Numerical study of water ice and molecular contamination build up during JWST deployment

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Motivation

- Water contributes a large fraction to spacecraft material loss due to outgassing. It is also present on surfaces, which makes components with a large surface area (such as a folded-up sunshield) major sources of water.
- Water deposition is not considered in “typical” space missions. Temperatures around 150 K needed for water to freeze in the low pressure environment. “Typical” spacecraft use heaters and “sun rotisserie” to maintain near-room temperature.
- Unlike its predecessor, the Hubble Space Telescope (HST), the James Webb Space Telescope (JWST) operates in the infrared regime.
- This operational regime requires maintaining extremely cold temperatures in the vicinity of the detectors to avoid saturating the faint signal with spurious thermal radiation from the spacecraft.
- A five layer sun shield divides the telescope into a cold space-facing “observatory” and a warm sun-facing “spacecraft”. The telescope is rotated into this configuration shortly post launch.
- JWST design thus introduced a risk of water icing on the cold observatory side. The objective of this analysis was to determine the amount of ice, along with volatile condensable material (VCM), deposited after 180-days post launch.

- This work builds upon a prior Contamination Sources and Effects Analysis (CSEA), JWST-ANYS-019440, 2012
Background

• Computing molecular deposition involves determining how much material reaches, and sticks to, each target surface element due to outgassing from all other elements.

• Using notation from the CSEA, mass deposition rate can be written as

\[
\dot{m}_i(t) = \sum_{j \neq i} [\nu_j(t) + \gamma_j(t)] A_j F_{ji} - \nu_i(t)
\]

- \( \nu \) is the mass desorption rate, \( \gamma \) is surface outgassing rate, \( A \) is the source area, and \( F \) is the area-normalized black-body “form factor”

• This time variation of surface mass can be numerically integrated using a scheme such as the first order Forward Euler,

\[
m_i(t + \Delta t) = m_i(t) + \dot{m}_i \Delta t
\]
Numerical Model

- Historically, commercial thermal radiation tools such as TSS or Thermal Desktop have been used to determine the black-body form factors. This was the approach taken in the CSEA.

- This approach is valid since in the absence of collisions in the low pressure environment, molecules move in straight lines between surfaces, like photons.

- In this work, we use an alternate approach. We utilized our in-house Contamination Transport Simulation Program (CTSP) to directly simulate the “gray-body” molecular transport.

- CTSP uses simulation “macroparticles” to represent the gas population. Particles are injected from source elements, and their positions (and velocities) through small time steps. Upon contacting a surface, they stick or reflect back based on the surface adhesion model.

- Particle positions and velocities can be interpolated to a volume grid to visualize number densities, partial pressures, and stream velocities. This is in addition to surface properties, such as deposition thickness or mass flux, available by legacy heat-transfer based tools.
Performing the analysis required ingesting a large number of inputs:

- 17 TSS geometry files covering distinct deployment phases
- 7 SINDA binary files providing element temperatures
- 2 .tssop optical property files
- 105 .nod and 9 .arr files containing material information
- 2 Tecplot files containing CSEA material assignments
- Material fluxes from CSEA analysis report
- ISIM outgassing rates
- Powerpoint slides listing timing of deployment phases

17 deployment geometries
Geometry Preparation

- Geometry preparation was a significant part of the overall modeling effort.
- Involved modifying a legacy TSS loader to take into account algebraic expressions, variable substitution, transformations, and additional shapes.
- Also had to address lack of watertightness arising from tessellation of conics and small gaps between shapes. Could lead to non-physical transport paths. Addressed by adding internal sinks.
- Required assigning surface material types. Highly time consuming manual process.
Continuity

- Transition between geometry phases modeled by saving surface deposition to a restart file according to TSS element node ID, tessellation index, and front/back side.

- Mass conservation requires that all node IDs from a prior phase exist in the new one.

- Not always the case, required some geometry modifications and specifying of node IDs maps.

sunshield cover rolls were not present in phase 8/9

single layer sunshield in phase 9 used different node IDs from tensioned version
Thermal Variation

- Surface temperature progression set by ingesting binary SINDA files
Thermal Variation

- Animation of surface temperature change:

**ANIMATION (.mp4)**

- Days: 2.30, 3.16, 5.51, 6.87, 7.71, 10.15, 12.22, 20.61, 180.00
Mass Sources

- CSEA analysis used analytical fits to ASTM-E-1559 measurements to set source outgassing fluxes.
- Retained the same models in this work.
- Water and VCM mass fluxes computed using surface element material type, temperature, and time.
- Material sources also included 5 vents on the sun-facing side, and 8 vents on observatory side, also temperature and time varying.
- Vent rates derived by project CCE team based on historical data, mass of vented components, and vacuum chamber measurements, as applicable.
Mass Conservation

- Initial simulations showed non-physical outgassing near hot SLI elements
- Issue traced down to provided outgassing flux models, given as functions of time and temperature
- Warmer temperature increases outgassing rate, but total mass loss (integrated to infinity) should remain constant assuming initial temperature warm enough to liberate all species
- Not the case, some materials (such as SLI) produced orders of magnitude higher total mass loss when hot, possibly >100% TML
- Equations adjusted to enforce 100% TML as exposure period increases to infinity.
Water Surface Model

- Water surface behavior determined according to a partial pressure model

- First, water vapor computed per model of Murphy and Koop (2005):
  \[ P = \exp \left( 9.550426 - \frac{5723.265}{T_{el}} + 3.53068 \ln(T_{el}) - 0.00728332T_{el} \right) \]

- Next, use Langmuir flux to compute desorption flux:
  \[ \Gamma = \frac{\alpha P}{\sqrt{2\pi m_{water} k_B T_{el}}} \quad \alpha = 1.0 \]

- The number of molecules leaving a surface element in a time step is
  \[ N_{cap} = \Gamma A_{el} \Delta t \]

- Whenever a simulation particle hits a surface, the “capacity” is decreased by the particle’s macroparticle weight. Particle reflected (fully or partially) as long as capacity remains positive, otherwise sticks.

- This model also used at the beginning of each CTSP simulation to desorb water from surfaces that have warmed up. It allowed us to resolve flash off of ice collected on the UPS post actuation, for example.
VCM Surface Model

- VCM deposition modeled with a temperature-dependent sticking coefficient:
  - 100% at -60 °C, 50% at -40 °C, 25% at -25 °C, 10% at 0 °C, 0.01% at 10 °C, and 0% at >10 °C
- Also assumed 10% of molecules impinging on sun-facing surfaces photopolymerize. Percentage scaled by cosine of angle between surface normal and sun direction.
- Used Paraview to identify sun-facing elements for each geometry phase. Photopolymerization used with these elements if sufficiently warm (>10 °C). Allowed us to eliminate elements oriented towards the sun but shadowed by the sunshield.
Time Marching

- Not computationally feasible to simulate the 180 day interval of interest directly
  - Time steps around 1 μs needed to resolve molecular motion, would require 15,000 billion simulation steps

- Used each simulation to establish molecular deposition rate. This rate then used to advance surface molecular count
  \[ N^{k+1} = N^k + N^k \Delta t_{\text{step}} \]

- Validated against direct integration with parallel plate configuration, excellent agreement as long as small time steps used during the initial high-outgassing period

- Analysis consisted of 200 integration steps (CTSP simulations), each consisting of 5000 time steps, with 3000 steps used for averaging.

- About 2 weeks of run time on a 10-core 64 Gb Xeon workstation.
Sensitivity Study

- Performed sensitivity study of the time marching algorithm by comparing 200 (baseline) and 100 (reduced) step cases.

- Comparable results with some small ($\leq 10$ Å) localized differences

- More steps: *lower* deposition, conservative
Results: Water (1/3)

• Animation below and snapshots show progression of water ice over the first 180 days, log scale (Å)

• Values within acceptable limits of CCP

ANIMATION (.mp4)
• This slide shows some additional views and contour plots of water molecular number density.

• Illustrates a capability that radiation heat transfer techniques can't match.

• Water initially concentrated in the “cocoon” of the folded-up configuration.
Results: Water (3/3)

- Additional Plots of selected components:

  primary mirror

  ISIM attic radiators

  core area

  secondary mirror: 0K (left) and actual modeled temperature (right)

  harness radiator deposition (left) and temperature (right)
Results: VCM

- This slide shows the predicted VCM deposition.
- On the observatory side, we mainly see VCM deposition arising from the cold surface temperature, although there is some photopolymerization along primary mirror backplane.
- On the warm, sun-facing side, VCM deposition arises from photopolymerization.
Conclusion

● Numerical simulation of water ice and molecular contaminant redistribution during the commissioning phase of JWST was recently completed.

● Utilized 17 different deployment configuration deployment files. Solution advanced forward through discrete time steps and restart files used to advance across geometry changes. Temperature set per thermal solver solution data.

● Surface adhesion modeled with Murphy-Koop partial pressure relationship for water, and temperature based sticking coefficient for VCM. Photopolymerization on sun-facing surfaces also considered.

● Analysis predicted contaminant deposition thickness compatible with the cleanliness requirements specified in the mission contamination control plan.

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● Questions? Contact lubos.brieda@particleincell.com