State-of-the-Art Modeling of Contaminant Transport in Vacuum Chambers and Space Environments

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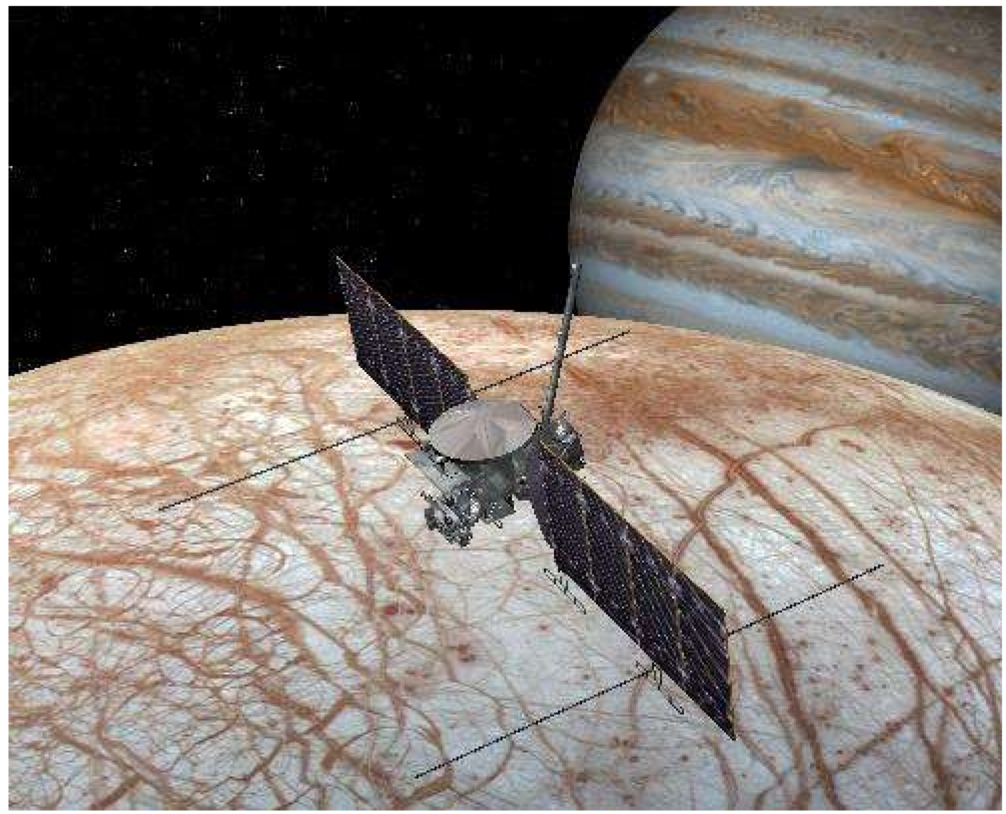
Contamination Control at NASA JPL:

As planned and proposed space exploration missions grow ever more ambitious in their scientific objectives their instruments necessarily increase in performance – as well as in sensitivity to contamination.

Contamination control is critical to ensuring the success of such missions, particularly:

- Missions that fly *sensitive mass spectrometers.*
  - Europa Clipper (inset)
- Missions intended to *detect organic samples*.
  - E.g. Mars 2020



Contamination Control at NASA JPL:

Characterizing contamination vectors with testing and modeling.

Spacecraft self-induced contamination – many sources, e.g.:

- Molecular outgassing or desorption from external surfaces.
- Propulsion systems:
  - Conventional mono- / bi-propellant engines: plumes with gas and liquid phase byproducts; leaks of unburnt propellant.
  - Electric propulsion: sputtering of incident surfaces.
- Venting of internal emissions through blanketing seams.

During fly-bys, **molecular outgassing** is the dominant source.

- Testing: monitoring of thermal vacuum chamber hardware bakeouts.
- Modeling: transport vectors include *direct*, *reflected*, and *return* flux.

Standard testing and modeling practices **can not capture** the rates and vectors relevant to highly-sensitive scientific missions.

Required Outgassing Rates

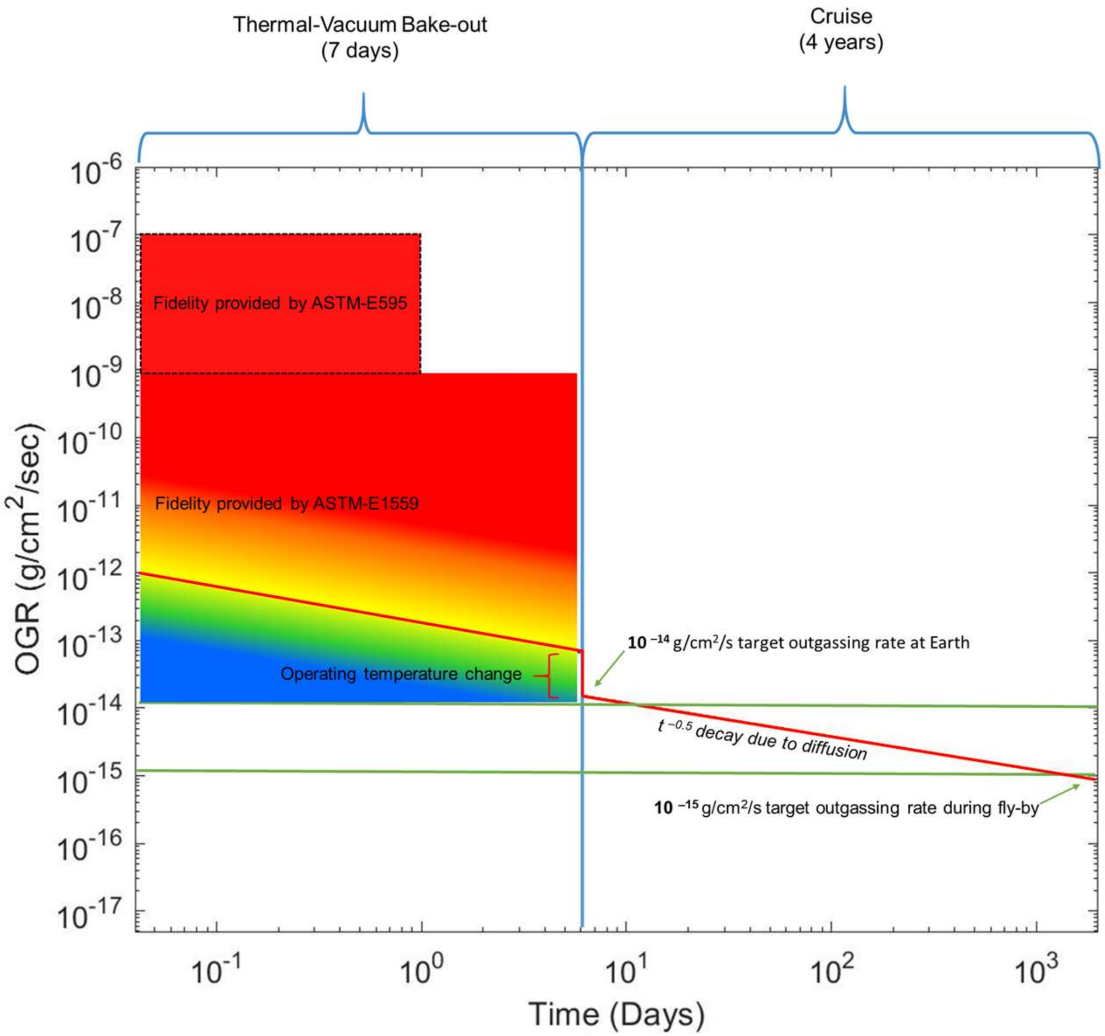
Motivating novel tools for monitoring and modeling bakeouts.

Example: OGRs for a mission with a sensitive mass spectrometer.

How can rates of this order be measured for spacecraft materials?

- At Europa, the radiation environment required a novel test campaign…

For more detail, refer to Dr. Anthony Wong's presentation, "Evaluating the In Situ Outgassing Characteristics of Silicone Adhesives in an Europa-Like Environment"

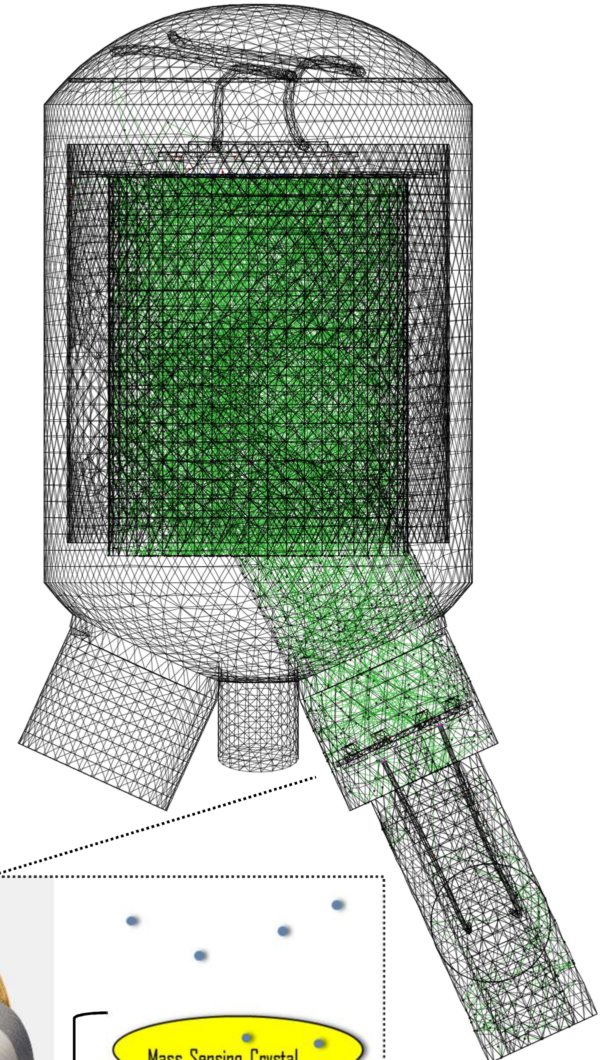


Vacuum Chamber Molecular Transport

Measuring outgassing rates during thermal vacuum chamber operations requires **modeling transport in the chamber environment** and deposition onto an instrument, i.e. a quartz crystal microbalance (QCM).

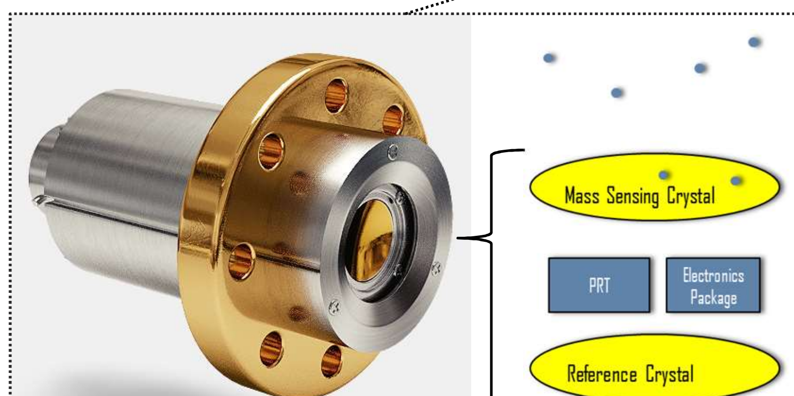
Pressures during thermal vacuum chamber operations are sufficiently low for transport to be entirely free-molecular ($< 10^{-5}$ torr; MFP > 1 m).

- Molecules do not collide with one another – instead transport is line-of-sight between surfaces.
- Each surface interaction is well-modeled as an instantaneous re-equilibration to the surface and Maxwellian emission (cosine-distributed angle).



Modeling tools:

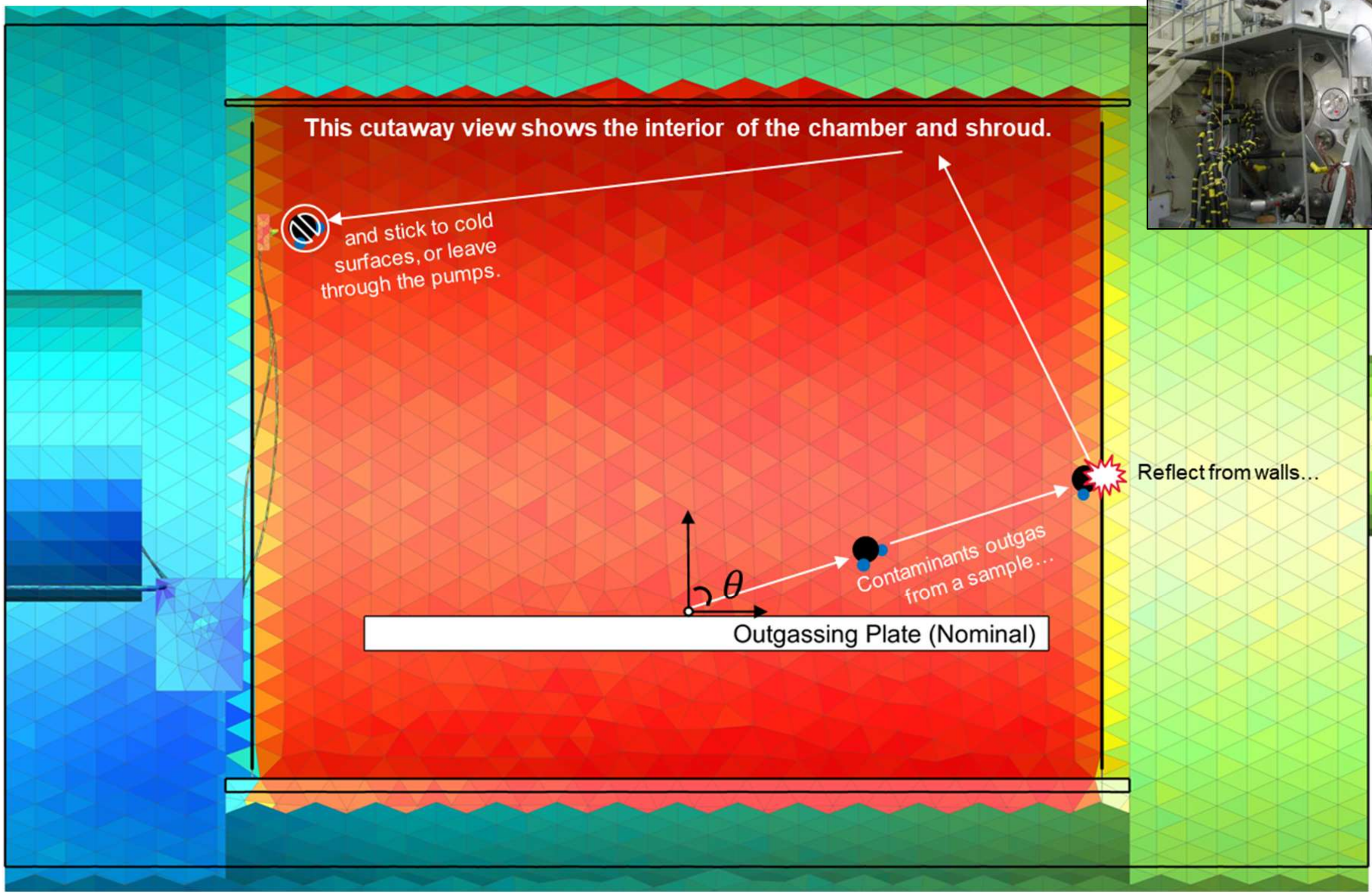
- ray-tracing Monte Carlo schemes (e.g. CERN's MOLFLOW+ code)
- view factor matrix calculation (JPL CC in-house solvers)



Photograph: QCM Research Mk. 10 TQCM.

Thermal Vacuum Chamber Operations:

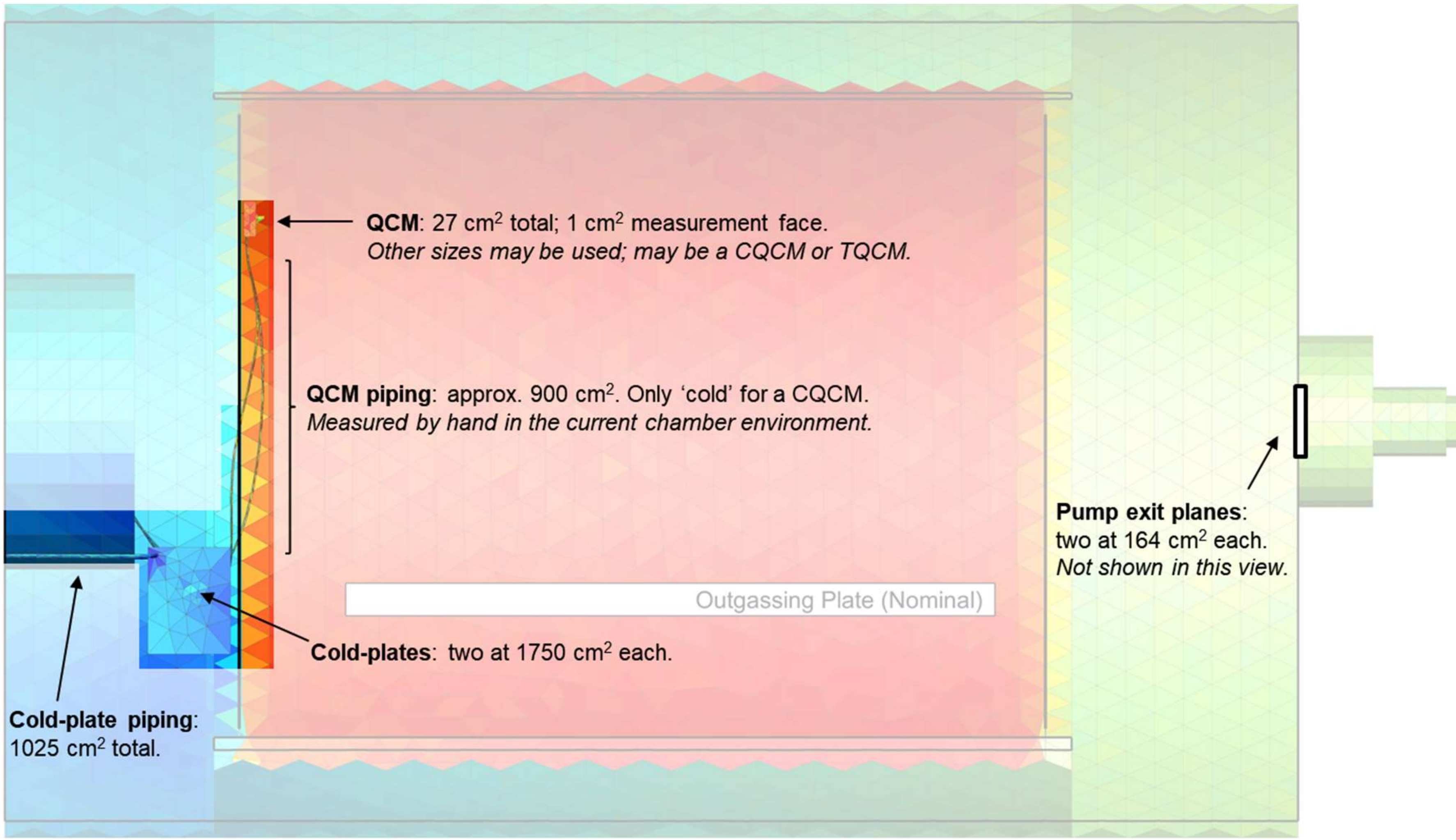
Molecular outgassing, free-molecular transport.



Photograph of this JPL chamber from Fields, K. 2009. "The certification of environmental chambers for testing flight hardware," 25th Aerospace Testing Conf.

Thermal Vacuum Chamber Operations:

Sinks: vents, pumps, and cryogenically-cooled surfaces.

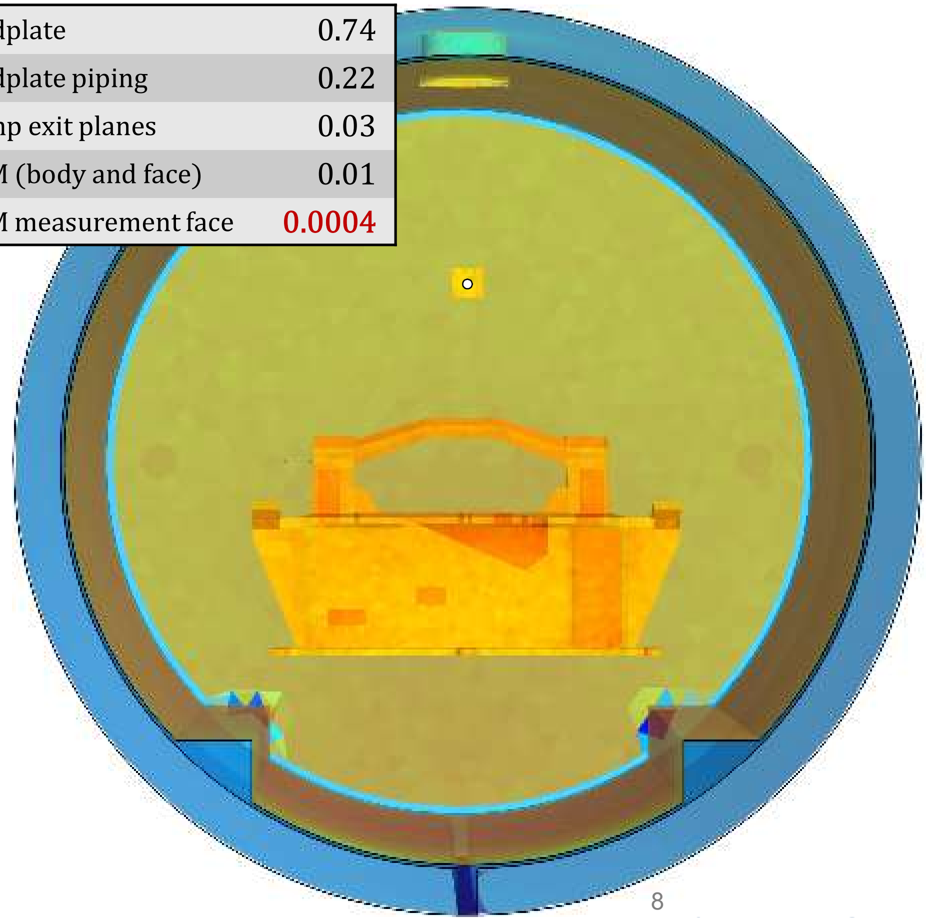


Converting Measurements to OGRs:

$$\boldsymbol{OGR}\left[\frac{\mathrm{g}}{\mathrm{cm^2\,s}}\right] = \left(QCM\ Measurement - Ch.Background \left[\frac{\mathrm{Hz}}{\mathrm{hr}}\right] \right) * \left(\frac{QCM\ Measurement\ Constant \left[\frac{\mathrm{g}}{\mathrm{Hz\,cm^2}}\right] * QCM\ Face\ Area\ [\mathrm{cm^2}]}{\boldsymbol{QCM\ Transmission\ Fraction,\ \alpha} \left[\frac{\mathrm{g}}{\mathrm{g}}\right] * Hardware\ Surface\ Area\ [\mathrm{cm^2}]} \right)$$

$$\boldsymbol{\alpha}\text{:}\ \frac{mass\ onto\ loss\ surface}{total\ mass\ from\ hardware}$$

Coldplate	0.74
Coldplate piping	0.22
Pump exit planes	0.03
QCM (body and face)	0.01
QCM measurement face	0.0004



Methodology:

- Creation of vacuum chamber geometric models, including the identification and measurement of critical hardware – e.g. position, size of vents; of cryocooled piping; of coldfingers and QCMs; and
- FM transport simulations to calculate QCM transmission (pictured).

Benefits:

- **Quantifies chamber geometric and temperature / getting** effects, and is therefore an improvement over transport modeling with area-fraction estimates.
- It also allows for **novel test configurations** – e.g. multi-QCM measurements during bake-outs – and for **iterative chamber designs** to optimize transport.

Iterative Vacuum Chamber Design:

Optimizing QCM transport for low-outgassing-rate testing.

In an example test: **1 × 10 $^{-4}$** of total outgassed mass lands on each QCM (α).

- Typical of QCM transmission in large chambers without effusion cells (i.e. predominantly line-of-sight)

Applying nominal values for a RIOT sample OGR, area, and test time:

$$m_{QCM} = [Sample\ OGR] * [Sample\ Area] * [Test\ Time] * \alpha$$

$$e.g.\ m_{QCM} = \left[10^{-13}\,\frac{g}{cm^2\,s}\right] * [50\ in^2] * [12\ hrs] * \alpha$$

Integrated over the test, just $\boldsymbol{m_{QCM}}$ **≈ 0.1 ng** would deposit per QCM!

- If you want to resolve O[$10^{-13}\,\frac{g}{cm^2 s}$] outgassing:

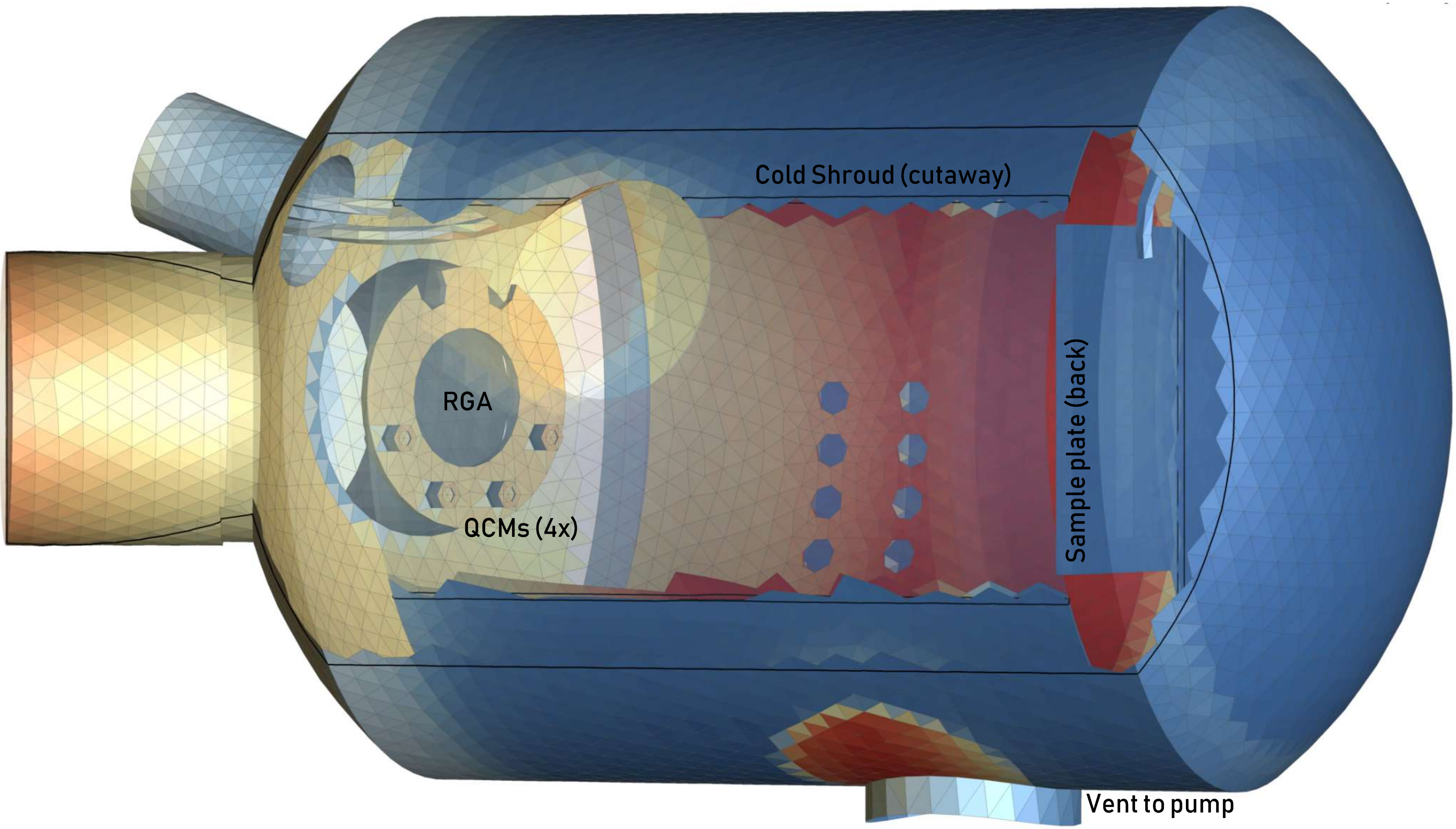
  sample area could be increased by at most a factor of two...

  test time could be extended by at most a factor of two…

  past experience shows that transmission fraction α can be increased by at least an order of magnitude with chamber geometry / boundary condition changes.

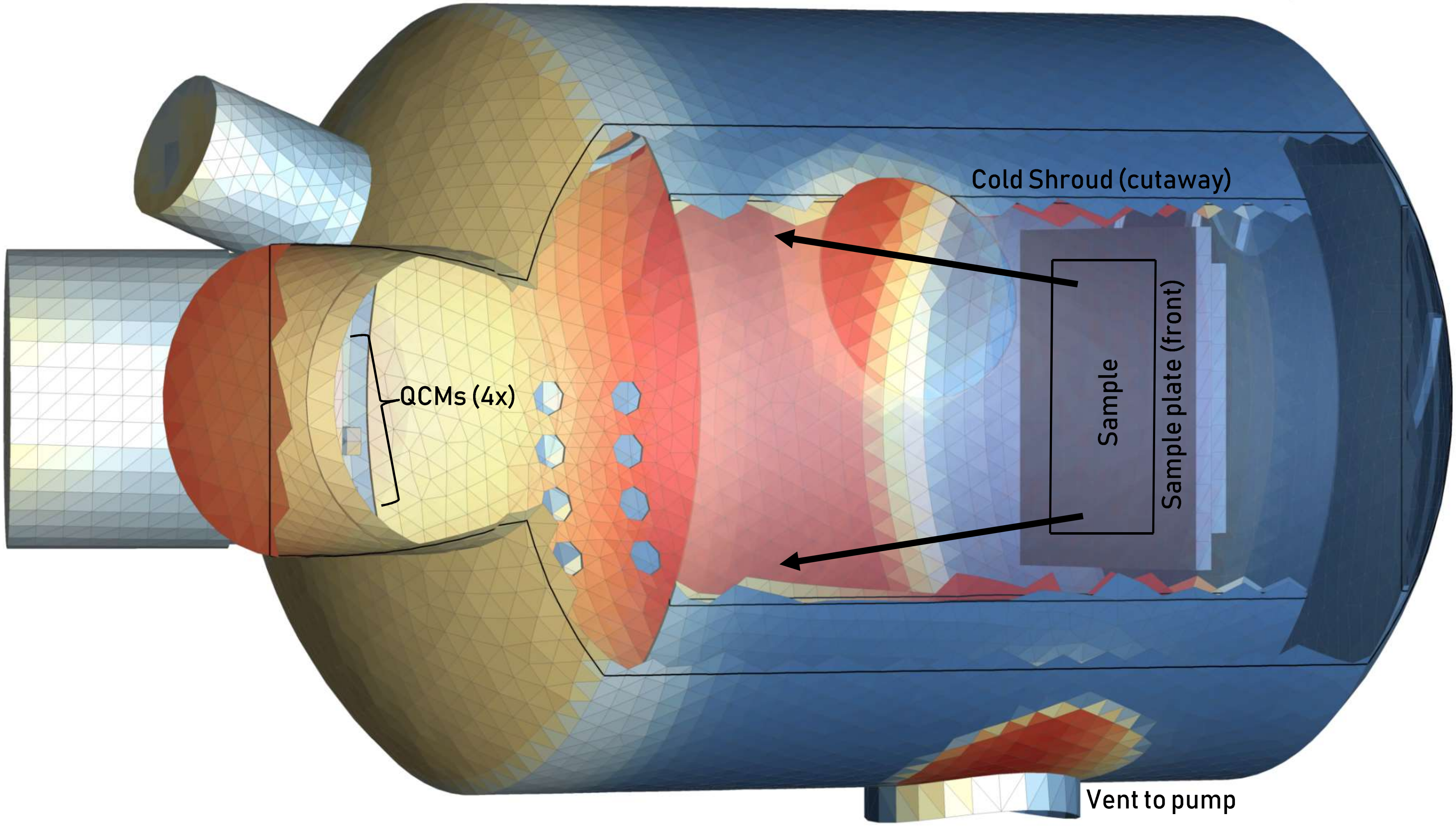
The optimal strategy to increase measurements to detectable levels:

Increase QCM transmission fraction.



JPL Dynamitron chamber free-molecular transport: Modeling results, baseline configuration.

Figure: 3-D cutaway of the chamber interior, colored by fluence of sample-outgassed molecules per unit area. Cutaway regions shown translucent.



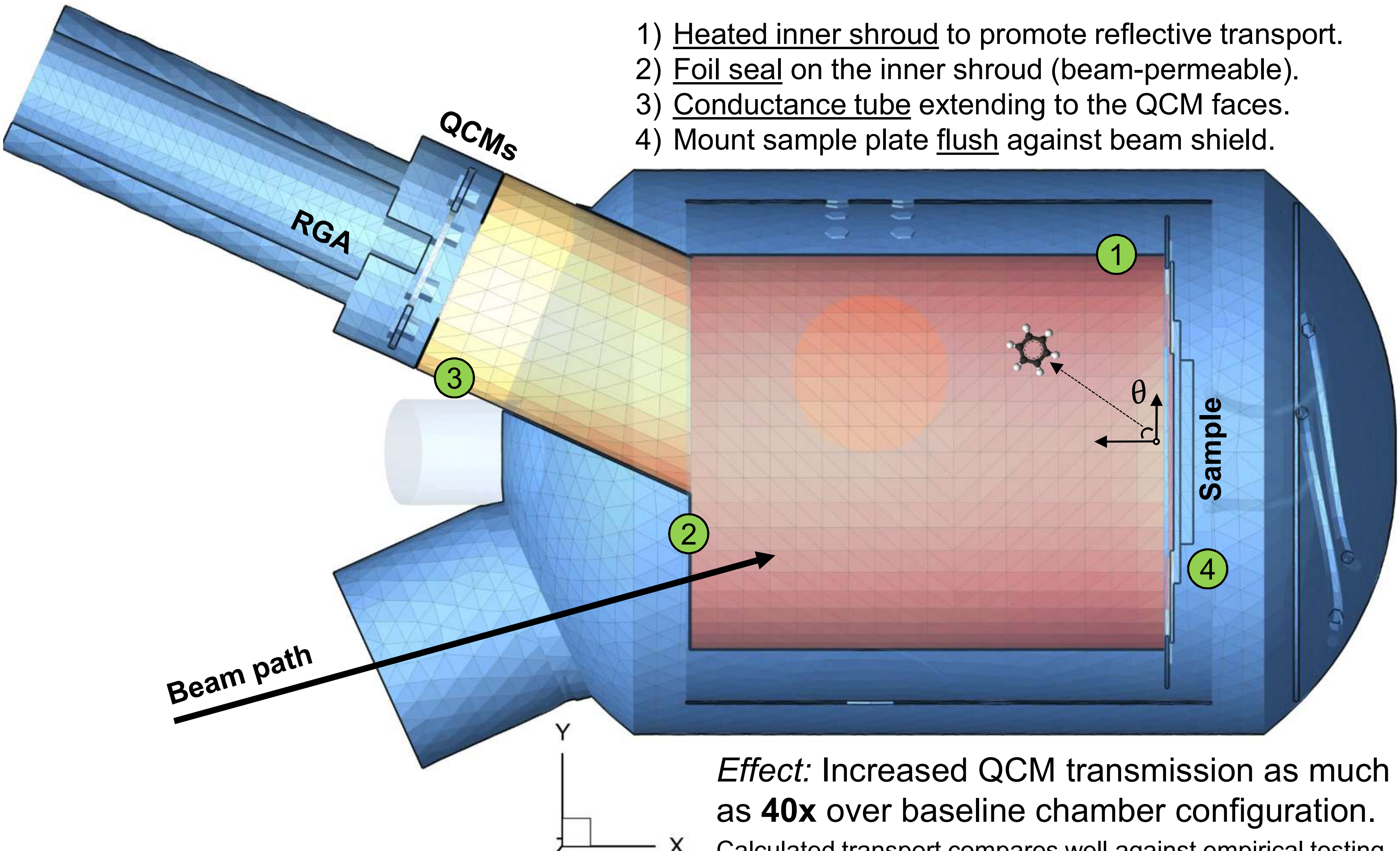
JPL Dynamitron chamber free-molecular transport: Modeling results, baseline configuration.

Result: A cold (80K) shroud collects **> 99 %** of outgassing, **< 1 %** to the pump vent.
1×10^{-4} of total outgassed mass deposits onto each QCM (α).

Iterative Vacuum Chamber Design

Optimizing QCM transport by simulating efficacy of ***modifications:***

1) Heated inner shroud to promote reflective transport.
2) Foil seal on the inner shroud (beam-permeable).
3) Conductance tube extending to the QCM faces.
4) Mount sample plate flush against beam shield.



Effect: Increased QCM transmission as much as **40x** over baseline chamber configuration.

Calculated transport compares well against empirical testing.

Spacecraft Contamination by Return Flux:

Molecular contaminants that outgas from a spacecraft “reflect” from an ambient exosphere during fly-bys and return to impact sensitive instruments.

This *return flux* is a primary vector for the self-induced contamination of instruments with low view factor to the spacecraft (e.g. mass spectrometers).

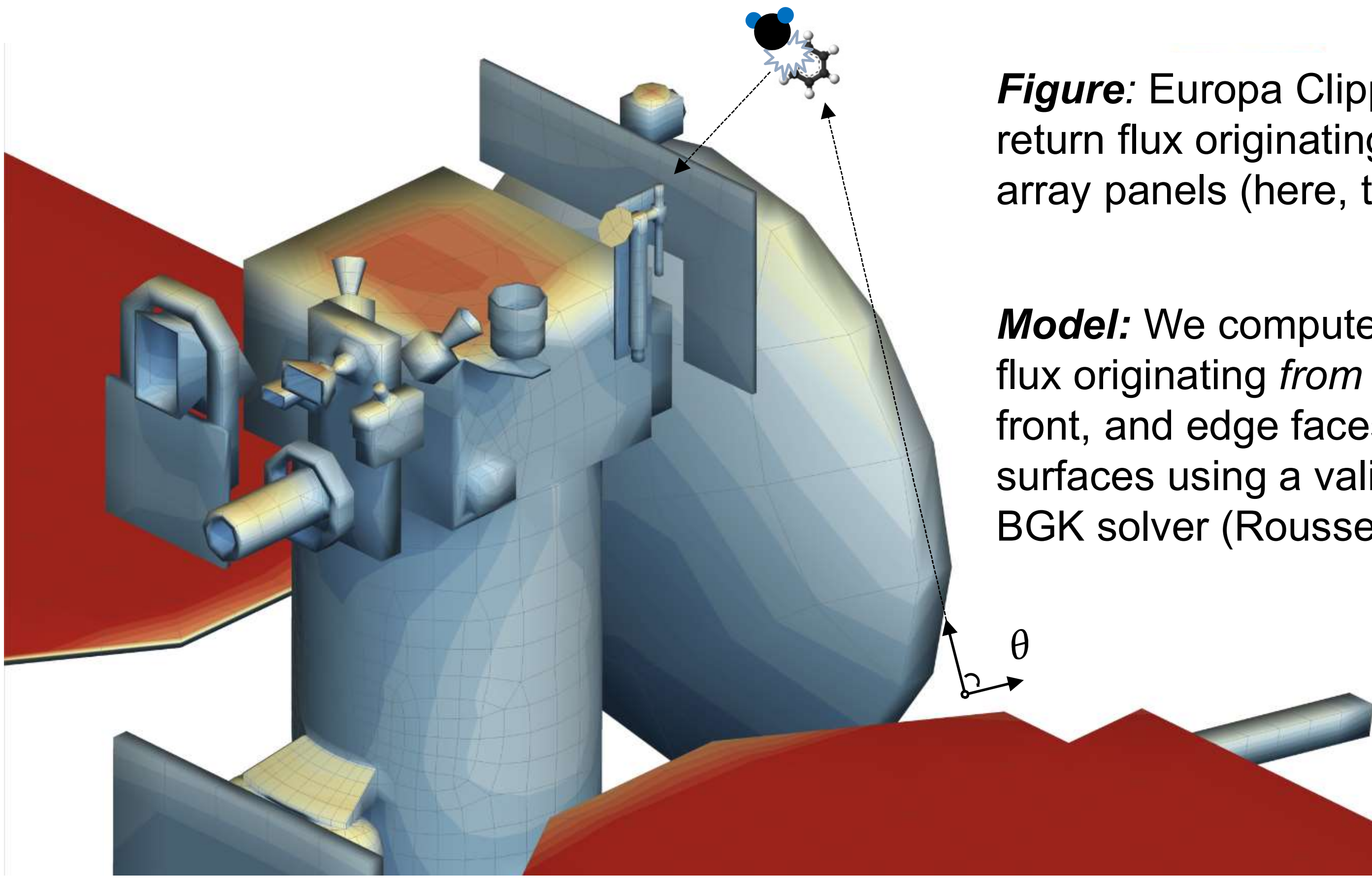


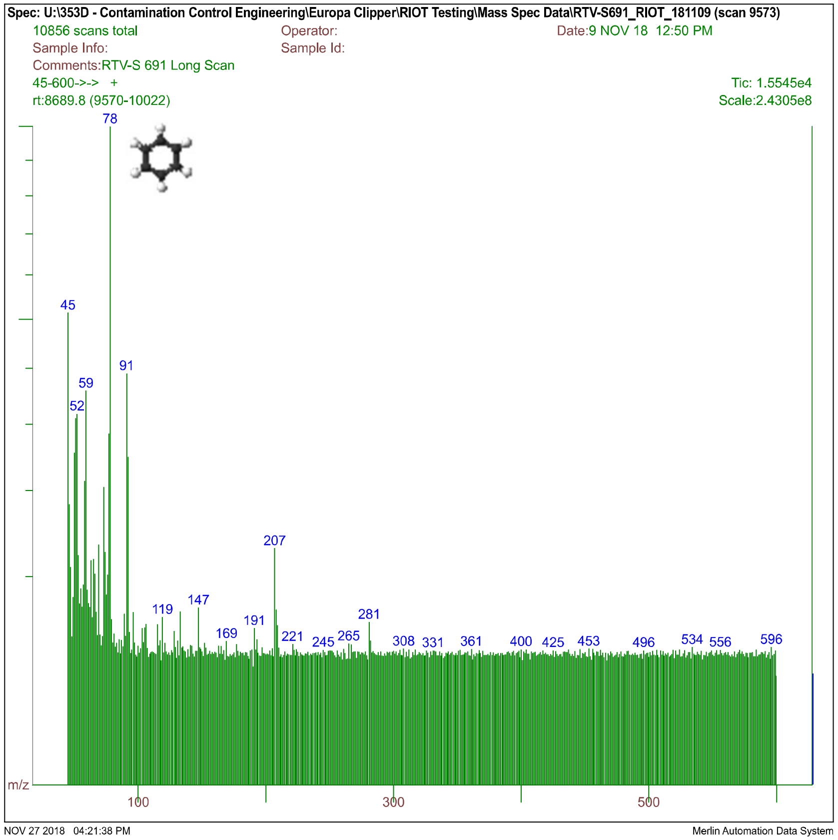
***Figure**:* Europa Clipper, colored by the return flux originating from RAM-facing array panels (here, the array backside).

Model: We compute contaminant return flux originating *from* solar array back, front, and edge faces *to* all spacecraft surfaces using a validated Boltzmann BGK solver (Roussel et al., 2002).

Return Flux Boundary Conditions:

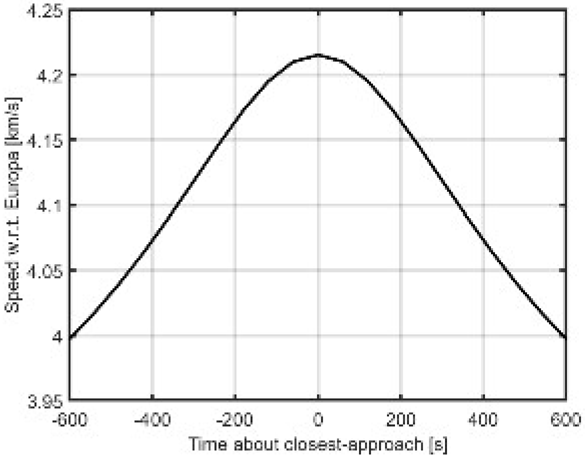
Outgassing Material Composition

RIOT mass spectrometer measurements show abundance of benzene (78 amu, $ø_{KD}$ 585 pm).

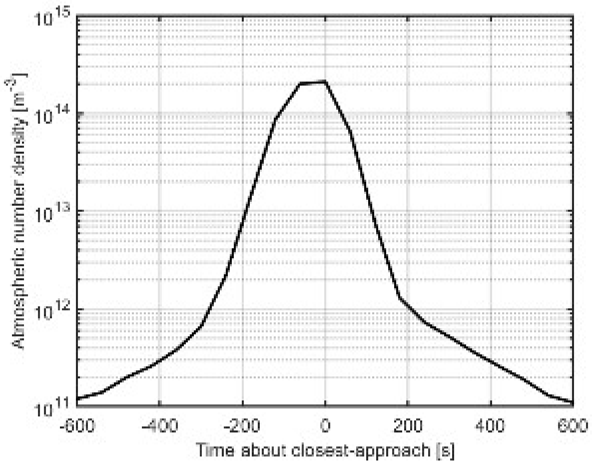


Trajectory, Atmospheric Interaction

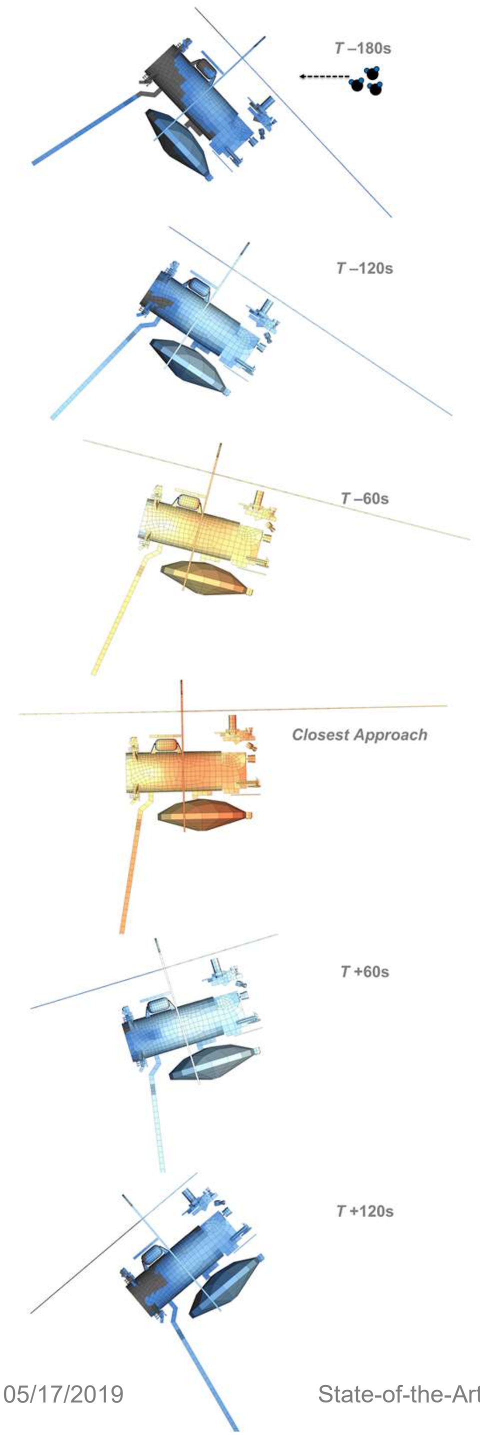
Spacecraft speed relative to body, RAM angle.

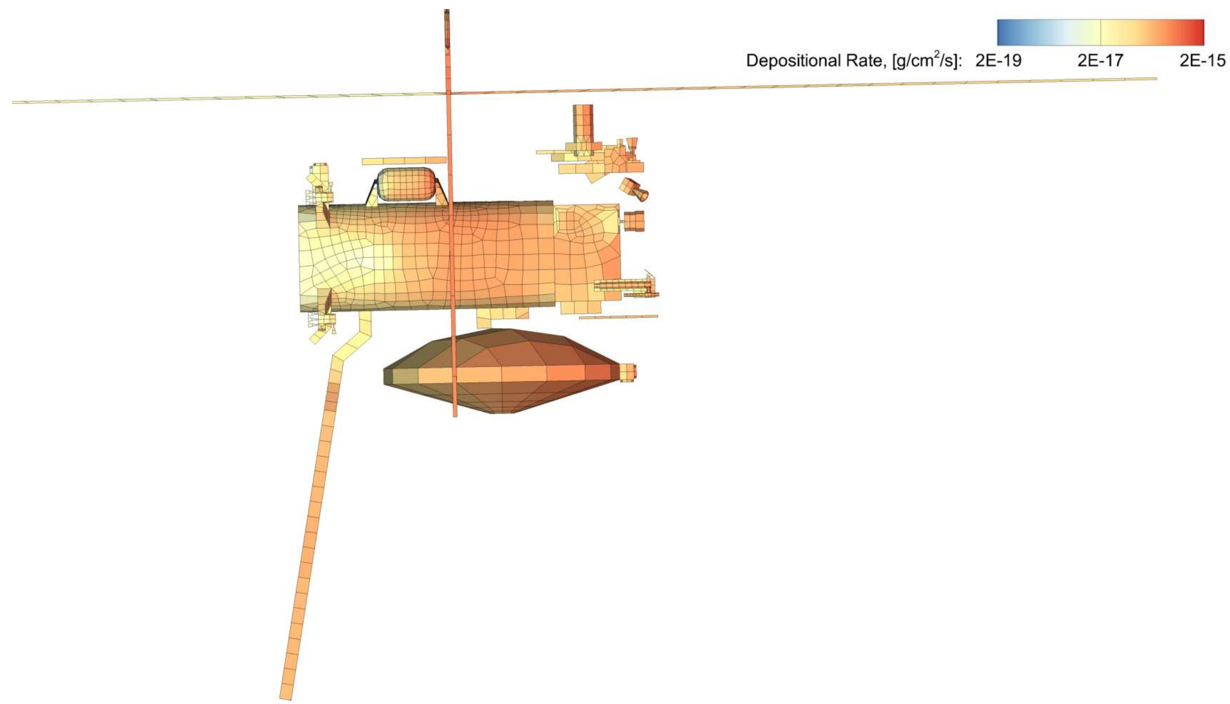


Atmospheric density and composition.



(Column) return flux originating from solar array thermal side during a close-approach fly-by; frames spaced by minute. **Note the preferential return of ram-directed outgassing to instrument surfaces.**





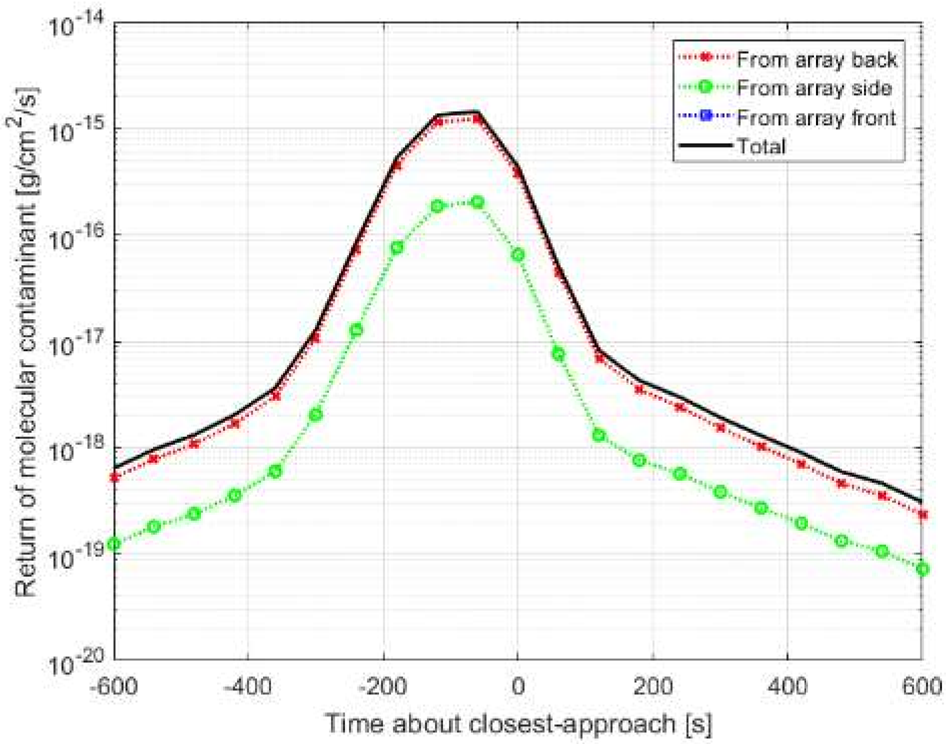


Figure: Return flux to an instrument from a typical Europan fly-by: the solar array's **ram-facing** thermal side dominates return flux to the instrument suite.

Active-side (solar cell, facing away from ram) contributions are minimal.

Table: Representative outgassing rates for a typical flight system's solar array and resultant peak molecular return flux rates per Europan fly-by.

Contaminant Source	Representative array outgassing rates [g/cm^2/s]	Peak return flux to an instrument, per source [g/cm^2/s]	Peak return flux to an instrument, **total** [g/cm^2/s]
Solar array active (solar cells)	1.0E–14	< 1.0E–20	
Solar array thermal (backside)	3.0E–14	4.0E–16	**5.0E–16**
Solar array edges (panel venting)	2.0E–12	9.0E–17	

Conclusions

- JPL Contamination Control has developed sophisticated capabilities for simulating free-molecular transport in vacuum chamber environments.
  - We demonstrate a methodology for determining hardware outgassing rates from Quartz Crystal Microbalance (QCM) measurements that enables the verification of bake-out exit criteria through the quantification of chamber geometry and temperature effects on free-molecular transport.
  - These capabilities allow us to characterize outgassing rates of concern to high-sensitivity scientific missions that could not be resolved in standard testing.

- Spacecraft self-induced contaminant return flux contributions to science instruments can be significant – especially to next-generation and state-of-the-art mass spectrometers intended to detect organics – and must be characterized to ensure that mission science objectives can be achieved.
  - The cases illustrated here, generated for a typical Europan fly-by, show a return flux of approximately 1 % of the effective outgassing rate from a solar powered spacecraft configuration. Hence, selection of low-outgassing materials (e.g., exhibiting rates of 1.0E–14 to 1.0E–15 $g/cm^2/s$) is desired to limit molecular return flux from the flight system to science instruments.

BACKUP: Quartz Crystal Microbalances

- Measures changes in mass by monitoring changes in resonant beat frequency between two matched crystals
- Crystal specifies the resonant frequency and therefore the mass calculation
- 15 MHz crystals: 1.964×10^{-9} g/cm^2/Hz
- QCM Hz/hr exit criteria are set based on chamber layout and outgassing rate requirements
- QCMs are very sensitive to small temperature changes, vibrations