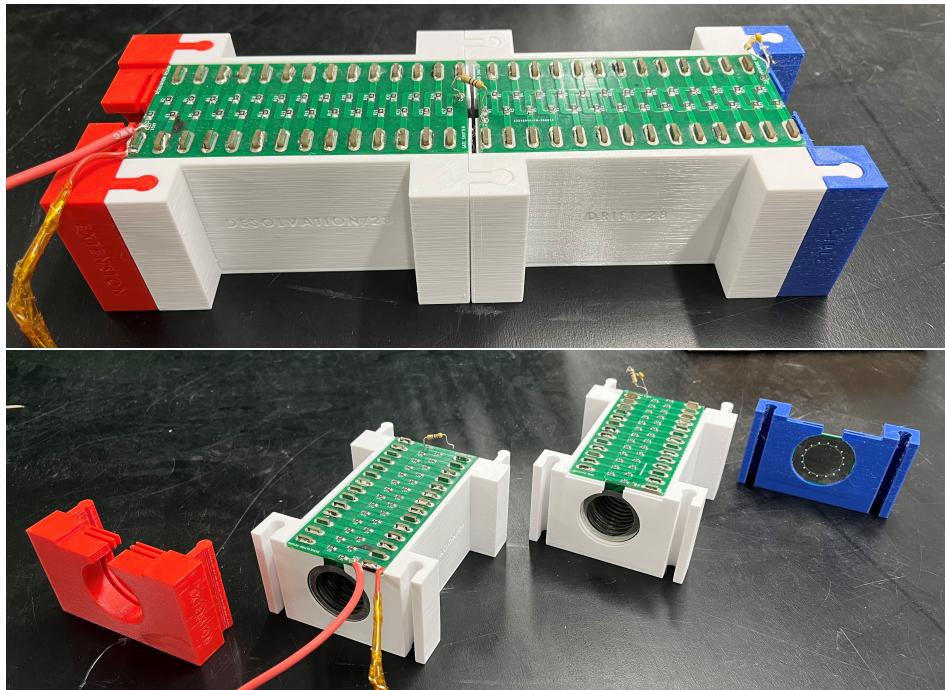
For the moment, the 4 parts shown on figure 3 have been printed :

1. **Desolvation zone** : this section contains 28 slots, meaning 28 electrodes can be placed. Every 2 electrodes have the same distance in between them, i.e. 0.8 mm. This ensures that the electric field is linear and continuous throughout the whole device.
2. **Drift zone** : this section also contains 28 slots. It is the same casing as the desolvation zone and has the same purpose.
3. **Target (also named "cible")** : this section contains a slot to insert the Faraday plate and a pocket to hold the amplifier PCB. It's important to keep the distance between the amplifier and the PCB as short as possible to limit noise.
4. **Extension** : this section contains 2 slots in order to increase the number of electrode if needed.

The parts containing the electrodes have a through-hole in the middle, revealing only the conductive part of the electrode. And they are attached to each other by a complementary design to ensure a good grip between them.



**Figure 4:** Picture of the casing with the electrodes inserted. The hole in the middle of the casing is big enough to reveal the conductive part of each electrode. In addition, the opening above the circle to facilitate 3D printing is visible.



**Figure 5:** Pictures of the current IMS with the 4 separate printed parts. The first part on the left in red is the extension, followed by the two white parts containing the 28 electrode slots, the desolvation and drift regions respectively. The PCBs and electrodes have been placed here. The blue part on the right is the target part, with the Faraday plate inserted. The photo illustrates the modularity of the IMS casing.

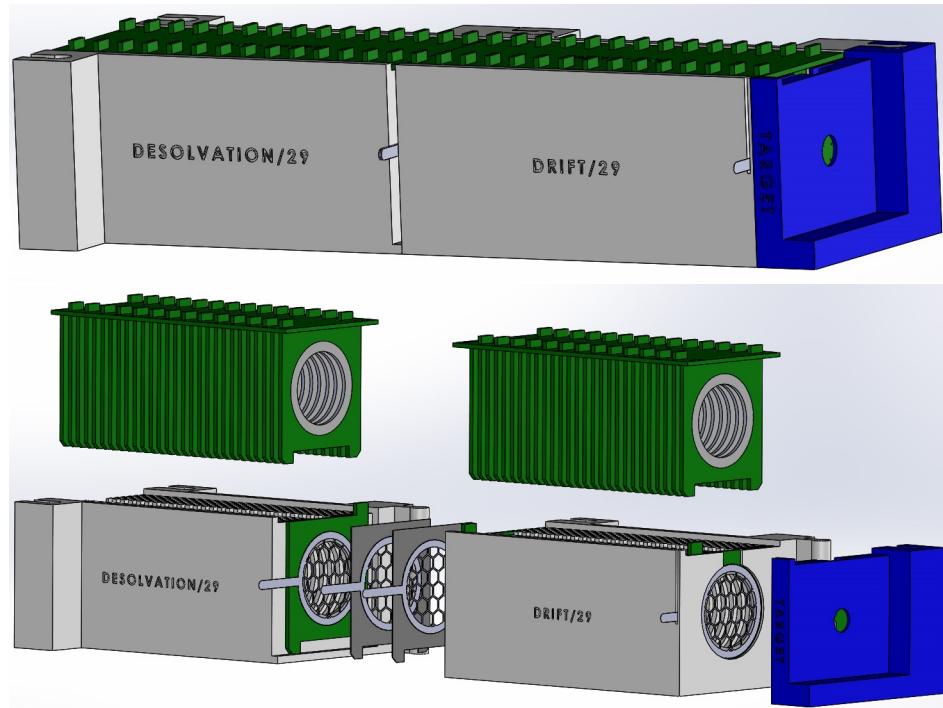
### 3.1.2 CAD V3 (not printed yet)

Here is shown the model of the V3 version of the CAD casing. It is a revised version with room to accommodate for the 3-grid on shutter, the aperture grid and the gas chamber for the target. The desolvation and drift regions have here 29 electrode slots each (the extension is thus not needed here and the ESI needle can be put in front directly).

The *target* part has a hole on its top to let a Teflon tube of buffer gas (air or nitrogen) flow into the gas chamber, as well as a small hole on its back to connect an SMA connector (the objective is to have the shortest path possible between the target and the amplification, thus reducing noise and

unwanted disturbance on the output signal).

Room has been made at the end of the *desolvation* part to accommodate for the 3-grid ion shutter. The same has been done for the aperture grid at the end of the *drift* part.



**Figure 6:** Pictures of the IMS V3. The figure illustrates the added modules of the casing.

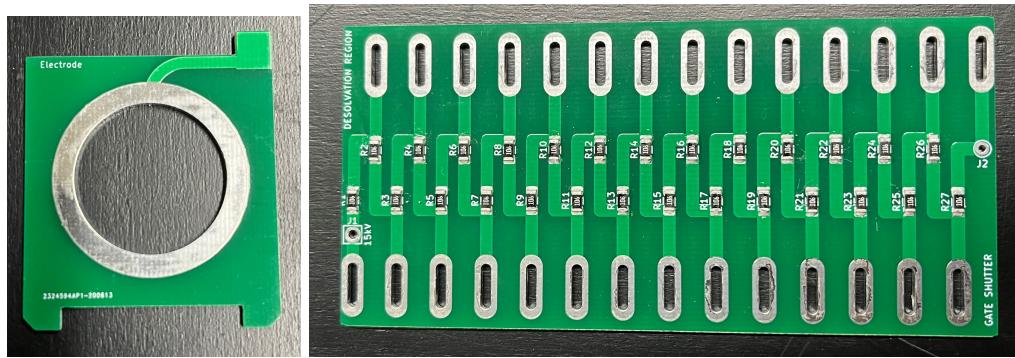
### 3.2 Electronics (PCBs)

#### 3.2.1 Dividers, electrodes and target

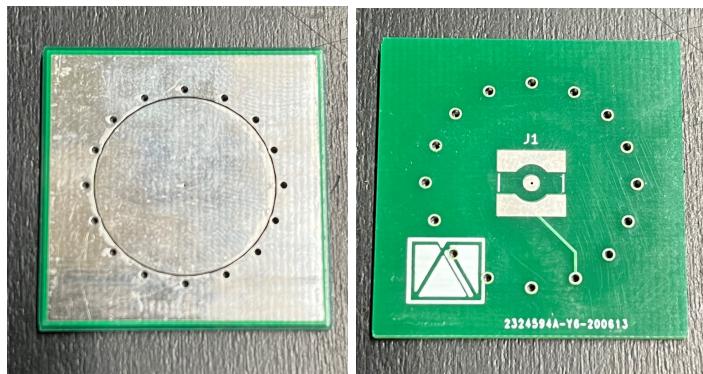
The dividers, electrodes and target PCBs represent the core of the IMS. The dividers are simple voltage dividers that will set the right potential to the electrodes throughout the IMS, creating a continuous potential gradient that will accelerate the ions.

The target is then placed at the end of the device, where the ions will hit it, creating a tiny current that can be processed and analyzed to be able to tell which molecule is inside the sample.

These PCBs are pretty straightforward, and their specifications rely mostly on their shape and size. The dividers contain only  $10\text{ M}\Omega$  resistors and holes where the electrodes can be slotted in. The electrodes are squared with holes in the middle with an exposed electrically conductive ring that, when set to the right potential, will accelerate the ions passing through. Finally the target is a small squared Faraday plate PCB with an open conductive surface on one side, facing the acceleration tunnel, and a connection pad for the amplification stage on its backside. 12 small holes can be seen to allow the drift gas to come in front of the target.



*Figure 7:* PCB of one electrode and of the desolvation region (mounted with resistors).



*Figure 8:* PCB of the target/cible.

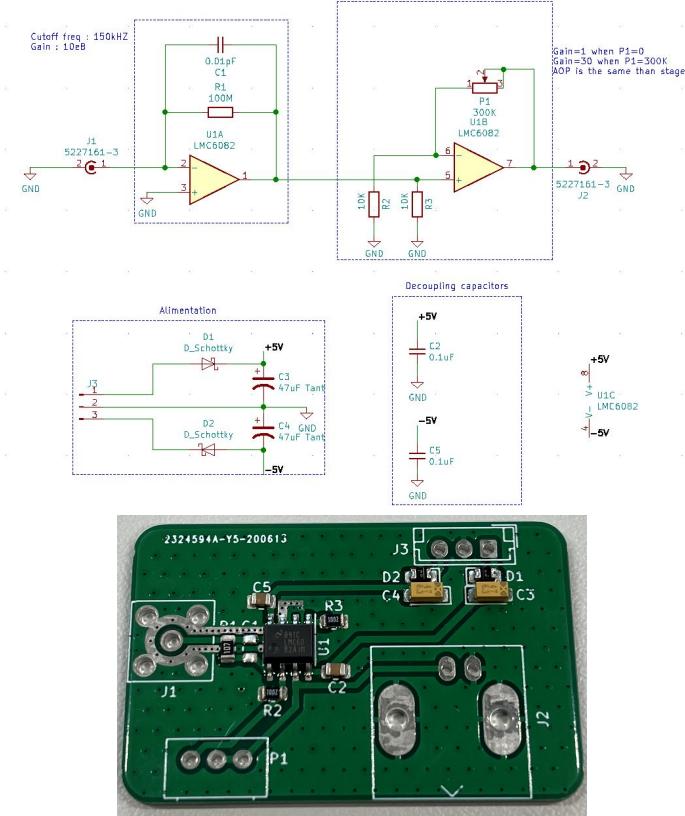
#### 3.2.2 Amplification stage

The amplification PCB is a more difficult PCB. The shape and size don't matter here, but there are many relevant specifications to be accounted for.

First, this PCB is a [transimpedance amplifier](#) [5] that will transform the tiny current coming from the target (scale is approximately a tenth of a nA) to a readable voltage (scale around 0.3-0.5 V). A big gain in a transimpedance amplifier also amplifies the noise present in the signal. With a very big resistor ( $100\text{M}\Omega$ ) like we have here, the problem is to avoid amplifying the noise to the point where our signal becomes unreadable. A very precise medical operational amplifier is thus needed with very low

bias current and low noise (which can be expensive). Lastly, the PCB should be as close as possible to the target to have the shortest signal path and limit the noise.

The amplification PCB is then composed of a transimpedance stage (100MΩ resistor) and a voltage follower stage (with an additional gain of 300-500 via a potentiometer for instance).



**Figure 9:** Schematic of the amplification PCB, with the two different stages highlighted. PCB, with a dual operational amplifier for the two stages. The SMD components are mounted on the PCB, and lacks only the connectors and potentiometer.

This PCB can be tested by applying a voltage of 1V over a 100 MΩ resistor at the input J1, thus creating a current of 1nA, and checking if an output voltage of 1V can be measured when the voltage follower doesn't have any additional gain (potentiometer is shorted). This was tested but unfortunately the C3 capacitor was grinded, probably resulting from a bad set up (component is easy to replace, the rest is still working as connections were tested).

The equivalent can be in theory tested on a breadboard but the bad/longer connections of the coupling of jumper cables on a breadboard could add a lot of noise and disrupt the detection of the signal.

### 3.2.3 Link between the Faraday plate and the amplification stage

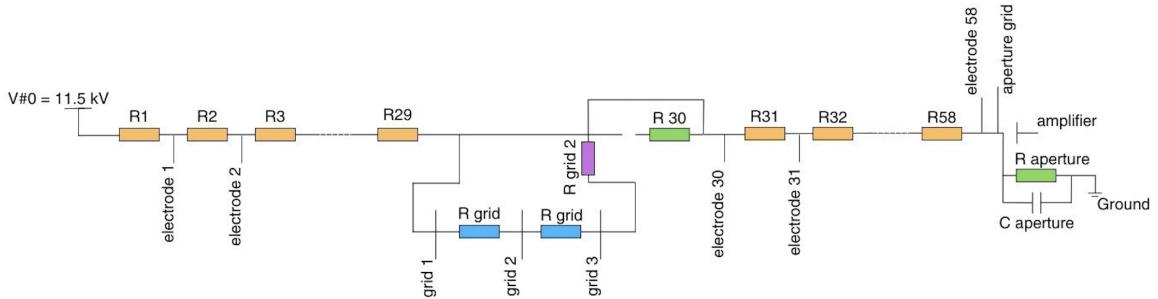
In chapter 3.2.2, we mentioned that the PCB should be as close as possible to the target to have the shortest signal path and limit the noise. Two options are available :

1. **SMA connectors** : In the paper, they suggest to use an SMA connector to connect the back of the Faraday plate to the amplification's PCB. This way of connecting the two PCBs allows for a gap between them. This can be useful for implementing a drift gas supply but would potentially add noise to the signal. In our case, since the current detected is only of the nA order, noise is not negligible and would therefore be a problem.

2. **Direct soldering** : Another option is to solder the back of the target directly to the amplification PCB. In this case, we would have to find another solution for the drift gas input (although at this stage of the project, we are not using one). However, this would considerably reduce noise. Soldering can be complicated because of the positioning of the connections. One possibility would be to apply solder paste to the back of the target, which would then be placed in a 3D printing mold. This mold would enable the two PCBs to be properly aligned. The amplifier PCB could then be placed correctly. Since the mold is made of plastic, it cannot go into the oven, which is the last step in the soldering process. The PCBs must therefore be carefully taped in this position with non-conductive tape.

### 3.3 Electronic circuit

In order to better understand the overall electrical diagram and the paper's resistance choice, an equivalent electrical diagram of the IMS from the first electrode to the amplifier is shown on figure 10.



**Figure 10:** Equivalent circuit.  $V_0$  is the voltage at the input, the resistances in orange are the ones on the divider PCB, and the resistances in blue and violet are the resistance of the grid shutter.

With :

$$R_1 = R_2 = R_3 = \dots = R_{58} = 1M\Omega$$

$$R_{aperture} = 500k\Omega \quad C_{aperture} = 0.22\mu F \quad R_{grid} = 150k\Omega \quad R_{grid2} = 700k\Omega$$

$$\text{gate opened} = \begin{cases} V_{grid1} = V_{#29} = 5.8kV \\ V_{grid2} = \frac{V_{grid1} + V_{grid3}}{2} = 5.75kV \\ V_{grid3} = \frac{V_{#29} + V_{#30}}{2} = 5.7kV \end{cases}$$

$$\text{gate closed} = \begin{cases} V_{grid1} = V_{#29} = 5.8kV \\ V_{grid2} = \frac{V_{grid1} + V_{grid3}}{2} + \text{small} = \langle 5.78 - 5.83 \rangle kV \\ V_{grid3} = \frac{V_{#29} + V_{#30}}{2} = 5.7kV \end{cases}$$

And :

$$\text{small} = \langle 30 - 80 \rangle V$$

Thanks to those equations, we see that when the gate is closed, the potential of the second grid is higher than when it is opened. In the paper, they recommend adding 30 to 80 V (referenced to "small" in the equations) to stop the flow of electrons. According to the calculations, a value of 50V or higher would result in a reverse electric field and effectively close the gate.

These calculations are based on the paper's values, not those of the current prototype. For the moment, the resistors on the divider PCB are  $10\text{ M}\Omega$ , designed to reduce power consumption. But this does not seem necessary, since with  $1\text{ M}\Omega$  resistors, power consumption is already only 160 to  $200\text{ }\mu\text{A}$ , and changing the resistor of the dividers would also mean adapting the other resistors of the circuit.

### 3.4 Nafion membrane

A Nafion membrane is commonly used in IMS to separate ionized gases from other gas and prevent interference with results. Here are some of the membrane's properties:

1. **Ion selection** : the membrane selects the ions of interest for measurement, while rejecting other non-ionized or uncharged gaseous species.
2. **Impurity removal** : the membrane can remove impurities from gases. It is therefore useful for eliminating contaminants that could interfere with results.
3. **Gas separation** : the membrane only allows high-mobility gases to pass through. It therefore prevents low-mobility gases (noble gases for example) from entering the drift zone and interfering with the results.

In our case, the membrane is mainly used for ion selection. In fact, it allows us to have only the species of interest in our spectrometer, and therefore more reliable results. The membrane is placed between the needle and the first electrode.

Our membrane specifications:

Model: Nafion 117

Thickness: 183  $\mu\text{m}$

Density: 360  $\text{g/m}^2$

Conductivity: 0.083  $\text{S/cm}$

Exchange capacity: 0.89  $\text{meq/g}$

Size: 40 mm diameter circle

## 4 Conclusion

This is a difficult multidisciplinary project with many different skills needed, such as : understanding the physics behind the working principle of the IMS (gas separation, ion acceleration and molecule drift, Electrospray Ionization), Computer Assisted Design for the 3D printed casing, electronic circuitry and high voltage supply handling (10-15kV), PCB design and potentially programming for the monitoring of the microcontroller to process the signal and analyze it. A lot of different parts of the IMS are built and work in principle in a stand alone fashion, but bringing them together for a fully working device is an intricate task.

The electrodes, dividers PCBs and target PCB are made and their connections are tested and working. The CAD 3D casing can accommodate them well, but the printed V2 version currently lacks a way to insert the 3-grid ion shutter gate. The V3 version on how to overcome this issue is ready for implementation, but without the physical grids themselves we cannot test it.

The target is made and ready and needs only a way to implement a sealed and controlled injection of a buffer gas on its back, in addition to a way of connecting it (probably SMA is best) to the amplification PCB with a path as short as possible (as discussed earlier).

Lastly, once everything before the microcontroller works, the monitoring of the signal needs to be done with a program capable of recognizing the sample from its spectrometry/signal. It can then say which molecules are present in the sample. The MCU must also controls each part of the IMS to synchronize the needle, the opening of the ion gate (<50  $\mu$ s ion packets) and the reading of the signal.

## References

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