Optimization of Outgassing Test Methods for Contaminant Species Extraction, Characterization and Modeling

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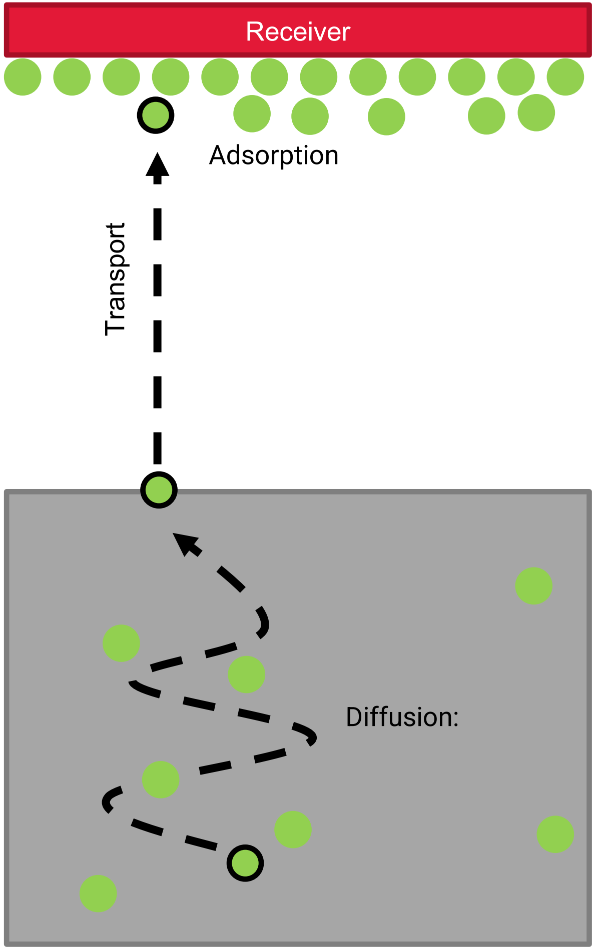
Introduction

- Current and future concept space exploration missions seek to determine past and present capability to support life and presence of life outside of Earth
- Knowledge of molecular constituents outgassed from spacecraft is needed to analyze the probability of a mission to meet its science objectives
- Outgassing analysis methods are needed to further current predictive capabilities
- JPL and collaborators are currently working on the development of multispecies formulations for materials outgassing to allow more accurate extrapolation to mission conditions.

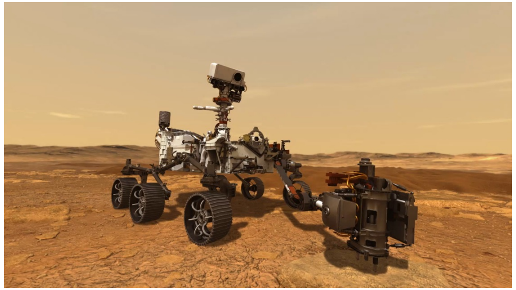
Outgassing

- Outgassing is the spontaneous evolution of atoms or molecules from a material
- Outgassing contamination is governed by several processes
  1. Diffusion of contaminant through the source material
  2. Viable Transport Mechanism
  3. Adsorption to the receiver material
  - 1,2,4 All of these physical processes have an exponential, Arrhenius, dependence on temperature
- Transport depends on environment (vacuum/continuum) and geometry
  - Continuum: Diffusion/Convection transport
  - Rarefied: Intermediate Knudsen number
  - Vacuum: Ballistic (line of sight) transport



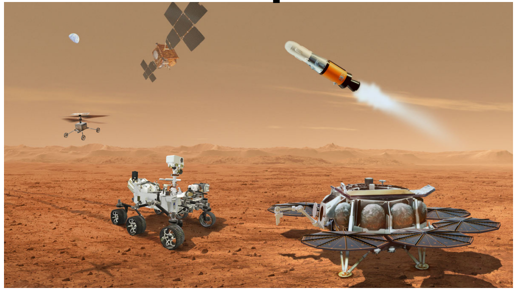
Outgassing Sensitivities Examples

Mars 2020



- Sampling Mars with objectives to detect organic signatures
- Outgassing contaminants condensing within sample tubes could jeopardize detection

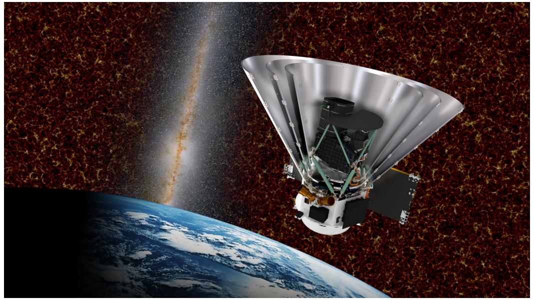
Mars Sample Return



- Returning sample tubes intended to detect organic signatures
- Outgassing contaminants leaking through sealed tubes could jeopardize scientific objectives

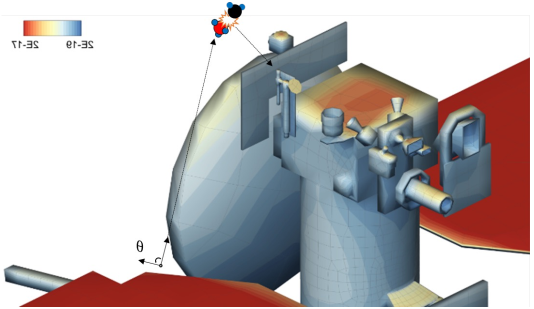
Outgassing must be characterized and quantified over the mission to guarantee scientific objectives

SPHEREx



- Scientific objectives to image biogenic molecules in the universe
- Water outgassing condensing in telescope causes severe attenuation of throughput

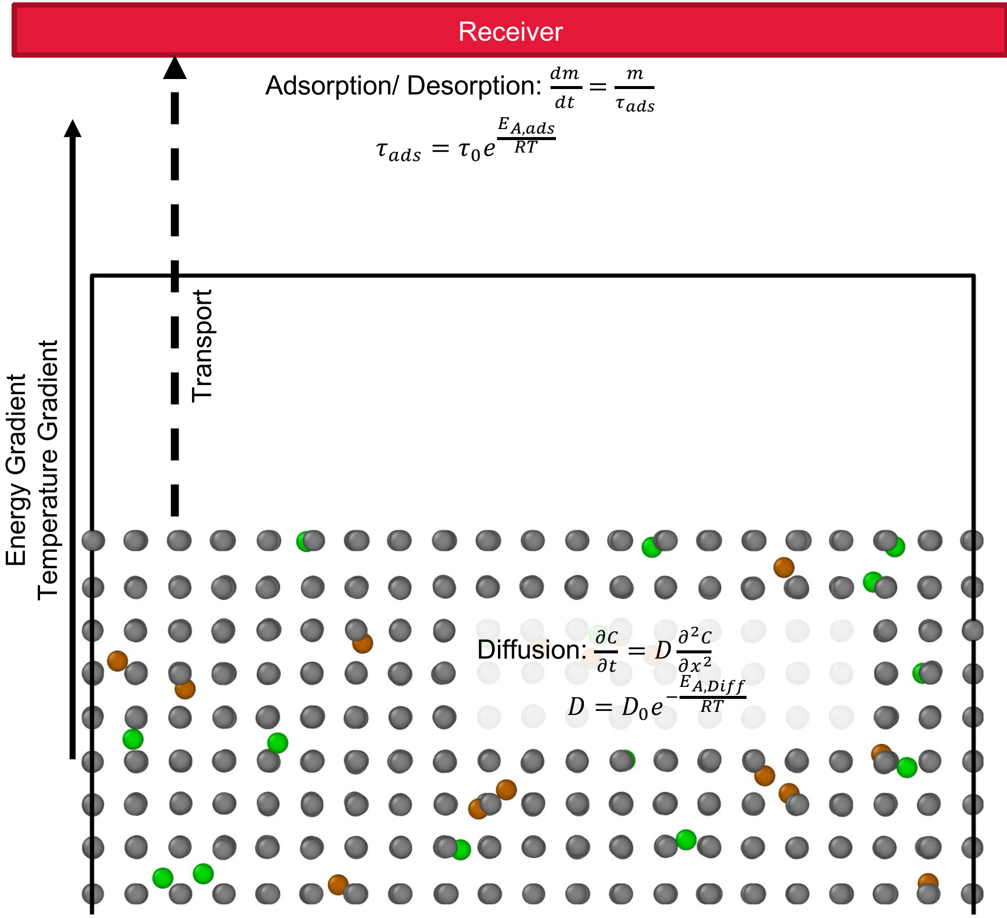
Europa Clipper



- Mass spectrometer instrument with objectives to sample Europa's atmosphere
- Outgassing contaminants reflected off atmosphere induce spurious mass spectra

Outgassing Kinetics

- Diffusion: $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$
    - Diffusion coefficient: $D = D_0 e^{-\frac{E_{a,diff}}{RT_{source}}}$
    - Initial Concentration: C_0
- Desorption/Adsorption: $\frac{dm}{dt} = \frac{m}{\tau}$
    - Residence time: $\tau_{ads} = \tau_0\, e^{-\frac{E_{a,ads}}{RT_{reciever}}}$
- Variables in red are the kinetic contaminant parameters which characterize a contaminant species outgassing behavior
    - Per contaminant species: $\{C_0, D_0, E_{a,diff}, \tau_0, E_{a,ads}\}$
    - In this model desorption from source material is not considered

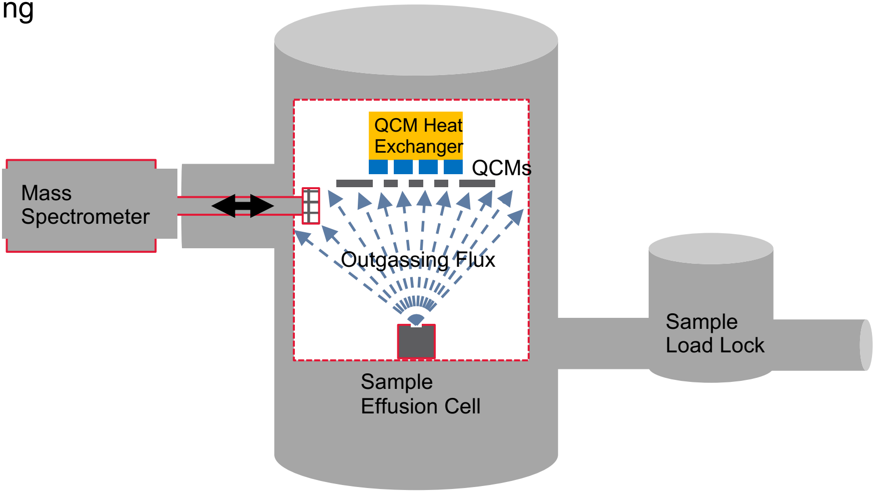


Molecular Dynamic Simulation of Outgassing

Outgassing Testing

- Outgassing materials testing is typically performed in specialized vacuum chambers designed for precise measurements of outgassing.
- Typically two test exercises to characterize outgassing kinetics
  1. Outgassing:
     - Sample is held at constant temperature or predefined temperature steps. Controls diffusion of outgassing out of sample material
     - Multiple QCMs at different temperatures measure outgassing collection over time. Controls residence time on different QCMs
  2. Reemission / QCM Thermo Gravimetric Analysis (QTGA):
     - QCM temperature is slowly raised (1C/min). Slowly changes residence time so contaminant species desorb.

- ASTM E1559: Standard Test Method for Contamination Outgassing Characteristics of Spacecraft Materials
- ECSS-Q-TM-70-52a: Kinetic outgassing of materials for space

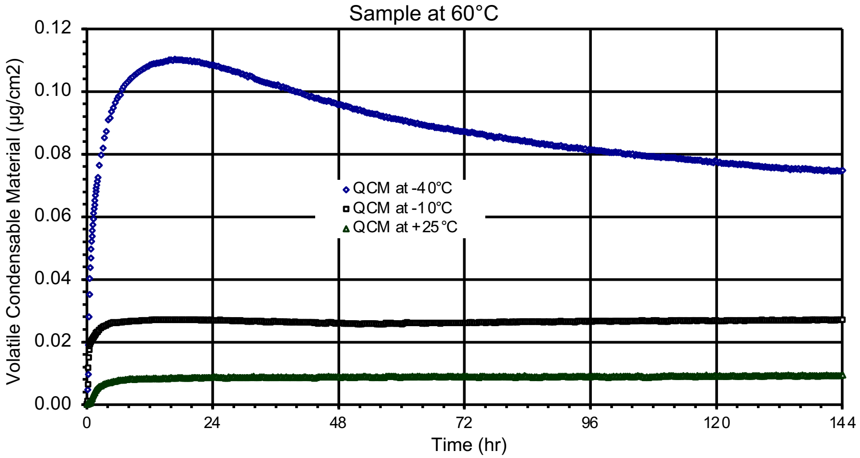


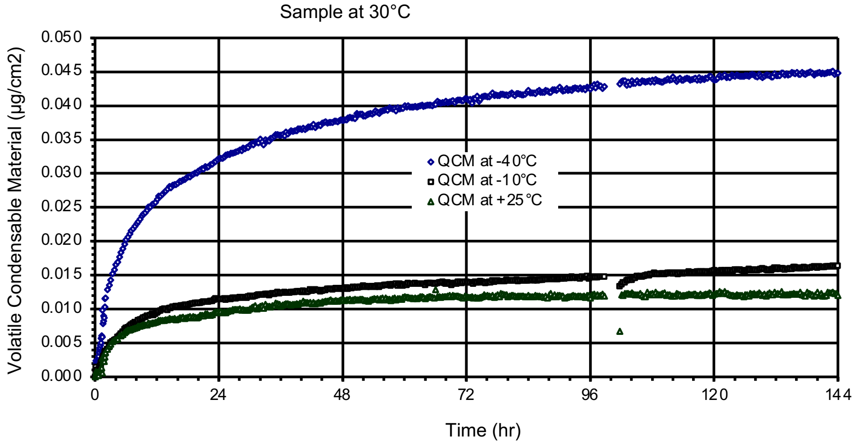
Testing Methodology Comparison

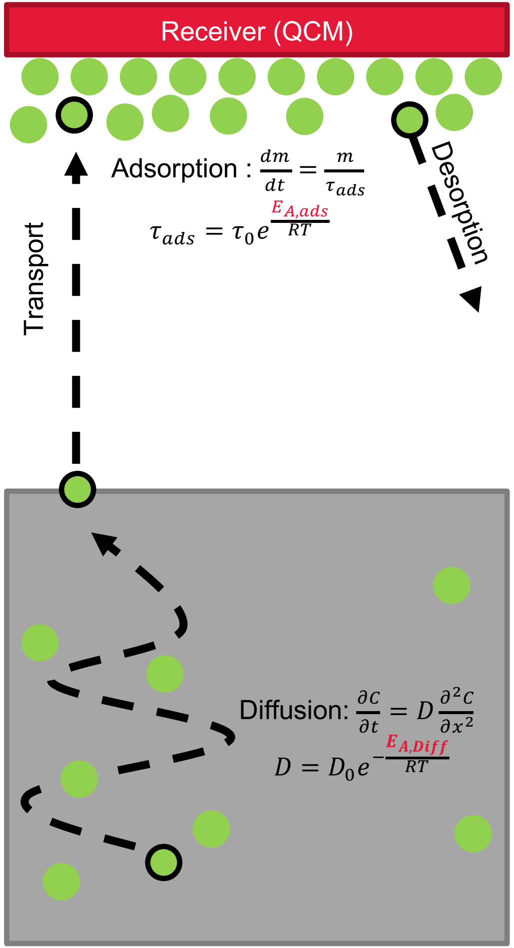
- ASTM E1559
  - Standard Test Method for Contamination Outgassing Characteristics of Spacecraft Materials
  - Outgassing test exercise is typically a single temperature isothermal outgassing
  - Method A: Prescribed source/source temperature and QCM temperatures
  - Method B: Allow variance of temperatures for application specific data
  - Includes a QTGA test exercise at the end of the test
  - Does not provide modeling recommendations
- ECSS-Q-TM-70-52a
  - ECSS-Q-TM-70-52A: Kinetic outgassing of materials for space
  - Outgassing test exercise is primarily temperature steps every 24 hours from 25C to 125C
  - Includes a QTGA test exercise at the end of the test
  - Provides several recommendations of outgassing modeling methods (ESTEC, ONERA)

Outgassing Isothermal Test

- More typical of ASTM-E1559 method
- Sample is held at constant temperature. Controls diffusion of outgassing out of sample material
- Multiple QCMs at different temperatures measure outgassing collection over time
- Net rates of accumulation on different temperature QCMs provides information on residence time: $E_{a,des}$
- Total accumulation on QCMs provide information on initial concentrations C_0


Sample at 60°C


Sample at 30°C



Adsorption : $\frac{dm}{dt} = \frac{m}{\tau_{ads}}$

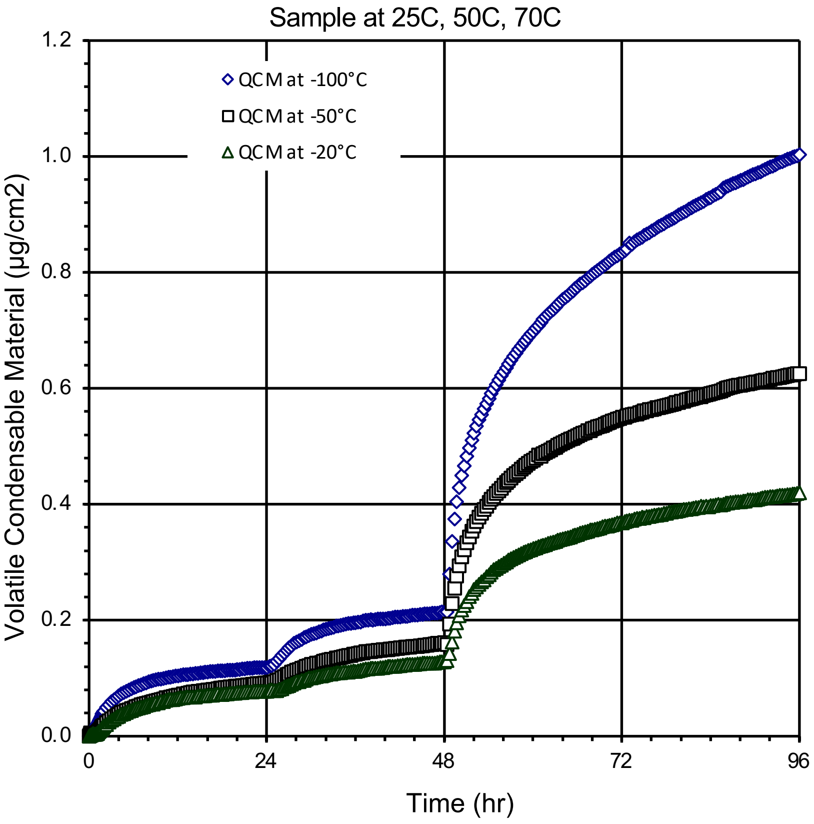
$\tau_{ads} = \tau_0 e^{\frac{E_{A,ads}}{RT}}$

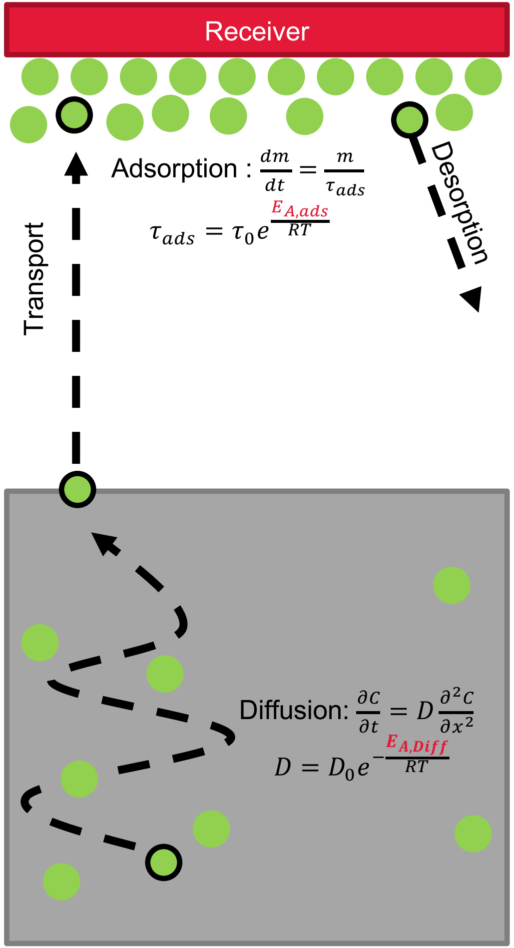
Diffusion: $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$

$D = D_0 e^{-\frac{E_{A,Diff}}{RT}}$

Stepped Outgassing Test

- Typical for ECSS-Q-TM-70-52a method
- Sample is held predefined temperature steps.
- Multiple QCMs at different temperatures measure outgassing collection over time
- Total accumulation on QCMs provide information on initial concentrations C_0
- Net rates of accumulation on different temperature QCMs provides information on residence time: $E_{a,des}$
- Change in sample temperature probes $E_{a,diff}$





Adsorption : $\frac{dm}{dt} = \frac{m}{\tau_{ads}}$

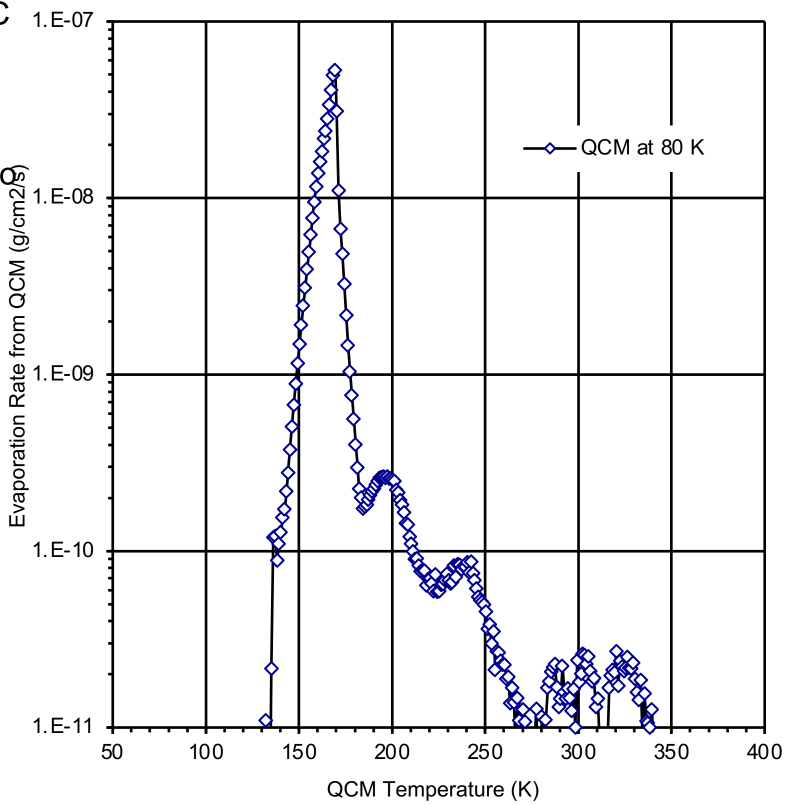
$$\tau_{ads} = \tau_0 e^{\frac{E_{A,ads}}{RT}}$$

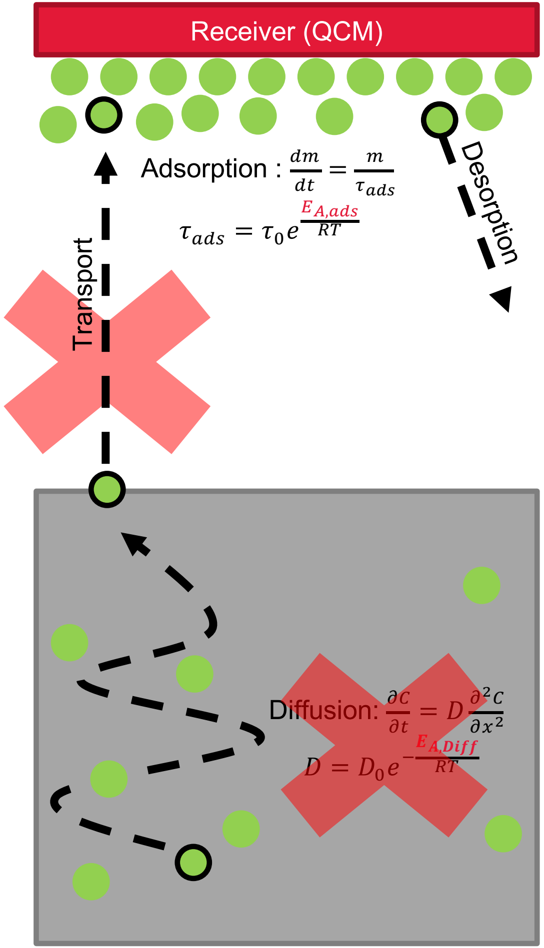
Diffusion: $\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$

$$D = D_0 e^{-\frac{E_{A,Diff}}{RT}}$$

QCM Thermo Gravimetric Analysis Test

- Common to ASTM and ESCC test methods
- Outgassing sample is removed from test chamber into load lock so QCMs are no longer accumulating
- QCM temperature is slowly raised (1C/min). Slowly changes residence time so contaminant species desorb
- Provides information on residence time in in much higher granularity, $E_{A,ads}$
- As temperature of QCM is raised slowly, contaminant species desorb sequentially due to their residence time

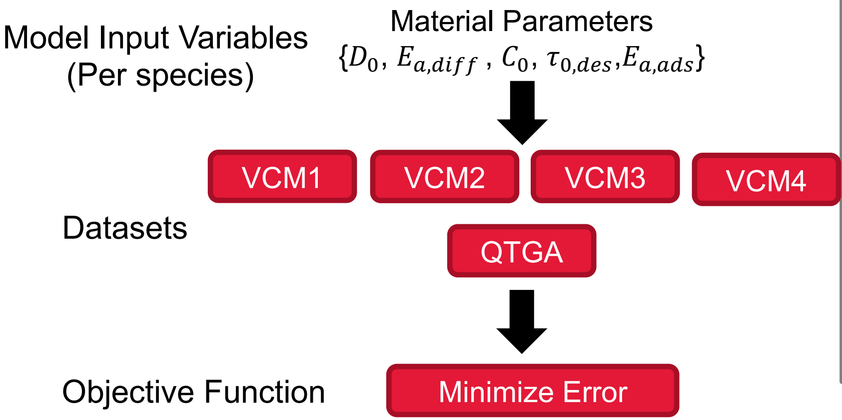


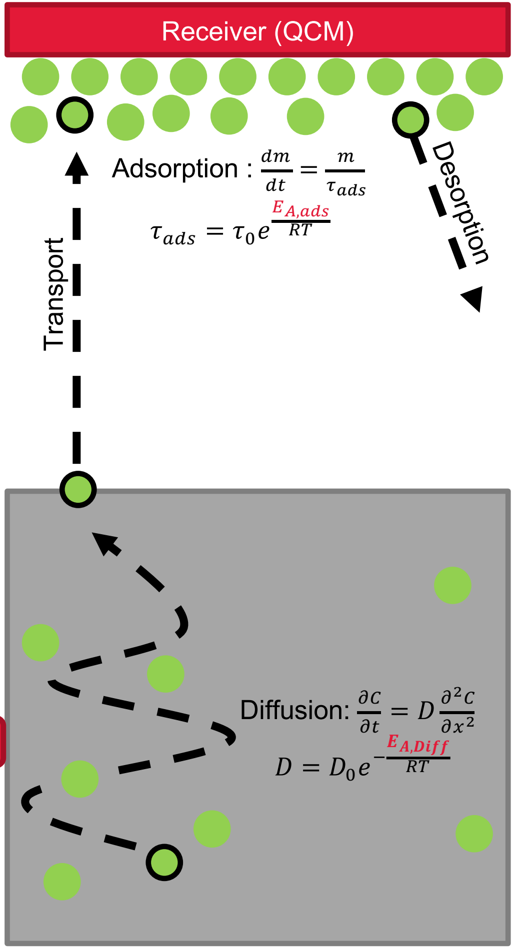


Multispecies Model Kinetic Fitting Scheme

- All available datasets are fit to minimize error between model and data
- VCMs datasets:
  - Modeling both diffusion and adsorption/desorption collection.
  - Critical to model both to describe desorption.
- QTGA datasets:
  - At least 1 QTGA at the end of the test. May contain many QTGA datasets
  - Modeling adsorption/desorption

- Result from a good fit is a set of kinetic contaminant parameters (per contaminant species) which characterize outgassing from that material and adsorption/desorption





$$\frac{dm}{dt} = \frac{m}{\tau_{ads}}$$

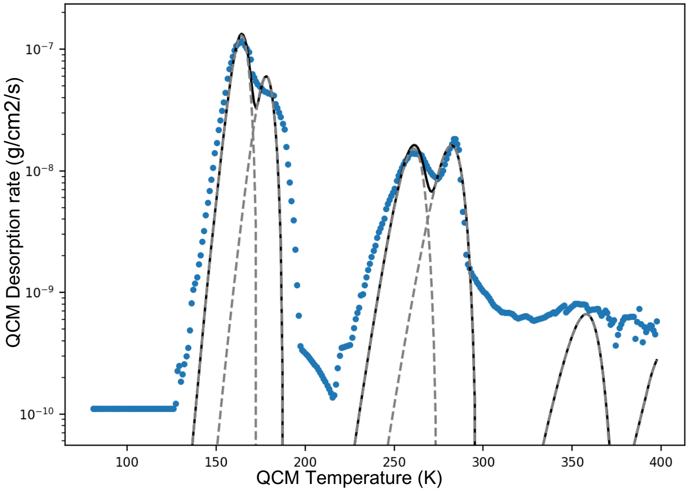
$$\tau_{ads} = \tau_0 e^{\frac{E_{A,ads}}{RT}}$$

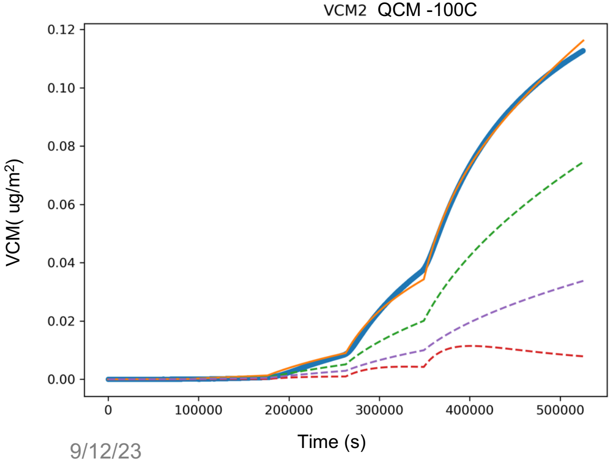
$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

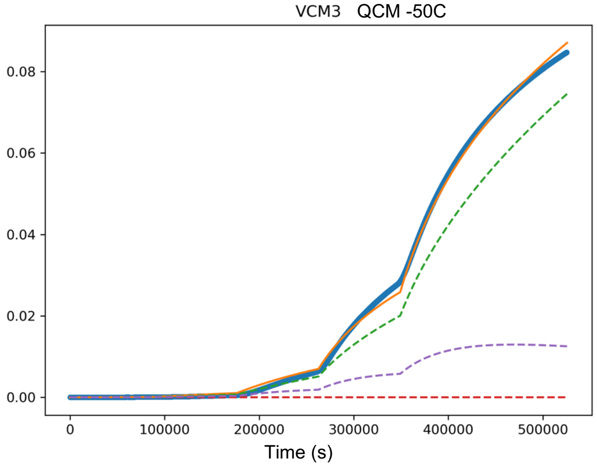
$$D = D_0 e^{-\frac{E_{A,Diff}}{RT}}$$

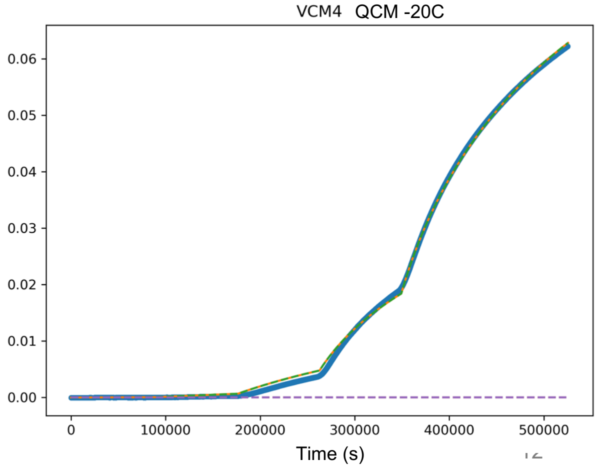
Example Multispecies Model Fit

- Test material isothermal has temperature steps at 20C 40C and 70C with QCMs collecting at 80K, -100C, -50C, -20C
- Model simultaneously reproduces key outgassing and collection features
  - QTGA and reemission residence times
  - Temperature behavior of outgassing
  - Decay of outgassing due to diffusion of contaminants
  - Collection of outgassing on different QCM temperatures




VCM2 QCM -100C


VCM3 QCM -50C

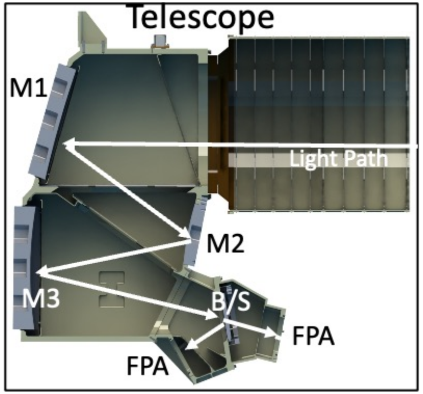

VCM4 QCM -20C

Testing Methodology Comparison

- Outgassing model *needs* be able to describe all scenarios and extrapolate to mission specific scenarios
    - Temperature change is outgassing source
    - Depletion of contaminant in source material
    - Adsorption/desorption of contaminant on receiving surface
    - Temperature change in receiving surface
- Multiple Isothermal tests
    - More typical of ASTM E1559
    - Less transferable
    - Commonly prebaked
    - More tailored to mission specific conditions. (worst case hot, worst case cold, etc...)
    - Multiple tests need to be performed to characterize material. Single isothermal test cant characterize temperature dependence of outgassing source
- Temperature steps
    - ECSS-Q-TM-70-52a
    - More transferable
    - Not mission specific
    - Single test extracts all kinetic parameters
    - Can extrapolate to mission specific conditions with correct modeling approach
- From development and usage of JPL multispecies model planned approach is to design test to extract material parameters and rely on model to extrapolate to mission conditions (temperature steps)

SPHEREx Example

- One of the primary objective of SPHEREx is to measure the existence of water in the universe
- Water molecules have a very strong adsorption peak in 2.75-3.35 μm wavelength
- Instrument is very sensitivity to water condensing onto the optical elements
- Attenuation of water contamination on instrument is exact wavelengths instrument is intended to detect
- Initial prediction of water accumulation led to unacceptable attenuation of scientific data



	Initial Requirements [2]
Mirror 1 (x2 surfaces)	100Å
Mirror 2 (x2 surfaces)	100Å
Mirror 3 (x2 surfaces)	100Å
Beamsplitter (x2 surfaces)	100Å
Detector (x1 surface)	100Å
Optical path thickness	900Å
Total absorption at α_{peak}	24%

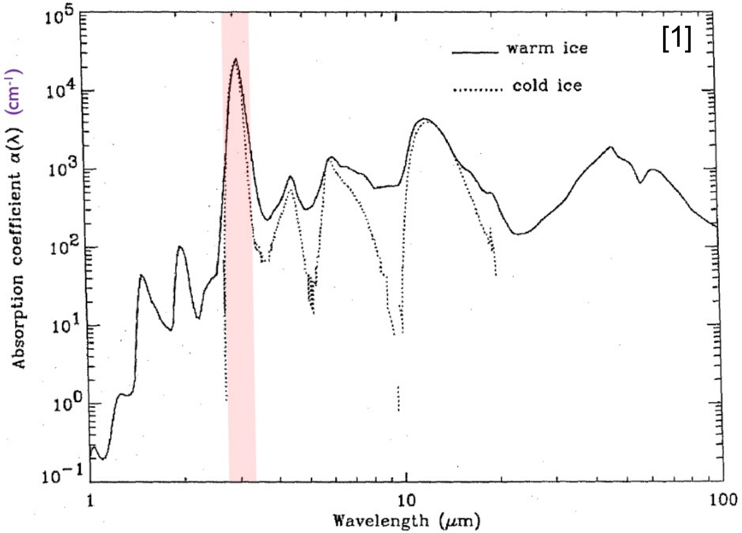


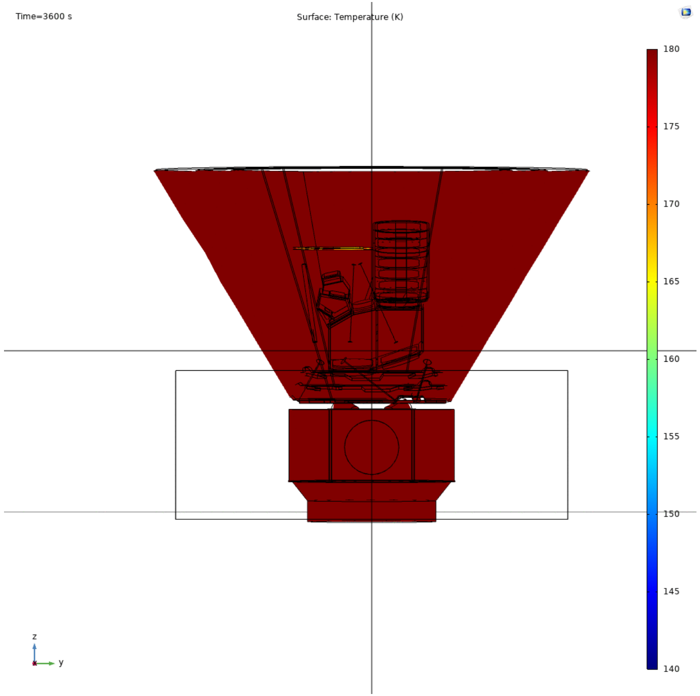
Figure 2. Absorption coefficient α(λ) of warm (250K)[6] and cold (80K)[8] ice based on tabulations of Warren[6] and Hudgins et al.[8]

[1] Lynch, D. K. The infrared spectral signature of water ice in the vacuum cryogenic AI&T environment. AEROSPACE CORP EL SEGUNDO CA, 2005.
[2] Alred, John M., et al. "Designing a Decontamination Solution for the Low-Earth-Orbit, Cryogenic SPHEREx Mission." 2021 IEEE Aerospace Conference (50100). IEEE, 2021.
[3] Alred, J. M., et al., 2022. "Modeling Contaminant Outgassing and Free Molecular Transport Processes for the Cryogenic SPHEREx Observatory." Presentation, 32nd International Symposium on Rarefied Gas Dynamics (RGD32).

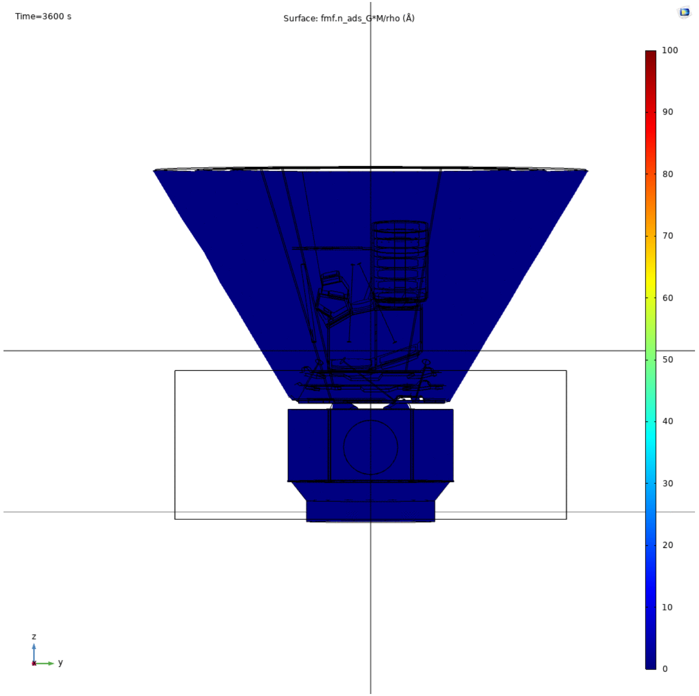
SPHEREx Example

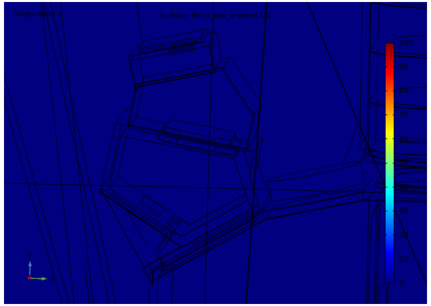
- Water outgassing transport simulation of the SPHEREx observatory
- Fully time/temperature resolved

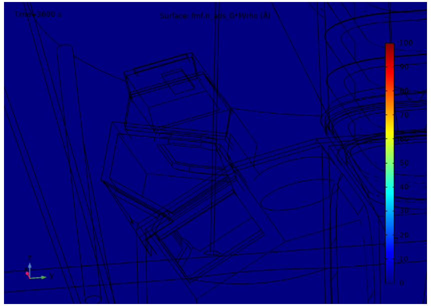
Temperature 0-180K



Accumulation 0-100 Angstroms



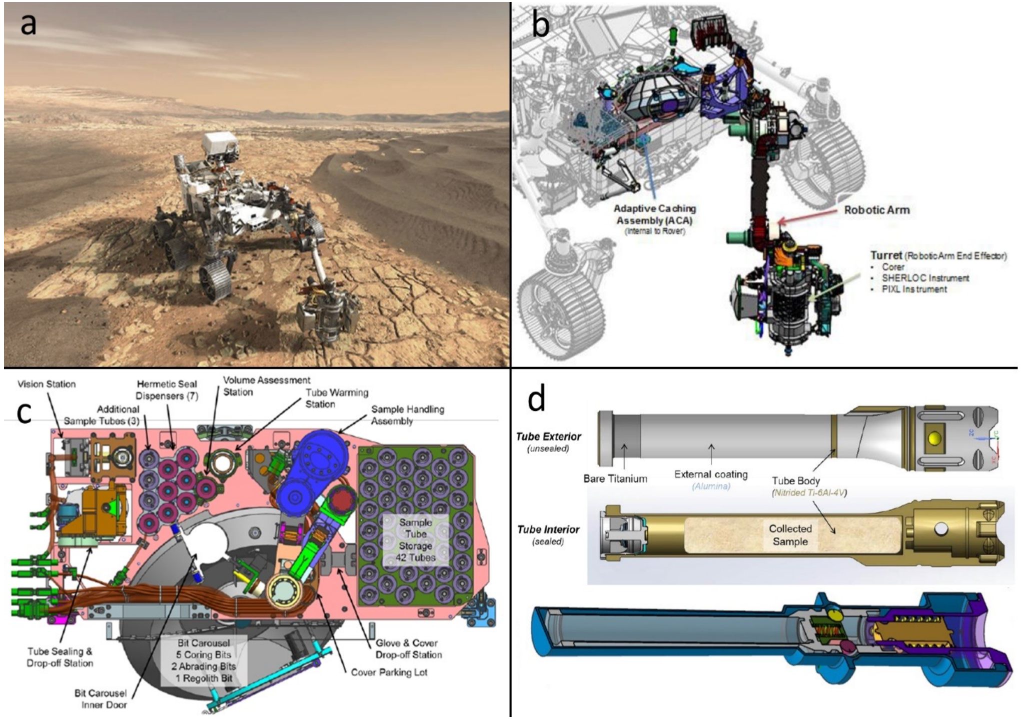




Alred, J. M., et al., 2022. “Modeling Contaminant Outgassing and Free Molecular Transport Processes for the Cryogenic SPHEREx Observatory.” Presentation, 32nd International Symposium on Rarefied Gas Dynamics (RGD32).

Mars 2020 Example

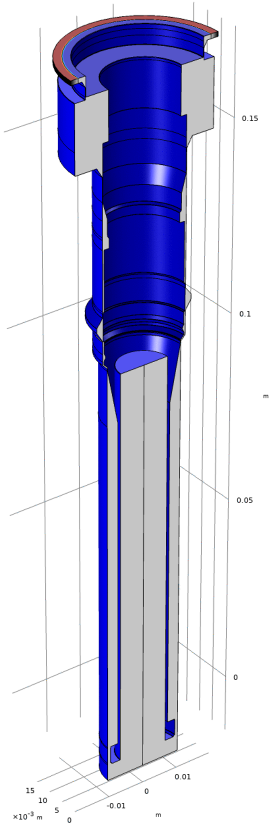
- Scientific requirement of less than 10 parts per billion (PPB) Total Organic Carbon (TOC) of terrestrial origin within the cached samples
- Each sample is nominally 15g which means less than 150ng of contamination can be tolerated
- This is less than a single layer of adsorbed contaminant molecules within the sample tubes
- More complicated than just cleaning sample tubes before launch. Outgassing can easily exceed this budget

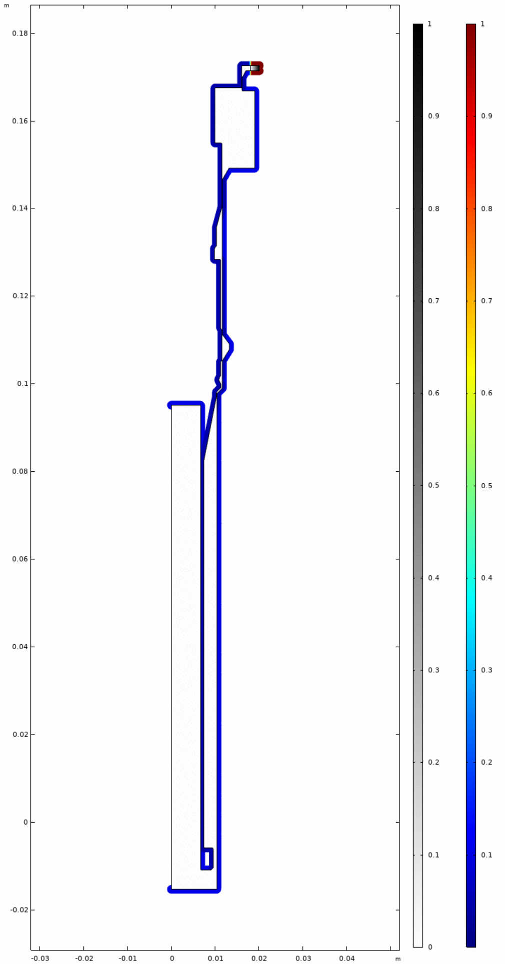


1. Alred, J., Martin, M., Hoey, W., Wong, A., White, L., Boeder, P., Cofer, S., Dias-Ribeiro, A., Soares, C., 2020. “Predicting Terrestrial Contamination of the Mars 2020 Sample Caching System with Novel Multispecies Outgassing and Transport Models.” Proceedings vol. 11489, Systems Contamination: Prediction, Control and Performance; 1148904.

Mars 2020 Example

- Simulation of contamination and accumulation transport in the sample tube Fluid Mechanical Particle Barrier (FMPB) during Assembly test and launch operations (ATLO)
- Contamination is mainly adsorbed by the high energy surfaces and cannot diffuse into the sample intimate surfaces
- Up through launch it is predicted that the sample tubes remained at their as-cleaned cleanliness
- This is expected to significantly improve estimates over the previous model





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1. Alred, J., Martin, M., Hoey, W., Wong, A., White, L., Boeder, P., Cofer, S., Dias-Ribeiro, A., Soares, C., 2020. "Predicting Terrestrial Contamination of the Mars 2020 Sample Caching System with Novel Multispecies Outgassing and Transport Models." Proceedings vol. 11489, Systems Contamination: Prediction, Control and Performance; 1148904.

Conclusions and Future Work

- JPL has been working, with several collaborators, to develop a multispecies kinetic outgassing model to allow for high fidelity characterization and prediction of outgassing
- The model has been applied to fit several different outgassing test profiles
- Heritage outgassing tests commonly test materials several times at mission conditions
- Current plan is to use multispecies kinetic model and optimize test profiles for extraction of material parameters

- Test campaign planned to compare heritage testing approach to newer test profiles to validate relying on model extrapolation to mission conditions
- Currently working on incorporation of mass spectrometry to obtain chemical information of outgassing species

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Recent Relevant Publications by JPL

Europa Clipper:

- *Soares, C., Wong, A., Hoey, W., Fugett, D., Anderson, J., Alred, J., Thorbourn, D., 2022. "High-Energy Radiation Induced Outgassing Testing and Modeling for Jovian System Missions." Presentation, ISMSE 15.*
- Ricchiuti, V., Fugett, D., Soares, C., 2022. "Modeling of Contamination Vent Path for Outgassing Components Underneath Thermal Blankets on Europa Clipper." Presentation, SPIE Optical Engineering + Applications Conference, San Diego, CA.
- Fugett, D., Soares, C., Wong, A., Anderson, J., Ricchiuti, V., Hoey, W., 2022. "Contamination Control Approach to Mitigating Radiation Induced Outgassing on Europa Clipper." Proc. IEEE Aerospace Conference.
- Anderson, J., Wong, A., Fugett, D., Hoey, W., 2020. "Modeling Radiation Influence on Spacecraft Materials Outgassing." Proc. IEEE Aerospace Conference.
- Soares, C., Hoey, W., Anderson, J., Ferraro, N., 2019. "Spacecraft Return Flux Considerations for Missions Targeting Detection of Organics with Mass Spectrometers." Proc. 70th International Astronautical Congress.
- Soares, C., Wong, A., Fugett, D., Hoey, W., Alred, J., Ferraro, N., Thorbourn, D., 2019. "High-Energy Radiation Testing and Effects on Spacecraft Materials Outgassing." Proc. 70th International Astronautical Congress.
- Wong, A., Fugett, D., Thorbourn, D., Martin, E., Hoey, W., et al. 2019. "Evaluating the *In Situ* Outgassing Characteristics of Silicone Adhesives in a Europa-Like Environment." Presentation, Applied Space Environments Conference, Los Angeles, CA.
- Hoey, W., Anderson, J., Soares, C., 2019. "State-of-the-Art Modeling of Contaminant Transport in Vacuum Chambers and Space Environments." Presentation, Applied Space Environments Conference, Los Angeles, CA.

Psyche Asteroid Mission:

- Martin, M., Alred J., Hoey, W., Ly, C., Soares, C., 2022. "Contamination Control Program for the Psyche Asteroid Mission." Presentation, SPIE Optical Engineering + Applications Conference, San Diego, CA.
- Martin, M., Hoey, W., Alred, J., Soares, C., Ferraro, N., 2021. "Understanding Spacecraft Test Environments in JPL's Twenty-Five-Foot Space Simulator." Presentation, Applied Space Environments Conference, Los Angeles, CA.
- Martin, M., Hoey, W., Alred, J., Soares, C., 2020. "Novel Contamination Control Model Development and Application to the Psyche Mission." Proc. IEEE Aerospace Conference.
- Martin, M., Wong, A., Hoey, W., Alred, J., Boeder, P., Soares, C., 2019. "Advancements in Monitoring and Operating Thermal Vacuum Environmental Test Chambers for Next-Generation Space Exploration Hardware." Presentation, 66th International Symposium of the American Vacuum Society, Columbus, OH.

Recent Relevant Publications by JPL

Mars 2020 Perseverance:

- Wong, A., Martin, M., Hoey, W., Soares, C., Hurst, K., Roberts, E., Perkins, R., Maltais, T., Shiraishi, L., Boeder, P., Alred, J., 2022. “Understanding Sampling Hardware Cleanliness from Perseverance Lessons Learned, and Forward Approach to Biosignature Missions.” Proc. AIAA SciTech Conference.
- Alred, J., Martin, M., Hoey, W., Wong, A., White, L., Boeder, P., Cofer, S., Dias-Ribeiro, A., Soares, C., 2020. “Predicting Terrestrial Contamination of the Mars 2020 Sample Caching System with Novel Multispecies Outgassing and Transport Models.” Proceedings vol. 11489, Systems Contamination: Prediction, Control and Performance; 1148904.
- Katz, I., Anderson, M., White, L., Boeder, P., Hoey, W., 2018. “Mars 2020 Sample Cleanliness Molecular Transport Model.” SPIE Opt. Eng. + Appl. Proceedings 10748, Systems Contamination: Prediction, Control and Performance 107480A.
- Soares, C., Hoey, W., Anderson, J., Anderson, M., Boeder, P., Ferraro, N., Liao, S., Sylvia, M., 2018. “Spacecraft Contamination Control Challenges for Space Missions with Organic Compound Detection Capabilities and for Potential Sample Return.” Proc. International Symposium on Materials in the Space Environment.

SPHEREx Observatory:

- Alred, J. M., et al., 2022. “Modeling Contaminant Outgassing and Free Molecular Transport Processes for the Cryogenic SPHEREx Observatory.” Presentation, 32nd International Symposium on Rarefied Gas Dynamics (RGD32).
- Alred, J. M. et al., 2021. “Designing a Decontamination Solution for the Low-Earth-Orbit, Cryogenic SPHEREx Mission,” Proc. IEEE Aerospace Conference.

Europa Lander Mission Concept:

- Hoey, W., Soares, C., Alred, J., Anderson, J., Martin, M., Shallcross, G., Wong, A., 2022. “Spacecraft Engine Plumes in Near-Vacuum: Earth’s Moon and Beyond.” Presentation, 32nd International Symposium on Rarefied Gas Dynamics (RGD32).
- Conte, A., Hoey, W., Wong, A., Soares, C., Grabe, M., Hepp, C., 2022. “Europa Lander Plume-Induced Contamination: Monopropellant Thruster Plumes Modeling in STG-CT High-Vacuum Chamber.” **(Manuscript in review)*
- Hoey, W., Lam, R., Wong, A., Soares, C., 2020. “Europa Lander Engine Plume Interactions with the Surface and Vehicle.” Proc. IEEE Aerospace Conference.
- Lam, R., Maghsoudi, E., Hoey, W., 2019. “Numerical Study of Lander Engine Plume Impingement on the Surface of Europa.” Proc. 66th JANNAF Propulsion Meeting / 37th Exhaust Plume and Signatures (EPSS) Meeting.

Recent Relevant Publications by JPL

Gateway:

- *Hoey, W., Soares, C., Martin, M., Shallcross, G., Steagall, C., Worthy, E., 2022. "A Predictive Model of Lunar Gateway Molecular Contamination." Presentation, ISMSE 15.*

Roman Space Telescope Coronagraph Instrument (CGI):

- Sylvia, M., Martin, M., Anderson, M., Cardines, J., Aldrich, D., Zhou, C., Hoey, W., Soares, C., 2021. "Contamination Requirements and Mitigation Strategies for the Nancy Grace Roman Coronagraph Instrument (CGI)." Presentation, 2021 NASA Contamination, Coatings, Materials, and Planetary Protection Workshop (CCMPP).

Fairing Particle Redistribution:

- Alred, J. M., et al., 2022. "Particle Contamination Launch Redistribution and Effects on the Low-Earth-Orbit Infrared SPHEREx Telescope." Presentation, SPIE Optical Engineering + Applications Conference, San Diego, CA.
- Hoey, W., Shallcross, G., Martin, M., Soares, C., Cooper, M., 2022. "Launch recontamination: planetary protection models for particle transport in spacecraft payload fairing environments." Presentation; 44th Committee on Space Research (COSPAR).
- Shallcross, G., Hoey, W., Soares, C., Cooper, M., 2022. "Launch recontamination: the evaluation of particle adhesion and removal mechanisms in spacecraft payload fairing environments." Presentation; 44th Committee on Space Research (COSPAR).
- Hoey, W., Alred, J., Anderson, J., Martin, M., Soares, C., Droz, E., Shallcross, G., 2021. "Toward Predictive Models of Launch Ascent Depressurization and Induced Particle Redistribution." Presentation, 2021 NASA Contamination, Coatings, Materials, and Planetary Protection Workshop (CCMPP).
- Anderson, J., Hoey, W., Alred, J., Soares, C., Brieda, L., 2020. "Space Launch Vehicle Transient Particle Redistribution Modeling and Implications for Optically Sensitive Payloads." Proceedings v. 11489, SPIE Systems Contamination: Prediction, Control and Performance; 114890D.

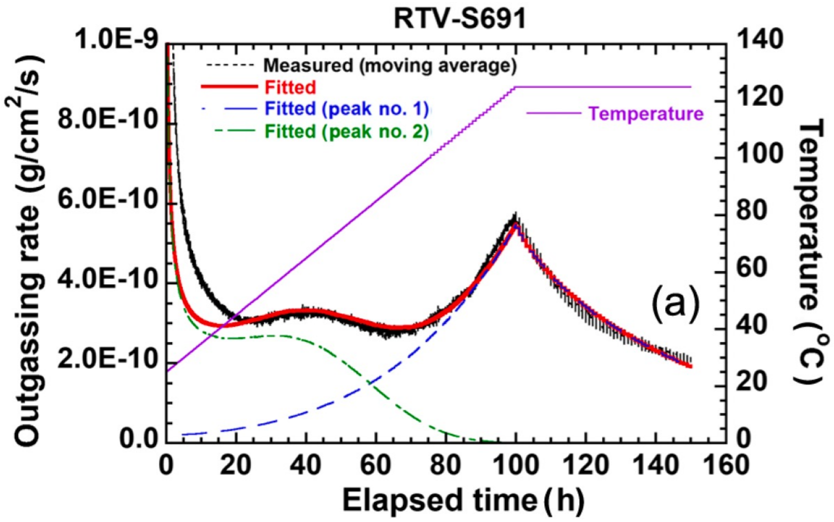
Modeling Methodology Comparison

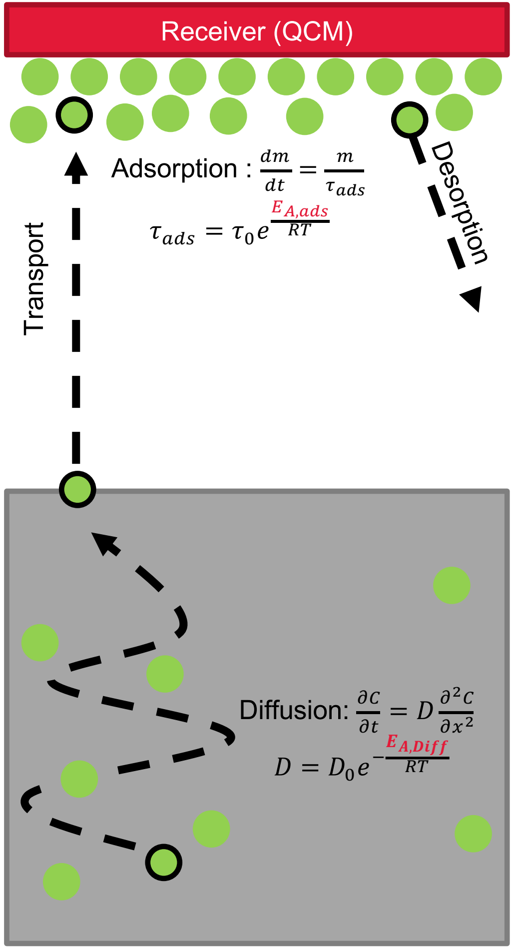
- **ECSS-Q-TM-70-52a 7.2 ESTEC Method**
- Fundamental differential equation of outgassing is desorption. First order time ODE.
- $\frac{dm_i}{dt} = -\frac{m_i}{\tau_i}$ [4-1]
  - t: time
  - $m_i(t=0) = m_{0i}$: the initial mass of contaminant species i
  - m_i: contaminant available mass
  - τ_i: $\tau_i = \tau_{0i} e^{-\frac{E_{ai}}{RT}}$: outgassing time constant of species I (s)
  - τ_{0i} : Arrhenius pre-exponential factor (s)
  - E_{ai}: Activation energy (desorption)
- $TML = \sum_i m_{0i}(1 - e^{-\frac{t}{\tau_i}})$ [7-1]
- Dimension: $\{t\}$
- Solved variable: $\{m_i\}$
- Physical parameters per contaminant species $\{\tau_{0i}, E_{ai}, m_{0i}\}$
- Environmental parameters: $\{T\}$

- **Proposed JPL 353d multispecies model**
- Fundamental differential equation of outgassing is diffusion. Second order partial differential equation.
- $\frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i}{\partial x^2}$,
  - t: time (s), x: space *within* outgassing material (s)
  - $C_i(t=0,x) = C_{0i}$: initial condition contaminant density (kg/m3)
  - $C_i(t, x=0) = 0$: *Vacuum boundary condition*
  - C_i: Concentration of species i (kg/m3)
  - $D_i = D_{0i} e^{-\frac{E_{ai}}{RT}}$: Diffusion coefficient (m2/s)
  - D_{0i}: Arrhenius pre-exponential factor (m2/s)
  - E_{ai}: Activation energy (diffusion)
- $r_i = \frac{4\, D_i\, C_{0i}}{L} \sum_{j=0}^{\infty} e^{-t\frac{D_i}{L^2}(2j-1)^2\,\pi^2}$
- Dimension: $\{\mathrm{x}, t\}$
- Solved variable: $\{C_i\}$
- Physical parameters per contaminant species $\{D_{0i}, E_{ai}, C_{0i}\}$
- Environmental parameters: $\{T\}$

JAXA Approach

- Linearly ramp temperature during outgassing portion
- Different approach to modulate sample temperature during test





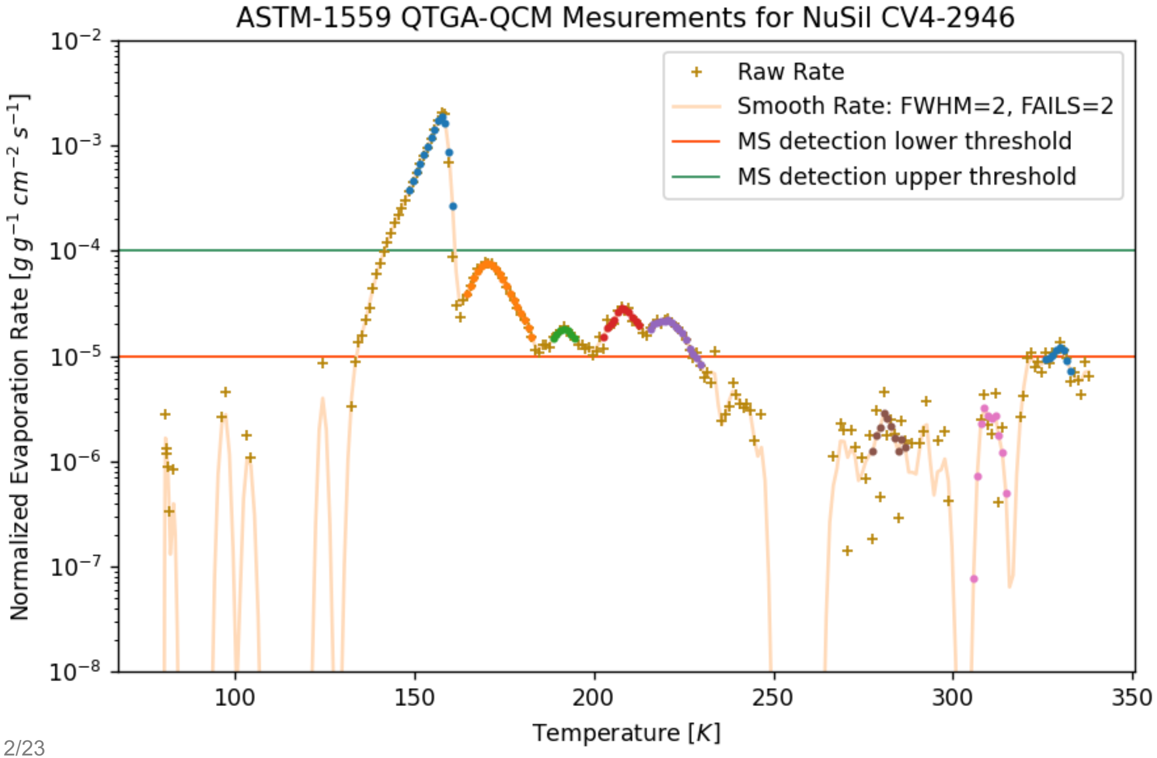
Shimazaki, Kazunori, et al. "Outgassing test methodology for contaminant emission model based on diffusion theory." *Journal of Astronomical Telescopes, Instruments, and Systems* 7.1 (2021): 018001-018001.

Mass Spectrometry

- Species from kinetic multispecies fit are “mathematical” model species.
  - Can connect activation energy of desorption to molecular weight, AMU, but no information from chemical composition can be derived from QCM data
- In the ASTME1559 setup the mass spectrometer has view to both the sample and QCM. Subsequently mass spectra data is collected during both isothermal test and QTGA test
- Mass spectrometer provides information of molecule chemical composition, but fragments parent molecules into smaller molecules or ions
- Mass spectra measurement is a combination of many outgassing molecules each possibly being fragmented
- Very challenging to processes in automated way

Why looking at QTGA is a natural first approach

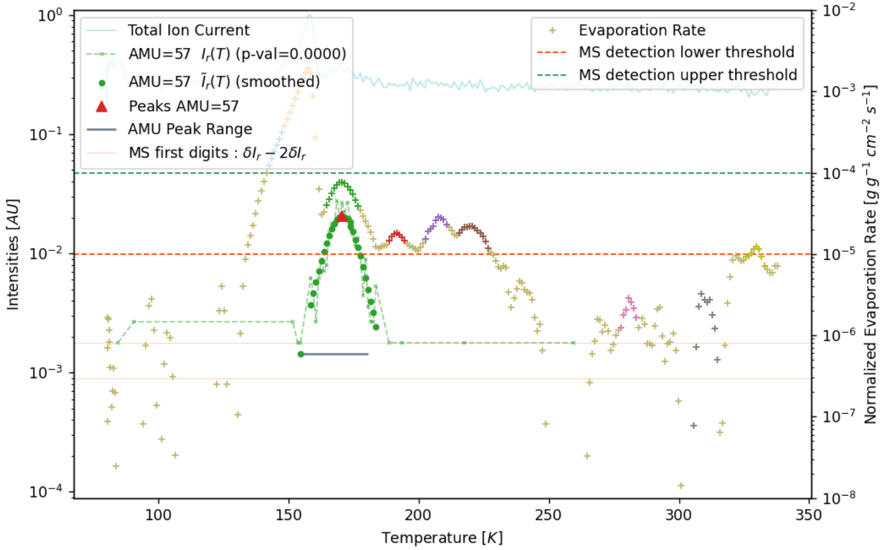
Recognizing species through desorption rate physical separation

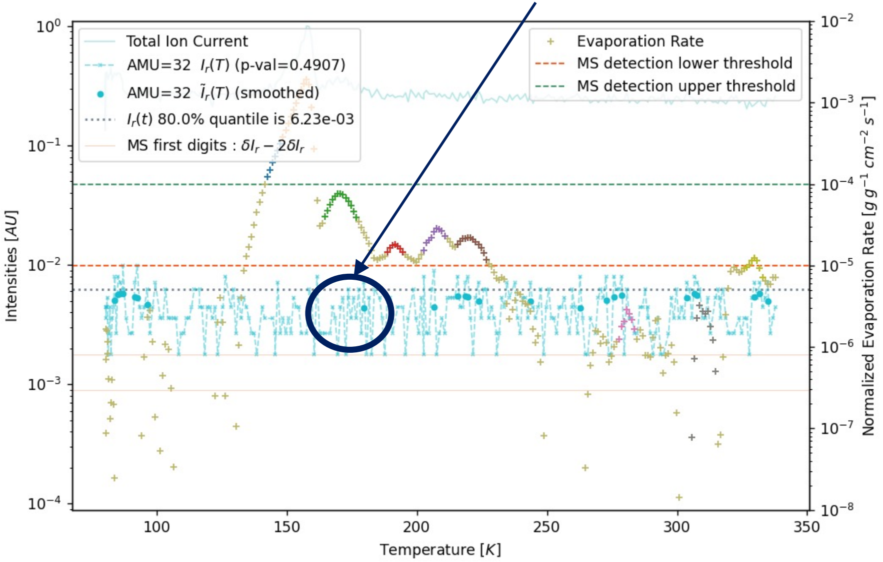


Controlled temperature gradient helps **separate species** in the **QTGA section** of the 1559 test

Filling the gap between 1559-QTGA and experimental spectrum

What makes a mass channel relevant to an outgassing species



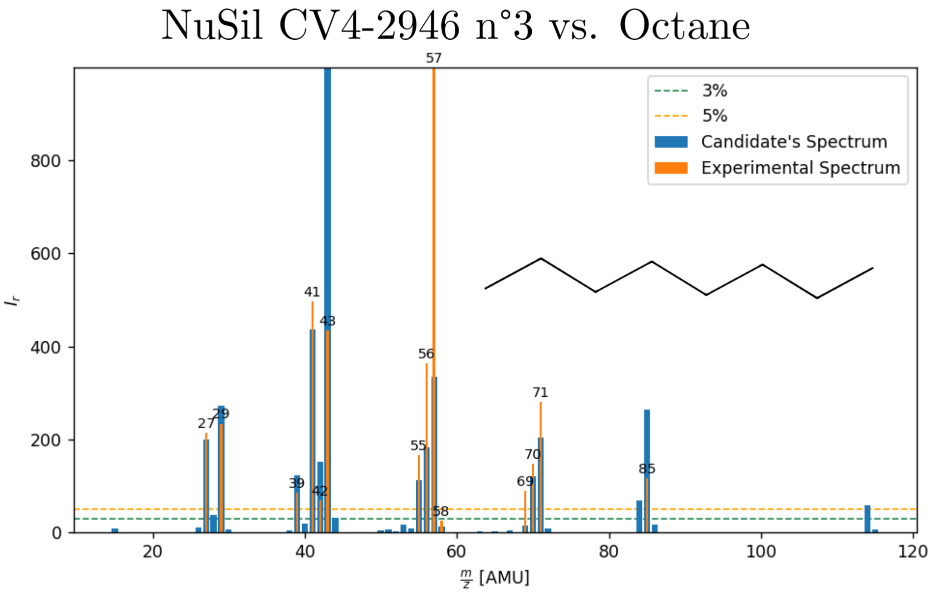


Low Signal-to-Noise Ratio

Correlation between **MS** and **QCM signals indicate** that a mass **channel** is **relevant**

What information can be inferred from a mass spectrum

Working with indirect information about a chemical species


NuSil CV4-2946 n°3 vs. Octane

Method	Score	Rank
RMSLE 3%	-2.364	6
Spec2Vec 3%	2.209	2
MS2DeepScore 3%	1.320	2
Composite 3%	**1.393**	**2**

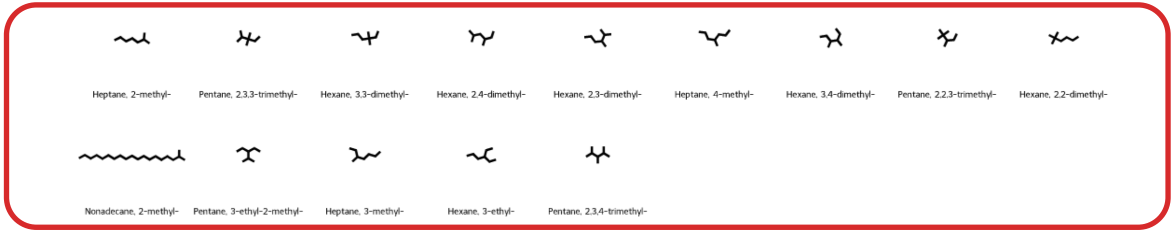
Diverse Scores → Unique Composite Score

Florian Huber et al., 2021

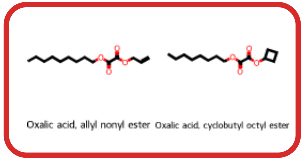
Spectrum similarity used as a proxy for molecular similarity helps us determine what the contaminants are most likely to be

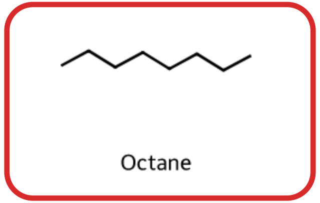
How to make sense of the result

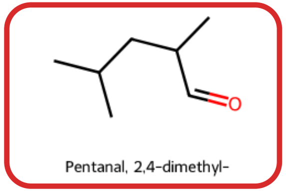
In the end, what can be known of a given outgassing species

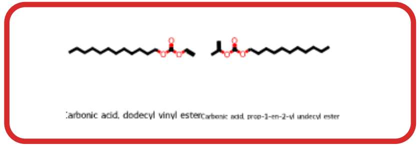

Heptane, 2-methyl- Pentane, 2,3,3-trimethyl- Hexane, 3,3-dimethyl- Hexane, 2,4-dimethyl- Hexane, 2,3-dimethyl- Heptane, 4-methyl- Hexane, 3,4-dimethyl- Pentane, 2,2,3-trimethyl- Hexane, 2,2-dimethyl-

Nonadecane, 2-methyl- Pentane, 3-ethyl-2-methyl- Heptane, 3-methyl- Hexane, 3-ethyl- Pentane, 2,3,4-trimethyl-


Oxalic acid, allyl nonyl ester Oxalic acid, cyclobutyl octyl ester


Octane


Pentanal, 2,4-dimethyl-


arbonic acid, dodecyl vinyl ester Carbonic acid, prop-1-en-2-yl undecyl ester

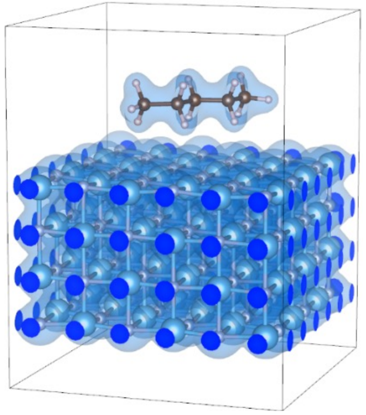
- Similar Top Ranking Results
- Few and related molecular groups
- Relative Confidence

Molecular clustering allows for a **comprehensive understanding** of an outgassing **species' identity**

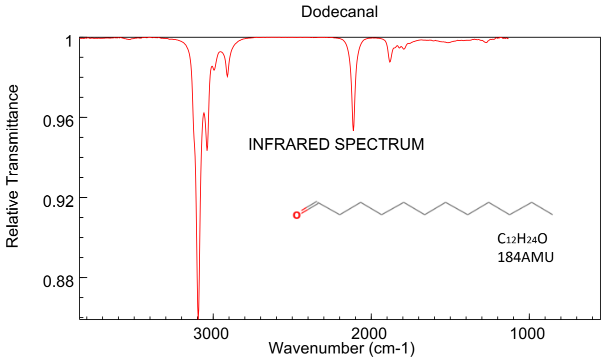
Mass Spectrometry Benefits

- By connecting kinetic multispecies model to mass spectrometry the kinetic contaminant parameters, $\{D_0,\ E_{a,diff}\ ,\ C_0,\ \tau_{0,des}, E_{a,ads}\}$ of outgassing molecules can be determined
- This kinetic multispecies model allows the capability of extrapolating outgassing for specific mission time and temperature conditions
- Knowledge of the contaminant chemical composition allows for a much more comprehensive understanding of the effects of outgassing contamination on scientific objectives
    - Molecular properties such as IR or UV spectra can be used to assess the impact to optical instruments and throughput (Example: SPHEREx, CGI, Psyche/DSOC)
    - Chemical composition can be assessed for the impact on sampling missions and detection of organics (Examples: Mars 2020, Mars Sample Return, Europa Lander)
    - Chemical composition can be assessed for the impact on mass spectrometers flown on missions intending to study atmospheric composition (Example: Cassini, Europa clipper)
- Additionally with the knowledge of chemical composition molecular properties can be calculated directly using computational material science techniques
    - Density functional theory was used to calculate the adsorption energy, $E_{A,ads}$, to TiN, the low surface energy coating in the Mars 2020 sample tubes[1]

DFT simulation of alkane adsorption to TiN



NIST IR Adsorption Spectra



NIST Chemistry WebBook (https://webbook.nist.gov/chemistry)

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1. Alred, J.M., Martin, M.G, Hoey, W.A., Wong, A.T., White, L.M., Boeder, P.A., Cofer, S.A., Dias-Ribeiro, A., Soares, C.E., "Predicting Terrestrial Contamination of the Mars 2020 Sample Caching System with Novel Multispecies Outgassing and Transport Models," Proc. SPIE 11489, Systems Contamination: Prediction, Control, and Performance 2020, 1148904, 21 August 2020.