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

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Outline

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

Directions:
- Have a QCM data file ready from a SITB Thermal Vacuum chamber.
- Enter information that is necessary for calculations in the "Error" tab for the cells that are highlighted in yellow.
- The cells that are in grey need outside calculations, which may be hard to calculate.
- The cells in green are the outputs of the model.
- The graph of the model and boundary conditions are on the "Graphs" Tab.

* After completing the preliminary inputs, press the "QCM Analysis" button to begin the program. Select a file then wait for the program to carry out its calculations.
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
  \[
  J = D \frac{\partial c}{\partial x} = \frac{2c_0 D}{L} \sum_0^\infty e^{\frac{-D(2i+1)^2\pi^2 t}{4L^2}}
  \]
  o Derived mass flux out of the surface of a plate

• Simplify by using power and exponential fits
  \[
  \frac{dm}{dt} \approx At^{-b}
  \]
  \[
  \frac{dm}{dt} \approx Ae^{-bt}
  \]
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]

\[
A = \frac{\sum X^2 \sum Y - \sum X \sum XY}{N \sum X^2 - (\sum X)^2}
\]

\[
B = \frac{N \sum XY - \sum X \sum Y}{N \sum X^2 - (\sum X)^2}
\]

• Correlating sigma values are calculated to the fitted models

\[
\sigma_Y = \sqrt{\frac{1}{N-2} \sum_{i=1}^{N} (Y_i - A - Bx_i)^2}
\]

• 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

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<th>Gaussian</th>
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<td>0.159</td>
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<tr>
<td>Below 1 sigma</td>
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Gaussian check OK? TRUE
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
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

Delta Data Plot
Acknowledgements

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