Developing Outgassing Models of Space Hardware through Interpretation of Quartz Crystal Microbalance Data

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Engineering Directorate
Concept-to-Flight

http://engineering.larc.nasa.gov/

Outline

- Introduction
- Background
- Description of the Outgassing Modeling Program
- Current Implementation and Results

Introduction – Troy Gustke

Bio – Troy Gustke

- **Born and raised in Newport News, VA**
- **Graduated from Peninsula Catholic High School in 2017**
- **Junior at Virginia Tech**
  - Major: Chemical Engineering
  - Minors: Mathematics, Chemistry
  - Interests: Molecular Dynamics, Modeling, Transport Phenomena

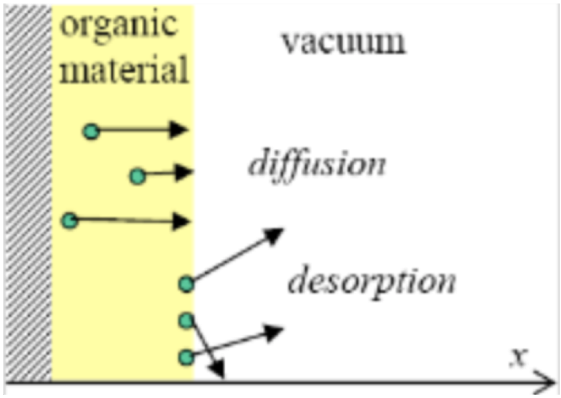
Currently:

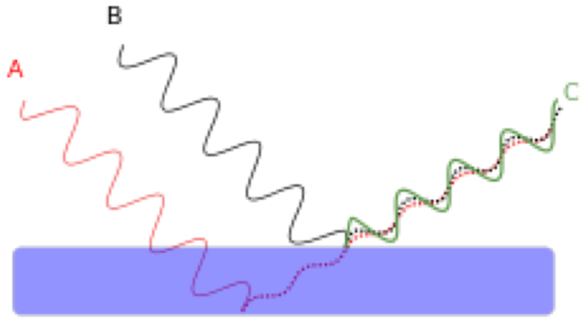
- **NASA - NIFS Intern (Contamination Control Engineering)**
  - Helped with integration and testing of space hardware for the MEDLI2 space flight project by providing molecular chemical analysis of non-volatile residue after thermal vacuum testing.
- **Virginia Tech – Undergraduate Researcher**
  - Developing accurate molecular dynamic simulations of metals using machine learning and optimization algorithms

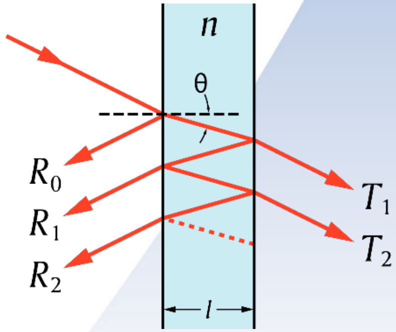
What is Contamination Control?

Contamination Control - The monitoring and prevention of material degradation due to environmental effects, more specifically related to sensitive optical materials.

- **Problems related to Space Hardware**
  - Outgassing - *"The emission of gasses trapped in materials"*
  - The outgassing of materials can bring up non-volatile products
  - Thin film deposition on optical systems can:
    - cause the laser to diffract, scatter, and reflect
    - Loss of thermal control and surface degradation
  - Alters optical material properties







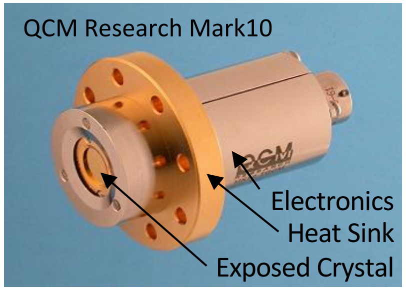
Space Environment Testing

- **Thermal Vacuum Chambers simulate space environment.**
  - 10^{-6} Torr
  - -190 to 130 °C
- **Sample Collection and Outgassing rate**
  - Cold Finger
  - Scavenger Plate
  - Hardware Swabs/Wipes
  - TQCM

Quartz Crystal Microbalance

Quartz Crystal Microbalance (QCM)

- Uses piezoelectric effect to vibrate quartz at a certain frequency
  - Isolated Crystal
    - Controlled environment
  - Exposed Crystal
    - Allows mass deposition to occur
    - Frequency slows down as mass deposition increases



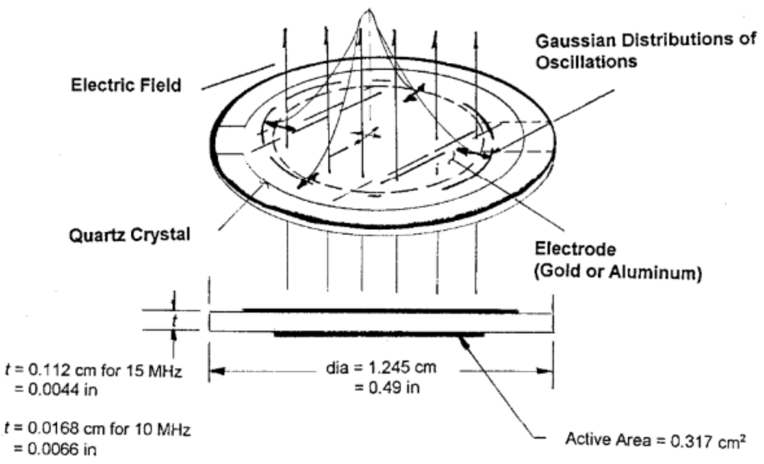


Figure 1 – Dissection of exposed crystal [2]

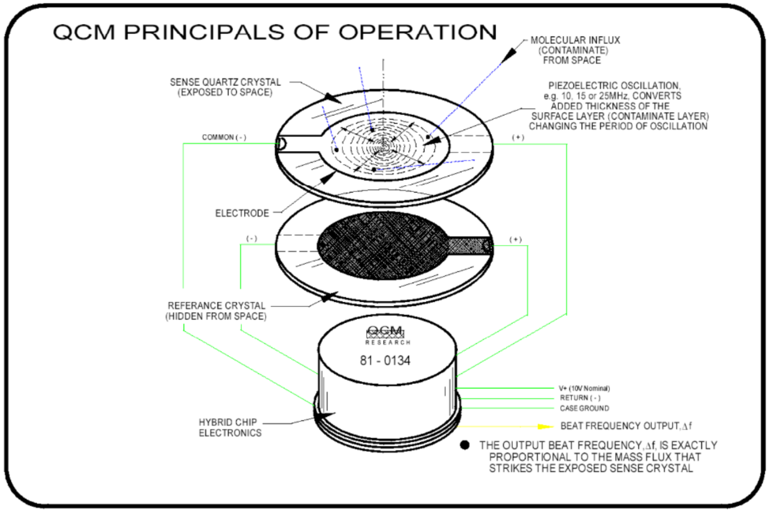
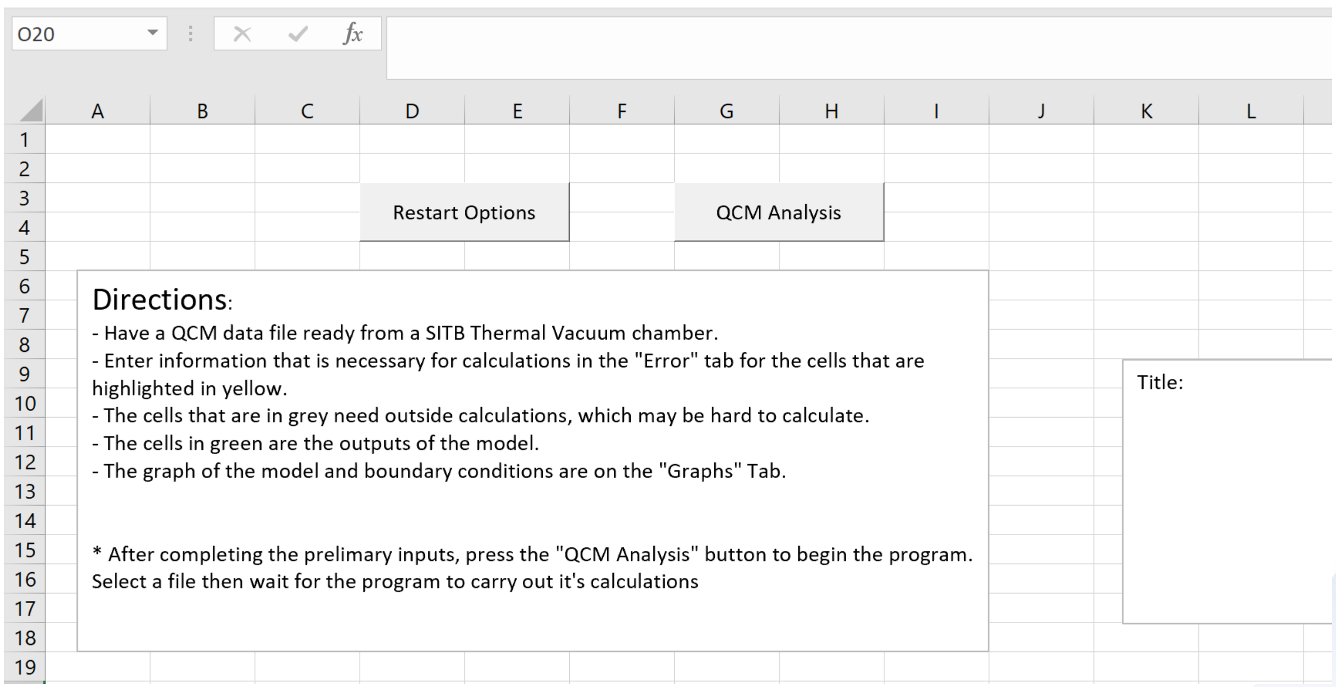


Figure 2 – Components of a QCM [2]

Outgassing Modeling Program

Run through Excel + Visual Basic

- Easy to navigate and run
- Widely used at NASA
- Relatively small amount of calculations
- Can be accessed on a share drive



Outgassing Modeling Program

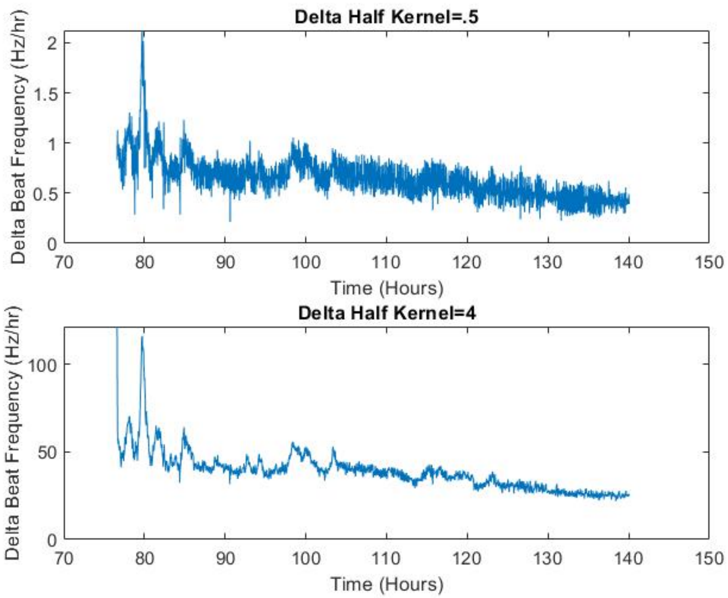
Bakeout Theory

- All Mass Flux out of the surface of the materials is described by Fick's Law [1]
  - $\frac{\partial m}{\partial t} = -D\frac{\partial m}{\partial x}$
- From this, further mass flux equations can be derived
  - $J = D\frac{\partial c}{\partial x} = \frac{2c_0 D}{L}\sum_0^\infty e^{\frac{-D(2i+1)^2\pi^2 t}{4L^2}}$
    - Derived mass flux out of the surface of a plate
- Simplify by using power and exponential fits
  - $\frac{dm}{dt} \approx At^{-b}$
  - $\frac{dm}{dt} \approx Ae^{-bt}$

Outgassing Modeling Program

Removing Noise

- QCM has many factors that affect the beat frequency
  - Temperature, mechanical, and electrical noise can cause error
- Since most noise is random noise, filtering over a designated kernel can reduce the noise drastically
  - If the data is noisy, increase the kernel



Error Analysis

- Mathematical computations are made to find A and b values for the fitted functions [1]

$$A = \frac{\sum X^2 \sum Y - \sum X \sum XY}{N \sum X^2 - \left(\sum X\right)^2}$$

$$B = \frac{N \sum XY - \sum X \sum Y}{N \sum X^2 - \left(\sum X\right)^2}$$

- Correlating sigma values are calculated to the fitted models

$$\sigma_Y = \sqrt{\frac{1}{N-2} \sum_{i=1}^{N} \left(Y_i - A - Bx_i\right)^2}$$

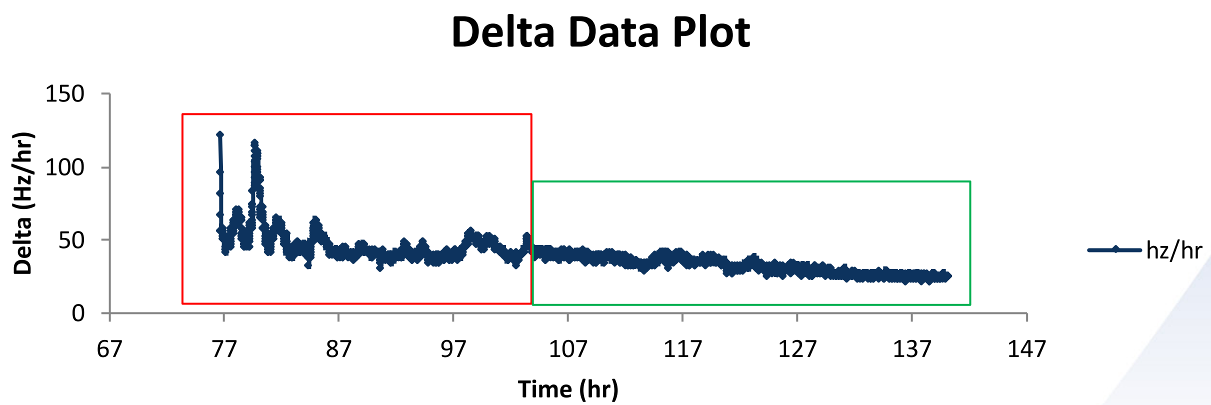
- As time increases, the uncertainty of the model increases
- A Gaussian distributive curve is taken of the data with the sigma bounds as the distribution bounds

	Number	fraction	Gaussian
Above 1 sigma	313	0.141	0.159
Below 1 sigma	180	0.081	0.159
Number of samples	2218		
Gaussian check OK?	TRUE		

Outgassing Modeling Program

➢ Systematic Error

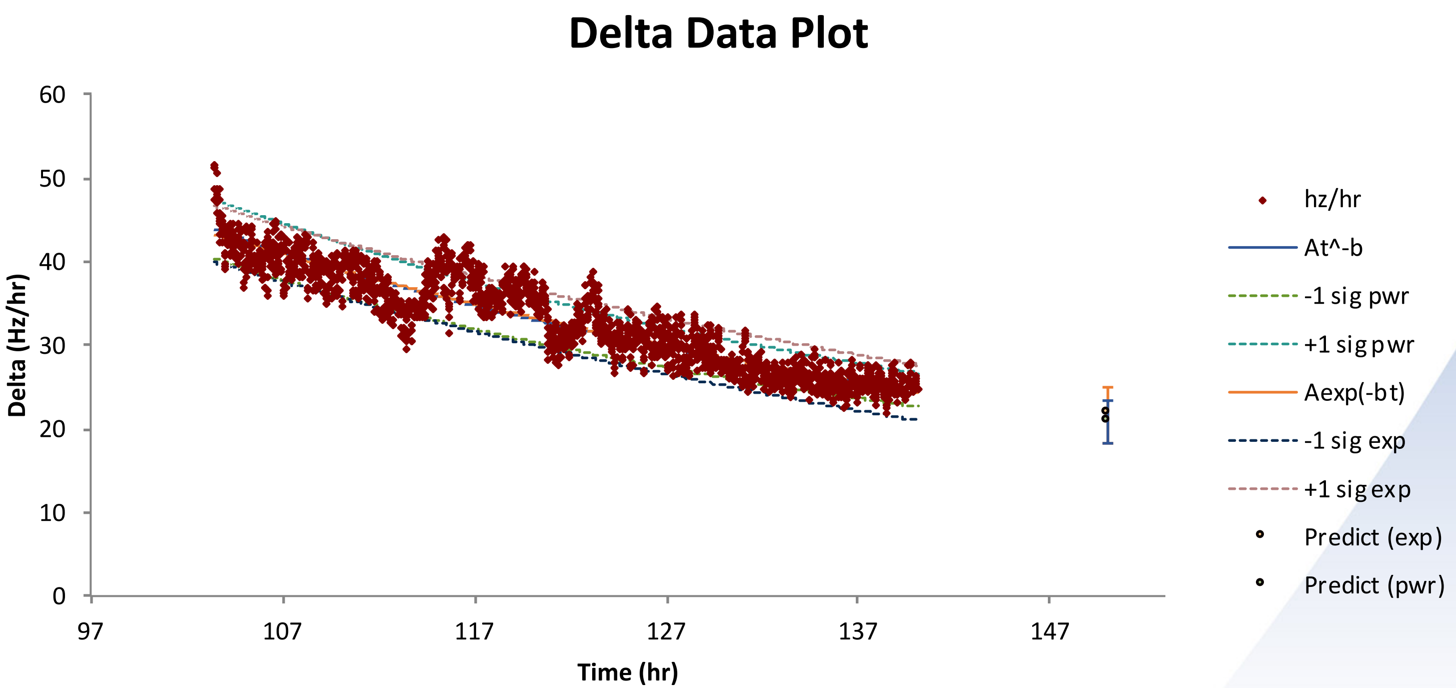
- Many data sets have systematic error that does not follow the material outgassing trend
  - Electrical noise
  - Thermal difference between the 2 crystals
  - Mechanical noise from LN2 pipes and gates
  - Grounding noise
- Since these data points do not represent material outgassing, this data can be disregarded when calculating the outgassing trend
  - Having many useless data points hurts the accuracy of the model



Results

Outputs

- Outgassing rate of hardware in Hz/hr and confidence value
- Time of stabilization
- Deposition rate of hardware in g/s and confidence value
- Graph of the Delta Beat Frequency vs. time with a power law and exponential law applied along with correlating sigma boundaries



Acknowledgements

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- Dave Hughes: NASA GSFC – Contamination Control Engineer

Other Acknowledgements

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Citations

- [1] Hughes, D. (2011). Contamination Control Course: Outgassing Certification (pp. 1–84). NASA Goddard Space Flight Center.
- [2] Wallace, S. (n.d.). *QCM: Theory and Practice*. Temecula, CA.
- [3] Huang, A. Y., Kastanas, G. N., Kramer, L., Soares, C. E., & Mikatarian, R. R. (2016). Materials outgassing rate decay in vacuum at isothermal conditions. *Systems Contamination: Prediction, Control, and Performance 2016*, *9952*, 995206. https://doi.org/10.1117/12.2241212