Breathing New Life into a Legacy: DIY Revival of an API 2000 Tandem Mass Spectrometer

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How this started

"Applications and techniques of high, ultra high and extreme vacuum technology - An introduction to vacuum technology" was the title of my pre-scientific paper written in high school. While writing this essay, I built and automated a high vacuum system at extremely low cost by buying used and often broken equipment from second-hand markets and repairing it.

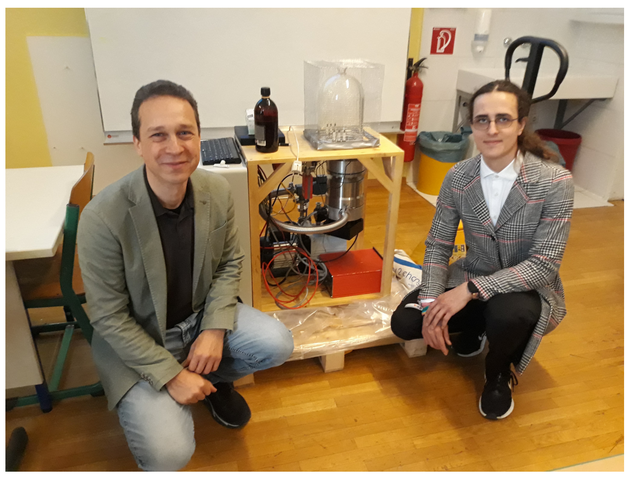


Figure 1. Pre-scientific paper presentation

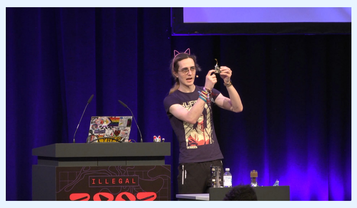
Getting the API2000 Ready

Before starting my new API2000 up for the very first time, some tasks were on my todo list:

- **Power Supply**. After many operating hours the switch mode PSU did not want to start up, all it ever needed was a good clean and it is working fine again.
- **Interface Heater.** Firstly I suspected the temperature control board on this one, but turns out the interface heater traces on the flex PCB were just rusted through, again an easy fix.
- **Software**. A copy of Analyst was needed to control this mass spectrometer.
- **A lot of learning** ...

... A lot of learning

I knew enough about vacuum systems and had enough hands-on experience with that, but using this new device was another difficult endavour. So the first big step was to learn about quadrupole mass spectrometers and how they function with a focus on my specific device. This then turned into a talk that I gave at 38c3 and can be watched here:



Interface Heater

The repair on the inteface heater was simpler than expected. After disassembling the vacuum interface, a lot of corrosion was visible on the flex PCB and the heater was destroyed.

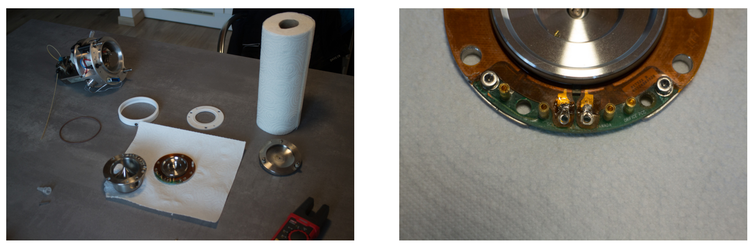


Figure 2. Interface heater repair

The fix was to scrape the solder mask off of the remaining traces and bridge the corroded metal. The interface heater has been working since then without any issues.

Software

Following extensive research on various forums, a person who is still active in the forum was identified. This individual was complaining about issues with Analyst 1.5.2, which included the API2000 as part of its supported hardware. Subsequently, an email was sent to them, enquiring about the possibility of obtaining a copy of the software. Following a period of back and forth communication, they went to the basement of their institute, powered up the Windows XP workstation, and proceeded to copy the necessary files.

The subsequent task was to locate the necessary hardware. Fortunately, I had the assistance of an individual with the relevant expertise: a retro computer enthusiast specialising on the MS DOS era to the Windows XP era. This individual possessed not only the ideal small form-factor PC for XP, but also the necessary GPIB card.

Math behind the stability in the quadrupole

With a few mathematical transformations and the assumption of a conservative force ($\vec{F} = -c \cdot \vec{r}$), one can easily write the equation of motion as a second order alternating differential equation, and with some further substituation it can be brought into a form known as "Mathieu's Equation".

$$\frac{d^2x}{d\tau^2} + (a + 2q \cdot cos(2\tau))x = 0$$

$$a = \frac{4qU}{mr_0{}^2\omega^2}, q = \frac{2qV}{mr_0{}^2\omega^2}, \tau = \frac{\omega t}{2}$$

Numerical stability solver

Unfortunately, solving this equation is not an easy task. Most engineering books that cover mass spectrometers would immediately present the solution graph and proceed with its interpretation.

Firstly, it is imperative to acknowledge that, within this particular context, a solution to the equation is not a prerequisite. Instead, the objective is to ascertain the stability regions of the equation.

The objective was to implement the numerical stability solver autonomously, a task which was successfully completed. Consequently, some of the most aesthetically pleasing plots of Mathieu's equation stability regions that have ever been published in the literature are presented herewith with great pride. A talk on the profound mathematical principles is currently in the works. For further information, please refer to my **website**.

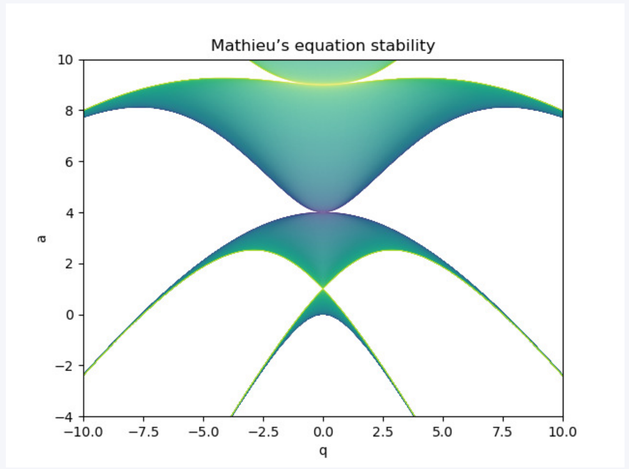


Figure 3. Stability of the Mathieu equation: white - unstable, colored - stable

The method implemented is known as "Hill's method solution".

First tests

Initial tests were conducted using two 10L nitrogen flasks, which were rapidly depleted, thereby validating the rationale for incorporating the nitrogen filter. Subsequently, a new issue emerged: the ionisation gauge **failed to power up**. Further tests with a multimeter indicated a loose connection at the filament within the tube as the likely cause. The resolution of this issue entailed charging a capacitor to 60V, establishing a connection between the gauge and the capacitor when it was in an open circuit state, and tapping the gauge against a surface. Spot welding the filament in place resulted in the gauge functioning optimally.

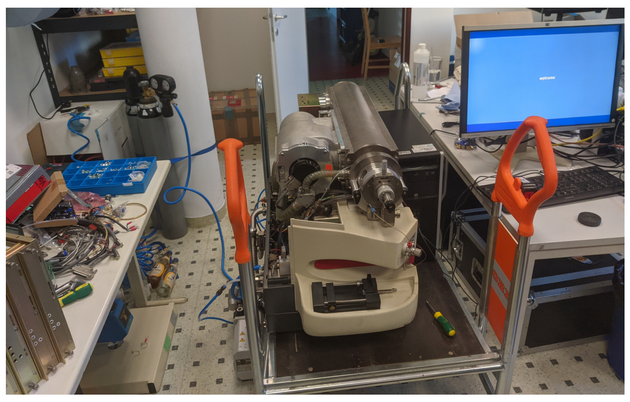


Figure 4. First tests

Following the rectification of the ionisation gauge, the mass spectrometer exhibited satisfactory functionality, thus indicating the viability of conducting a preliminary evaluation of its basic operational capabilities. Subsequent to the consumption of a coffee beverage, the decision was made to undertake a first functional test involving the direct injection of the coffee, in a diluted and filtered state, through the mass spectrometer. The objective of this experiment was to ascertain the presence of caffeine in the coffee sample.

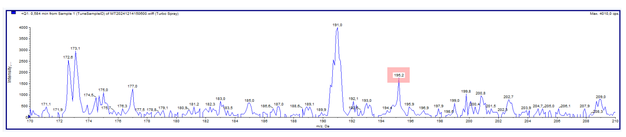


Figure 5. Q1 scan of coffee | +4.2 kV IS, 360 °C TEM, 5 min

The result was verified with a Q2 scan, with Q1 fixed at 195.2 Da. This process enabled the confirmation of the identity of the substance as caffeine.

Nitrogen gas supply

Buying Nitrogen was **too expensive** for the needed amount. After some research it was found that carbon molecular sieves can be bought cheaply from the far east. For the PSA[a] cycle two pressure chambers were needed with a volume of about 2L each. For this, old CO_2 fire extinguishers were used, as their pressure rating far exceedes the operating pressure of 8 Bar.

Figure 6. CMS[b] nitrogen filter

The analysis of the gas produced by the filter for quality purposes has not yet been conducted, due to the fact that my Balzers QMA 125 residual gas analyser is not yet equipped with all of its electronic components. Preliminary checks were conducted using electrochemical sensors to check for O2 concentration.

Upgrade to HPLC-MS/MS

Following the successful restoration of the mass spectrometer, the subsequent step was to integrate it with HPLC to make HPLC-MS/MS analysis possible. Utilising "sold as is" Shimadzu gear at a remarkably economical price in Vienna, I proceeded to procure autosamplers and pumps. I had previously repaired an UV/VIS detector, which I then utilised to verify the operational integrity of the HPLC equipment.

Following a more extensive search, the necessary controller was procured, and the requisite optical cables were constructed using Toslink plastic fibres and the necessary connectors from DigiKey. Thereafter, the setup was completed.

Figure 7. HPLC-MS/MS setup in my living room

Future work

1. **Mathieu's equation stability as an example of immense creativity in solving advanced mathematical problems**. A talk about the mathematics behind the stability of the quadrupole mass spectrometer.
2. **Blood analysis and measurement of hormone levels**. This will push the limits of what is possible with the API2000 instrument and may require a lot of tuning, cleaning and perhaps even modifications to the instrument.
3. **And so much more**... Regularly check my blog at gry.sh to follow my journey in science.

Special thanks

- **Martin de Wendt** - Sciex
- **Dickson Wambua**
- Everyone supporting me at **TU Graz**

[a] Pressure swing adsorption
[b] Carbon molecular sieves