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Application of contaminant species separation by TGA/MS to unraveling outgassing physics and laws

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ABSTRACT

Progress was performed recently on the separation and characterization of the chemical species outgassed by space materials, relying on the assessment of thermogravimetric analysis (TGA) peaks by mass spectrometry (MS). A companion communication reports on this experimental technique and the first level processing of these MS data, which often allows determining which are the outgassed species, and their MS spectra. This communication focusses more on the second analysis step, *i.e.* the study of the MS data acquired during the initial outgassing phase. Ancient simpler outgassing analyses based on total mass measurements only, most of the time on quartz crystal microbalances (QCMs), cannot realistically determine the separate contribution of different species, even though some models consider the contribution of several species, which are indeed more “mathematical species” than physical ones. In contrast, this new approach, also taking into account the MS measurements during the outgassing, and known species spectra (from the TGA/MS analysis done previously), allows a more realistic determination of the contribution of each real chemical species to the total outgassing. Even though results are not yet final and perfect, measured outgassing fluxes from several species and materials are presented. Their physical analysis, through comparison and fit by diffusion or other possible outgassing laws are also presented. At this level, they clearly point to diffusion laws, rather than to any other outgassing law, although not necessarily always Fickian diffusion. This method was applied to typical US or European outgassing approaches, with either isothermal ASTM-1559 outgassing tests or multi-temperature VBQC-type tests.

Keywords: Contamination, outgassing, chemical species, species separation, mass spectrometry, thermogravimetric analysis, diffusion, desorption.

1. INTRODUCTION

Both the American and European dynamic outgassing tests, respectively based on ASTM-E-1559 standard [1] and ECSS-Q-TM-70-52A standard (*cf.* [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. 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 models under scrutiny. For example, concerning outgassing, a unique measurement dataset can usually equally be fitted by a sum of

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desorption laws (exponentials) or a sum of diffusion laws (Fick's law solutions). Indeed, practice 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. And determining this physics is the key to a realistic extrapolation from days-long experiments to years-long missions, and to mission temperature history.

This is why we have been working now for 15 years on what we often call "species separation", meaning an experimental determination of the deposit or flux of each contaminant 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 our 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 we showed that processing existing ASTM-1559 data could also lead to species separation provided good enough Mass Spectrometry data (MS) were collected during the tests [11]. Even though the American ASTM-1559 standard differs by some aspects from the ECSS standard (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 [12], this communication reviews all these efforts, including also more recent results. The *in situ* method we have been developing for species separation approach is based on coupling Thermogravimetric Analysis (TGA) and Mass Spectrometry (MS). The principle consists in first depositing contaminants on a QCM or a plate, then in a second step in reemitting this deposit by heating it at a 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 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.

The companion paper [12] focusses on the first step of the data processing. MS and QCM data during the deposit reemission (TGA) are analyzed to separate the contribution of different species, and possibly identify them from chemical species databases. This paper focusses on the second step of data processing, the determination of each chemical species outgassing law, thanks to the study of the relevant fragments, characteristic of a given species, during the first outgassing phase.

Next section explains our methodology, and gives the basis of diffusion theory (and solutions). The following main section reviews most per-species outgassing data we have, and compares them to diffusion laws, or other outgassing laws. It is organized historically, material by material. A conclusion, and perspectives for this still-to-be-developed approach, terminates this paper.

2. THEORY AND METHODOLOGY

In the companion paper [12], we saw that for most species, we could find some fragments (values of m/z in their MS spectra) that looked to be present only in this species spectrum. These are the specific fragments that we shall now consider during the outgassing phase. Of course, this approach relies on the assumption that the global sensitivity of the transfer system and mass spectrometer is sufficient. We will see on the examples presented thereafter, that it is often the case. We will not enter into the experimental features permitting this, essentially the hot-shroud transfer method (here directly from the Knudsen cell to the MS), since they were thoroughly discussed in the companion paper. Here we shall more focus on outgassing and its theory.

In the past many different physics and laws were considered to rule outgassing. In Europe, since the 1980s, surface desorption and its residence time law, leading to an exponential decay, was most often favored [3]. Yet, no experimental evidence really supported this assumption and some attempt were performed to discriminate between a desorption-ruled

outgassing and a diffusion-ruled outgassing. Unfortunately, based on QCM cumulated measurements, discrimination between either physics was poor and not very conclusive [5]. This assumption must thus be revisited now that experiments can characterize outgassing of each chemical species separately.

In the USA, the most common theoretical processing of the ASTM-1559 data consisted in extrapolating the cumulated QCM data from 5-7 days to years with some power law for the outgassing flow rate versus time. The exponent was usually in the range between -1 and -0.5, and often quite close to -0.5. Even though this approach can be considered as an empirical fit, the $t^{1/2}$ behavior is typical of the short-term asymptotic behavior of Fick's law solutions (*cf.* below).

In the next section, we review several species-level outgassing data from several materials and compare them to relevant outgassing laws. Since in all cases, data prove consistent with diffusion-type laws, and not desorption-type exponentials, we first briefly review diffusion laws in this theoretical section.

Fick's law describes diffusion:

$$\frac{\partial c(x,t)}{\partial t} = D \frac{\partial^2 c(x,t)}{\partial x^2} \quad (1)$$

ruling the concentration of one species of contaminant $c(x,t)$ within a material depth (space coordinate x) over time (t). The diffusion coefficient is thermally activated and should follow an Arrhenius law:

$$D = D_0 e^{-E_a/kT}. \quad (2)$$

The solution of the partial differential equation (1) can either be computed numerically, or expressed as series developments if the initial conditions are uniform ($c(x,0) = c_0$ for x in $[0,L]$, L the diffusion length). There are two developments. The series converging better for large times

$$c(x,t) = \frac{4c_0}{\pi} \sum_{i=0}^{\infty} \left\{ \frac{(-1)^i}{2i+1} \exp[-D(2i+1)^2 \pi^2 t / 4L^2] \cos \left[\frac{(2i+1)\pi x}{2L} \right] \right\} \quad (3)$$

gives the long term asymptotic behavior of the solution by keeping only its first term ($i = 0$), decaying exponentially as $\exp(-\pi^2 D t / 4L^2)$. Similarly, and more interestingly for our forthcoming data analyses, the outgassed flux at the material surface, $f(t)$, is given by:

$$f(t) = D \left. \frac{\partial c(x,t)}{\partial x} \right|_{x=L} \quad (4)$$

and follows this exponential decay for large t ($t \gg L^2/D$):

$$f(t) \sim \frac{2c_0 D}{L} e^{-\frac{\pi^2 D t}{4L^2}}. \quad (5)$$

This regime is reached when contaminant depletion becomes deep, reaching the bottom of the material. The space dependence of the density is a simple $1/4$ of a period of a cosine.

Similarly, the short times development of Fick's law for uniform initial conditions

$$c(x,t) = c_0 \left\{ 1 - \sum_{i=0}^{\infty} \left[(-1)^i \operatorname{erfc} \left(\frac{(2i+1)L-x}{2\sqrt{Dt}} \right) \right] - \sum_{i=0}^{\infty} \left[(-1)^i \operatorname{erfc} \left(\frac{(2i+1)L+x}{2\sqrt{Dt}} \right) \right] \right\} \quad (6)$$

gives the short term asymptotic behavior of the outgassed flux (for $t \ll L^2/D$):

$$f(t) \sim c_0 \sqrt{\frac{D}{\pi t}} \quad (7)$$

In this regime, only the upper layers of the material started being depleted in contaminants. This flux is not dependent at all of the material thickness L , which is no surprise since deeper layers were not yet depleted at all.

3. OUTGASSING DATA AND PHYSICS

Here, we review the outgassing data and the modeling we were able to carry for all materials we studied over time. They include two epoxy glues, EC2216 and EC9323-2, one silicone glue CV4-2946 and Black Kapton, the first two

characterized in Europe, the last two in the USA, following their respective test standards (adding MS measurements during outgassing and TGA phases of course).

3.1 EC2216

The first material we studied, during the years 2010, was the Scotch-Weld 3M™ epoxy glue EC2216. In these earlier years of development of our species separation technique, most efforts were devoted to the TGA/MS part of the experiments, specifically dedicated to species separation. Yet, the mass spectrometer was sometimes turned on during the outgassing phase also, leading to some interesting data and analyses. Here we only report about the $m/z = 91$ a.m.u. signal and its modeling with a Fickian diffusion law. This fragment is typical of toluene ($C_6H_5CH_2$ radical) and not very much present in other species spectra. Clearly, the fit by a diffusion model exhibited on Figure 1 is really convincing that the outgassing of toluene from EC2216 is ruled by its diffusion throughout this epoxy glue.

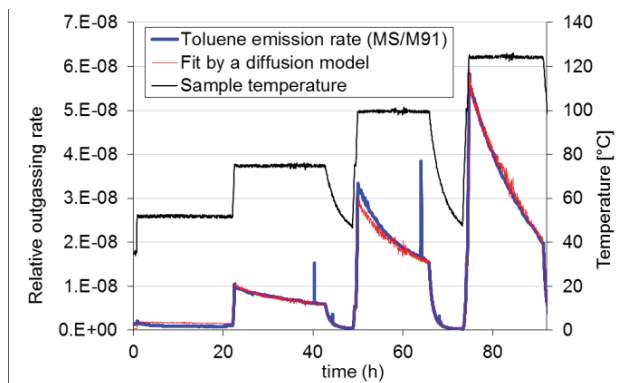


Figure 1: Mass peak 91 measurement (blue) during temperature step outgassing of EC2216 (black), considered to be representative of toluene, compared to a diffusion-limited outgassing model (red).

3.2 EC9323

More recently, we started studying the outgassing of other materials, in particular the other Scotch-Weld 3M™ epoxy glue EC9323-2. As reported in the companion paper [12], advances in the experimental setup allowed separating and identifying as many as seven species. They all had in their spectra some specific fragments with a signal large enough to be followed during the outgassing phase, which we discuss here. As examples, we present two chemical species, each with two fragments (m/z values) with a satisfying signal-to-noise ratio. All of them could also be fitted quite satisfactorily with Fick's laws.

Figure 2 displays the outgassing rate of two main fragments of 1'-(butyn-3-one-1-yl)-menthol spectrum, of masses 165 and 180 a.m.u. respectively. The temperature steps are given in Figure 3, while Figure 4 gives the spectrum and formula of this molecule. The fit is quite convincing that Fick's diffusion is the right physics ruling menthol outgassing from EC9233-2.

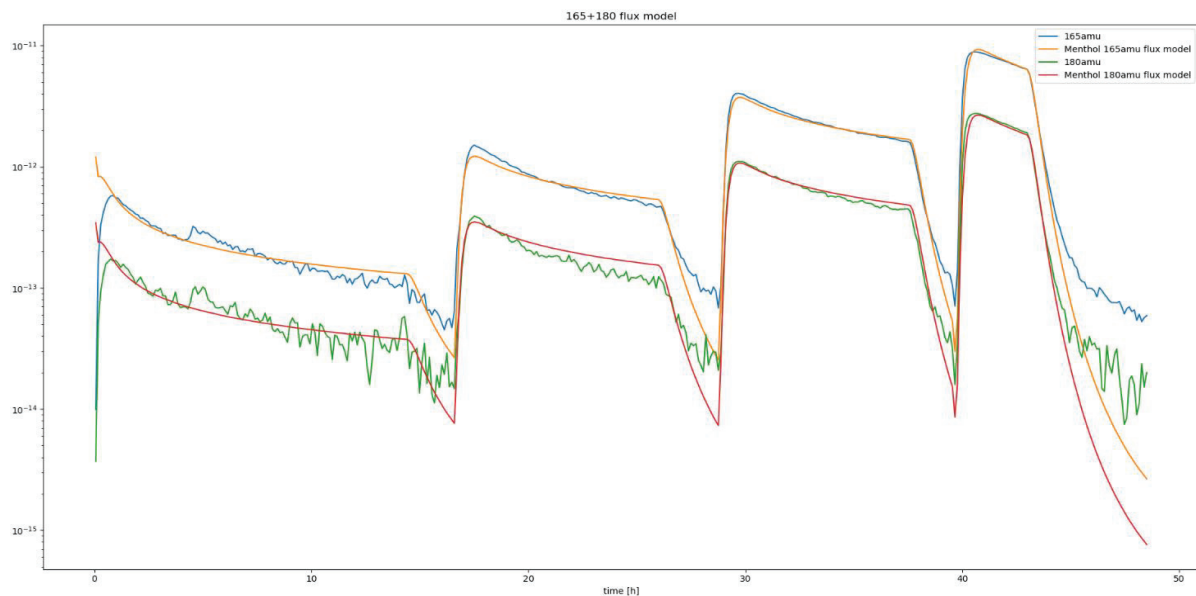


Figure 2: Outgassing MS signal for two fragments (165 and 180 a.m.u.) of 1'-(butyn-3-one-1-yl)-menthol spectrum (arbitrary MS units), and their fit by Fick's law, with $E_a = 110$ kJ/mol and diffusion coefficient $D_0 = 680$ m²/s (diffusion length = 1 mm, half of the bulk sample thickness).

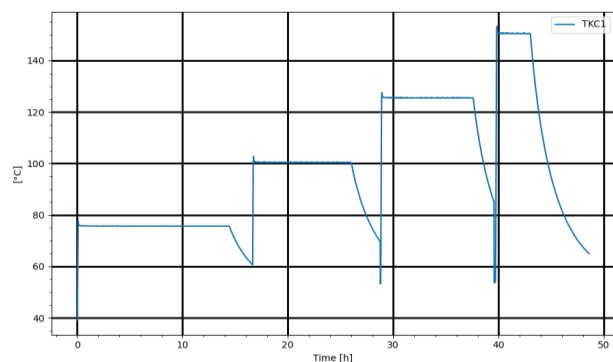


Figure 3: Temperature steps of the Knudsen cell during the EC9323 outgassing tests reported here. At the end of each step, the Knudsen cell is cooled down passively to reduce the outgassing signal to allow TGA/MS measurements (the TGA/MS time intervals are removed from these data, both from the temperature profile here, and the flux histories above)

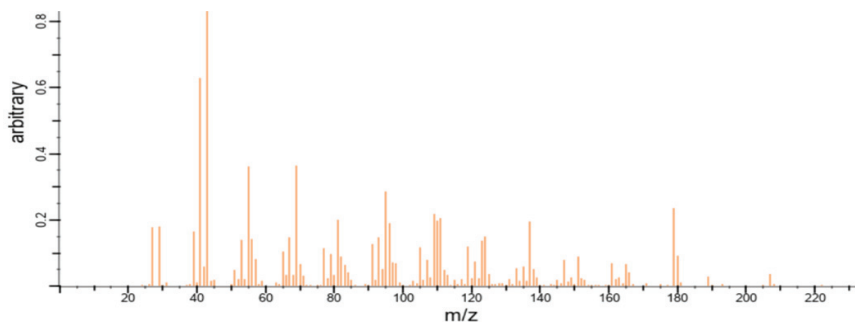


Figure 4: MS spectrum and chemical formula of 1'-(butyn-3-one-1-yl)-menthol.

Next figures similarly represent the outgassed flux of two fragments of another identified species outgassed by EC2216, the butylated hydroxytoluene, and its MS spectrum and formula (for the same temperature profile, this is the same experiment). Fick's law again gives a good fit of the data. The experimental data might be overestimated in the first 18 hours since 10^{-14} is close to the noise level of the mass spectrometer. The lower panel of the figure also gives the partial integral of the flux measurement and modeling (their primitives, the molecule fluence), which is similar to the direct QCM signal for the mass cumulated over all species. Its fit is also correct, showing that both the flux and fluences are correctly estimated by Fick's law.

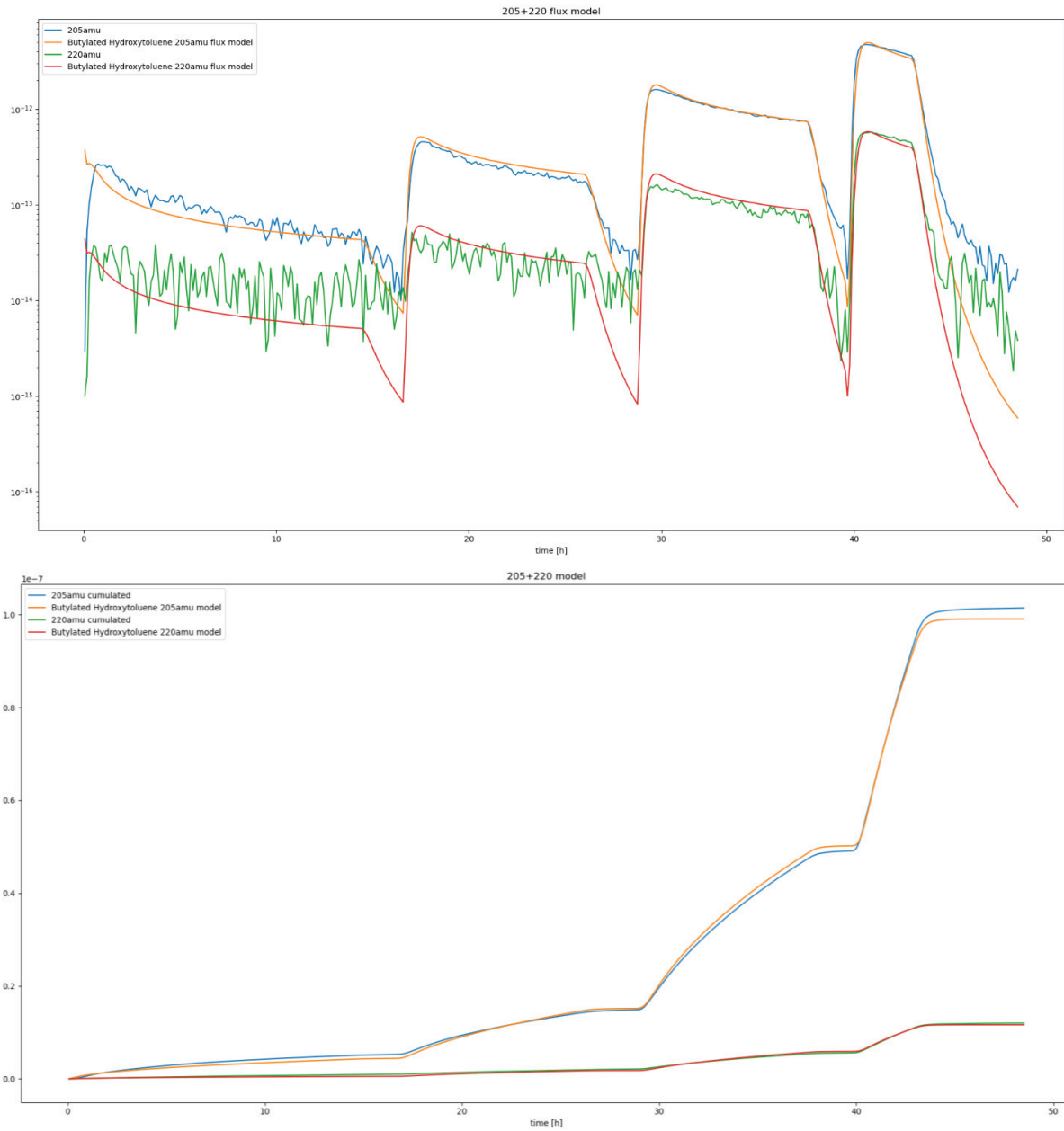


Figure 5. Outgassing MS signal for two fragments (205 and 220 a.m.u.) of butylated hydroxytoluene spectrum (arbitrary MS units), and their fit by Fick's law, with $E_a = 120$ kJ/mol, $D_0 = 4000$ m²/s; the flux on upper panel (direct MS signal), and its partial time integral on lower panel (its primitive).

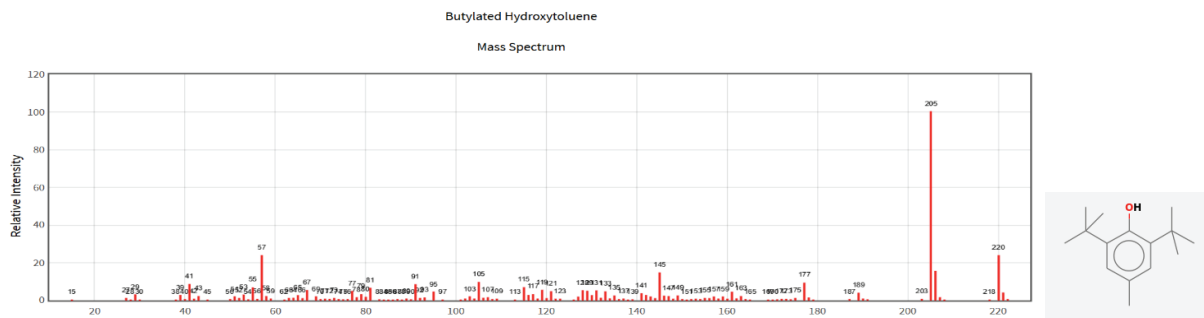


Figure 6: MS spectrum and chemical formula of butylated hydroxytoluene.

3.3 Nusil CV4-2946

In parallel, data collected during preexisting ASTM-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 this peak and identified thanks to its (partial) mass spectrum, and its outgassing behavior studied. This section reports our analysis of Nusil CV4-2946 silicone glue, while next ones deals with Black Kapton.

In spite of the low temperature of this CV4-2946 test (isothermal at 45 °C), two species were detected (beyond water), and more or less reliably identified [11][12]. Figure 7 represents the outgassing fluxes of three fragments belonging to their spectra, for an ASTM-A559 isothermal 45°C test. They are again quite well fitted by a Fick's law, each with its own set of parameters (E_a , D_0 , c_0). Here, the MS noise level is supposed to be close to the “1st digit” line, which corresponds to the first digitalization level above zero.

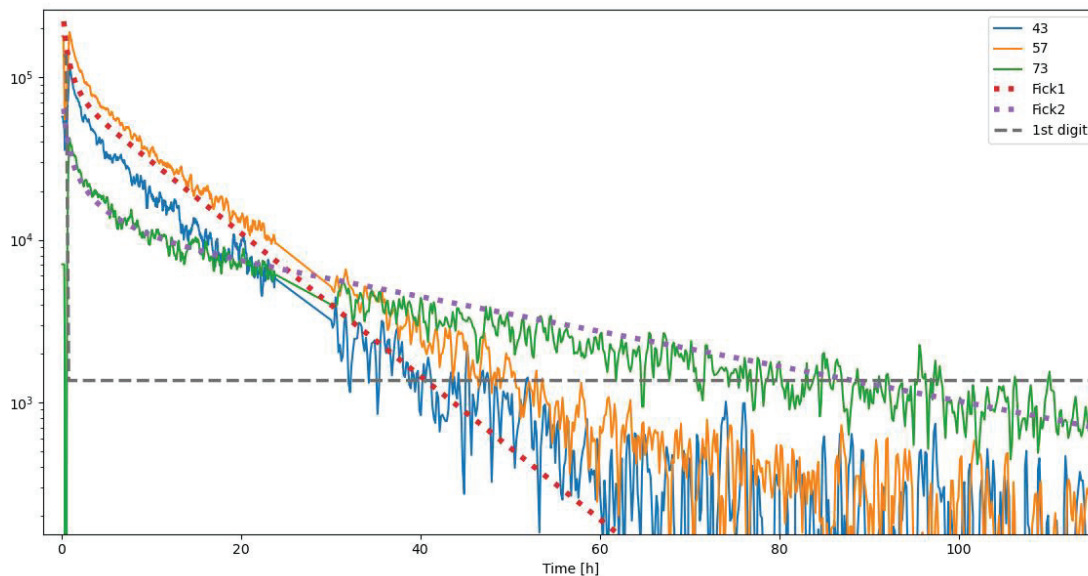


Figure 7. Outgassing MS signal for three fragments outgassed by CV4-2946, two (43 and 57) considered as part of the octane spectrum (or similar alkane), one (73) of less established origin (maybe the trimethylsilyl radical), and their fits by two different Fick's laws, with two diffusion coefficients $D=3\ 700\ \text{m}^2/\text{s}$ and $900\ \text{m}^2/\text{s}$ respectively (no temperature dependence needed for these isothermal experiments)

It is interesting to note that for the first time in the data and models displayed so far, both the short-times and long-times regimes are clearly visible. As in most previous graphs, the first few hours of data are convex in this semi-log plot, which is characteristic of the short-times $t^{1/2}$ asymptotic behavior for Fick's law solutions (Eq. (7)). After this, and for the first time (except maybe for the last step of Figure 5), the linearity of the curves shows that the exponential decay of the long-term development of Fick's law solutions is reached (Eq. (5)). In spite of the low temperature of the test, these species reach the exponential regime where they come close to a full depletion throughout the material, because they are much more volatile than those detected in the previous materials (molecular weights below 100 a.m.u. versus around 200 a.m.u.).

3.4 Black Kapton

This section deals with similar data and analysis for Black Kapton (25 μm), on the basis of isothermal 105 $^{\circ}\text{C}$ ASTM-1559 test. Two species were detected here again (beyond water) [11][12].

This time, the attempts to fit these measurements by Fick's laws, as depicted on Figure 8, failed. The attempt 1 (dotted purple curve) fits correctly the long-term exponential decay of 42-43-60 a.m.u. fragments, but completely fails to do so in the short-term.

Indeed these fits involve very few free parameters and very few degrees of freedom: beyond a global factor (total concentration, shift a curve vertically on the plot), the only free parameter is the (isothermal) diffusion coefficient D . Once fixed by the slope of the final linear/exponential decay in this semi-log plot (time constant = $(4L^2/\pi^2D)$, cf. Eq. (5)), the transition between the initial $t^{1/2}$ regime and the final linear/exponential regime is automatically fixed (for $t \sim L^2/D$), without extra freedom.

When rather trying to fit the short-time part of the data (attempt 2, dotted brown curve), by increasing D , the transition to the final linear/exponential regime comes too early. No good fit of these measurements looks feasible by solutions of Fick's law.

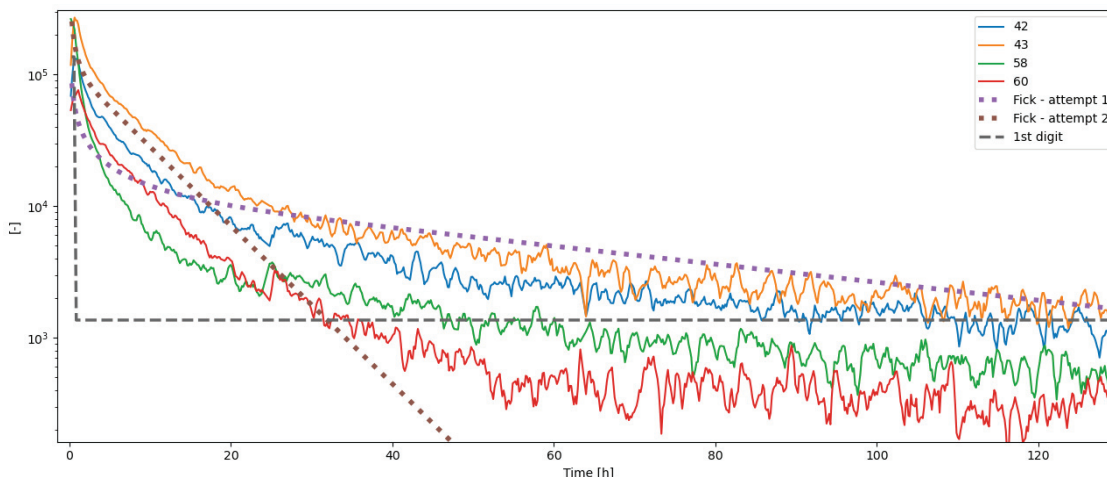


Figure 8. Outgassing MS signal of four fragments outgassed by Black Kapton, three (42, 43 and 60) considered as part of the propanal spectrum (or maybe acetone), one (58) of less established origin (maybe N,N-dimethylhydroxylamine), and an attempt to fit them by two different Fick's laws.

Other attempts to fit these data by empirical laws are reported on Figure 9. The $t^{1/2}$ law (purple dotted) can do a decent job in the short-times (no surprise since it is typical of diffusion in the short-times), but does not decay quick enough in the long-times regime. The t^{-1} law (brown dotted) does a better job over the whole timeframe, with some discrepancy in the intermediate time range (5-20 hours) yet. A pure desorption law, giving an exponential decay over the whole timeframe, *i.e.* a straight line in this semi-log plot, would visibly not do a better job.

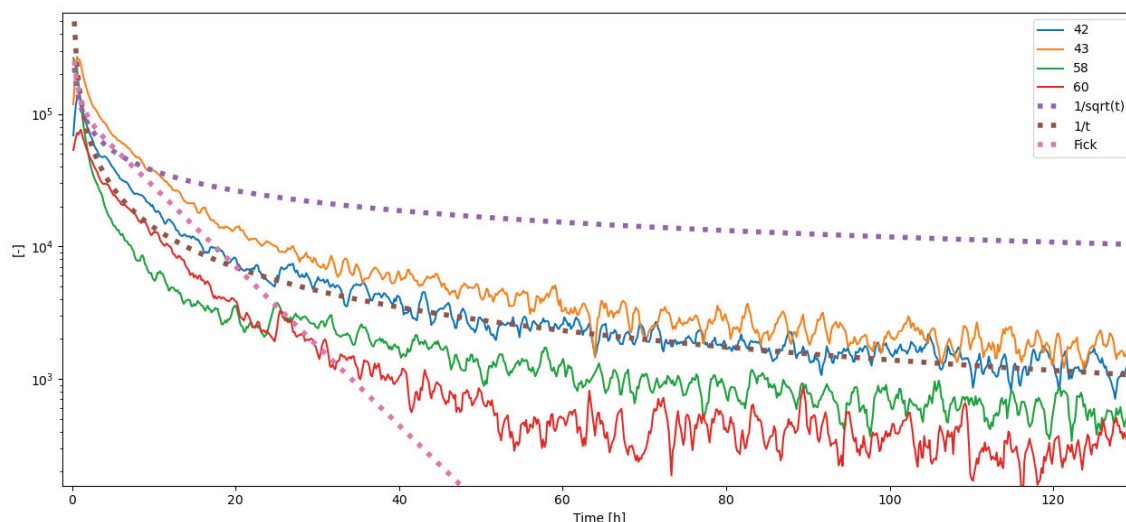


Figure 9. Same experimental data from Black Kapton, with different attempts to fit them, by empirical power laws here.

An alternative explanation of these data could be non-Fickian diffusion [13]. Phenomena like polymer swelling can change the diffusion coefficients of contaminants between beginning and end of test, thus modifying the diffusion solutions from purely Fickian diffusion. It cannot be excluded yet that the very small thickness of this sample, or a specific wrapping shape could be at the origin of this difference. In any case, the global behavior of these species outgassing from Black Kapton remains similar to previous data. A fast initial decay, somewhat close to a $t^{-1/2}$ law, is followed by a final decay close to an exponential. This behavior is likely to be general to non-Fickian diffusion models (simply by considering smaller time frames over which D changes little, and for which Fick's law is a good approximation). Some non-Fickian diffusion might thus be the physics ruling the outgassing of these species from Black Kapton. This aspect still needs further investigations.

4. CONCLUSION AND PERSPECTIVES

We reviewed the progress of molecular-species-level analysis of outgassing done in the last decade or so. Thanks to the species separation TGA/MS technique described in the companion paper, the mass spectra of the main species outgassed by the studied materials could be determined. Most of these species were even identified in chemical databases. Depending on the mixture of outgassed species (and chamber background) some of the spectra fragments only belong to one species spectrum, and could thus be tracked during the outgassing phase as proxies for the outgassed flux of this species.

Next achievement was the comparison of these one-molecular-species outgassing fluxes to possible outgassing physics and laws. And there, the answer was quite clear. Most data could be very satisfactorily modeled by diffusion laws, most often Fick's law solutions, maybe a non-Fickian diffusion law in the last case (Black Kapton). The species-level experimental data we were able to gather and study did not look like matching any other outgassing law, in particular the exponential desorption decay.

Many steps and difficulties were overcome until now, but many more remain on the path. Given these promising results, species separation looks to be only path towards a real breakthrough towards a finer contamination analysis, and is well worth some more efforts.

Many different directions look very promising. First, to ascertain these results, we must clearly study other materials and outgassed species, improving the accuracy and extensiveness of the experimental data collected and modeled. The improvement of many experimental aspects can concur to the general objective, as e.g. more experimental sensitivity (better matter transfer factors, MS sensitivity...), a better species separation, which depends e.g. on the deposit thickness. One tested material, a silicone paint (unpublished results), did indeed not allow a good species separation, maybe due to strong interactions between species in the deposit. This shows a direction of progress. Testing a given material with several

diffusion thicknesses is another interesting idea to validate the physics ruling outgassing. Diffusion through a fraction of a millimeter, or many centimeters, although based on the same diffusion parameters, should give very different outgassing fluxes, to be matched by fitting only a couple of parameters for one species. If successful, diffusion law will be definitely confirmed as ruling outgassing in these cases.

Many aspects of the numerical processing of these data are also to be improved. Treating fragments belonging to several spectra is one of them. Automating more this complex data processing, to use it quasi automatically at the end of a “MS-improved” VBQC or ASTM test, is another one. Investigating other outgassing laws, like non-Fickian diffusion, needs both physical and mathematical progress.

Finally, once the species separation and identification becomes robust enough, more applications can be studied. Here, on the basis of species identification during TGA/MS phase, we studied outgassing species per species. The applicative objective is clear, we want to be able to predict 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 (in the companion paper) that reemission physics of a given species was somewhat influenced by other species in the deposit, but these inter-species 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 species presents in a deposit. The improvement of this status could also give a new impetus to that other topic of research.

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