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# Separation of contaminant species by TGA/MS in European and U.S. approaches to outgassing

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## ABSTRACT

Well-established procedures for the characterization of contamination during outgassing usually involve total mass measurements through quartz crystal microbalance (QCM). Recently, the addition of mass spectrometry (MS) measurements to these data has become more common. The combination of both high sensitivity QCM and MS data may lead to a better understanding of the physics taking place during outgassing contamination processes. The way to do so is to complement the basic measurements of total mass loss on QCMs by the identification of each species and the quantitative determination of each species contribution.

In a first characterization step, the thermogravimetric analysis of contaminants deposited on QCMs allows a partial species separation that helps exploiting mass spectrometry data. In return, these data permit a finer species separation. The key to these measurements is to obtain sufficient signal to noise ratio in the mass spectrometer. Though outgassing of space materials is not done the same way in Europe (multi-temperature steps, ECSS-Q-TM-70-52A) and in the US (isothermal, ASTM E-1559-09), both tests could be used to perform a first species separation, as reported here. Most species outgassed by a few common materials were identified (and quantified) through TGA and MS coupling. As reported in a companion paper, the knowledge of these species' spectra then allows the analysis of the MS data during the initial outgassing phase, determining the quantitative outgassing of each species and leading to the improved comprehension of the physical laws ruling outgassing.

**Keywords:** Contamination, outgassing, chemical species, species separation, mass spectrometry, thermogravimetric analysis, quartz crystal microbalance.

## 1. INTRODUCTION

Both the American and European dynamic outgassing tests, respectively based on ASTM-E-1559 standard [1] and ECSS-Q-TM-70-52A (cf standard [2], and some underlying theory from the 1980s in [3]), mostly rely on the measurements of deposits on Quartz Crystal Microbalances (QCM). These deposits, depending on the QCM temperature, are considered representative of the Total Mass Loss (TML) on cryogenic QCMs, or of Collected Volatile Condensable Material (CVCM) on warmer QCMs. Since most materials outgas several different contaminant species simultaneously, these deposits are a cumulative deposit, summing up the contributions of all chemical species.

Determining these cumulative deposits, at any temperature, is already very valuable, and most mission contamination budgets are consistently defined in terms of similar cumulative mass deposits per surface unit. Yet, ignoring the composition of a deposit in terms of its chemical species has several drawbacks. Since any QCM measurement corresponds to the cumulated masses of several species, when testing a theory, it must be compared to a sum of laws. Stated differently, these data must be fitted by a sum of physical laws. In practice this turns out to bring little constraint to the theoretical

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models under scrutiny. For example, concerning outgassing, a unique measurement dataset can equally be fitted by a sum of desorption laws (exponentials) or a sum of diffusion laws (Fick law solutions). Indeed, experience shows that only the outgassing rate of a single species gives enough constraints on its single outgassing law to determine which physics is involved. If, in a dedicated experiment, we are able to determine the outgassing rate of a single species, out of a single desorption law and a single diffusion law only one will allow fitting these data, telling us the physics at play. Determining this physics is the key to a realistic extrapolation of mission duration, to mission temperature history.

This is why we have been working for 15 years on what we often call “species separation”, meaning an experimental determination of the deposit or flux of each chemical species individually. These finer experimental data can also bring very valuable insights on other physics like the deposit dynamics and reemission, photo-catalysis, photolysis, etc. Older publications announced the working program [4] and first promising results [5] obtained by ONERA, in collaboration with CNES or sometimes ESA. Later activities dug into the physics of contaminant deposits and their reemission [6], species separation [7] or outgassing again [8][9][10]. More recently, JPL also joined the effort in that direction, and it was showed that processing existing ASTM-E-1559 data could also lead to species separation provided that good enough Mass Spectrometry (MS) data were collected during the tests [11]. Even though the American ASTM-E-1559 standard differs by some aspects (one long isotherm step instead of several successive increasingly warm steps, repeated with a new sample for several temperatures if needed), supplementing the QCM measurement of the cumulated mass by MS data is just as beneficial as for European VBQC-type dynamic tests.

With a companion paper, this communication reviews all these efforts, including also more recent results. The *in situ* method that has been developed for species separation approach is based on coupling Thermogravimetric Analysis (TGA) and Mass Spectrometry (MS). The principle consists in a first step in depositing contaminants on a QCM or a plate, then in a second step in reemitting this deposit by heating it at regular rate (1 or 2 K/min) to analyze the mass reemission rate but also individual partial pressures by MS. The data processing goes the other way around. The first processing step deal with the TGA/MS data (second step of the experiment). In good conditions, the TGA led to a good enough species separation, the molecular species being reemitted in separate peaks, at successive temperatures. In principle the MS gives the mass spectra of each species when it is being reemitted, allowing its characterization, and possibly its identification. The second processing step deals with the first outgassing step of the experiment. Once MS spectra are known for all species, MS data also collected during the outgassing phase allows tracking the behavior of their outgassing, hence their physics. And this is feasible both for the stepwise outgassing profile of ECSS-Q-TM-70-52A and for the longer isothermal outgassing of ASTM-E-1559, provided MS data are collected during the outgassing and the TGA with a good signal to background ratio.

This paper focusses on the first step of the data processing. MS and QCM data gathered during the deposit reemission (TGA) are analyzed to separate the contribution of different species, and possibly identify them in chemical species databases. Its companion paper [12] focusses on the second step of data processing: the determination of each chemical species outgassing law.

In the next section—still somewhat introductory—this paper reviews the main experimental campaigns and materials that were studied. The following section follows a different path and reviews all the key steps of the TGA/MS approach to species separation, namely measurement sensitivity, actual species separation by TGA and, finally, species identification thanks to their MS spectra. A conclusion, and perspectives of this still-to-be-developed approach, terminate this paper.

## 2. TEST CAMPAIGNS

The first material studied following our TGA/MS approach was the Scotch-Weld 3M™ epoxy glue EC-2216. Many experimental aspects had to be improved over time to reach a good signal level (and SNR). Due to the principle of contaminant transfer throughout a hot shroud as explained next in section 3.1, the suppression of any cold point was one of the challenges. At the end of the road, about half of the chemical species outgassed by the EC2216 could be identified [7]. Some fragments of their MS spectra could also be tracked during the outgassing phase (e.g.  $m/z = 91$  amu for toluene) and were shown consistent not with desorption but with diffusion law [10]. Another result worth noting was that the TGAs from QCMs at -75, -50, -25 and 0 °C respectively looked very much alike in their final warmer part (approximately above 0 °C), and only differed in their colder part, as if everything was similar except for most volatile species to have left the warmer QCMs (cf [5], Figure 21). This means that the presence of more volatile species did not affect the behavior of heavier ones in the deposit mixture in that case.

More recently, we started studying the outgassing of other materials, the other epoxy glue EC-9323-2 and the silicone paint MAP PNC. These results are still unpublished and are partly reported here. Globally, this other epoxy glue behaved similarly, with a reasonably good species separation by the TGA/MS method, which allowed identifying a large majority of the outgassed species (cf below) and their outgassing behavior (cf companion paper [12]). The silicone paint was a more difficult case, with many fragments seen in MS behaving similarly during the TGA, either because of poor physical species separation during the reemission during the TGA, or because many fragments are common to several chemical species.

In parallel, data collected during preexisting ASTM-E-1559 tests in possession of JPL were studied. Some had very small signal due to rather low-temperature outgassing, but some were usable [11]. Even though few reemission peaks were visible on TQCM TGAs, most of the times a species could be related to each peak and identified thanks to its (partial) mass spectrum, allowing its outgassing behavior to be studied. This success on standard ASTM-E-1559 test results gave good hope and confidence in this species separation method, which should prove even better in more specifically tailored experiments.

### 3. KEY STEPS OF THE APPROACH

Here, we review the important features of experiments meant to perform contaminant species characterization at chemical species level, not simply as a cumulated mass on a QCM. Let us first remember that the TGA/MS method relies on two successive processes:

- 1) the outgassing of contaminants from a source placed in an effusion cell, allowing the deposition of the outgassed species onto QCMs, possibly at different temperatures
- 2) the reemission, during heating of the QCMs at controlled rates (TGAs), of the deposited contaminants, which are then transported towards the mass spectrometer, allowing species separation and possibly identification

#### 3.1 Metrology

##### MS sensitivity

First, as it is a key instrument in the TGA/MS method, the mass spectrometer must fragment and/or ionize and count sufficient contaminant molecules for their output signal to raise above background level. That is to say that the partial pressure of each different species outgassed at an instant  $t$  must be high enough at the vicinity of the spectrometer to be transformed into electrons so that their signal over background level is high enough. This is currently done by two distinct ways, depending on the chosen approach.

In a first class of apparatus, such as the ones used in the U.S., the spatial proximity of the QCMs with the mass spectrometer allows good view factors between them. Only direct views between the QCMs and the MS are considered as all of them are placed in a cryogenic shroud. That is to say that any contaminant that does not reach directly the MS after being reemitted gets condensed on the shroud and is “lost” from the point of view of the experiment. One understands that to increase the signal, QCMs and MS must spatially be very close from each other, within a few centimeters. This complicates the first part of the experiment: the outgassing and measurement of TML and CVCMs. Indeed, if the QCMs must at some point face towards the MS, they must as well be able to collect the outgassed flux from the effusion cell, which mean that—as the shroud is at cryogenic temperature—they must have a good direct view of the effusion cell! This can be done by two manners: whether by allowing the rotation of the QCMs or by allowing close enough spatial proximity. In the first method, the QCMs face the effusion cell during outgassing, collecting the direct flux of contaminants; they then rotate to face the MS before being heated during TGA allowing reemission of the deposited contaminants towards the MS. In the second one, the three components are place in such a way that without any mobile parts they have satisfactory view factors (Figure 1).

In a second apparatus, as can be found at ONERA, France, the three main components (the effusion cell, the QCMs and the MS) are immobile. The main difference originates from the way contaminants are transported during the two phases above-mentioned. In such facility, the shroud enveloping the components is maintained at fairly high temperature, so that none of the contaminants can adsorb at its surface: any rebound is immediate (Figure 2). This has for consequence that there are only two ways for contaminants to stop travelling inside the shroud. Whether they reach the pumping system via dedicated holes or they are collected by any cold spot in the system. If designed properly, the chamber should ideally have only two cold spots, namely the QCMs and the MS. One downside consequence of such a system is that the calculation of TML and CVCMs is made a little bit more complicated as the calculation of the view factors is not anymore solely geometrical, but needs a calibration with a known substance first. Indeed, the knowledge of the sum of the surfaces of the

cold spots and pumping orifices in not so easy to obtain. As there are not only direct views between the different parts of the system but also contaminants transfers via rebounds on the shroud, we prefer using the term transfer factor to view factor. Besides, in order to increase the total amount of contaminants reaching the MS, collecting plates were added to the sample holder containing the QCMs. These collecting plates are kept at the same temperature than the QCMs but their surface is roughly 10 times higher. These plates can also be submitted to TGAs and release up to 10 times more contaminants, thus multiplying the signal in the MS by the same amount.

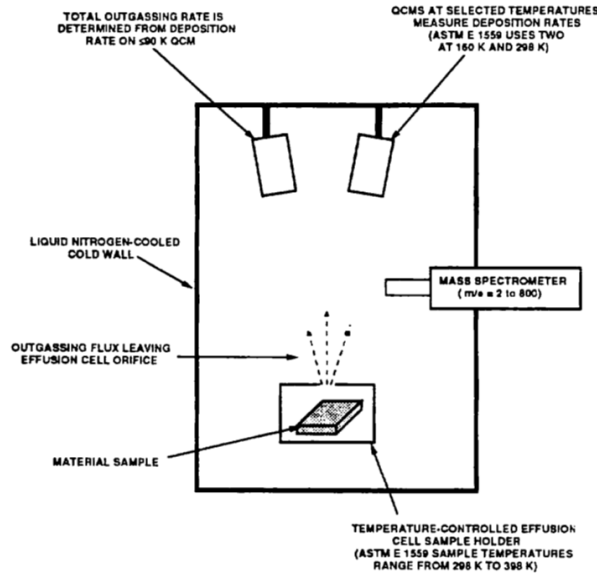


Figure 1: Schematic representation of a facility designed to study the outgassing properties of materials. This is an illustration of a vacuum chamber equipped with a cryogenic shroud where the different parts of the apparatus need to have direct view factors.

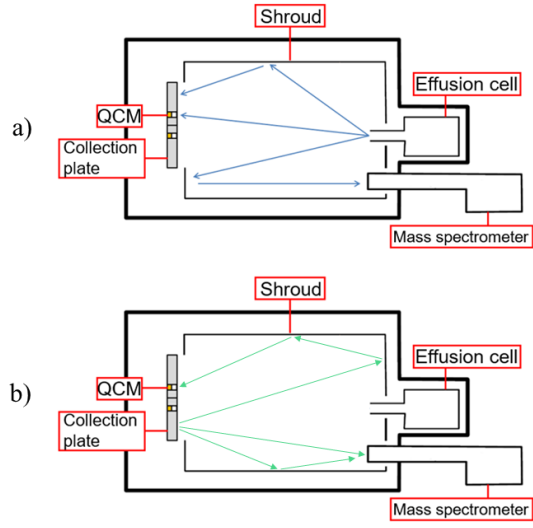


Figure 2: Schematic representation of another facility designed to study the outgassing properties of materials. This is an illustration of a vacuum chamber equipped with a hot shroud where the different parts of the apparatus do not need to have direct view factors. Due to the temperature of the shroud, immediate rebounds of contaminants occur allowing no direct view factors but so-called transfer factors between the different parts of the device a) during outgassing, b) during reemission.

### QCMs and outgassing temperatures

Another point worth mentioning is the way contaminant sources are heated to allow outgassing and the temperature of the QCMs collecting the outgassed flux. In the ASTM-E-1559 approach, Test Method A states that isothermal outgassing steps should be carried out at 3 different temperature (398, 348 and 323 or 373 K, depending on the contaminant deposition on the cryogenic QCM) though it is clearly stated that this point can vary a lot depending on materials specificity. There should be at least three different QCMs collecting the contaminants, at different temperatures:  $\leq 90$  K, 160 K and 298 K. The important point to remember here is that the outgassing tests are carried out isothermally during several days (up to a week).

In the approach adopted at ONERA until now, all the QCMs are kept at the same temperature, around 190 K while the outgassing is carried out using temperature steps. While the outgassing usually starts at relatively low temperature (often around 325 K), the latter is raised by steps of 25 K every 12 to 24 h until reaching fairly high temperatures of around 425-450 K. As most physics at play during outgassing (diffusion, desorption etc.) are thermally activated, this allows their artificial acceleration, useful for a better extrapolation of results on the long-term space mission duration.

### 3.2 Species separation through TGA

The idea of a TGA to perform species separation is simple. As species are meant to have a single reemission temperature, they should be reemitted successively as those temperatures are reached. While this ideal case is true when dealing with pure compounds or when the deposit on top of the QCMs is very thin (typically sub-monolayer deposits), leading to no intermolecular interaction, a larger deposit can be a source of problems. Indeed, it was shown in previous works [6], the presence of several different species with different volatilities in a deposit changes the way molecules are being reemitted. For example, it is conceivable that a less volatile species traps a more volatile one in a deposit: the reemission of the latter would then be postponed to when the first one would allow more mobility of the different species contained in the deposit. In practice, the fact is that after outgassing, the deposit on top of the QCMs and collecting plates is never sub-monolayer, nor close to one. Most of the time, the thickness of the deposit is evaluated to at least several hundred angstroms, meaning there are plenty of interactions possible.

One way to test if there are many intermolecular interactions is to look at the width of a reemission peaks. In the ideal case, the flux of reemitted molecules is proportional to  $e^{\frac{-E_a}{RT(t)}}$ , thus to  $e^{\frac{-E_a}{RT^2} \frac{dT}{dt}}$ . A standard width for a reemission peak would be when  $\frac{E_a}{RT^2} \Delta T$  is equal to 1 or at most several units. This leads to  $\Delta T = \frac{RT}{E_a} \cdot T$ . With a typical reemission temperature of 300 K one gets  $\Delta T = \frac{8.32 \cdot 300^2}{10^5} \sim 10$  K.

What we have here is some kind of criterion to know whether there are a lot of intermolecular interaction. The following Figures 3 and 4 extracted from previous studies carried out at ONERA show two examples. In the first one, the reemission peaks are quite narrow and the non-interaction criterion seems respected whereas in the second one, the reemission peaks are clearly too wide for the molecules responsible for them to be reemitted without interacting with other compounds.

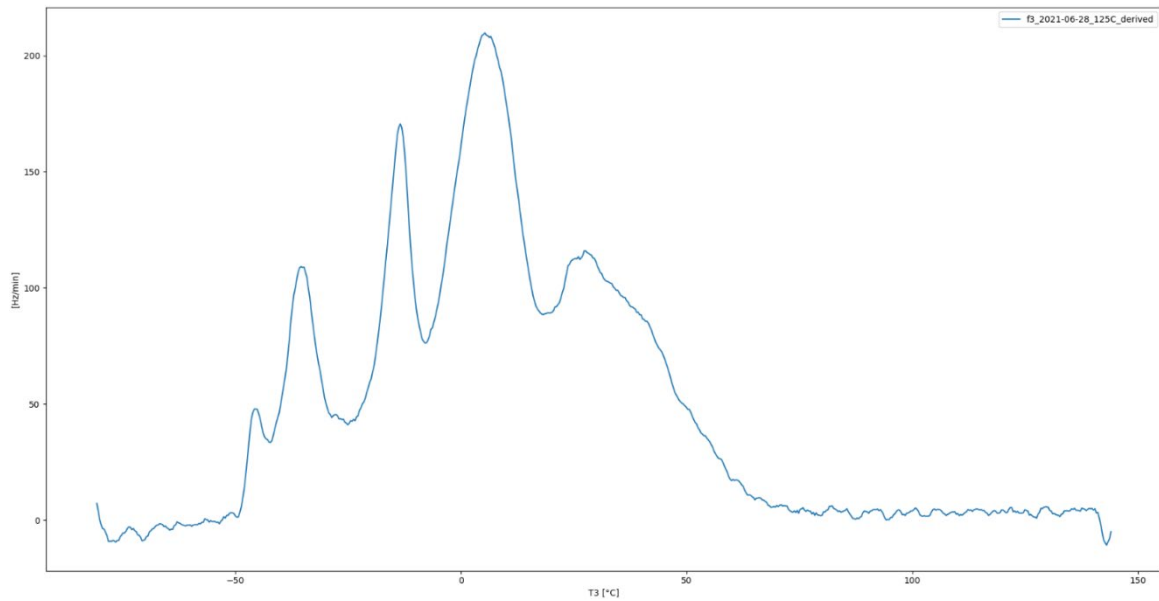


Figure 3: Derivative of a QCM frequency during a TGA at  $2 \text{ K}\cdot\text{min}^{-1}$  after a piece of Scotchweld EC-9323-2 was outgassed at  $125 \text{ }^\circ\text{C}$ . Several narrow reemission peaks can be observed with width of the order of magnitude of around  $10 \text{ K}$ , sign that few intermolecular interactions occurred.

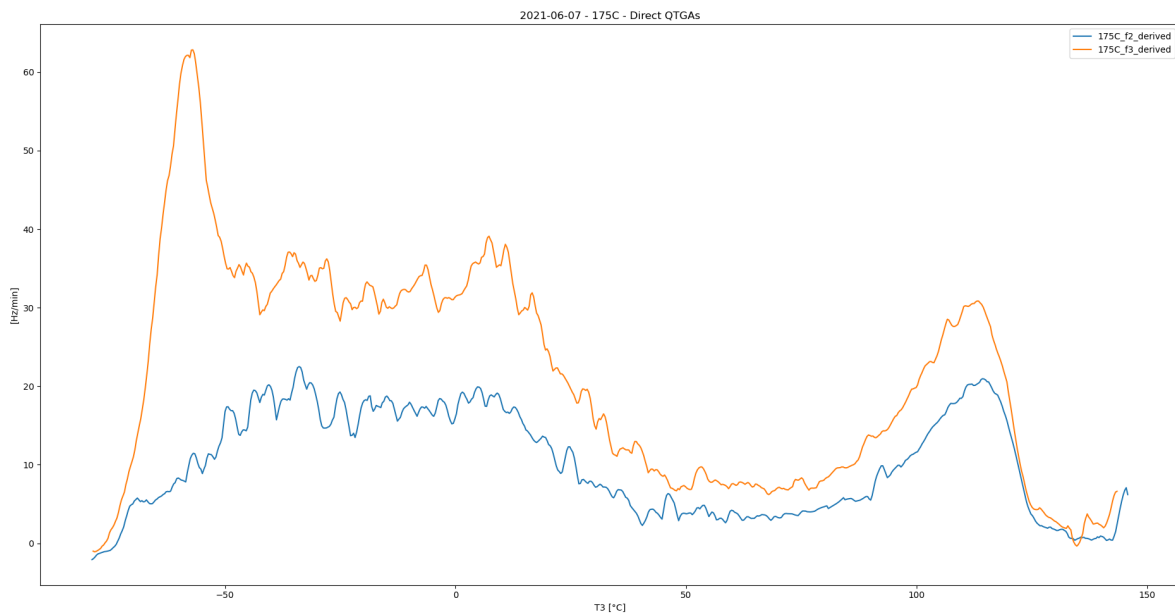


Figure 4: Derivative of two QCMs frequencies during TGAs at  $2 \text{ K}\cdot\text{min}^{-1}$  after a sheet of aluminum covered with the silicone paint MAP PNC was outgassed at  $175 \text{ }^\circ\text{C}$ . Several wide reemission peaks can be observed with width well above the order of magnitude of around  $10 \text{ K}$ , sign that many intermolecular interactions occurred.

### 3.3 Chemical species identification

If in the best case, contaminants were reemitted one after the other there is still a need for their identification. Indeed, let us keep in mind that the purpose of the work presented here is to unravel the physics at play during the outgassing of space materials. To do so, the total mass outgassed and detected must be separated into distinct species by deciphering the MS

data gathered during the TGA phase. Once individual molecules are identified, it becomes much easier to find specific fragments in the MS data and analyze their behavior during outgassing. This part of the work is very well described in the companion paper [12] that goes along this article.

The whole point is to be able to identify individual molecules thanks to the MS data. The first thing that allows identification of a single molecule is finding a relatively heavy fragment (high  $m/z$  ratio) that seems to present only a single peak during reemission. The high  $m/z$  ratio, coupled with the single peak criterion is what permits thinking that this peak is characteristic from a single contaminant. Knowing the reemission temperature of the molecule from which originates the fragment, one is able to find other fragments peaking at the same temperature. In order to distinguish two molecules that would be reemitted at the same temperature, one should look at the “shape” of the peaks. If all the fragments originate from the same molecule, their spectra should be proportionate during the entirety of the reemission. This means that in log-scale, their spectra should look parallel, as can be seen in Figure 5. A good example of discrimination between two molecules being reemitted at the same temperature is visible in Figure 6. There, all the fragments being looked at are peaking at the same temperature. Nevertheless, it is clear that there are two distinctive “shapes” of peak in these spectra, suggesting at least two different molecules were reemitted at the same time.

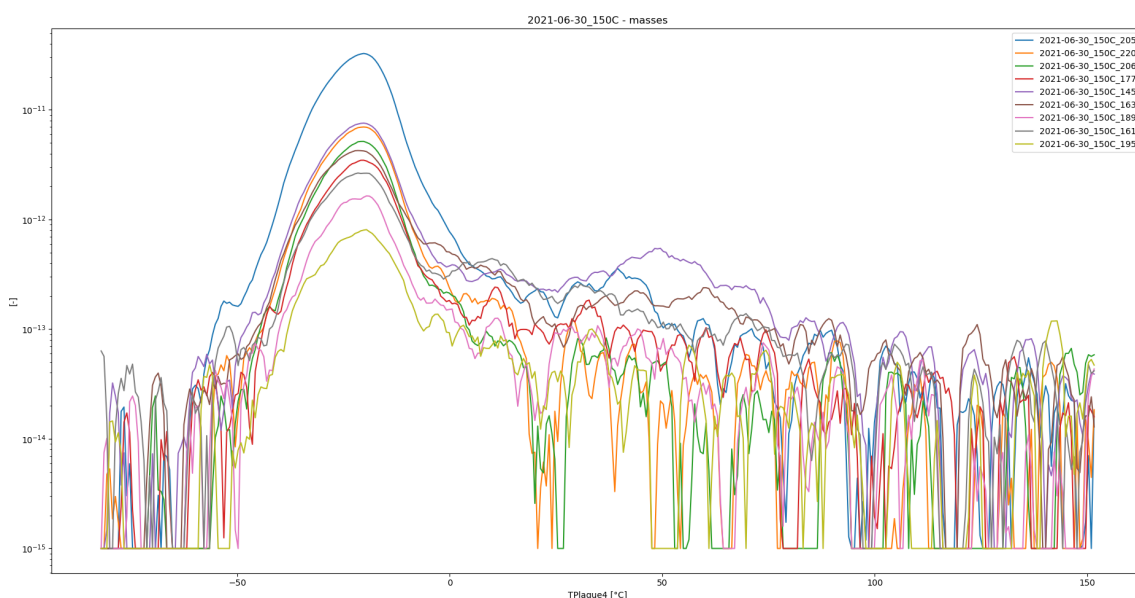


Figure 5: Mass spectrometry signals recorded during the TGA of a collection plate at  $2 \text{ K.min}^{-1}$  after a piece of Scotchweld EC-9223-2 was outgassed at  $150 \text{ }^\circ\text{C}$ . In log-scale, all these signals look parallel to each other: this is a strong signal that these fragments originate from the same molecule.



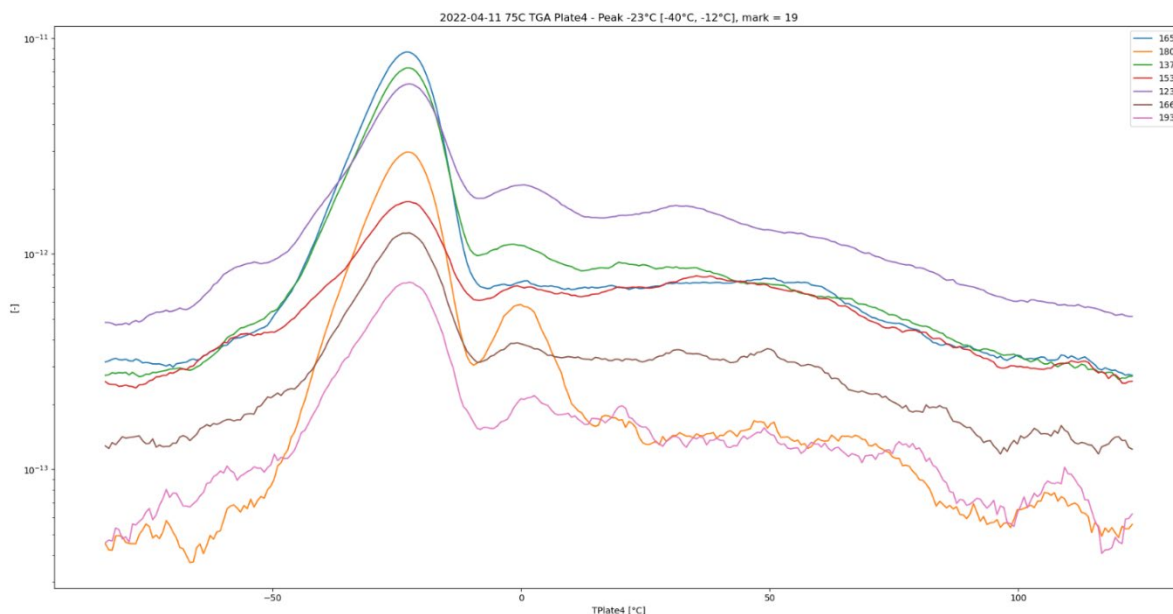


Figure 6: Mass spectrometry signals recorded during the TGA of a collection plate at  $2 \text{ K}\cdot\text{min}^{-1}$  after a piece of Scotchweld EC-9223-2 was outgassed at  $75 \text{ }^\circ\text{C}$ . Though all these signals peak at the same temperature, one can observe two distinctive shapes: a narrower one with the fragments 137, 165 and 180 amu, a wider one with the fragments 123, 153, 166 and 193 amu. This is a strong signal that these fragments originate from two different species reemitted then at the same temperature.

A stack of several parallel signals (Figure 7a) allows the reconstruction of a partial mass spectrum. An example of such spectrum is available in Figure 7b. It must be compared to a mass spectra database, such as the one maintained by NIST (Figure 7c) or to a gas chromatography coupled to mass spectrometry (GC-MS) analysis previously carried out. This way one is able to identify the contaminants reemitted during TGA with relative certainty.

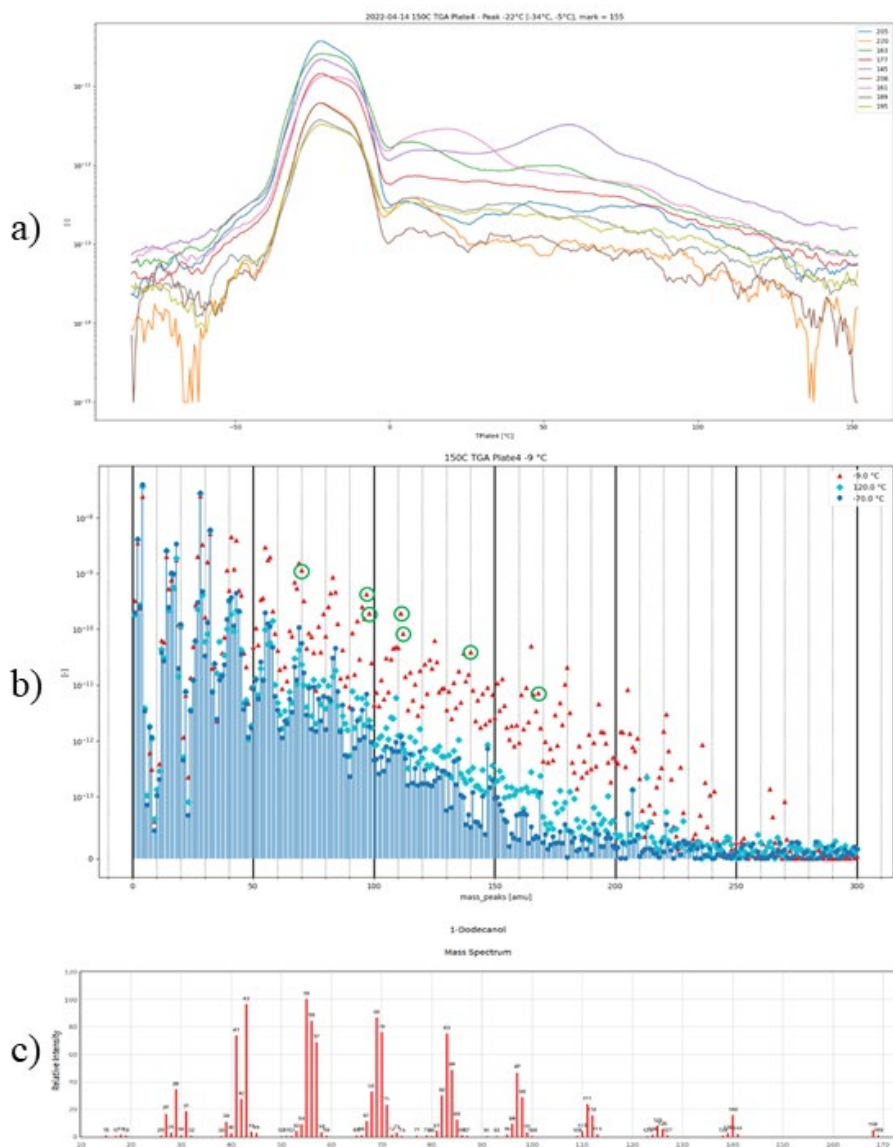


Figure 7: a) Stack of several parallel mass spectra signal obtained during a TGA at  $2 \text{ K.min}^{-1}$  after a piece of Scotchweld EC-9323-2 was outgassed at  $150 \text{ }^\circ\text{C}$ . b) Mass spectrum obtained at during the TGA of collection plate after a  $150 \text{ }^\circ\text{C}$  outgassing step. Two backgrounds are represented: one at low temperature ( $-70 \text{ }^\circ\text{C}$ , blue circles), one at high temperature ( $120 \text{ }^\circ\text{C}$ , cyan squares). The signal recorded is represented by red triangles. Among this signal, unique peaks detected in a) are circled in green. c) Mass spectrum of 1-dodecanol as can be found in the NIST mass spectra database [13].

The Figure 7 above illustrates the way the identification of molecules is done. In a first time, mass spectrometry signal are recorded, then transformed into mass spectra, which can finally be compared to different databases or sources such as GC-MS experiments previously carried out on the samples outgassed.

In the recent years, a very satisfactory species separation and identification of contaminants originating from the outgassing of the Scotchweld EC-9323-2 following the ECSS was carried out. It allowed the separation and identification of up to 7 outgassed species. Thanks to that, it was possible to look at the outgassing MS data with a novel eye and characterize the physics responsible for their kinetics and even predict accurately the outcome of a bake-out in terms of CVCMS. An insight of the method used for such physics determination is available in this article's companion paper.

Similarly, two species separation and identification were made possible with data shared by JPL following the outgassing of both Black Kapton and Nusil CV4-2946 following this time the ASTM-E-1559 protocol [11]. These experiments allowed the separation and identification of several molecules besides water in each material, even though their outgassing had been carried out at relatively low temperature (thus outgassing rates): 105 and 45 °C for Kapton and Nusil CV4-2946, respectively. With such data, it was possible to affirm that at least two contaminants identified in black Kapton did not follow a Fick's law during outgassing whereas the ones identified in Nusil CV4-2946 could all be satisfactorily be modelled with one.

This shows that whatever the standard followed for outgassing, the TGA/MS method could identify contaminants and lead to knowledge of the physics ruling their behavior during outgassing.

#### 4. CONCLUSION AND PERSPECTIVES

This paper reviewed the progress made in species separation and identification in the recent years in terms of experimental setup. The first ONERA attempt at species separation carried out on Scotchweld EC-2216 permitted progress with the hot-shroud technique and MS fragments tracking. It shown as well that species that are more volatile do not change the behavior of heavier ones during TGA. Following these results, new campaigns on Scotchweld EC-9323-2 and MAP PNC shown mixed results. Though both species separation and identification worked very satisfactorily on the former, the latter put the light on the limitation of such method on some materials where strong intermolecular interactions happen.

The differences that exist between the European and US approach both in terms of materials and methods were briefly shown, the point being that these differences are not so impactful as similar results can be obtained with both methods (see companion paper). Species separation and identification techniques were described with an accent put on the identification of outgassed compounds. Though some satisfying results could be obtain on some materials (here on Scotchweld EC-9323-2), other ones showed the limitations of the method (MAP PNC). Results from JPL analyzed at ONERA demonstrated that the analysis method is robust enough as species identification and study of outgassing behavior could be completed regardless of the standard used to carry out the tests.

On the one hand, focusing on the good results, the technique presented here seems promising for long-term prediction of space materials outgassing, of great interest for satellite manufacturers. On the other end, it must be improved for it to become a routine method of assessment of new space materials. As it was underlined with MAP PNC, the technique does not yet work well on all the materials tested. Many more tests will follow, consolidating the knowledge and allowing to improve the performance of both the device and the data processing. Indeed, in terms of experiments, efforts are put at the moment to increase the sensibility of the mass spectrometer and stabilize the temperature of the QCMs. Both these efforts pointing towards an increased SNR. In terms of data processing, a lot of work is put on the automation of peaks recognition and the reconstruction of mass spectra when several molecules reemission peaks are overlapping.

Finally, once the species separation and identification becomes robust enough, more applications can be studied. In the companion paper, based on species identification during TGA/MS phase, outgassing was studied species per species. The applicative objective is clear: the prediction of long-term in-flight outgassing for any temperature history of a material. Knowing the species composing a contaminant deposit is also a good basis to study the future dynamics of this deposit, its reemission, photo-polymerization, photolysis... Of course we saw that reemission physics of a given species was somewhat influenced by other species in the deposit, but these intermolecular interactions might be reduced in some cases (apparently for thinner deposits) and neglected, or studied if relevant for space situations. Molecular-species-level models were developed for photofixation [14][15] but progress remain difficult due to poor knowledge of the species present in a deposit. The improvement of this status could also give a new impetus to that other topic of research.

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