24th Space Simulation Conference

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Tutorial Abstract:

Hardware Outgassing Certification

This course will provide students with the understanding necessary to calculate certification requirements for and interpret the data from hardware undergoing vacuum bakeout. The fundamental physics that drive hardware outgassing and contaminant deposition will be explained, and data reduction techniques will be applied to examples.

Presentation Requirements:

2 hours
PC with projector

Bio:

David Hughes is the Contamination Engineering Manager for the Hubble Space Telescope. He has 15 years of experience in aerospace contamination control and has been involved in each of the Hubble servicing missions. In addition to project support, his research interests include photopolymerization, improved contamination modeling techniques, and the design of slide rules. David has a Masters of Engineering Management from George Washington University and a Bachelors of Science from Carnegie Mellon University.

Hardware Outgassing Certification

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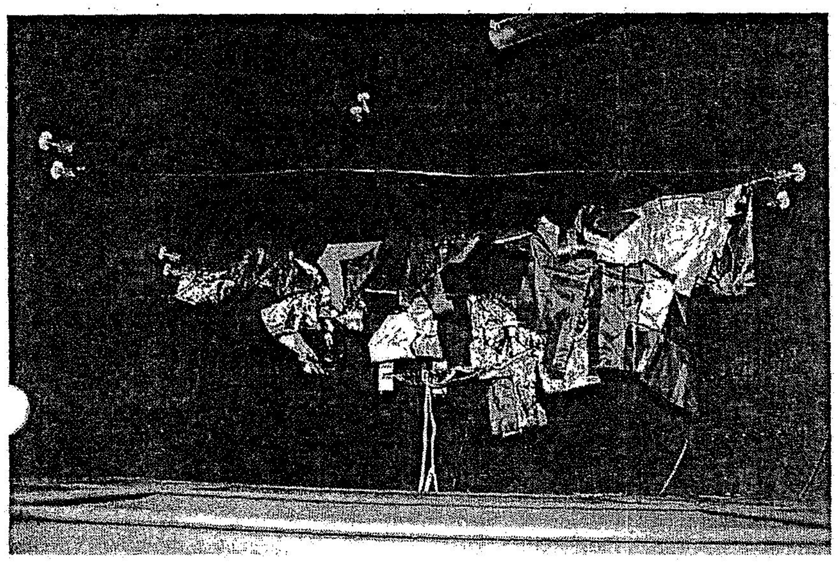
Theory

- Description
- Criteria
- Sequence
- Physics

Criteria Types

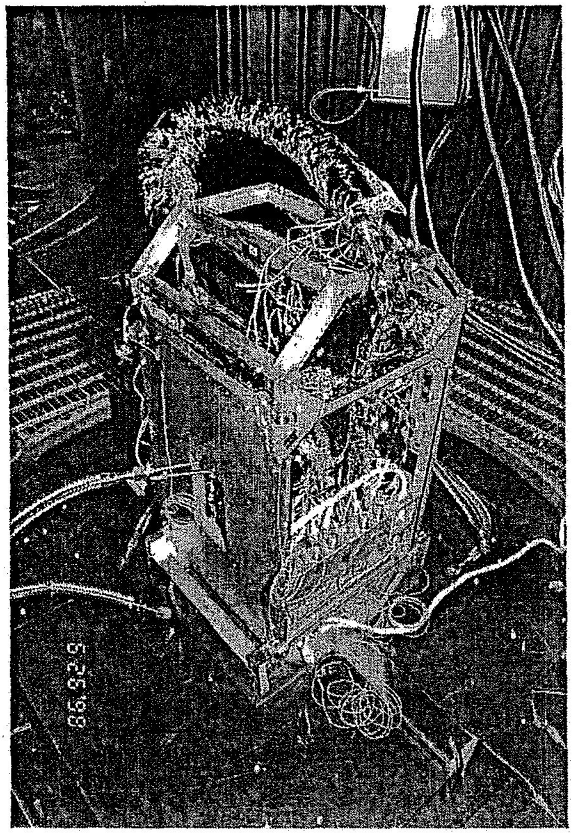
- Time/Temperature
- Coarse Bakeout
- Certification Conditions

- Applies to raw materials, components, or parts that have a history of monitored bakeouts and show good uniformity
- Specify the item temperature and the duration
- Outgassing rate data may or may not be collected but is not part of the certification
- Cost and schedule can be predicted



Criteria Types

- Time/Temperature
- Coarse Bakeout
- Certification Conditions



- Sample and collection temperatures should be representative of on-orbit conditions
- Rule of thumb
  - Hardware 10 degrees above maximum prediction
  - Collection 10 degrees below sensitive surface minimum prediction
- Outgassing requirement is converted to collection rate requirement based on chamber configuration
- Best characterization of hardware

Typical Sequence

Days to Weeks

- QCM criteria
  - As low as possible
  - As stable as possible
  - Below a fraction of the hardware criteria
- Species present
- Temperature
  - As high as possible for bakeout purposes
  - Match hardware criteria for background measurement purposes

Preparation	Chamber Cert	Hardware Bake	Hardware Cert	Data Analysis

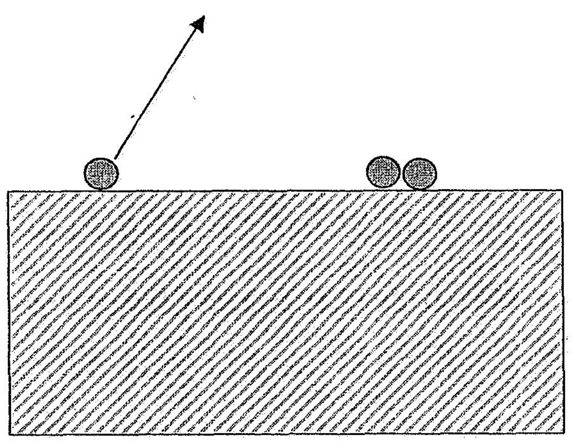
Typical Sequence

Days

- Set hardware temperature
  - Representative of on-orbit temperature
- Record data
- Terminate certification phase
  - Return to bakeout conditions if criteria was not met
  - Collect cold finger data if certification criteria was met

Physical Process

- Surface Desorption
- Bulk Outgassing
- Rate Equations



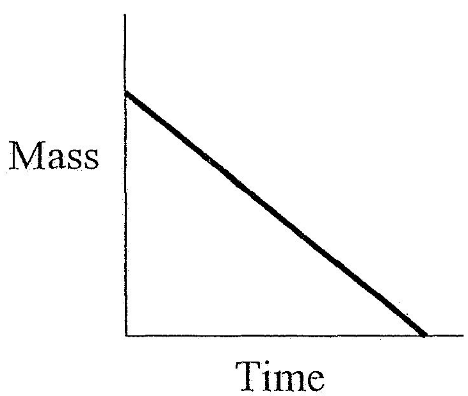
- Cleanroom Non-volatile Residue
  - Molecules are bound to the surface by Van Der Waals forces
  - Thermal energy can overcome the bonding and release the molecule
  - Small quantity
  - Quickly depleted
- Examples
  - Water
  - Mold release compounds
  - Fingerprints

Bakeout Theory

- Surface Desorption
- Bulk Outgassing
- Rate Equations

$$\frac{dm}{dt} = -k$$

$$m = -kt$$



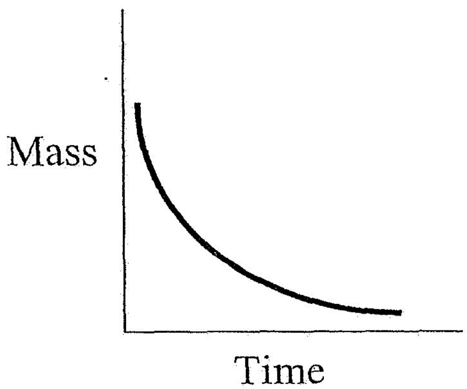
- 0th order evaporation or sublimation
  - evaporation rate is independent of how much is present
- 1st order desorption
  - rate is proportional to the mass present
  - exponential decay in mass remaining
  - tau is the time constant
  - Ea is activation energy and tau_0 is the fundamental vibration frequency of the molecules
  - rate = -A/tau e^-t/tau
- Diffusion limited bakeout
  - dc/dt = -Ddc/dx; Fick's law
  - solution is a function of t^0.5; power law
  - rate = At^-b

Bakeout Theory

- Surface Desorption
- Bulk Outgassing
- Rate Equations

$$\frac{\partial m}{dt} = -D\frac{\partial m}{dx}$$

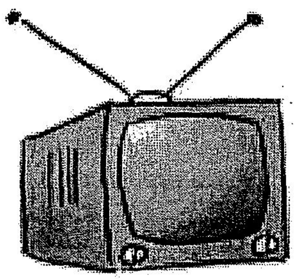
$$\frac{dm}{dt} \approx At^{-b}$$



- 0 order evaporation or sublimation
  - Dm/dt = -k; evaporation rate is independent of how much is present
- 1st order desorption
  - rate is proportional to the mass present
  - exponential decay in mass remaining
  - tau is the time constant
  - Ea is activation energy and tau_0 is the fundamental vibration frequency of the molecules
- Diffusion limited bakeout
  - dc/dt = -Ddc/dx; Fick's law
  - Numerical solution required
  - Short term rate follows a power law
  - Long term rate follows an exponential

Quartz Crystal Microbalance

- Theory
- Response
- Stability
- Types
- Field of View

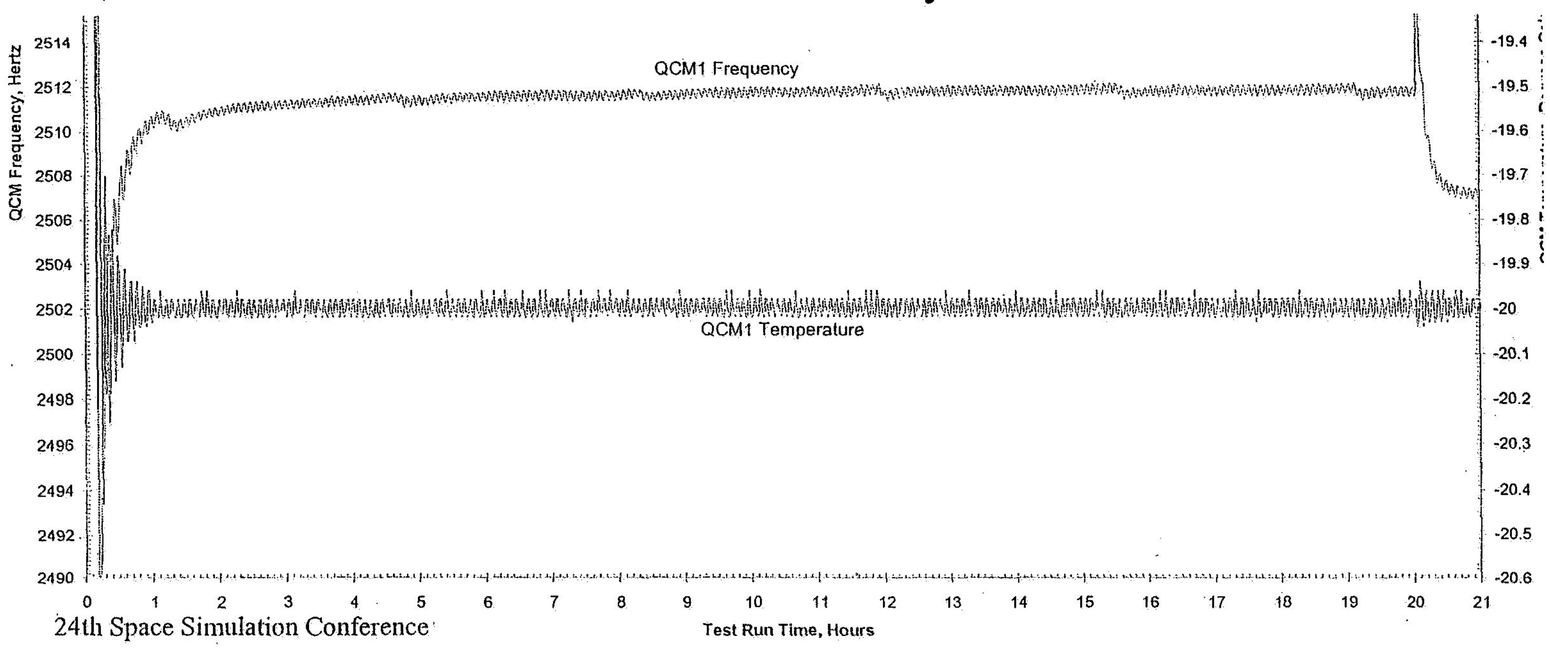


- Oscillating quartz crystal
  - Frequency inversely proportional to mass
  - Frequency varies with temperature
  - Range is MHz
- Two crystals of nearly equal frequency are used
  - One is exposed, the other is the reference
  - Beat frequency of the crystals is KHz
  - Because the reference crystal has nearly the same temperature, the effect of temperature changes is reduced

Quartz Crystal Microbalance

- Theory
- Response
- Stability
- Types
- Field of View

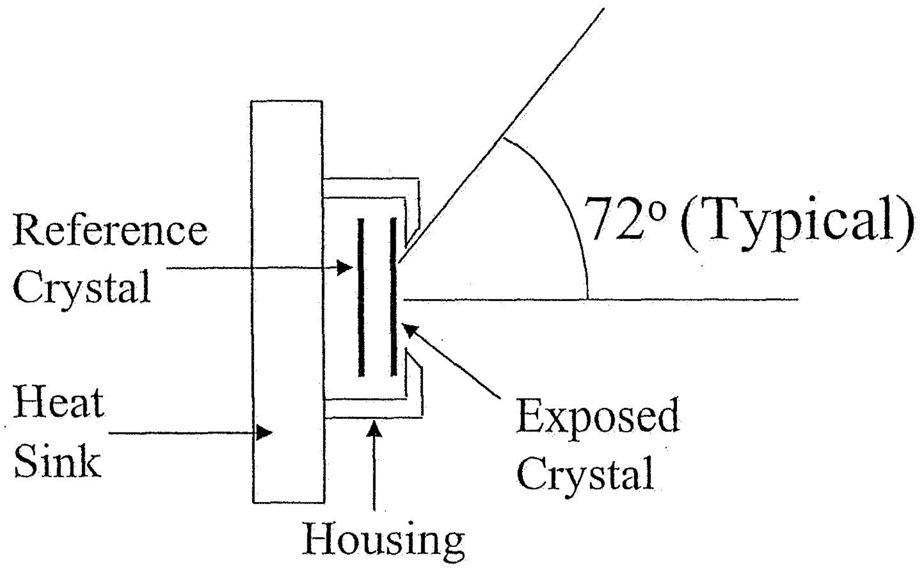
- Aging may cause drift in QCM output
  - Stress relief in resonators, electrodes, etc
  - Oscillator circuit aging
  - Quartz outgassing or absorption of gasses such as helium
  - Diffusion effects
  - Radiation effects on quartz
- Yearly rate of 5-51 Hz drift for 15 MHz



Quartz Crystal Microbalance

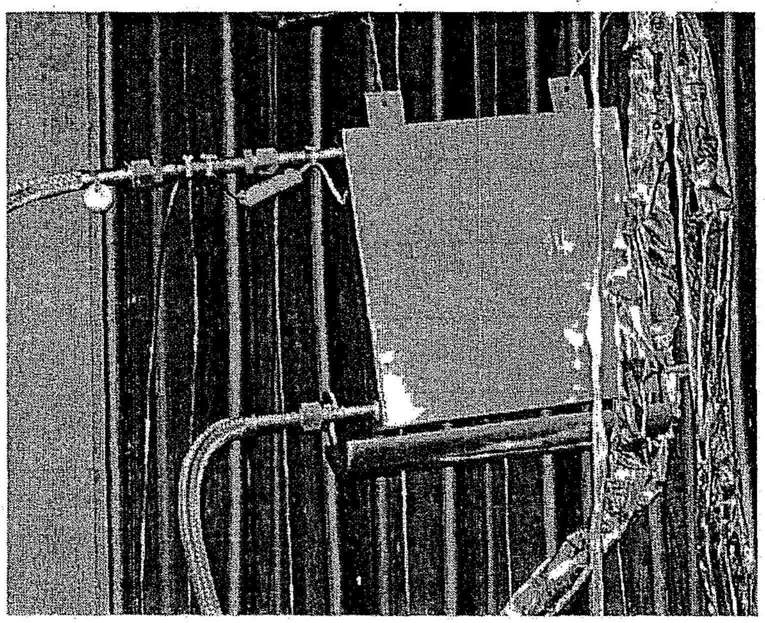
- Theory
- Response
- Stability
- Types
- Field of View

- Housing design determines FOV
  - Varies by manufacturer and model
  - Must be accounted for in modeling transport of molecules to the QCM
- Conversion factor from Hz to g/cm^2 is provided by manufacturer



Species Collection

- Coldfinger
- Scavenger Plate



- Larger version of coldfinger
- Cooled during entire test
  - Used to reduce molecular flux to pumps and QCM
  - Can be rinse sampled but will include species that are depleted by the end of the test
- Typically has a "drip tray"

Thermal Instrumentation

- Chamber Shroud
- Heater Plates
- Miscellaneous

- Cylindrical metal insert in the chamber
- Typically plumbed with LN2 lines for cooling
- May also have heaters installed
- May be painted or black anodized for high emissivity
- The chamber wall is not temperature controlled
  - Stays near room temperature
  - May heat up during shroud driven bakeouts

Thermal Instrumentation

- Chamber Shroud
- Heater Plates
- Miscellaneous

- Thermocouples
  - Required to monitor the temperature of the hardware
  - Difficult to keep free from particle contamination
- LN2 lines
  - May need to be baked out if they are new

Does any of this contribute to the chamber background?

Outgassing and Deposition

- Hardware Outgassing
- Background Outgassing
- Chamber Environment

- Outgassing rate (OGR) in g/cm²/s to Deposition Rate (DPR) in g/cm²/s
  - A is area in cm²
  - VF is viewfactor
  - Subscript HW for hardware

$$\frac{OGR_{HW} \cdot A_{HW} \cdot VF_{HW->QCM}}{A_{QCM}} = DPR_{QCM}$$

- Deposition rate (g/cm²/s) to Delta (Hz/hr)
  - CF is conversion factor from QCM manufacturer (g/cm²/Hz)

$$DPR_{QCM} \div CF \cdot (3600 \frac{s}{hr}) = Delta$$

Requirements

- Hardware Outgassing
- Background Outgassing
- Chamber Environment

If the background is high, it is likely to decrease over the course of the hardware test, making data interpretation difficult.

- Chamber history
  - Presence of undesirable species (eg, silicones)
  - High background outgassing rates
- Acceptable background rate
  - Rule of thumb (non-critical): half the hardware requirement
  - Rule of thumb (critical): 1/10th the hardware requirement
  - High backgrounds also mean that the coldfinger results are less representative of the hardware being tested
- Pre-test chamber bakeouts are used to reduce the background

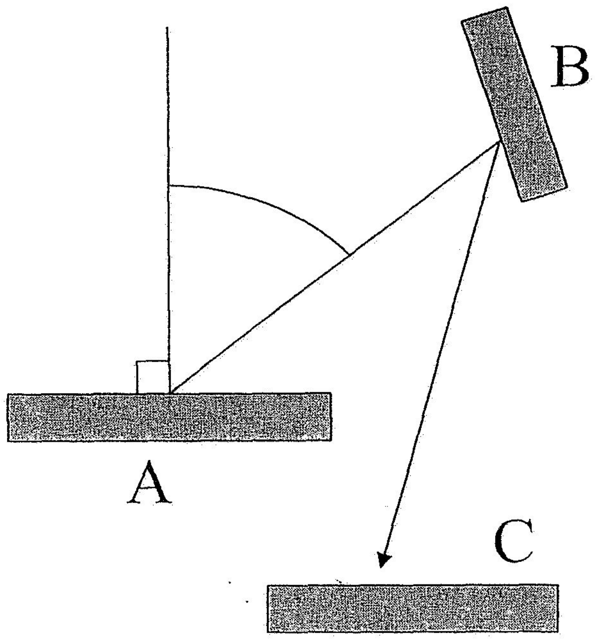
Configuration

- Molecular Transport
- Chamber Characterization
- Radiation Viewfactors
- Molecular Viewfactors

- Chamber configuration determines the relationship between sample outgassing and QCM readings
- Multiple QCMs may be required

Viewfactor Definition

- Random Walk
- Implications
- Radiation Viewfactors
- Molecular Viewfactors



- For molecular transport, we allow multiple bounces
  - The viewfactor from A->B must now include paths other than line of sight
  - Molecules that do not stop on a surface do not contribute to the viewfactor to that surface
  - The sum of all viewfactors is still 1

Viewfactors

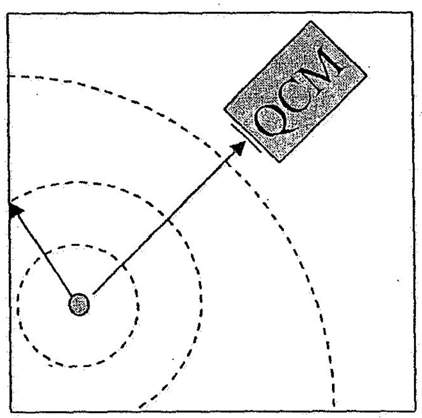
- Geometry Independent
- Simple Configurations
- Test Boxes

- Complex test configurations
  - Multiple hardware elements in view of QCM
  - Non-isothermal environment
  - Numerical analysis is required
- Ideal chamber configurations
  - Viewfactor to the QCM is nearly independent of hardware geometry
- Simple test configurations
  - Isothermal environment
  - Single hardware element
  - Viewfactor may be found statistically

Configuration

- Ideal "Hot Wall"
- Ideal "Cold Wall"

- The hardware is a point source
- All surfaces condense the outgassed species
- Molecules outgas as expanding sphere
- QCM crystal plane is tangent to the sphere



$$VF_{HW->QCM} = \frac{A_{QCM}}{4\pi \cdot d^2_{HW->QCM}}$$

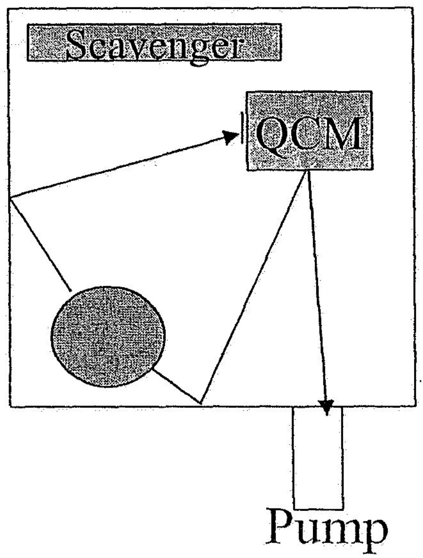
Effective Pump Area

- Hot Wall
  - Chamber Characterization
- Cold Wall
- Vented Cavity

$$VF_{HW->QCM} = \frac{A_{QCM}}{A_{QCM} + A_{Pump} + A_{Other}}$$

$$\frac{OGR_{HW} \cdot A_{HW} \cdot VF_{HW->QCM}}{A_{QCM}} = DPR_{QCM}$$

- Solve for unknowns: $OGR_{chamber}$, A_{pump}
  - Two equations required
    - Achieve a stable QCM reading
    - Then activate the cold finger or scavenger plate
- Pump effective area is a function of the ratio of before and after rates

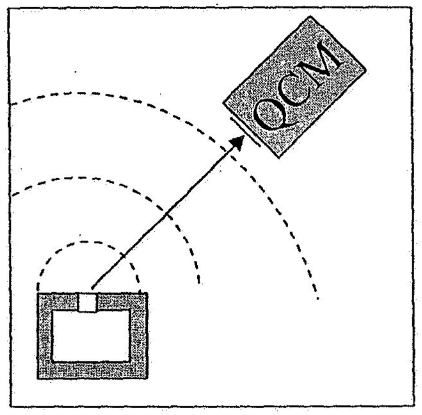


$$\frac{Rate_{NoScavenger}}{Rate_{WithScavenger}} = \frac{A_{QCM} + A_{Pump} + A_{Scavenger}}{A_{QCM} + A_{Pump}}$$

$$A_{Pump} \approx \frac{A_{Scavenger}}{Ratio - 1}$$

Simple Configurations

- Hot Wall
  - Chamber characterization
- Cold Wall
- Cold Wall, Vented Cavity



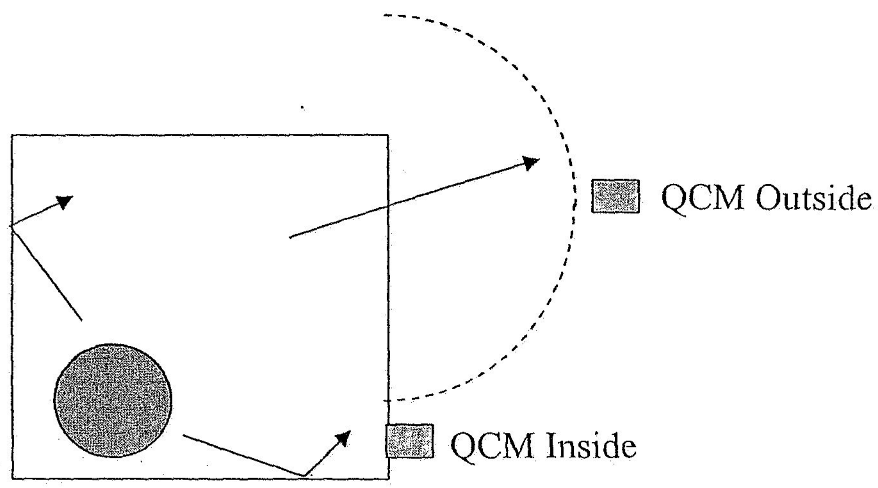
- Chamber wall is colder than the QCM
- Primary outgassing source is inside a cavity with one vent
- The QCM faces the vent
- Vent is small enough to treat as a point source
  - Diameter << distance to QCM
- Assume molecules exiting the vent are uniformly distributed over a hemisphere
  - Not the end of a tube

$$VF_{HW->QCM} = \frac{A_{QCM}}{2\pi \cdot d^2_{HW->QCM}}$$

Test Boxes

- Description
- Test Box w/ Cold Wall
- Test Box w/ Hot Wall

- QCM inside the box
  - Hot Wall equation applies
  - Use the box vent area as the chamber pump area
- QCM outside the box
  - Vented Cavity equation applies



Viewfactor Summary

- Hot Wall

$$VF_{HW->QCM} = \frac{A_{QCM}}{A_{QCM} + A_{Pump} + A_{Other}}$$

- Ideal Cold Wall

$$VF_{HW->QCM} = \frac{A_{QCM}}{4\pi \cdot d^2_{HW->QCM}}$$

- Vented Cavity

$$VF_{HW->QCM} = \frac{A_{QCM}}{2\pi \cdot d^2_{HW->QCM}}$$

- Test Box, Hot Wall

$$VF_{HW->QCM} = \frac{A_{QCM}}{A_{QCM} + A_{Vent} \cdot \left[1 - A_{Vent} / (A_{Vent} + A_{Pump})\right]}$$

$$\frac{OGR_{HW} \cdot A_{HW} \cdot VF_{HW->QCM}}{A_{QCM}} = DPR_{QCM}$$

Data

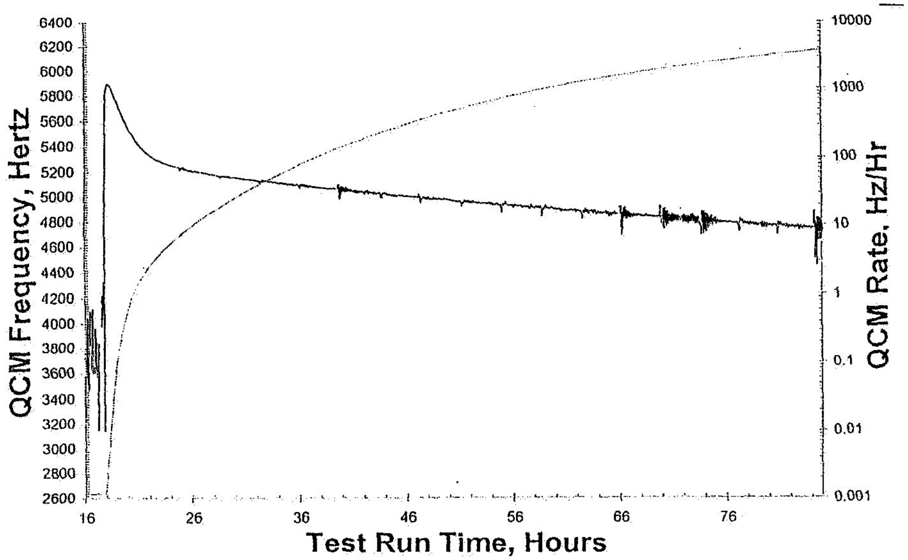
- Hourly Data
- Averaging

Time	Freq	Delta	Delta Delta	Shroud	Hardware
1:00	2787			30.1	46.2
2:00	2904	117		30.0	46.2
3:00	3010	106	-11	30.1	46.5
4:00	3108	98	-8	30.0	46.4
5:00	3200	92	-6	30.2	46.3
6:00	3220	20	-72	30.0	35.1
7:00	3225	5	-15	30.1	30.4

- Reported as
  - Frequency in Hz
  - Delta in Hz/hr
  - Delta Delta in Hz/hr/hr
  - Temperature in Celsius
- The rate (Delta) and derivative (Delta Delta) are backwards difference
  - Delta Delta depends on 3 hours of data
  - Make sure the temperatures are the same at each time step involved
    - Hardware
    - QCM
    - Coldfinger
    - Scavenger plate

Data

- Nominal
- Problems

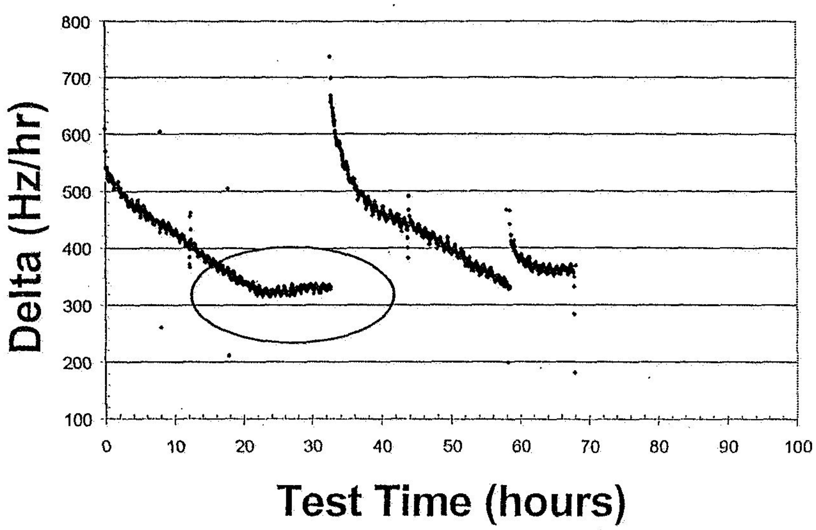


- In some cases, simply meeting a pre-determined QCM rate is sufficient to declare success
- If the background is non-negligible, or the rate is changing significantly, analysis of the data may be required
  - Enough background data must be collected to make statistically valid predictions
  - Curve fit the rate (Delta) vs. test hour
    - Exponential
    - Power Law

Crystal Saturation

- Nominal
- Problems
  - Examples

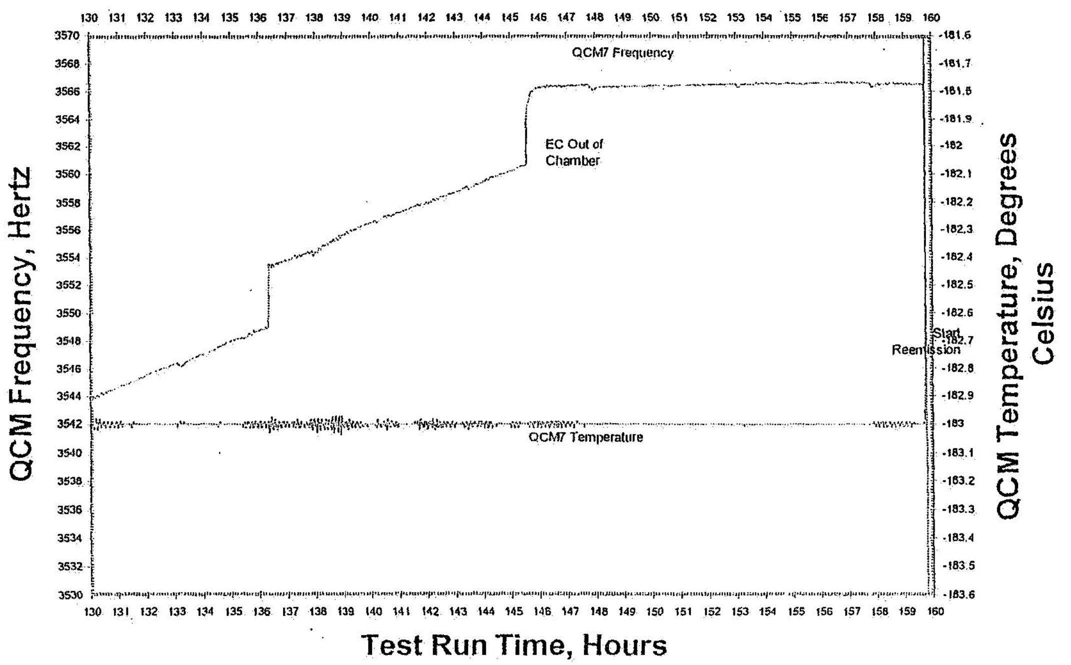
- QCM rate should decrease over time
  - Non-physical behavior was observed
  - Baking off the QCM corrected the behavior



Crystal Shift

- Nominal
- Problems
  - Examples

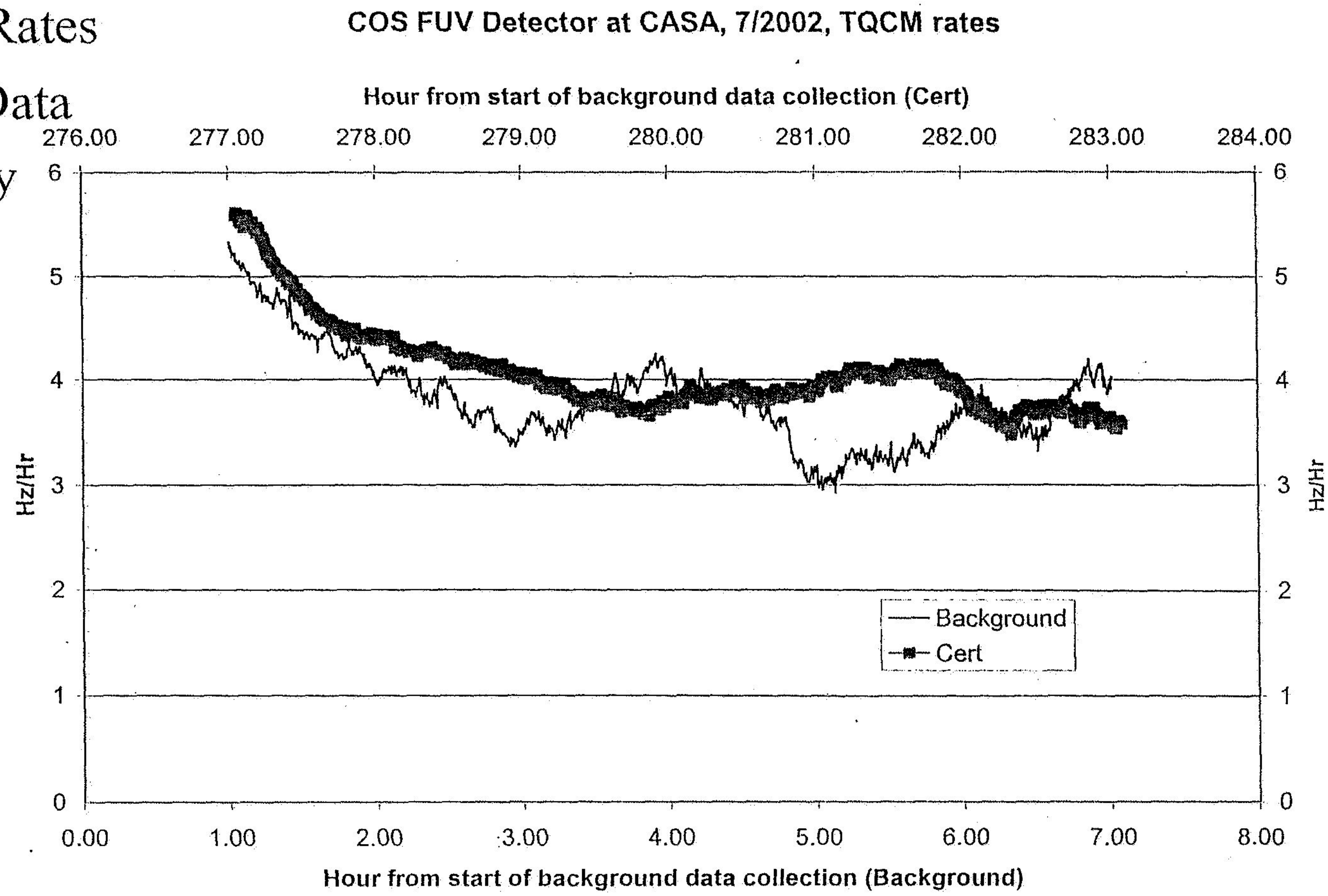
- Frequency should not jump instantaneously
  - Jump in frequency occurred over a single two minute data interval
  - Rate before and after jump was consistent



Collect Data

- Hot Wall Requirements
- Plot of QCM Rates
- Synchronizing Rates
- Analyzing the Data
- The Wrong Way

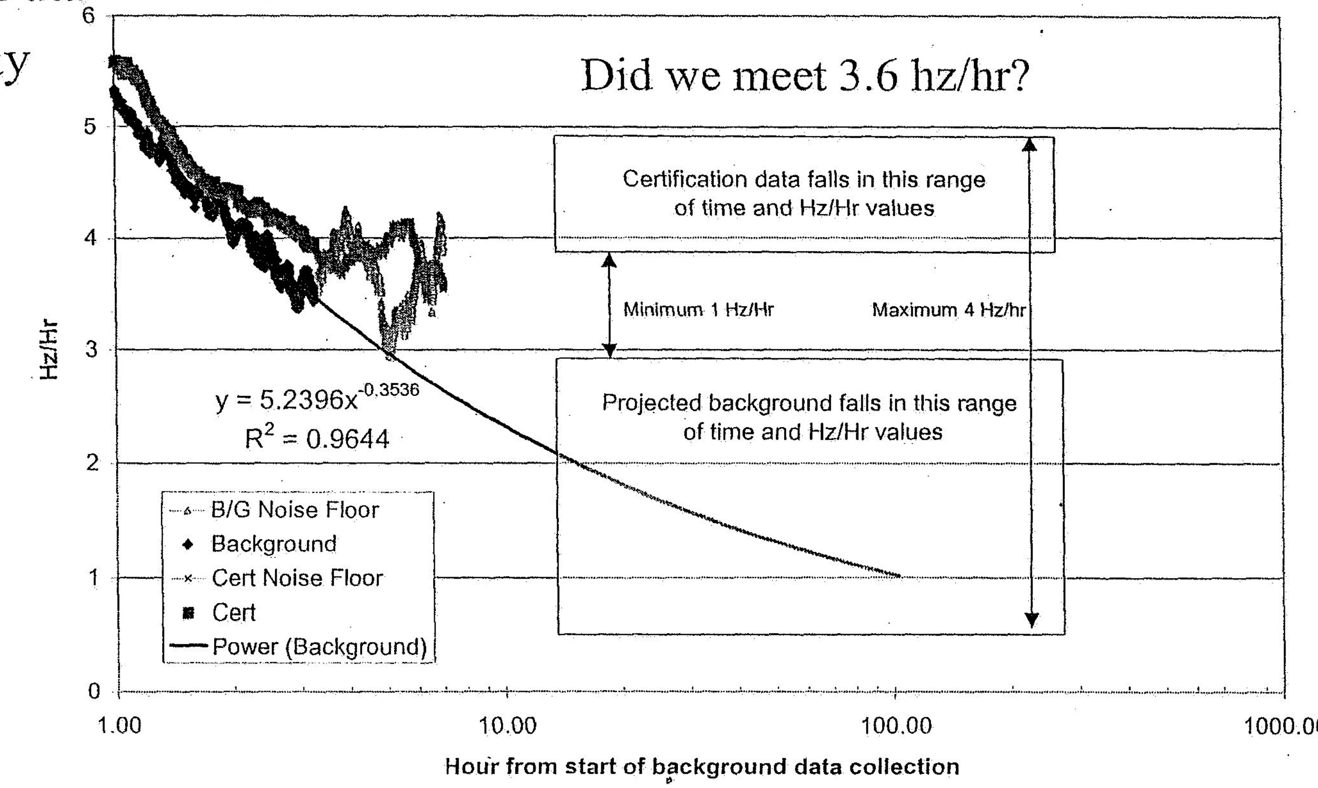
- Data aligned to superimpose time under vacuum for background and certification



Data

- Hot Wall Requirements
- Plot of QCM Rates
- Synchronizing Rates
- Analyzing the Data
- The Wrong Way

- Observation of sinusoidal behavior provides noise floor
- Exponential decay for surface outgassing of chamber extrapolated to certification time



Error Analysis

- Why Use Error Analysis
- How To Perform
- Example Spreadsheet
- Plot With Error Bounds

- Error analysis is the mathematical study of how random errors in the value of variables (measurements) affects the answer given by a formula
- Good reference text
  - "An introduction to error analysis", Taylor, J.

Error Analysis

- Why Use Error Analysis
- How To Perform
- Example Spreadsheet
- Plot With Error Bounds

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

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

- The representative outgassing equation and viewfactor equation (if used) must be analyzed first to determine the error equations
  - Convert to linear form (Y = AX + B) by working in logarithms
  - y=(a)x^b
  - log(y) = log(a)+(b)log(x)
  - Y: log(y), X: log(x)
  - A: b, B: log(a)
- A spreadsheet of the data can be constructed using the derived error equations
  - Least squares solution uses Excel functions SUM, SUMSQ and SUMPRODUCT
- The error bounds can be plotted over the data

$$\sigma_Y = \sqrt{\frac{1}{N-2} \sum_{i=1}^{N} \left(Y_i - A - Bx_i\right)^2} \qquad \sigma_A = \sigma_Y \sqrt{\frac{\sum x^2}{N \sum X^2 - \left(\sum X\right)^2}} \qquad \sigma_B = \sigma_Y \sqrt{\frac{N}{N \sum X^2 - \left(\sum X\right)^2}}$$

Error Analysis

- Why Use Error Analysis
- How To Perform
- Example Spreadsheet
- Plot With Error Bounds

- Data taken early in the test
  - Stronger response vs time
  - Lower uncertainty
- Data taken later
  - As asymptote is approached
  - More uncertainty for same data gathering length

OGR = A * t^(-b)
(time in hours by convention)

	measured or calculated value	sigma (errc	units	sigma/value
A	10.42866	0.51608	g/s	4.9%
-b	-0.133188	0.02512		19%
QCM Temp	233.15	0	K	0%
Src Temp	371.946	0.153867	K	0%
future time	20	1	hr	5%
future rate	6.997573	0.63197	g/s	9%

OGR = A * t^(-b)
(time in hours by convention)

	measured or calculated value	sigma (errc	units	sigma/value
A	10.60813	1.506953	g/s	14.2%
-b	-0.138984	0.055756		40%
QCM Temp	233.15	0	K	0%
Src Temp	371.9471	0.152869	K	0%
future time	20	1	hr	5%
future rate	6.995461	1.534665	g/s	22% ←

Summary

- Chamber configuration determines the relationship between hardware outgassing and the QCM reading
- Except in simple, clear cut cases, QCM data should be carefully analyzed before presenting the interpretation to the project
- Error analysis may be required in some cases