



# Modeling contamination migration on the Chandra X-ray Observatory — III

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# Outline



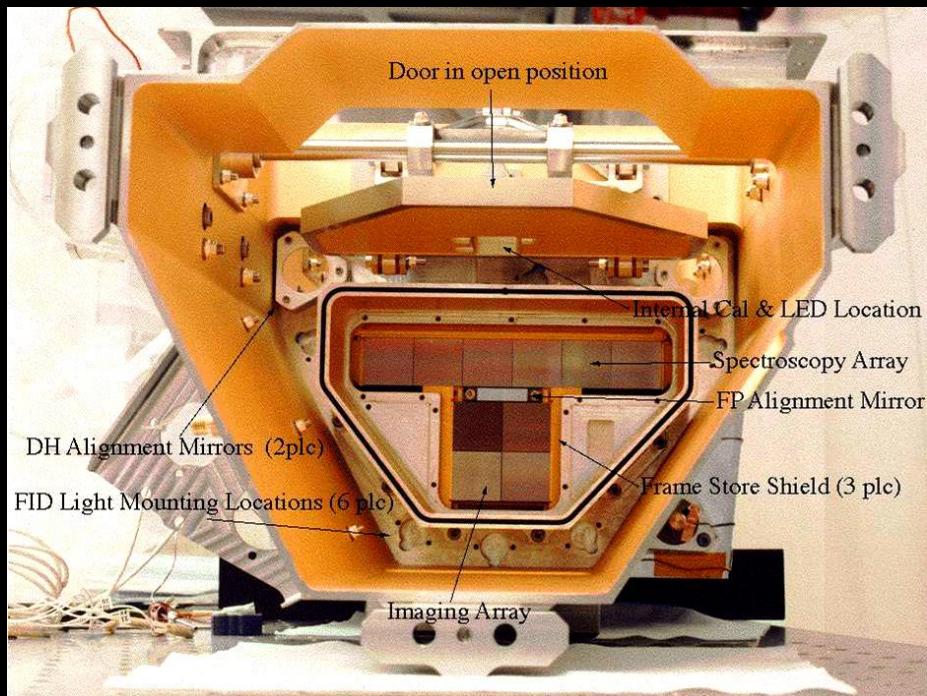
- Introduction
- Molecular contamination on ACIS filters
- Thermal model for ACIS cavity
- Molecular transport simulations
- Summary



# Chandra's Advanced CCD Imaging Spectrometer (ACIS)



- ACIS cavity
  - Collimator
  - Snoot & door
  - Camera top & filters (OBF)



- ACIS operating temperatures
  - Focal plane  $T_{FP} = -120^{\circ}\text{C}$
  - Camera housing  $T_{DH} = -60^{\circ}\text{C}$ 
    - $\approx 8^{\circ}\text{C}$  colder with heaters off
  - Optical blocking filters  $T_{OBF}$ 
    - $\approx T_{DH} \approx -60^{\circ}\text{C}$  near OBF edge
    - 5–20°C warmer near center depending on emissivity  $\epsilon_{OBF}$
- Contamination on cold OBFs
  - Mass column  $\approx 200 \mu\text{g cm}^{-2}$ .
    - $\leq 1 \text{ g}$  in entire *Chandra* optical cavity (calculated)
    - $\approx 30 \times$  pre-flight estimates
  - Thicker near OBF edge

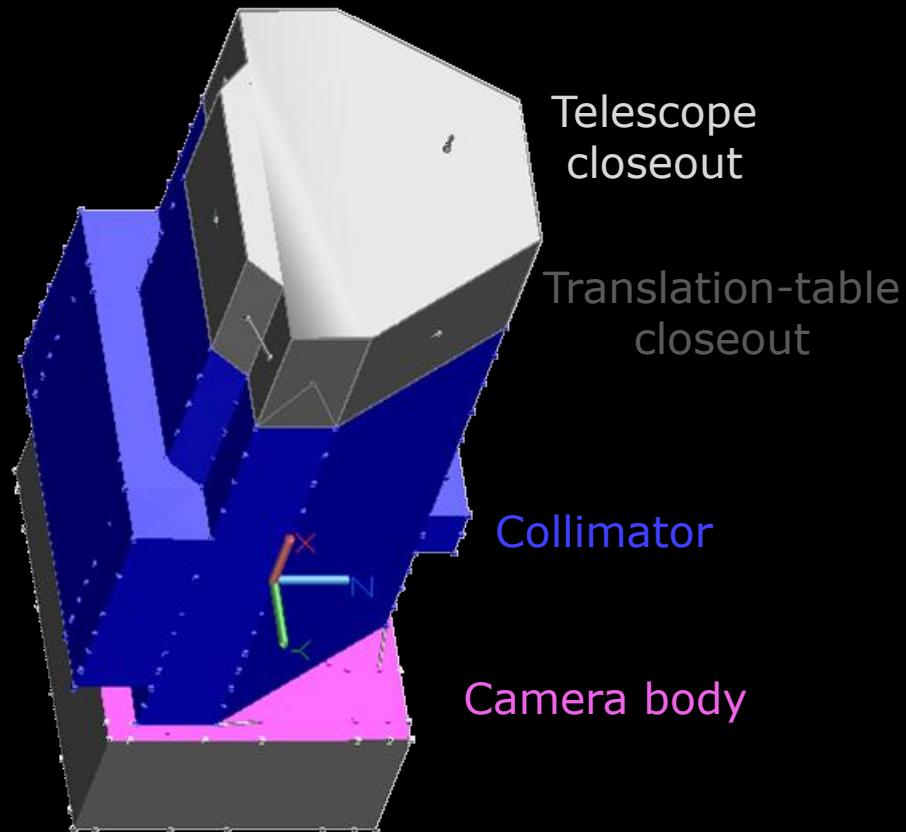


# Contamination-migration simulations for Chandra



- 2004 (I)
  - Low-resolution geometrical model for ACIS cavity
  - Supported bake-out decision in 2004
- 2013 (II)
  - High-resolution geometrical model for ACIS cavity
  - Higher emissivity for contaminated surfaces
- 2015 (III)
  - Same model as 2013
  - Will support bake-out decision in 2016

- ACIS geometrical model (exterior view)





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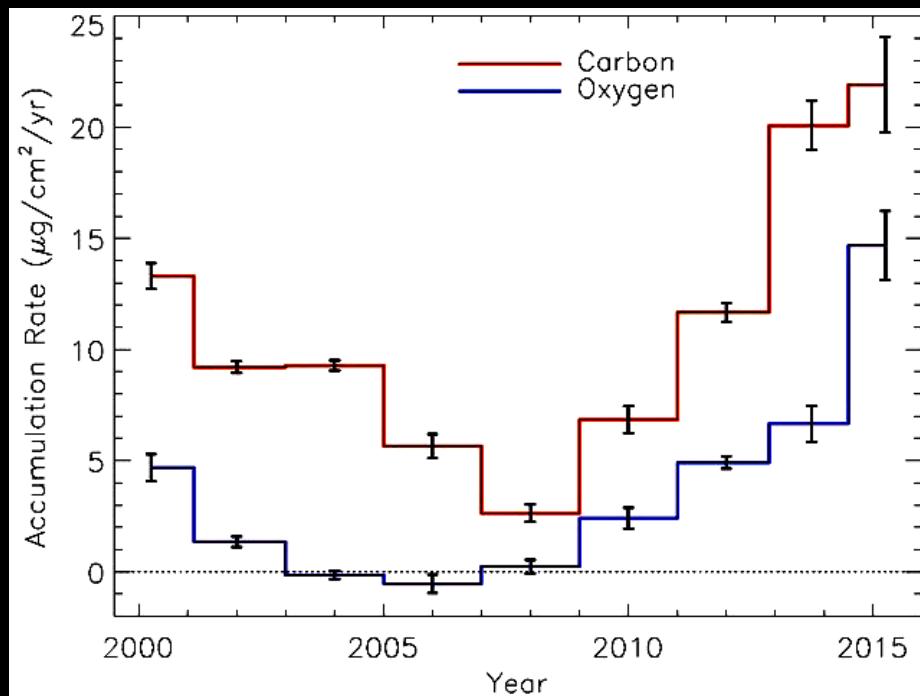
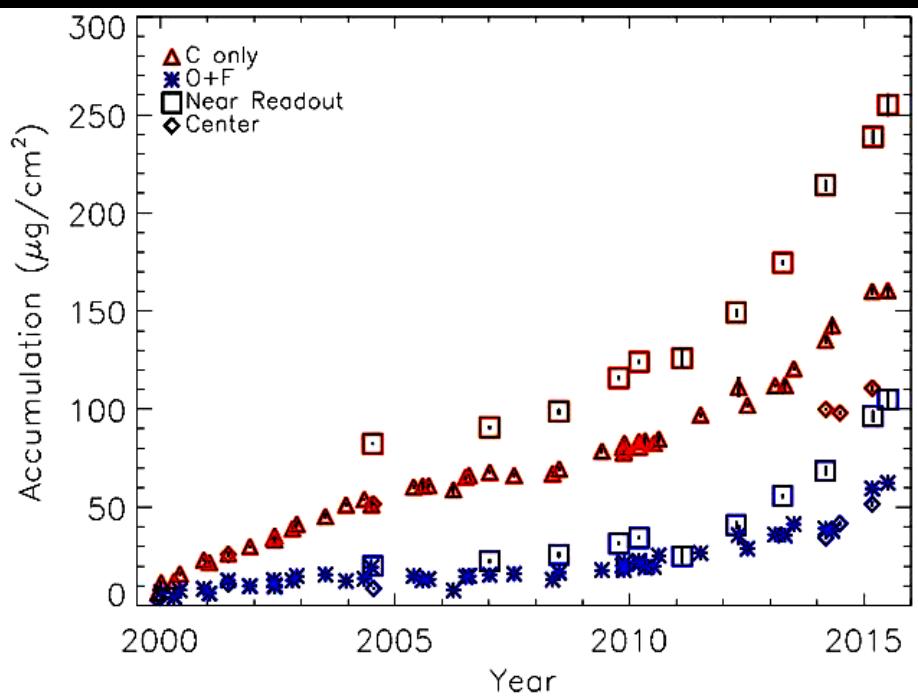


# Evolution of mass column, its rate, and composition



- Accumulation of contaminants
  - LETG/ACIS-S spectra
    - Atomic (C,O,F) edge depths
  - Thickest near OBF edges

- Rate fell until about 2009 then started rising.
- Composition changes indicate multiple species.

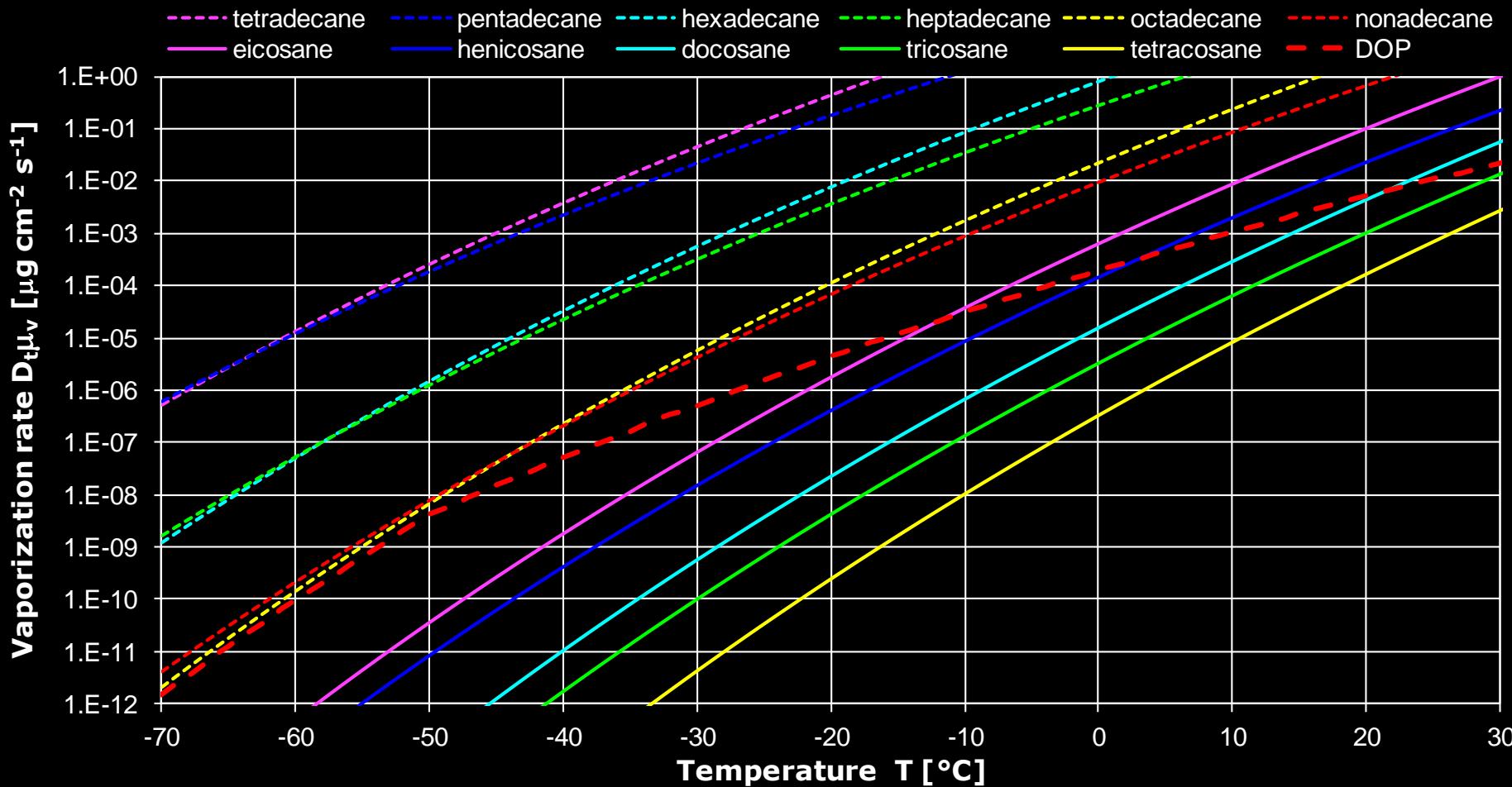




# Temperature dependence of mass vaporization rate



## Mass vaporization rates of some organic compounds

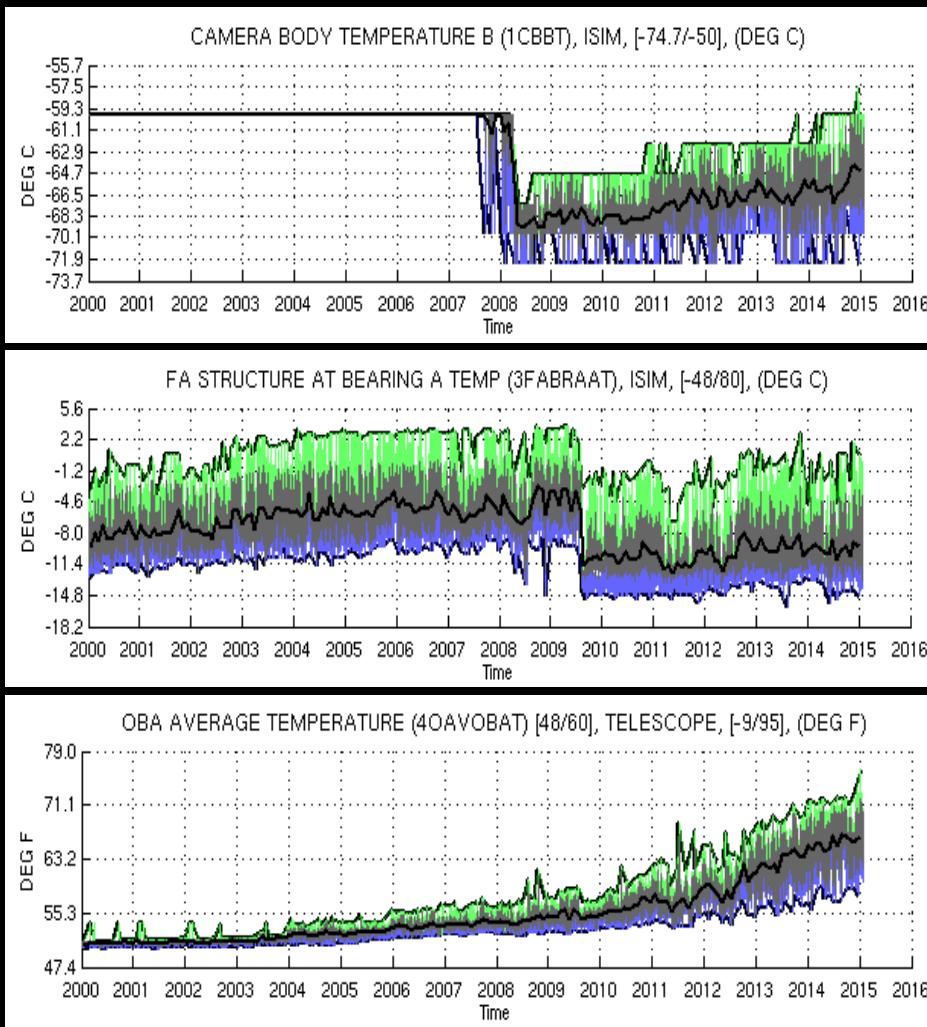




# Thermal history



- Most systems are warming.
  - Continuing degradation of external insulation (MLI)
- Strive to keep ACIS focal plane cold to preserve performance.
  - Carefully plan observations.
  - Disabled some heaters.
    - ACIS detector-housing heater (2008 April)
    - A SIM focus-assembly heater (2009 August)
- Optical bench has warmed rapidly since about 2010.
  - New contamination source?





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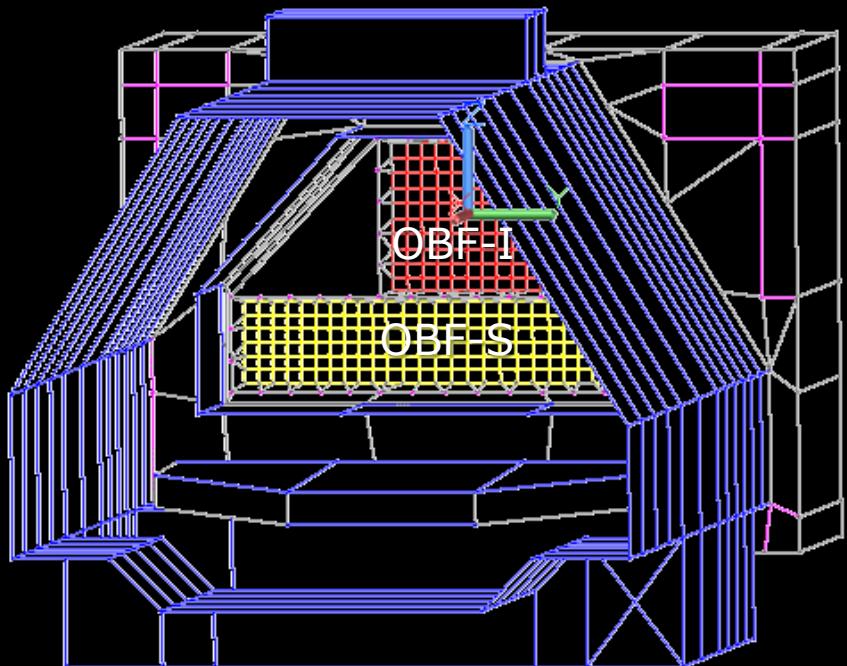
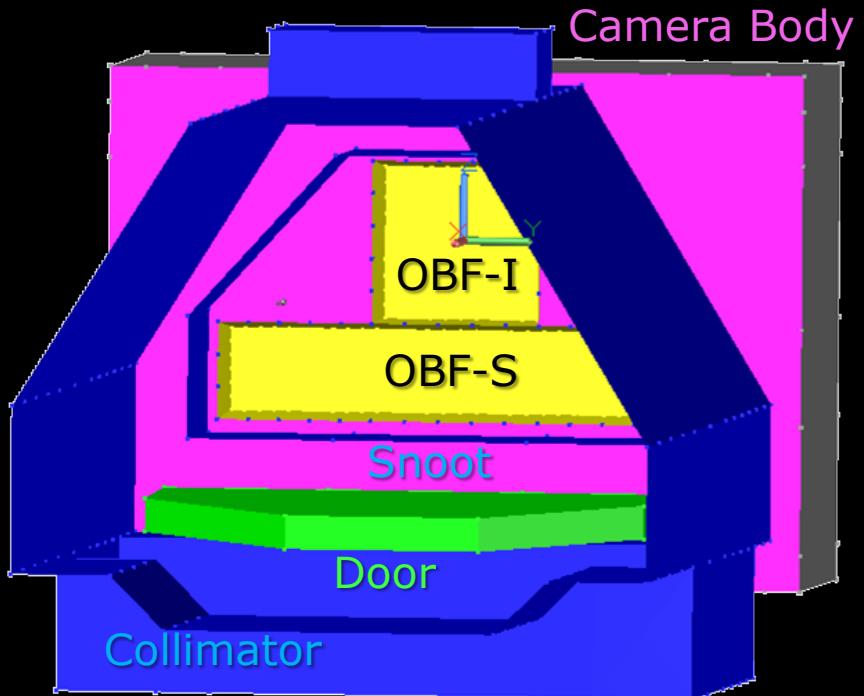


# ACIS geometric model (interior view)



- Interior view of ACIS cavity
  - Snoot & door inside collimator
  - Camera top with OBFs

- High-resolution model maps temperature gradients
  - OBF: 121 I & 203 S nodes
  - Collimator: 12 axial zones

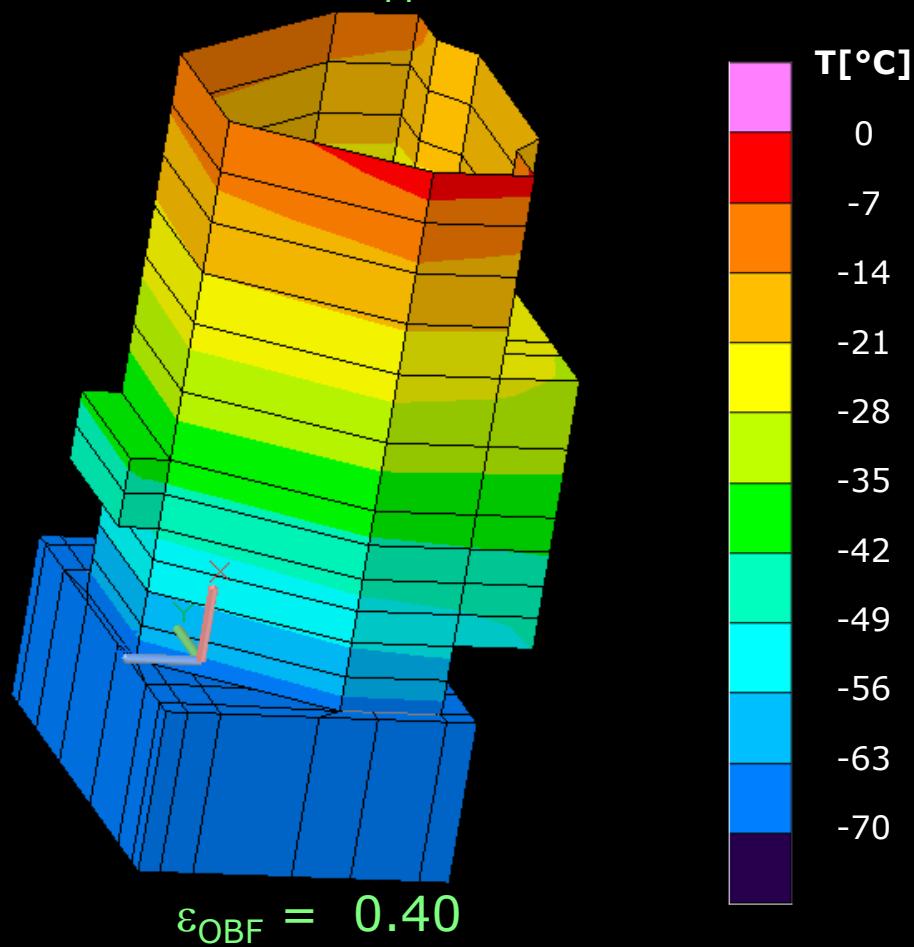




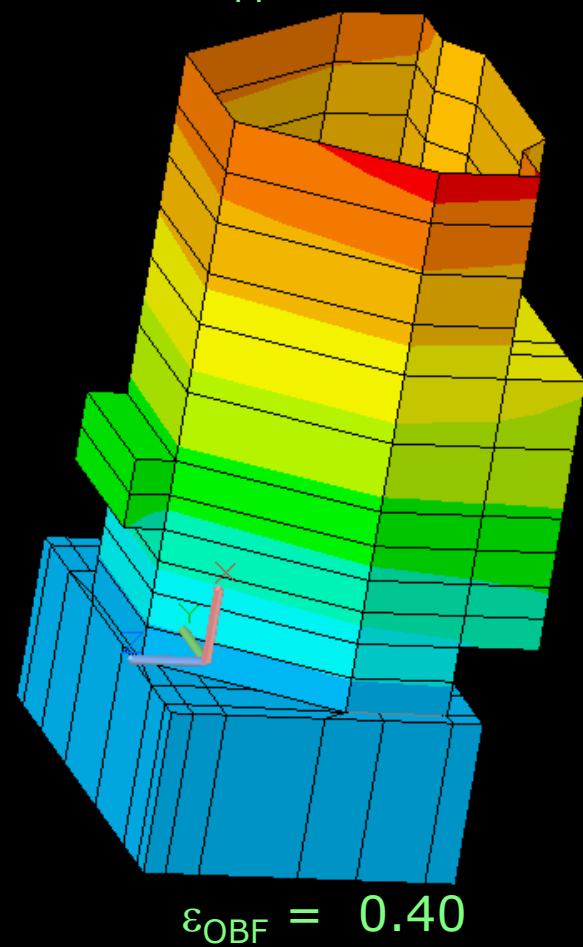
# ACIS temperature distribution (operational conditions)



➤ DH heater OFF,  $T_{FP} = -120^{\circ}\text{C}$



➤  $T_{DH} = -60^{\circ}\text{C}$ ,  $T_{FP} = -120^{\circ}\text{C}$

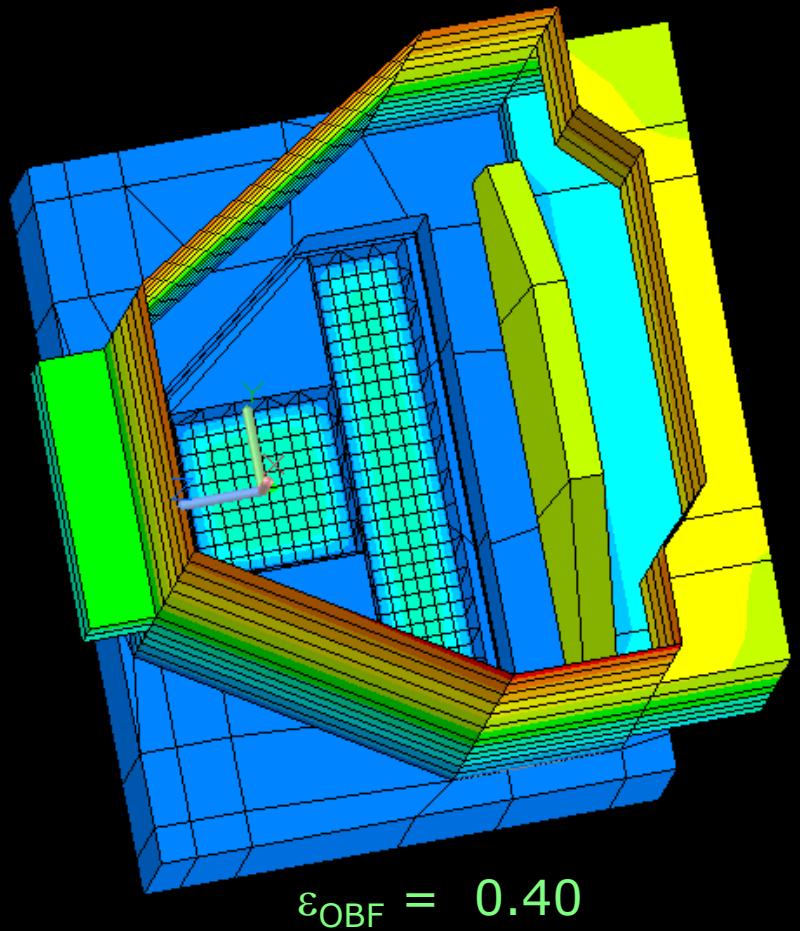




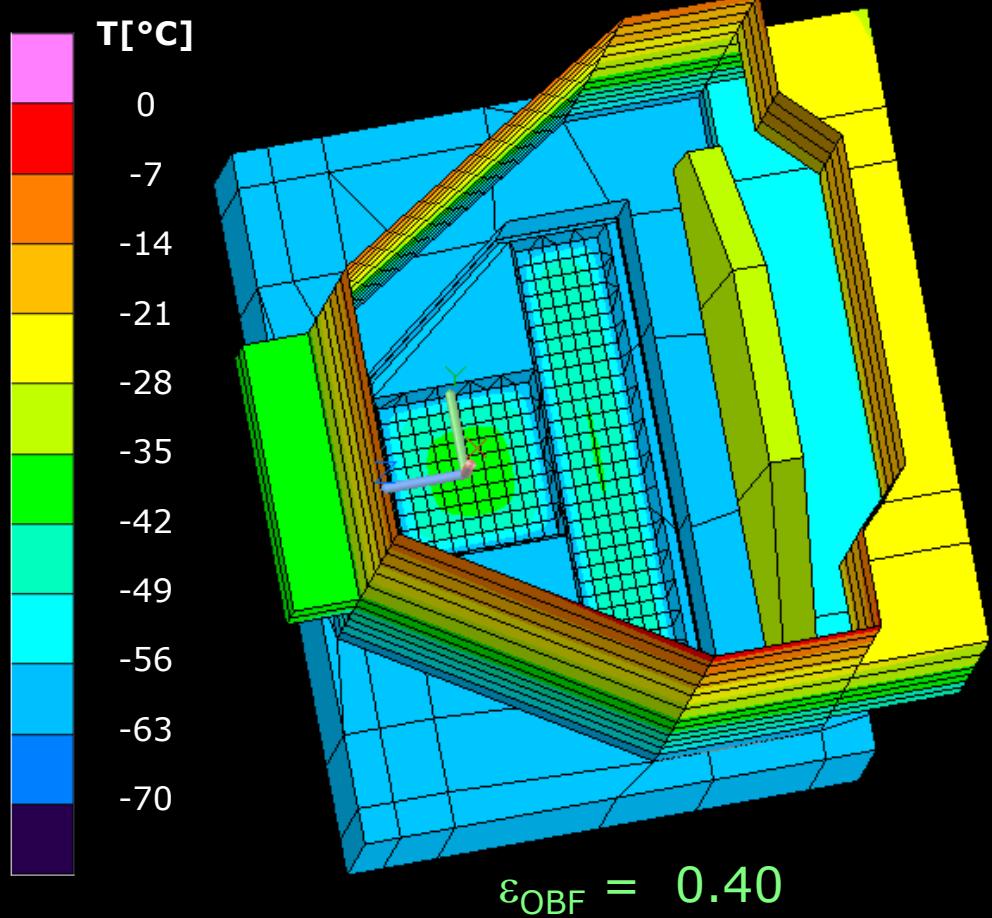
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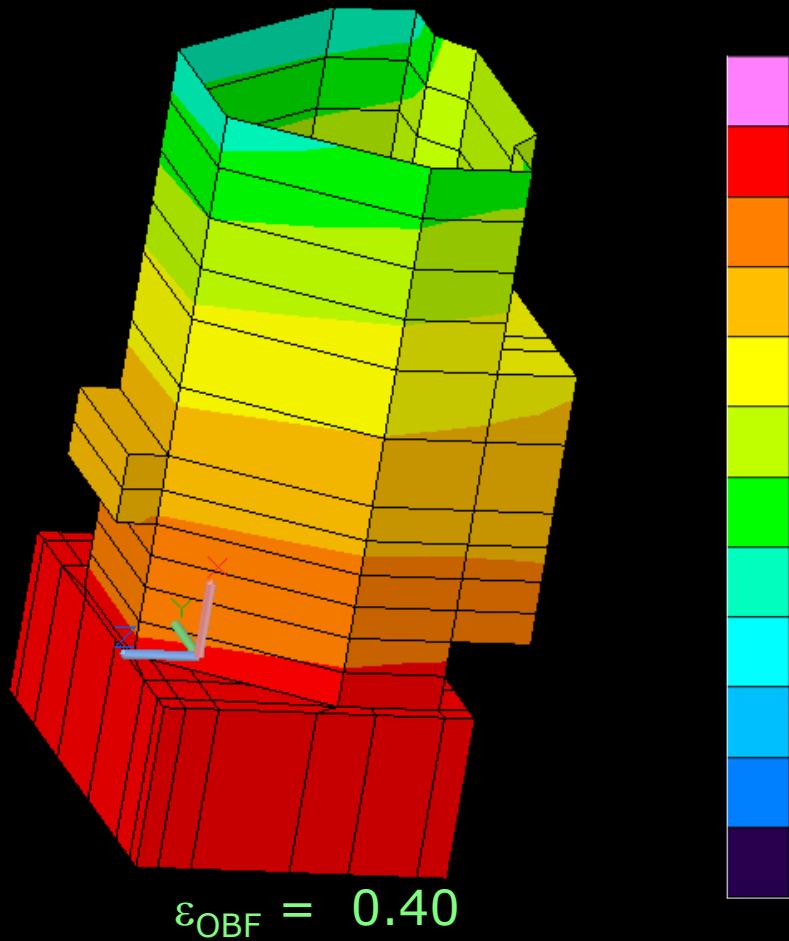




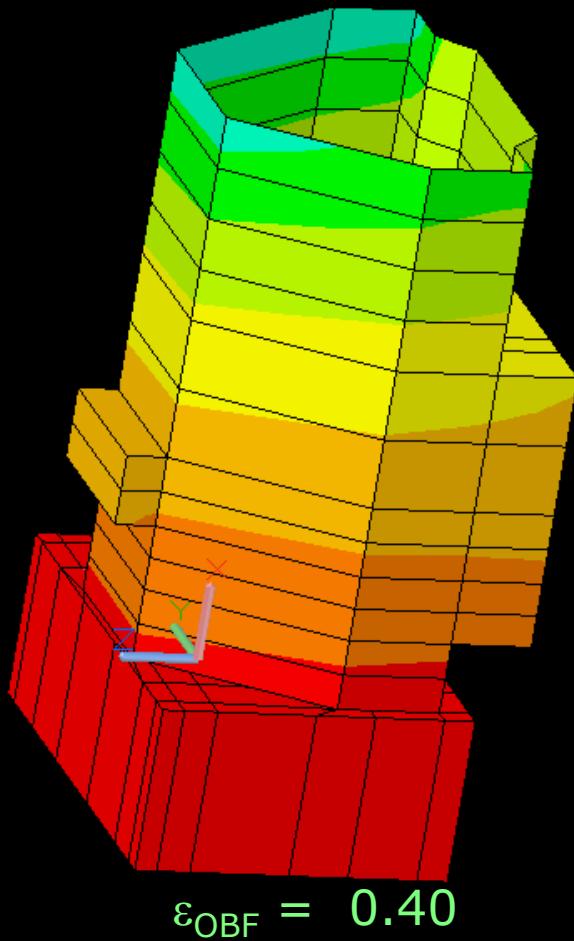
# ACIS temperature distribution (bake-out conditions)



➤  $T_{DH} = +25^\circ\text{C}$ ,  $T_{FP} = -60^\circ\text{C}$



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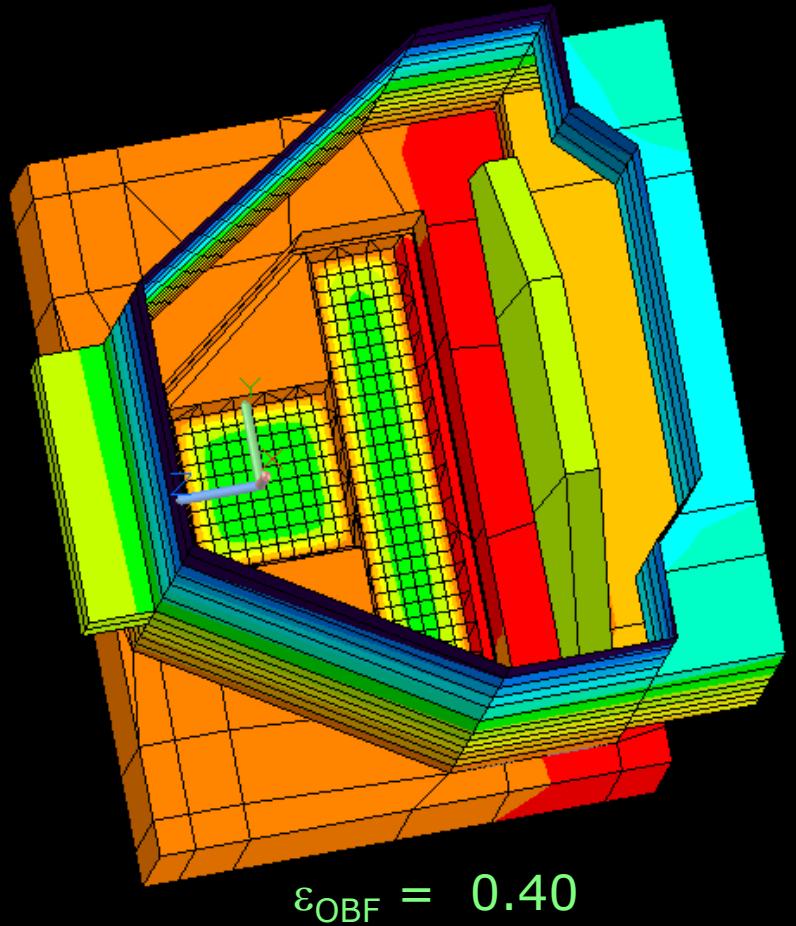




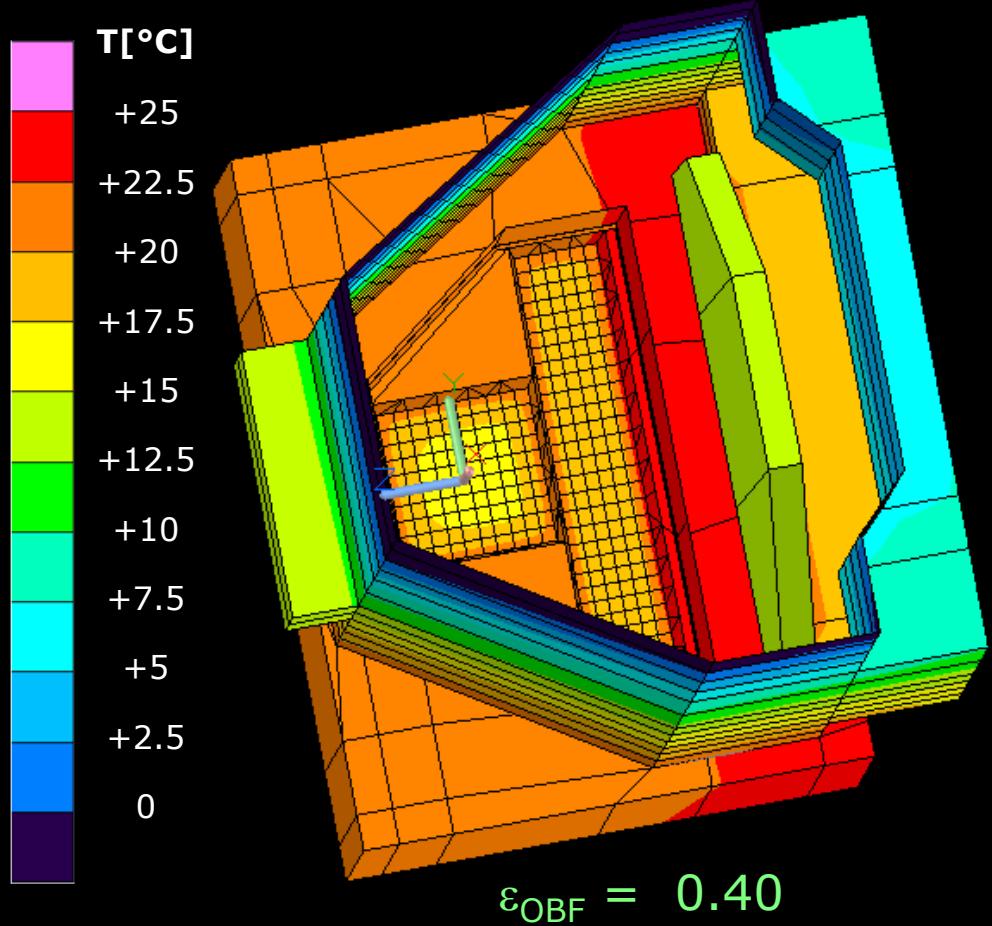
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# Molecular flux equations and geometric view factors



## ➤ Net mass flux onto node j

$$\frac{d\mu_j}{dt} = -\dot{\mu}_v(T_j)\Theta(\mu_j) + \sum_k \dot{\mu}_v(T_k)\Theta(\mu_k) f_{jk} \frac{A_k}{A_j}$$

## ➤ Mass vaporization flux

### □ Related to vapor pressure

$$\dot{\mu}_v(T) = \frac{P_v(T)}{\sqrt{2\pi RT/M}}$$

## ➤ Clausius–Clapeyron relation

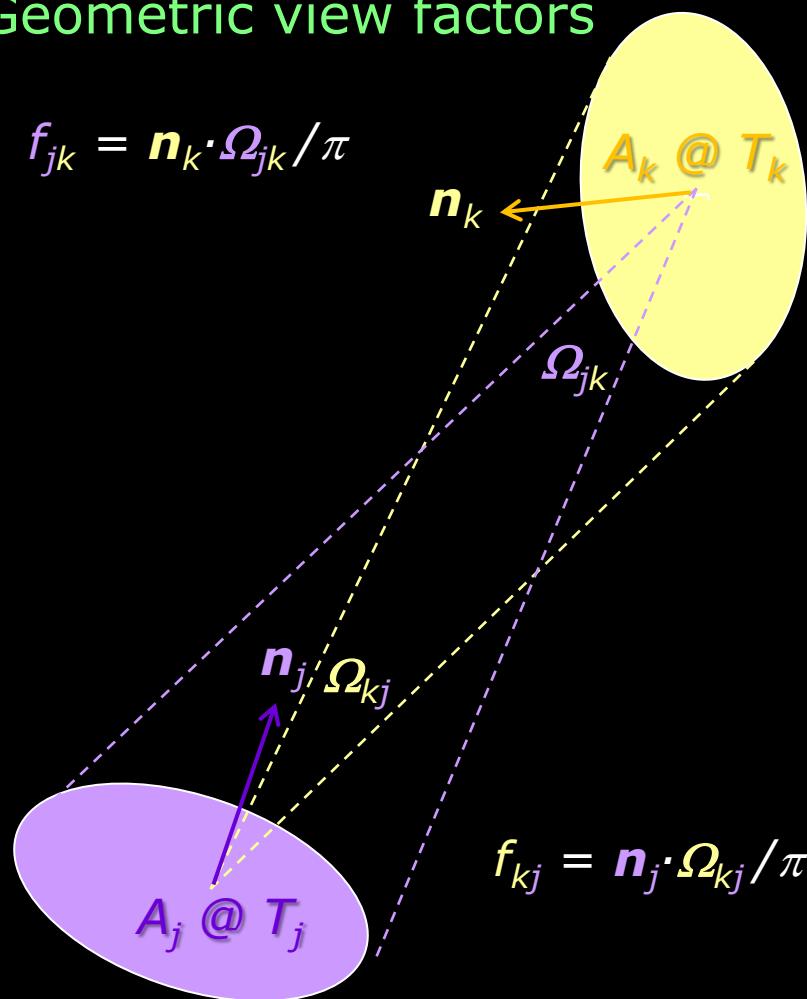
### □ Temperature dependence

### □ Vaporization enthalpy $\Delta_v H$

$$P_v(T) = P_v(T_\circ) \text{Exp}\left[-\frac{\Delta_v H}{R}\left(\frac{1}{T} - \frac{1}{T_\circ}\right)\right]$$
$$\dot{\mu}_v(T) = \dot{\mu}_v(T_\circ) \sqrt{\frac{T_\circ}{T}} \text{Exp}\left[-\frac{\Delta_v H}{R}\left(\frac{1}{T} - \frac{1}{T_\circ}\right)\right]$$

## ➤ Geometric view factors

$$f_{jk} = \mathbf{n}_k \cdot \Omega_{jk} / \pi$$

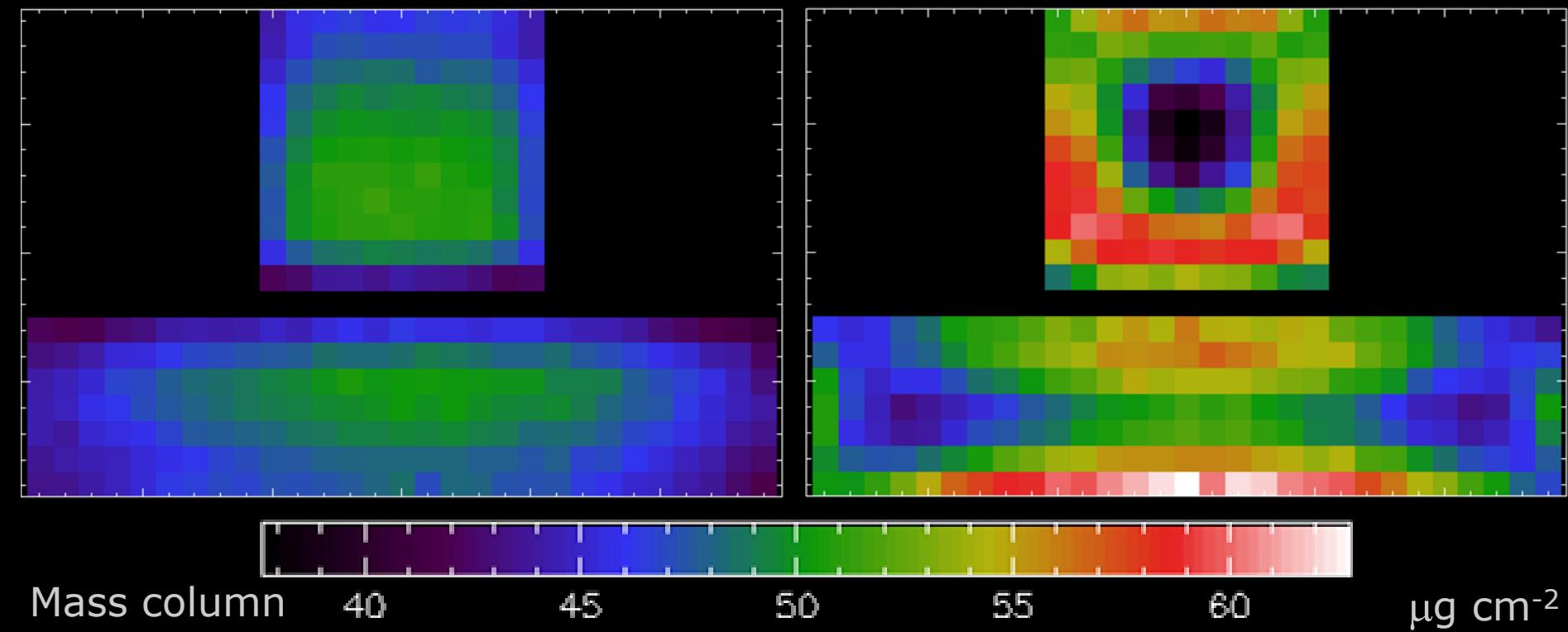




# Simulations of contaminant accumulation onto ACIS OBFs



- Lower volatility contaminant
  - Deposition dominates.
    - Accumulates most at center.
- Higher volatility contaminant
  - Vaporization is significant.
    - Accumulates most at edges.

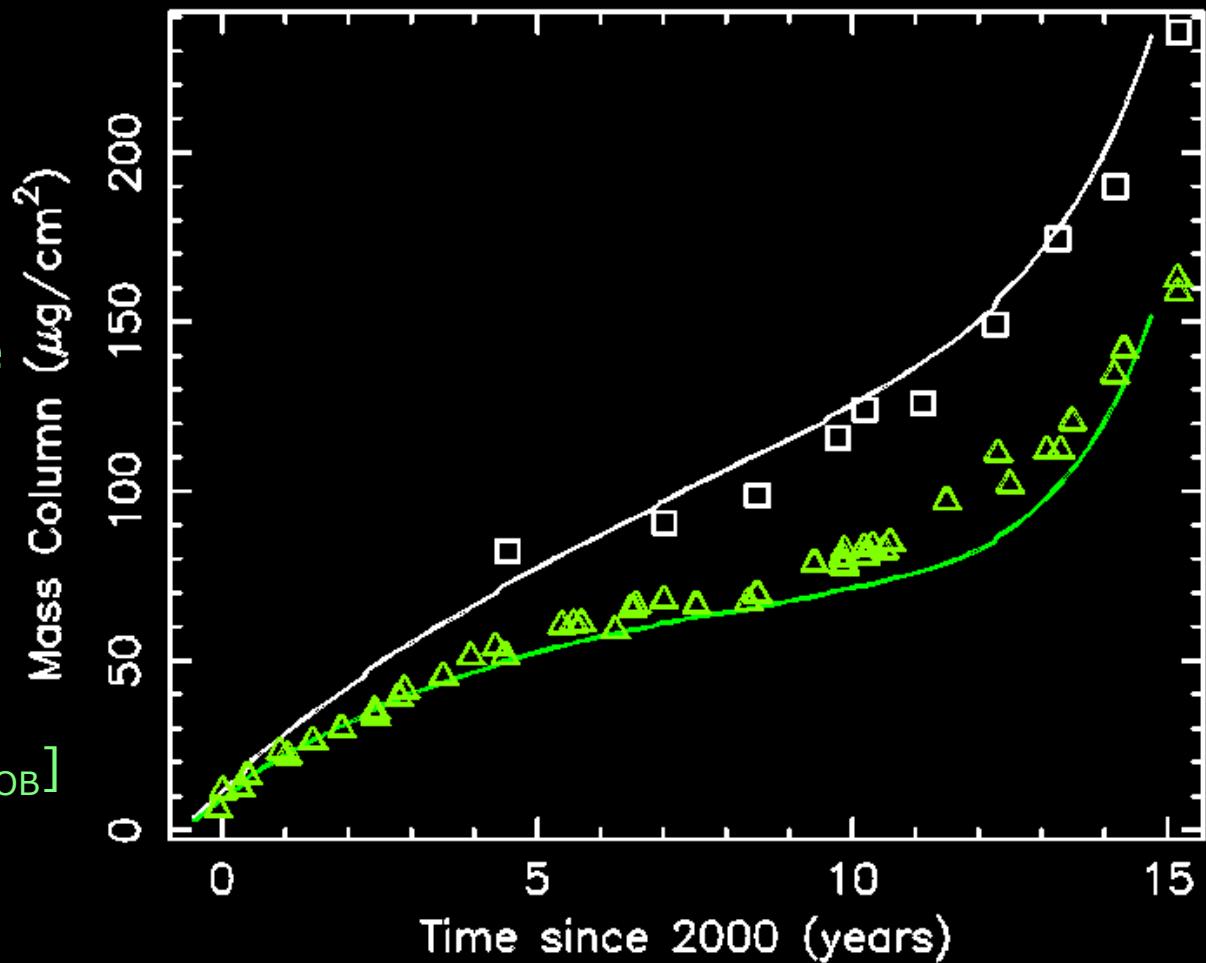




# Accumulation simulation: two components



- Low-volatility component
  - Source rate drops exponentially due to depletion.
    - 3.7-year timescale
- Medium-volatility component
  - Source rate rises with increasing optical-bench  $T_{OB}$ .
    - $\propto \text{Exp}[-\text{constant}/T_{OB}]$
    - Rises until source depletion occurs.

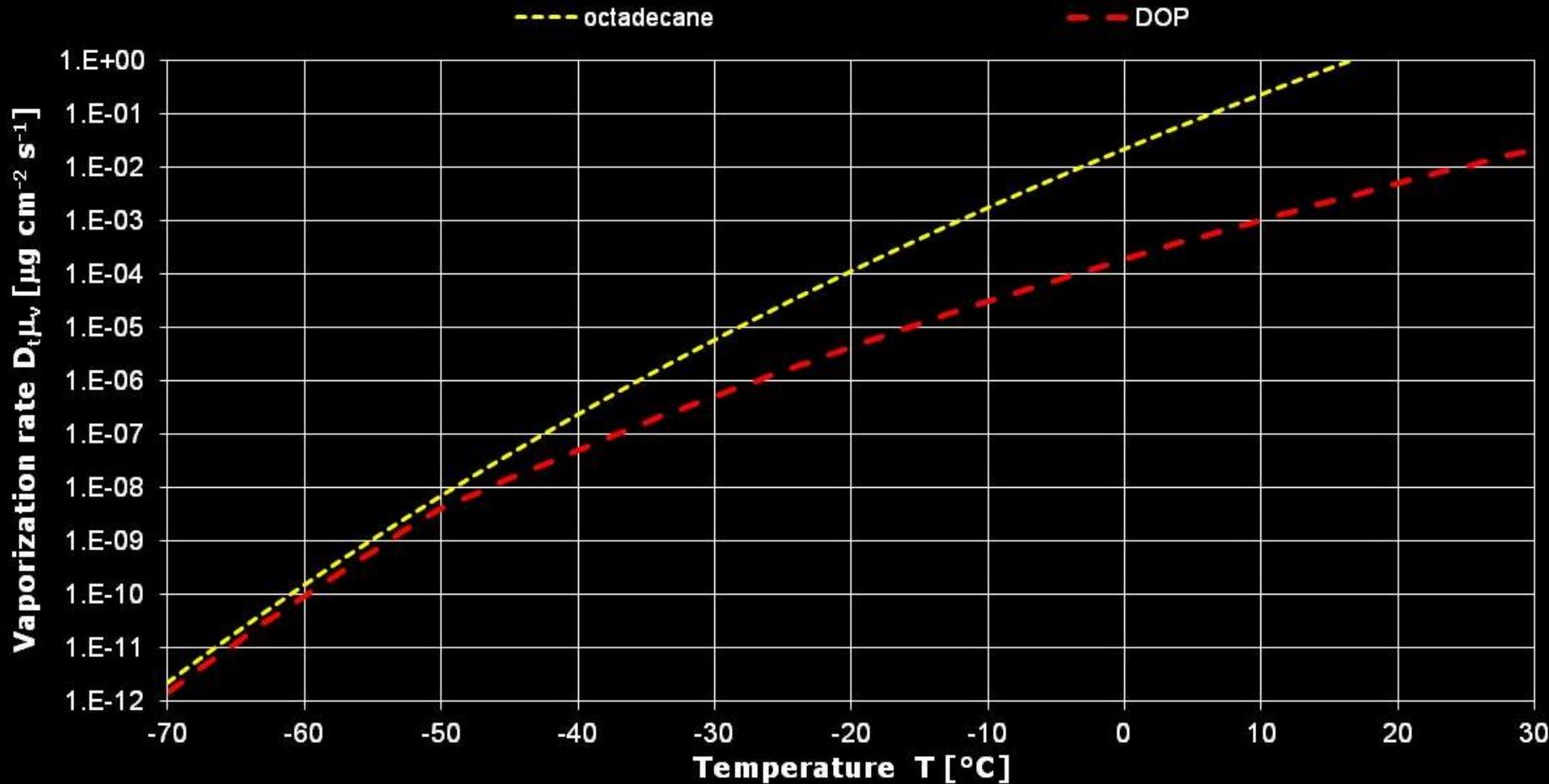




# Vaporization rate: Dependence upon phase state



**Mass vaporization rates of a solid and of a liquid**



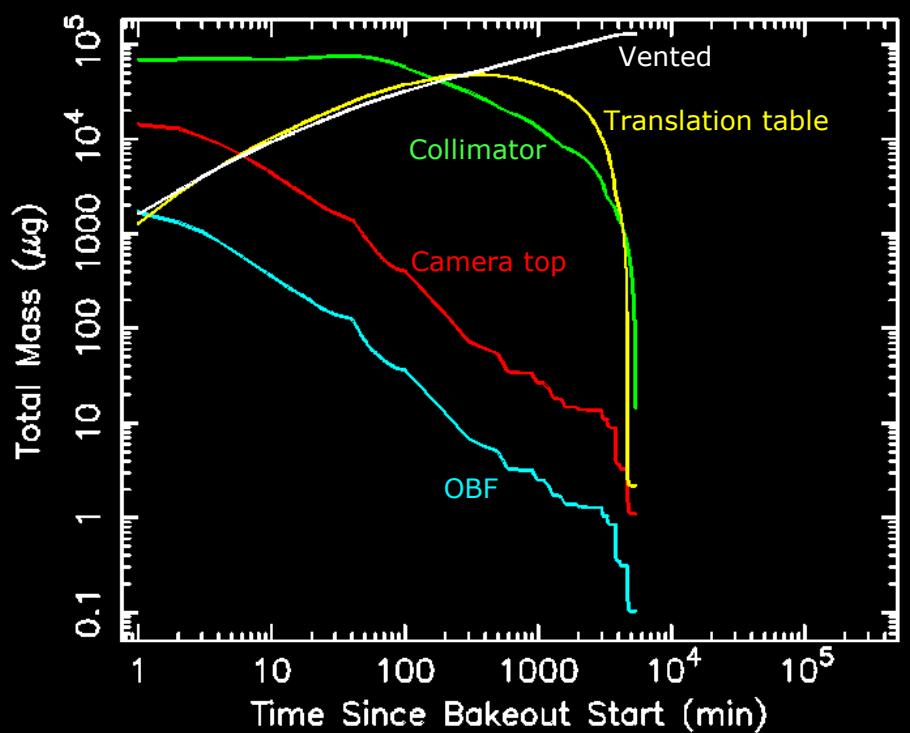


# Bake-out simulation: Octadecane mass



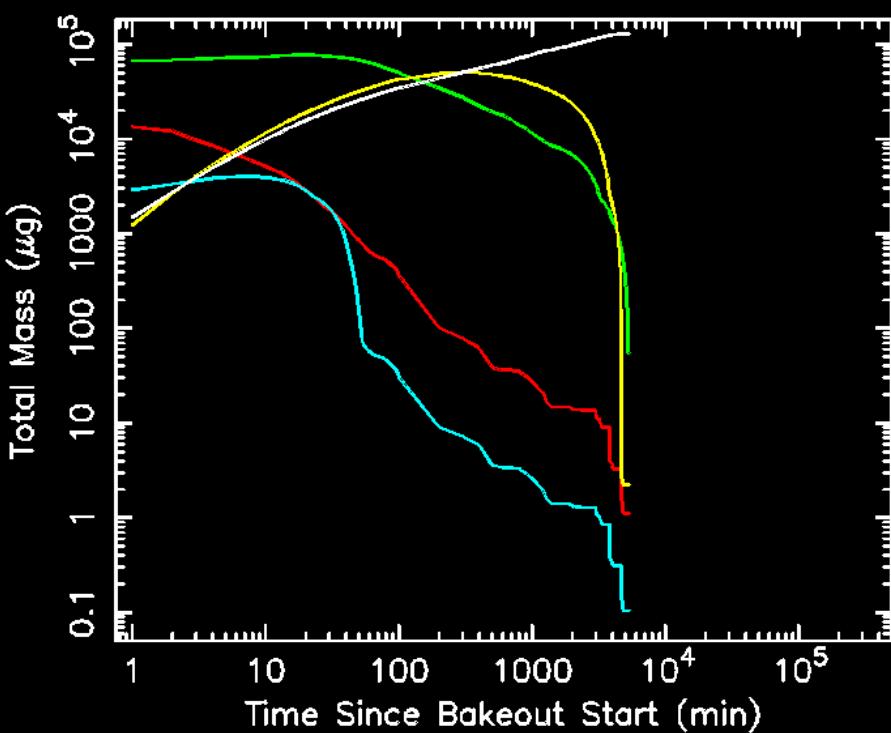
## ➤ Warm focal plane

- $T_{DH} = +25^\circ\text{C}$
- $T_{FP} = +25^\circ\text{C}$



## ➤ Cool focal plane

- $T_{DH} = +25^\circ\text{C}$
- $T_{FP} = -60^\circ\text{C}$





# Bake-out simulation: Octadecane column

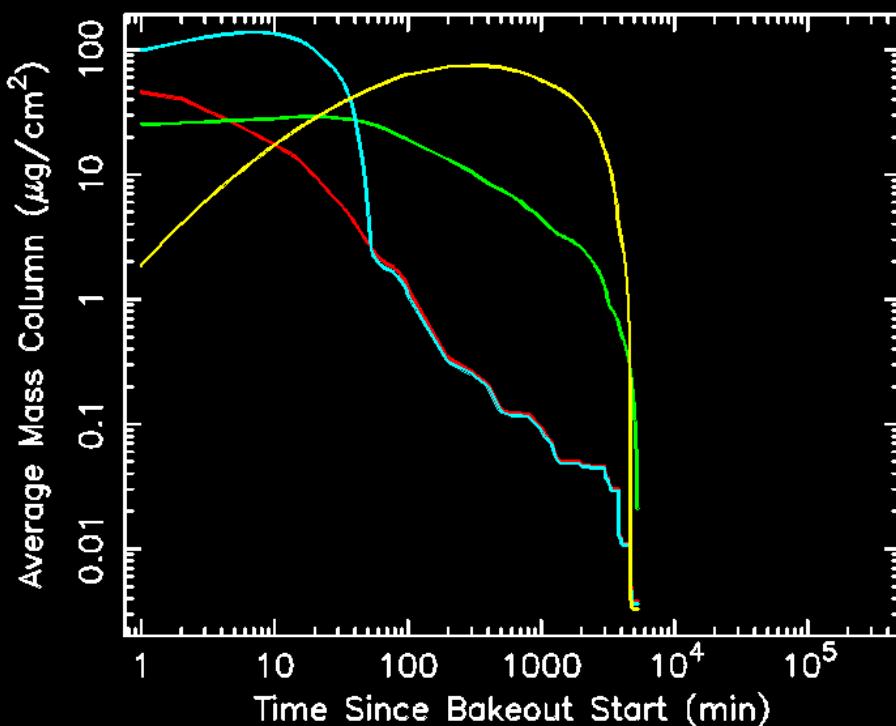
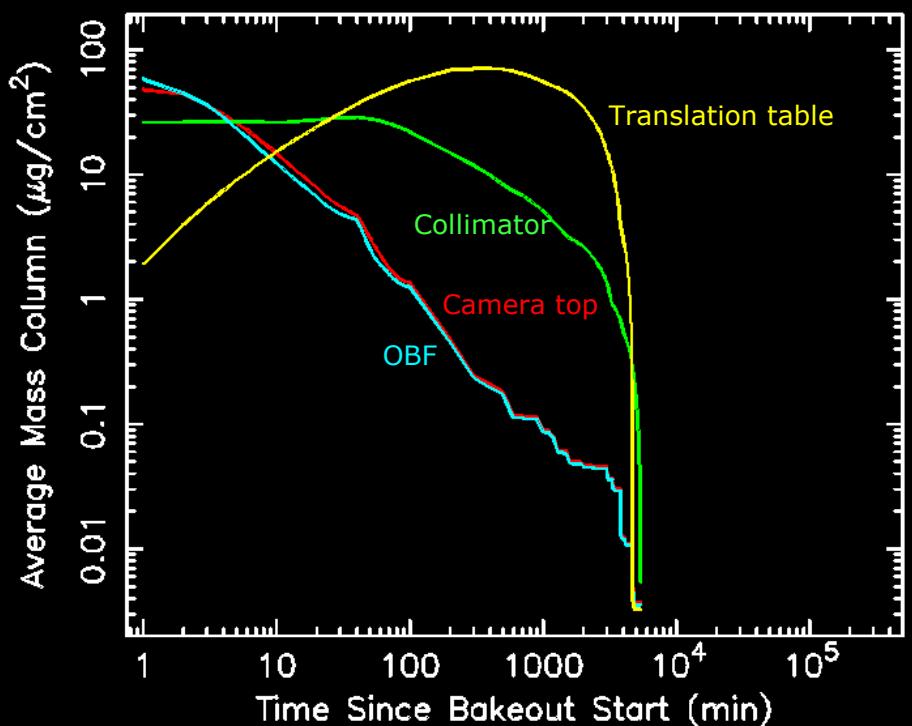


## ➤ Warm focal plane

- ❑  $T_{DH} = +25^\circ\text{C}$
- ❑  $T_{FP} = +25^\circ\text{C}$

## ➤ Cool focal plane

- ❑  $T_{DH} = +25^\circ\text{C}$
- ❑  $T_{FP} = -60^\circ\text{C}$



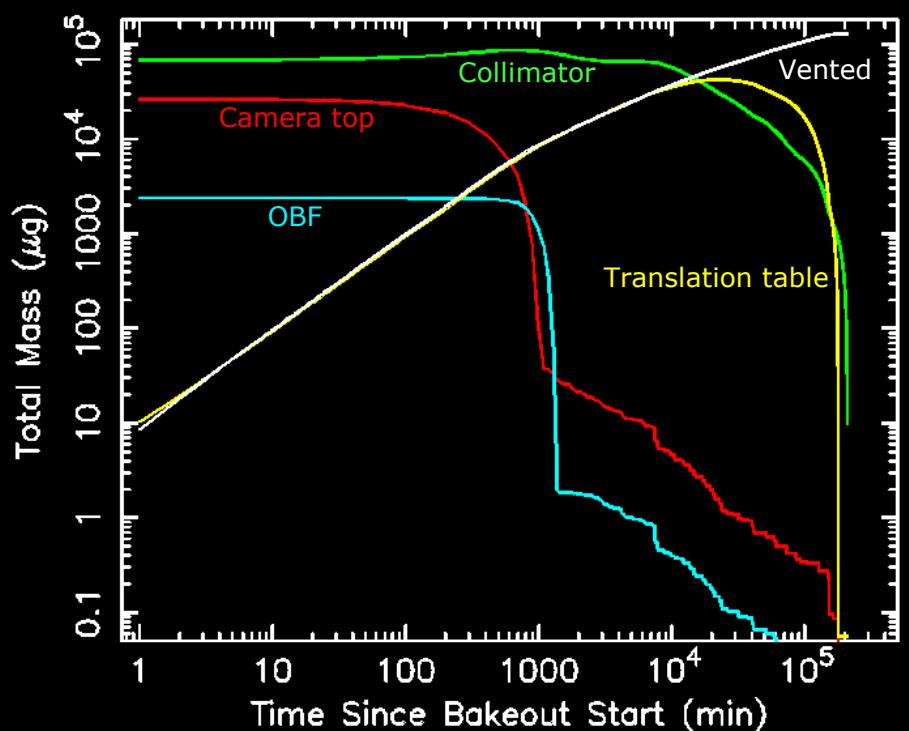


# Bake-out simulation: Dioctyl phthalate mass



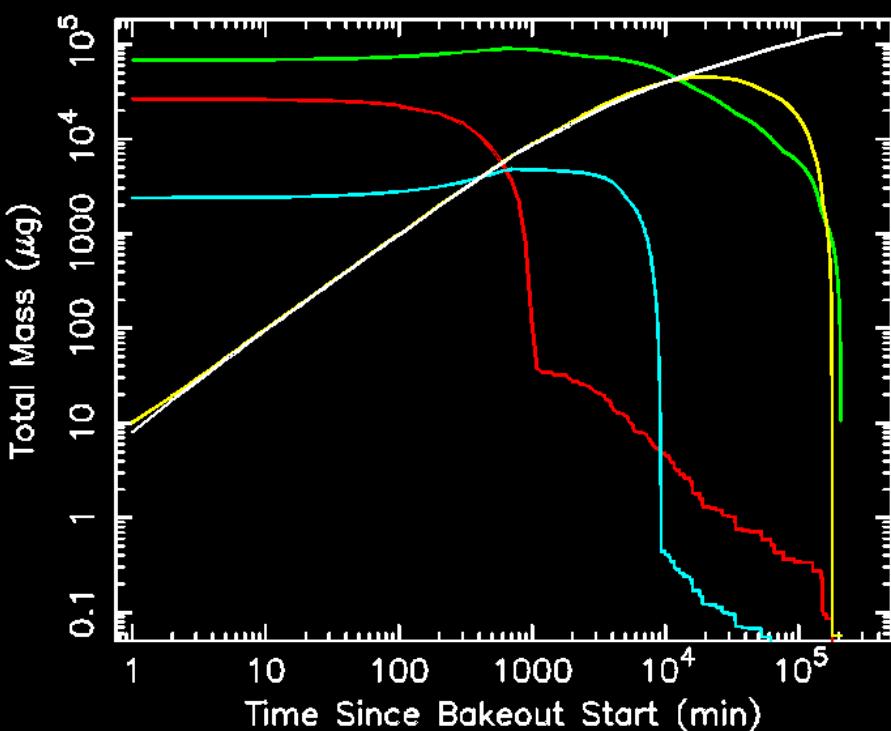
## ➤ Warm focal plane

- ❑  $T_{DH} = +25^\circ\text{C}$
- ❑  $T_{FP} = +25^\circ\text{C}$



## ➤ Cool focal plane

- ❑  $T_{DH} = +25^\circ\text{C}$
- ❑  $T_{FP} = -60^\circ\text{C}$





# Bake-out simulation: Diocetyl phthalate column

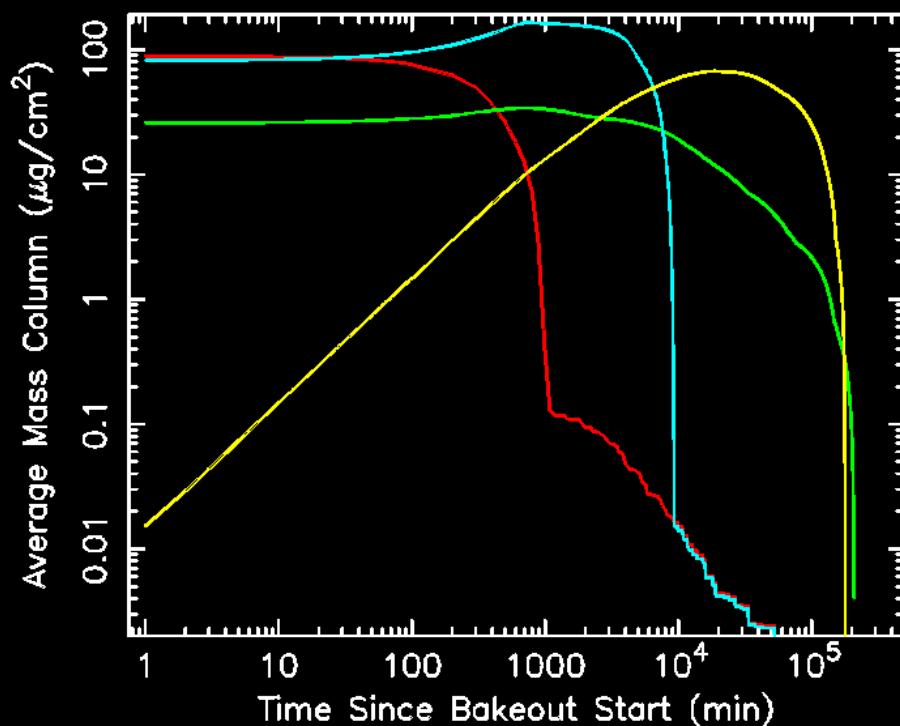
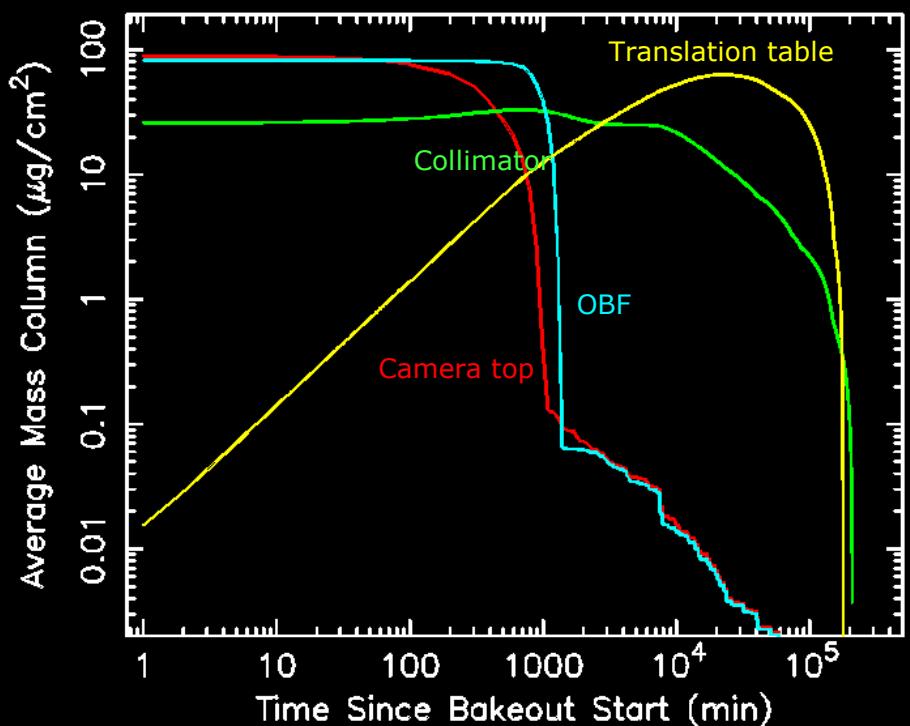


## ➤ Warm focal plane

- ❑  $T_{DH} = +25^\circ\text{C}$
- ❑  $T_{FP} = +25^\circ\text{C}$

## ➤ Cool focal plane

- ❑  $T_{DH} = +25^\circ\text{C}$
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- Contamination-migration simulation provides a useful tool.
  - Utility for absolute predictions is still limited.
    - Absolute predictions require knowledge of contaminant's volatility.
    - Uncertainty in temperatures propagates exponentially to rate error.
  - Model may require additional physics.
    - Treatment of multiple molecular species
    - Dependence of thermal emissivity upon contaminant mass column
      - Affects temperature distribution and thus mass vaporization rate
    - Surface redistribution, especially for a liquid contaminant
- Will use model to provide input for a bake-out decision.
  - Constrain properties of molecular contaminant(s).
  - Simulate contamination migration under potential scenarios.
    - Turning housing heaters back ON
    - Various bake-out conditions for ACIS