Prediction of Contamination Levels by Thermogravimetric Analysis

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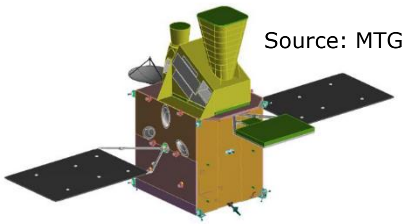
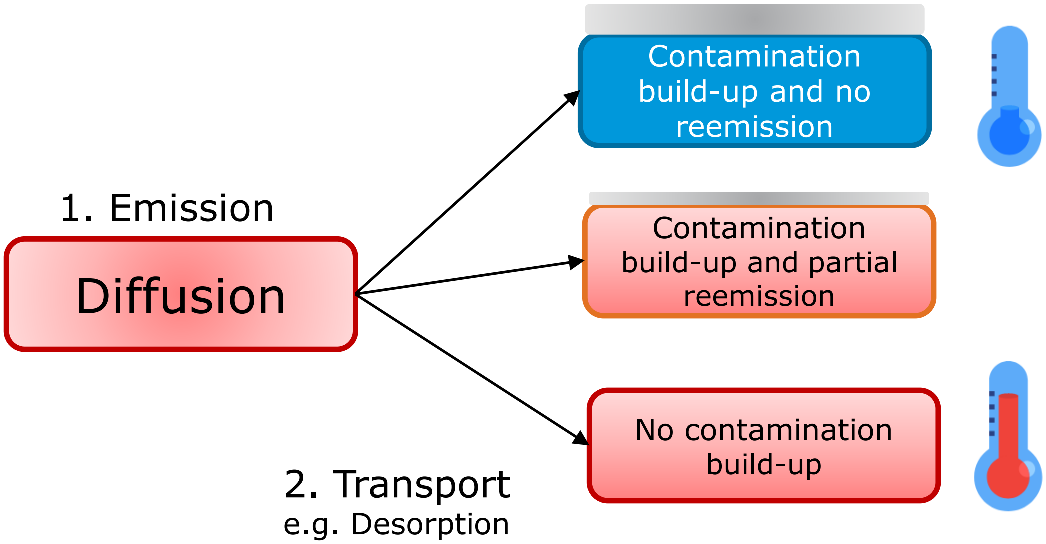
Presentation outline



1. Dynamic outgassing test at ESA ESTEC
2. Addition of TGA analysis to the test to estimate the contamination levels at specific regions of surface temperature
3. Introduction of sticking coefficient function to the prediction tool
4. Results of deposition rates obtained from the prediction tool vs. experiment
5. Conclusions and Future work

Contamination build up due to spacecraft outgassing



3. Probability of Sticking

Three main scenarios of contamination behavior on a surface

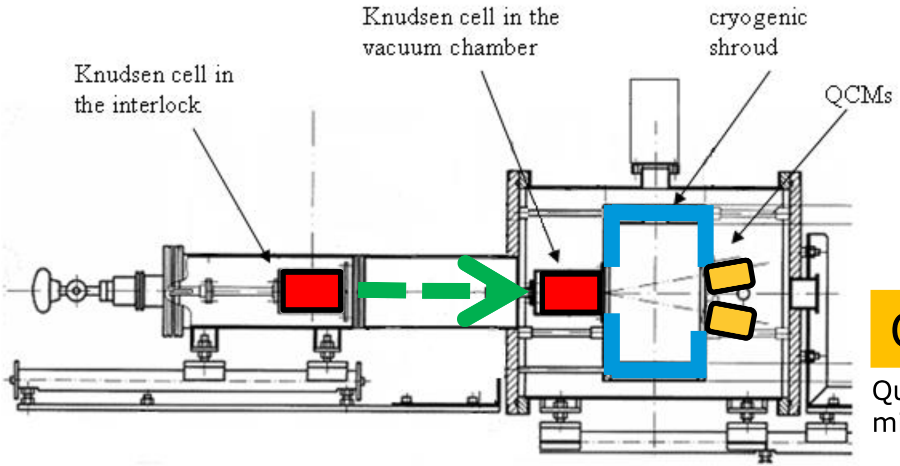
Full Sticking

Partial Sticking

No Sticking

Dynamic outgassing test method

Sample temperature is increased from 25°C to X°C by steps of 25°C every 24h. The number of steps and the duration at the max. test temperature is adjusted based on the real application temperature and the max. permitted test temperature of the sample.



QCMs

Quartz crystal microbalance

KC

$T_{max} \cong 450°C$

Liquid N_2

$\bar{T} \cong -175°C$

$$P < 5 \times 10^{-6} mbar$$

$$T_{QCM,1} \cong -170°C$$

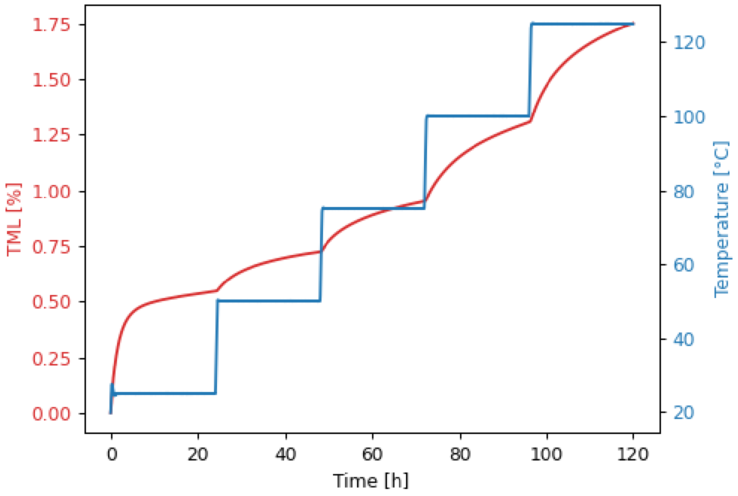
TML Total mass loss

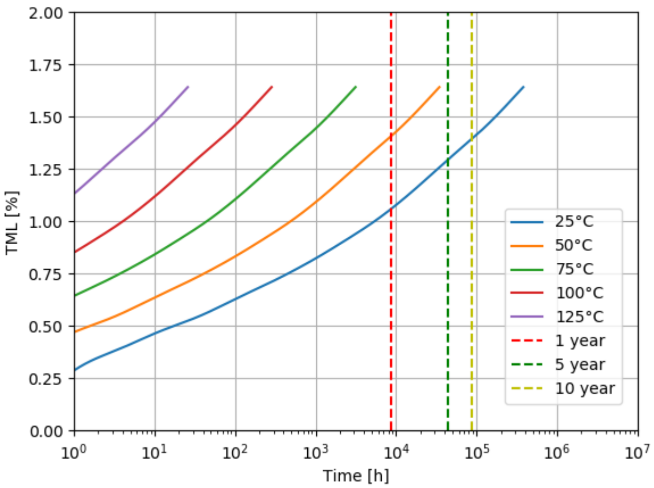
$$T_{QCM,2} \cong -25°C$$
$$T_{QCM,3} \cong -75°C$$
$$T_{QCM,4} \cong -50°C$$

CVCM Collected Volatile Condensable Material

Test according to: ECSS-Q-TM-70-52A

From dynamic outgassing testing to long-term predictions

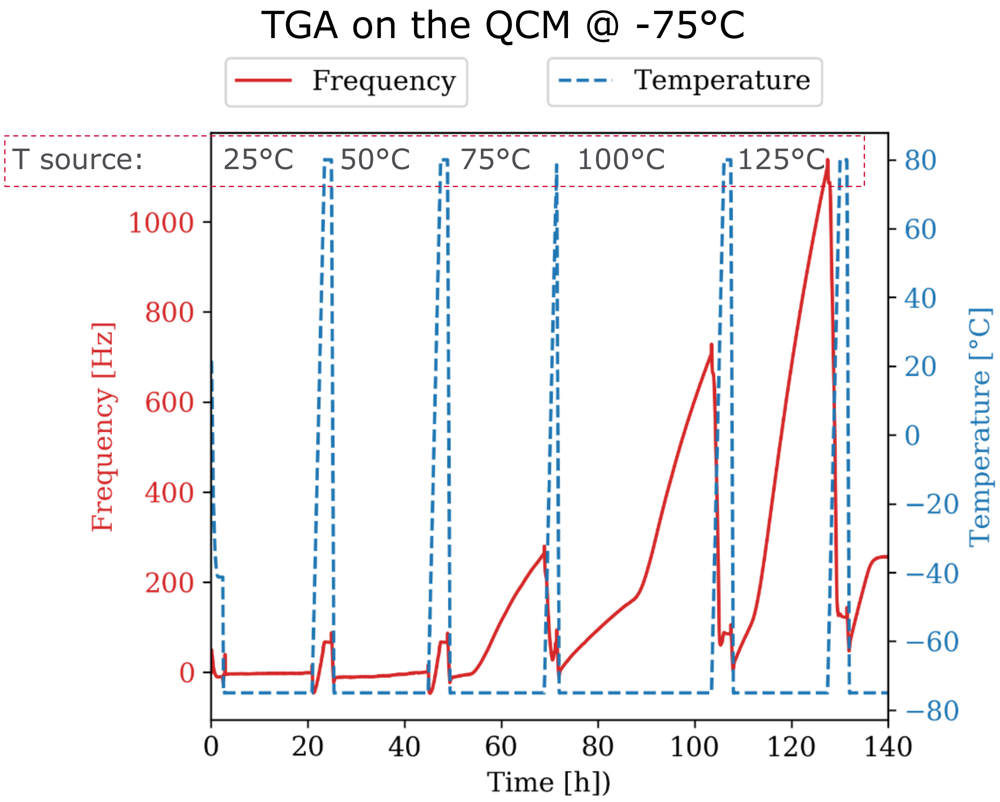




1) Mathematical species (fitted parameters to the desorption model)
2) Activation energies and temperature-time constant
3) TML, RML and CVCM of the sample
4) QTGA Analysis

1) Rampini, R., E. Ftaka, and M. Van Eesbeek. "Dynamic Outgassing Testing: A Revisited Mathematical Approach." *11th ISMSE, France* (2009).
2) Rampini, R., L. Grizzaffi, and C. Lobascio. "Outgassing kinetics testing of spacecraft materials." Materialwissenschaft und Werkstofftechnik 34.4 (2003): 359-364.

Modified standard outgassing test -QTGA



- Standard as per:

Kinetic outgassing of materials for space
ECSS-Q-TM-70-52A, ESA-ESTEC (2011)

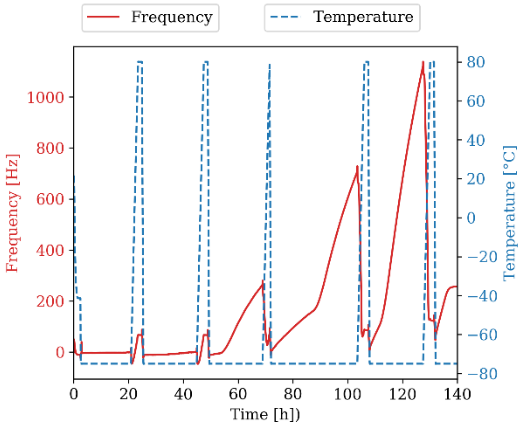
- Addition of QTGA analysis on the QCM at -75°C to the standard outgassing

- TGA performed after each outgassing step
- ($T_{outgassing}$ = 25,50,75,100,125°C)

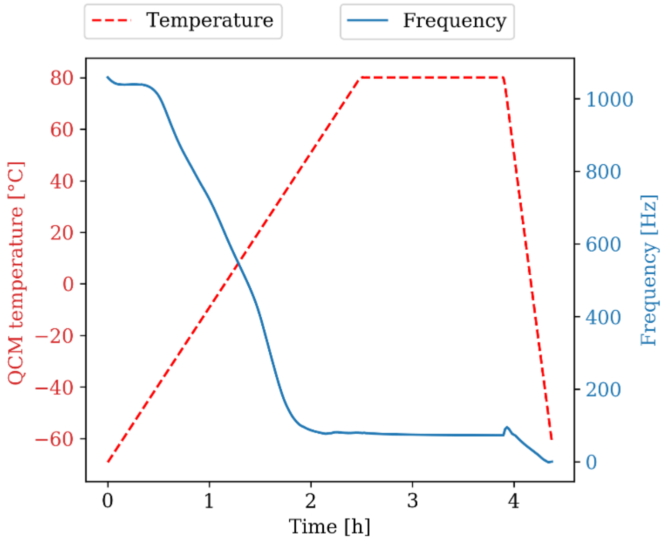
Modified standard outgassing test

Extraction of QTGA data into the mathematical species

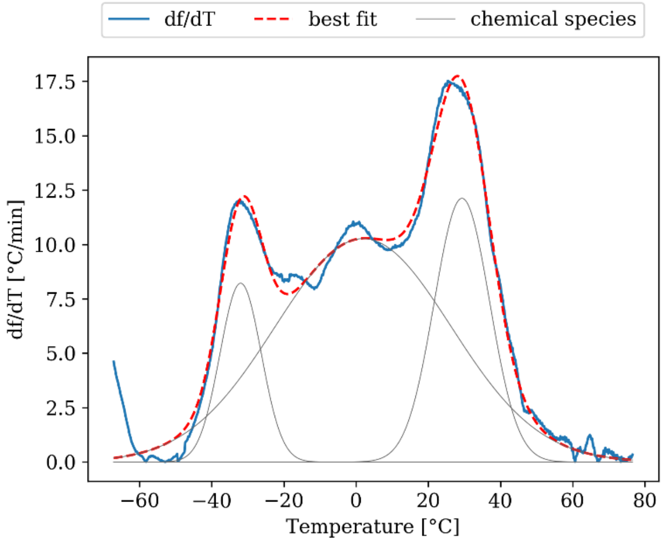
1. QTGA



2. TGA -> DTG



3. DTG -> Best fit



Species separation

3 chemical species + water

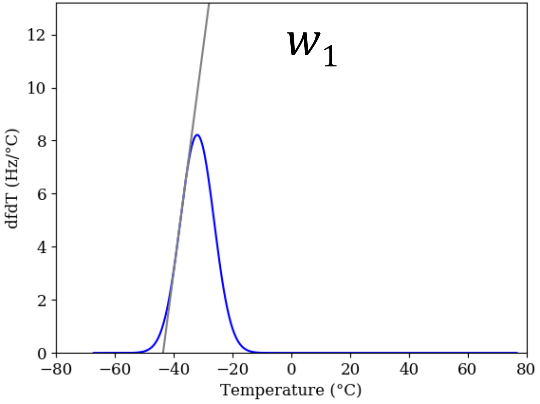
Tc_{α} – capitation temperature for specie α

$w1$ – weight factor for specie α

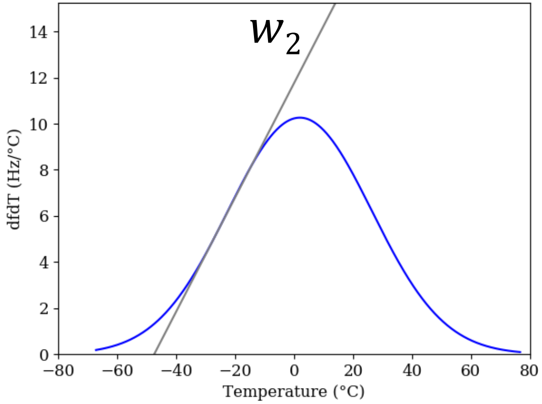
$$w_{aqua} = 1 - \frac{CVCM(-75°C)}{TML(-175°C)}$$

$$Tc_{aqua} = -112°C$$

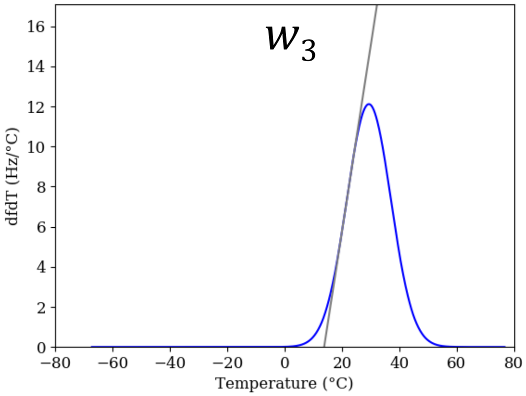
$Tc_{\alpha 1}$ = -43°C



$Tc_{\alpha 2}$ = -47°C



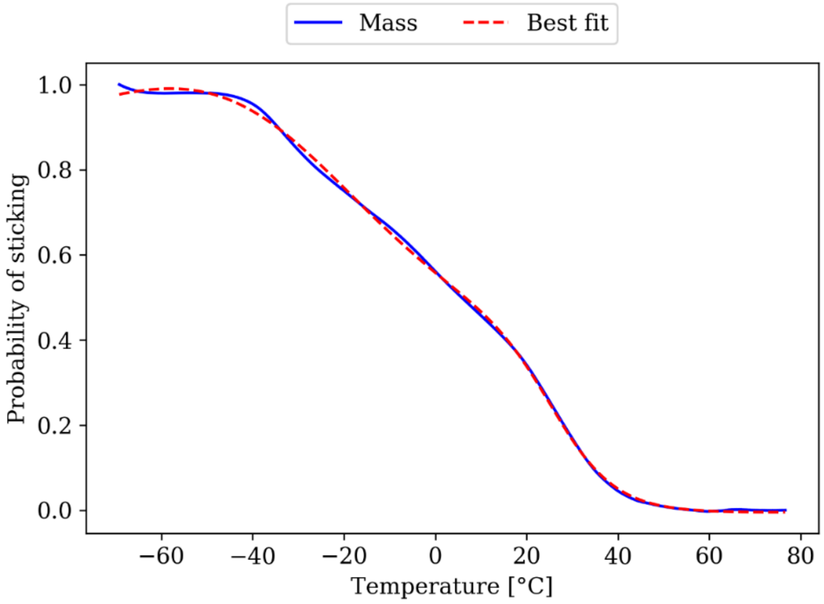
$Tc_{\alpha 3}$ = 14°C



$$w_a = \frac{A_\alpha}{\sum \alpha}$$

Probability of sticking

For a certain outgassing step and the range of surface temperatures



$$S(T) = \sum_{\alpha=1}^{\alpha} w_\alpha \cdot \frac{1}{1+e^{\frac{T - Tc\alpha}{\Delta Tc\alpha}}}$$

$$m_{deposit}(T_{QCM}) = TML \cdot (S(T)aq + S(T))$$

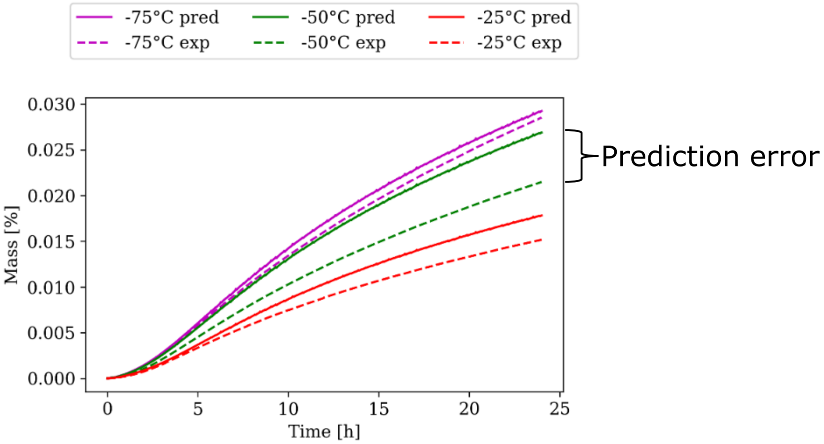
$S(T)$ - sticking coefficient for mixture of chemical species at given temperature

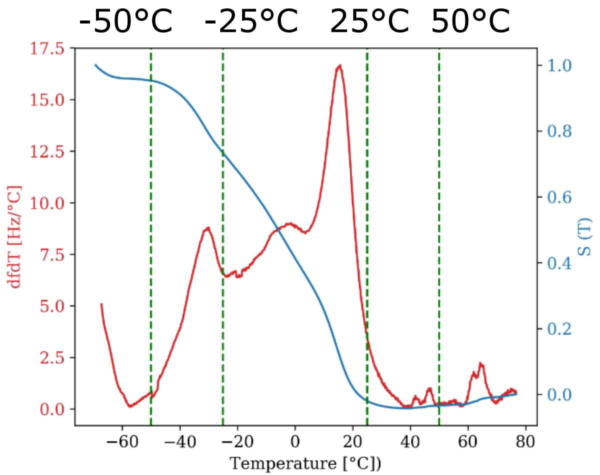
$w_{\alpha/aqua}$ - weight fraction of species α/water

Tc_α - captation temperature for species α

ΔTc_α - transition coefficient for species α

Results – step4, T outgassing = 100°C





Material A (adhesive) –low outgassing

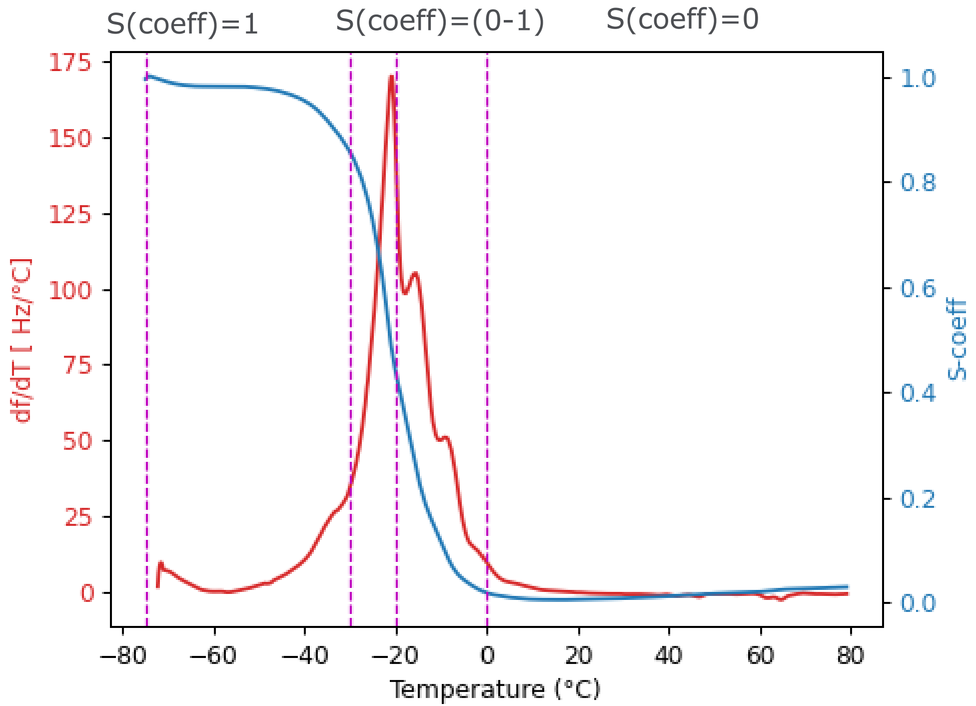
T [°C]	-75	-50	-25	25	50
S(T)	1	1	0.7	0.1	0
md (%) Predicted	0.029	0.027	0.017	0.003	0
md (%) Measured	0.028	0.021	0.015	0.002	0

Material B (silicone compound) – high outgassing

T [°C]	-75	-50	-25	25	50
S(T)	1	1	1	0.2	0
md (%) Predicted	0.278	0.275	0.273	0.045	0
md (%) Measured	0.276	0.276	0.244	0.01	0

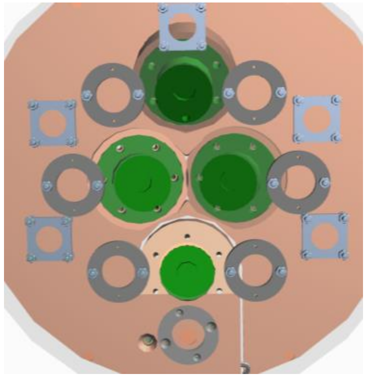
Sticking coefficients in the slope of TGA

Temperatures of 4 QCMs set to match specific S(coeff) values

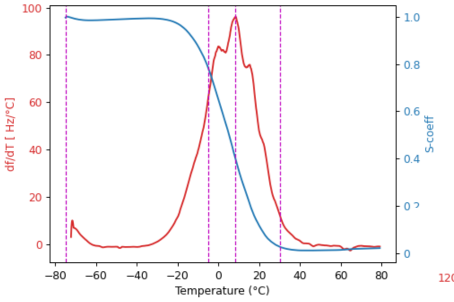


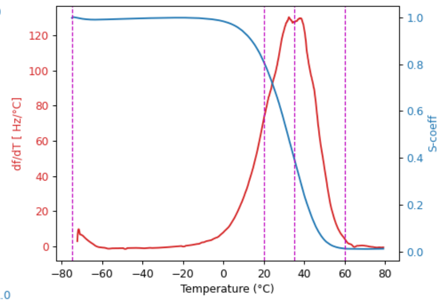
Silicone compound, Step 2 - 50°C				
T [°C]	-75	-30	-20 (peak)	0
S(T)	1	0.8	0.5	0
md (%) Predicted	0.14	0.12	0.07	0
md (%) Measured	0.10	0.01	0.01	0

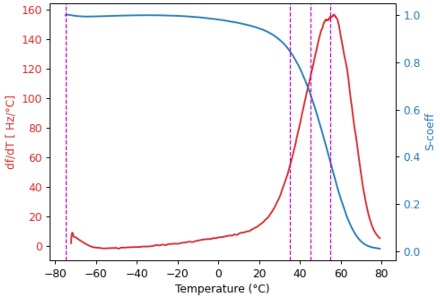
$$T_{QCM,1} \cong S(coeff) = 1$$
$$T_{QCM,2} \cong S(coeff) = 0.8$$
$$T_{QCM,3} \cong S(coeff) = DTG\ max$$
$$T_{QCM,4} \cong S(coeff) = 0$$



Reemission at higher temperatures







Step 3 75 ℃

T [°C]	-75	-5	8(DTG peak)	30
S(T)	0.99	0.8	0.4	0
md (%) Predicted	0.17	0.14	0.07	0
md (%) Measured	0.17	0.03	0.01	0

Step 4 100 ℃

T [°C]	-75	20	35(DTG peak)	60
S(T)	0.99	0.82	0.38	0
md (%) Predicted	0.28	0.23	0.11	0
md (%) Measured	0.3	0.04	0	0

Step 5 125 ℃

T [°C]	-75	35	45	55 (DTG peak)
S(T)	0.99	0.82	0.38	0
md (%) Predicted	0.35	0.29	0.13	0
md (%) Measured	0.36	0.10	0.03	0

Prediction of contamination levels

Current approach:

Test > Input parameters > Modelling tool (e.g. SYSTEMA/AIRBUS)

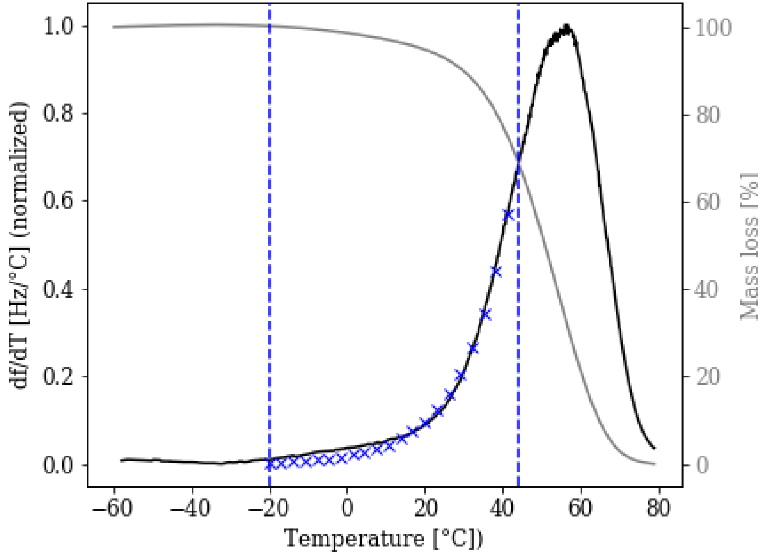
$$m_{deposit}(T) = TML - m_0 e^{\frac{-Ea}{RT}}$$

Reemission rate is dependent on Ea of chemical species – the energy required to initiate the reemission process according to the relation exp(- Ea/RT) – currently we do not calculate the kinetic parameters for each specie as there is no guarantee that the mathematical species overlap with physical species (Species separation work is ongoing with colleagues from Onera)

100 % if $T_s < Tc_{a1}$

(0 – 100%) if $T_s > Tc_{a1}$ & T_s , Tc_{an} -> Future work

0% if $T_s > T_{DTG}$



Conclusions

1 **QTGA** added to standard outgassing test **allows reasonable estimation of contamination levels** by assessing the probability of sticking at given surface temperature

2 **The prediction error is the most significant in the temperature region of the TGA slope**, where the QTGA reaction progresses fast, typically in a narrow temperature window, so adding more temperature points (QCMs) in this region can significantly improve the prediction accuracy

3 **The goal is to substantially simplify the extraction of reemission parameters**, so such procedure could be implemented more routinely for a variety of spacecraft projects

For more information please see:

Suliga, Agnieszka, Orcun Ergincan, and Riccardo Rampini. "Modeling of Spacecraft Outgassed Contamination Levels by Thermogravimetric Analysis." Journal of Spacecraft and Rockets (2021): 1-7.

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Modeling of Spacecraft Outgassed Contamination Levels by Thermogravimetric Analysis

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Outgassing from spacecraft materials is known to degrade performance of various components, of which particularly affected are cold and cryogenic surfaces. For those surfaces that suffer from performance losses due to molecular contamination, it is important to assess the contamination levels at an early stage of a project to apply necessary risk mitigation and/or risk avoidance. The focus of this work is on the reemission parameters of the molecular contamination model used in the simulations and improvement of the long-term predictions of in-flight contamination levels. This is realized by experimentally finding a number of sticking coefficients for a set of chemical species released from a contaminated surface during the thermogravimetric analysis. The predicted results are in good agreement with the experimental values.