Removing Misconceptions in Molecular Contaminant Transport Phenomena

Chung Wong*
Jesse D. Fowler
De-Ling Liu

The Aerospace Corporation
* Northrop Grumman, Azusa, CA

NASA Contamination, Materials and Planetary Protection Workshop
Nov 7, 2019

Introduction

Molecular Contaminant Transport Phenomena

- 3 misconceptions of molecular transport that we often hear
  - *Molecules are impervious through tortuous paths*
  - *Direct line-of-sight is needed for molecules to contaminate a surface*
  - *Molecules will shoot out straight from a gap*
- These misconceptions are related and can be explained by molecular flow
- Transport phenomena of molecular contaminants in the space vacuum environment are quite different from what we observed on the ground
  - *Mean free path of molecules is much larger, ~4 km for Argon at* 1×10^{-8} *Torr*
  - *Intermolecular interactions are rare events*
  - *Molecular interactions with the walls of a space structure occurs much more frequently*
- Molecular interaction with a surface causes a molecule to lose memory of its initial velocity and direction
- Molecules travels really fast
  - *E.g. mean thermal velocity of Argon at room temperature ~400 m/s*

Type of molecule, geometry, and temperature profile must be taken into account when modeling molecular transfer

Governing equations at the thermal walls

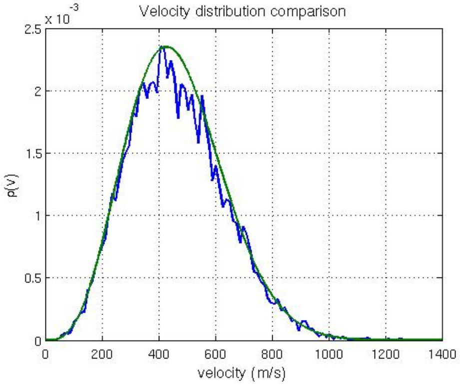
Microscopic view of molecular interaction with walls

- Molecular interactions with surfaces are complicated but usually modeled as a thermal wall interaction
- A molecule that reaches a surface will adsorb on the surface and subsequently re-emitted from the surface in a diffuse manner
  - *Total thermal accommodation*
  - *Initial velocity components are reset and the velocity governed by wall temperature*
  - *Velocity distribution at the wall is a biased Maxwell distribution function*

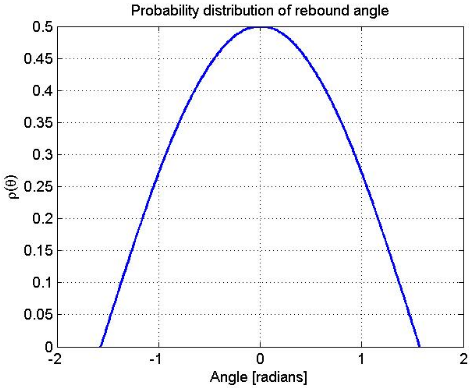
$$\rho_{\|}(v_{\|}) = \sqrt{\frac{m}{2\pi k_B T_W}} e^{-m v_{\|}^2 / 2 k_B T_W}$$

$$\rho_{\perp}(v_{\perp}) = \frac{m}{k_B T_W} v_{\perp} e^{-m v_{\perp}^2 / 2 k_B T_W}$$

$$\Longrightarrow \quad \rho(v) = \frac{1}{2}\left(\frac{m}{k_B T_W}\right)^2 v^3 e^{-m v^2 / 2 k_B T_W}$$



$$\rho(\theta) = \frac{\cos(\theta)}{2}$$



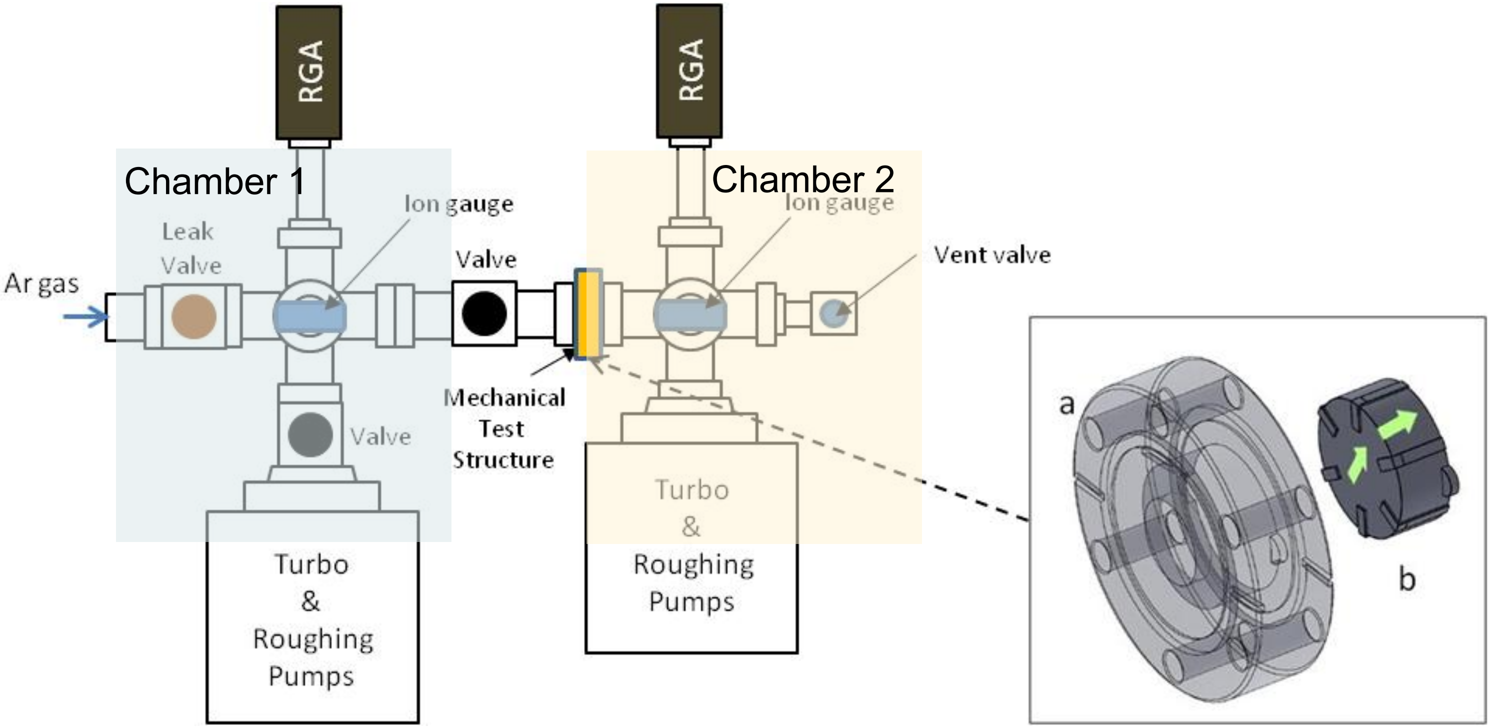
Misconception 1

Molecules are impervious through tortuous path

Model and Test showing pressure differential

Material transport through a tortuous path

- Fabricated a mechanical test structure with 20 mil stand-offs to create a narrow L-shaped path
- Use residual gas analyzers (RGAs) to monitor Argon pressure



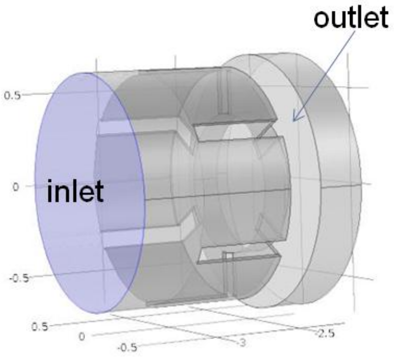
Both chambers being pumped by turbo pumps

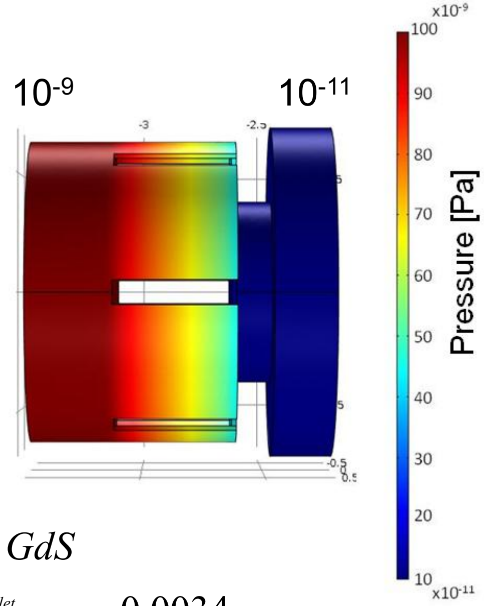
Using thermal wall model, we were able to reproduce our experimental results

Monte Carlo Method

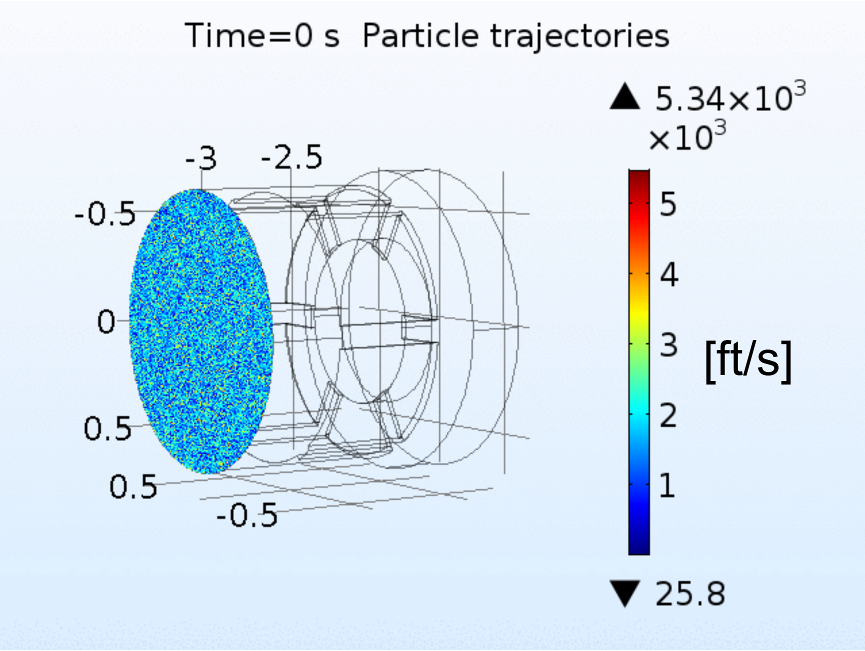
Time scale of material transfer

- Using Monte Carlo method, we predicted that the pressure differential across the structure is 2 orders of magnitude
- Gas molecules move extremely fast 1000 ft/s or ~300 m/s
- Argon gas arrives from inlet to outlet within 100’s of µs





$$\text{Transmission prob. } \alpha = \frac{\int_{S_{outlet}} GdS}{\int_{S_{inlet}} JdS} = 0.0034$$



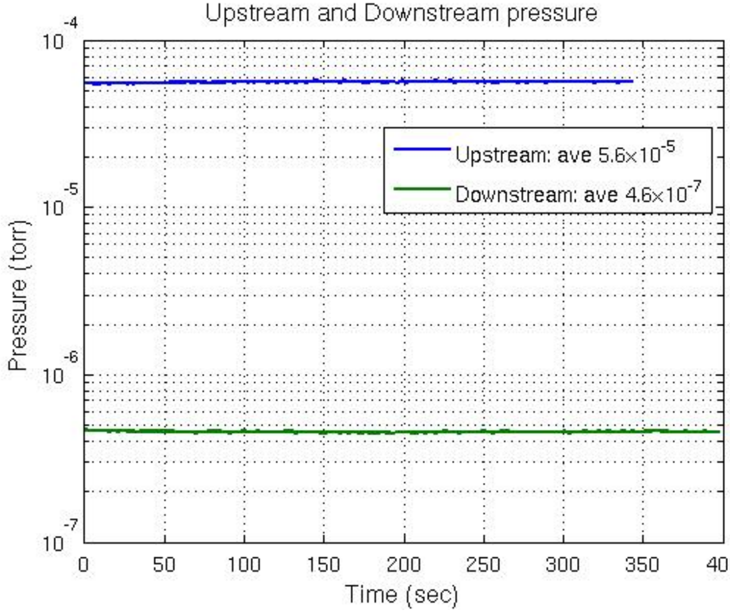
Molecular flow animation

Argon gas arrive at the outlet very rapidly due to the high mean thermal velocity

Pressure differential

Measurement and model

Experimental measurements



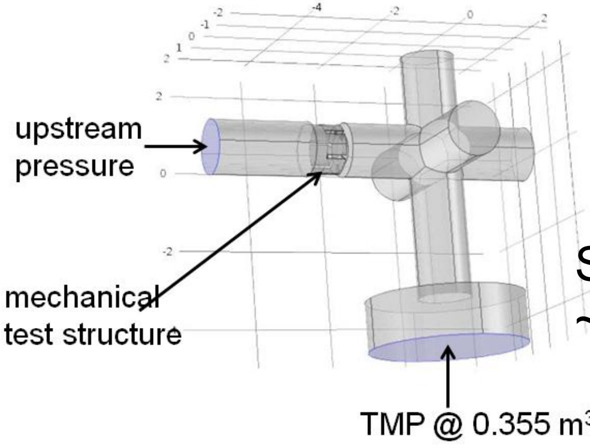
$$Q_{TS} = C_{TS}(P_1 - P_2)$$

$$Q = P_2 \cdot S_{eff}$$

$$C_{TS} = \alpha A \tfrac{1}{4}\langle v \rangle$$

Simple formula gave an estimated of 0.0023

Molecular flow simulation



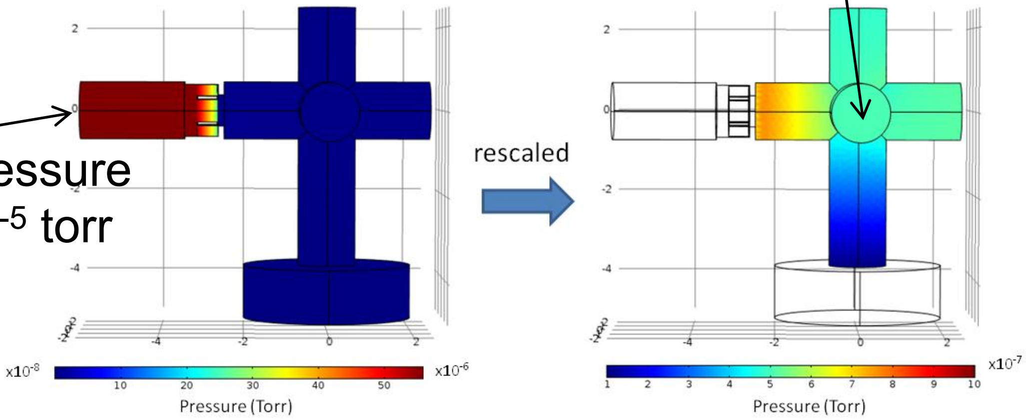
upstream pressure

mechanical test structure

TMP @ 0.355 m^3/s

Simulated pressure ~5x10^{-7} torr

Upstream pressure set to 5.6x10^{-5} torr



Simulated downstream pressure is in excellent agreement with measurements

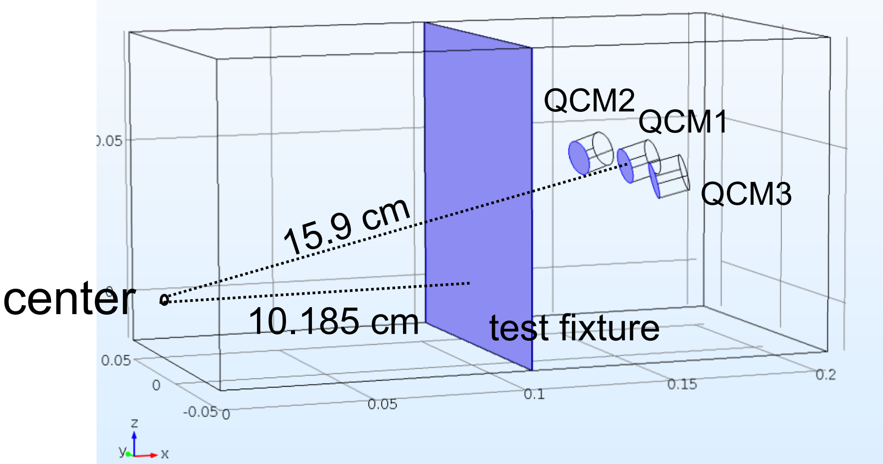
Misconception 2

Direct line-of-sight is needed for contamination

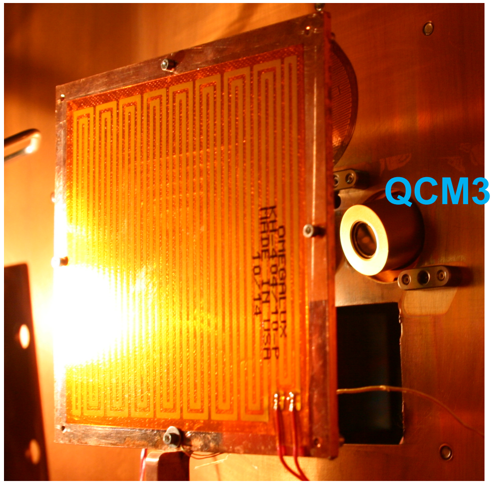
Outgassing experiment

Direct outgassing measurements of materials at 10°C

- We have tested outgassing from composite that was wrapped in MLI blanket
- The materials are placed on a 4” by 4” temperature control fixture located 10.185 cm away from the spherical center of 3 quartz crystal microbalances (QCMs)
- QCMs were surrounded by a large cold shroud
- We present water accumulated on QCM as a function of time
  - *Data are uncorrected for background that is low ~100 Hz or 20 Å per day*



dimension in meters



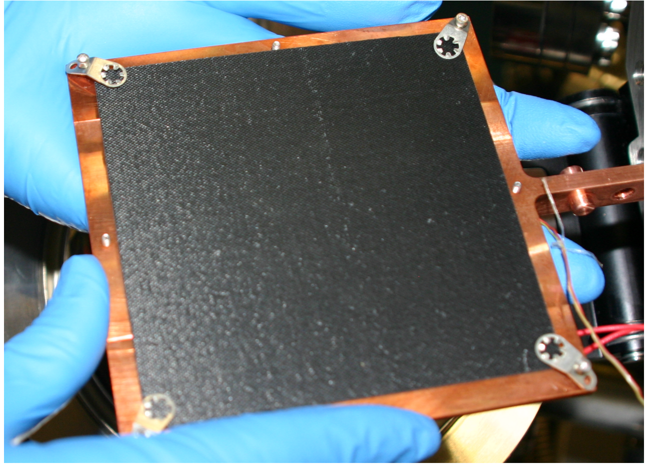
Test fixture in front of QCMs

There are gaps in the MLI blanket that are not directly seen by QCM1

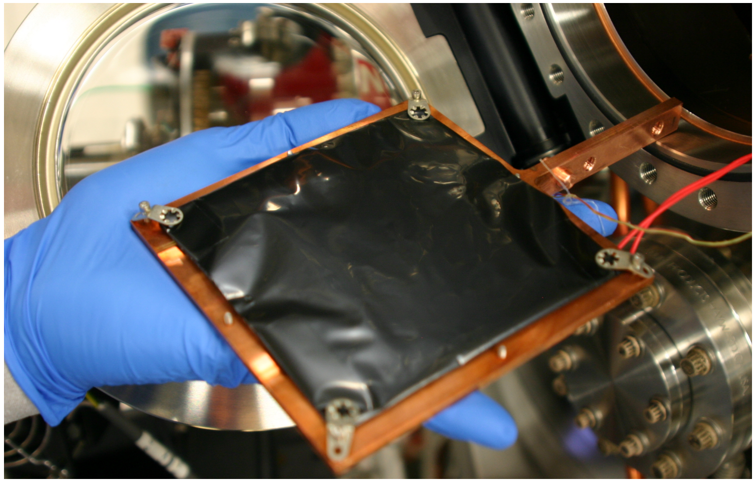
Material mounted on the temperature controlled fixture

3 materials/configurations were tested

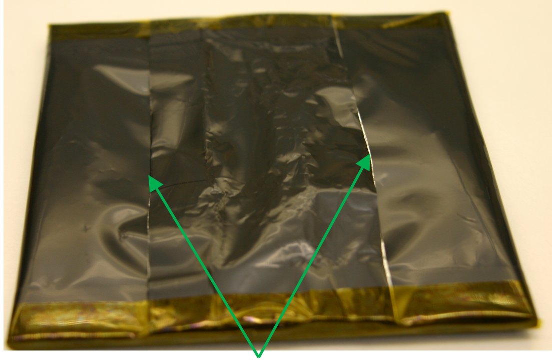
Composite on test fixture



8”x4” MLI (folded in half)

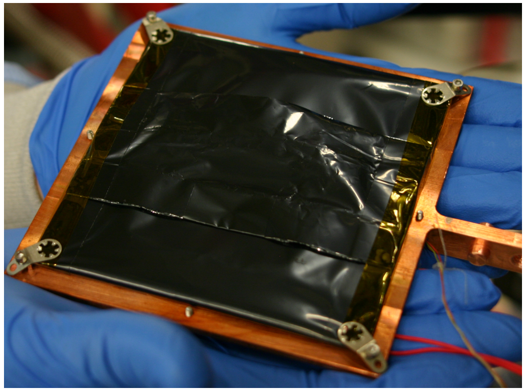


Composite Wrapped in MLI



gaps

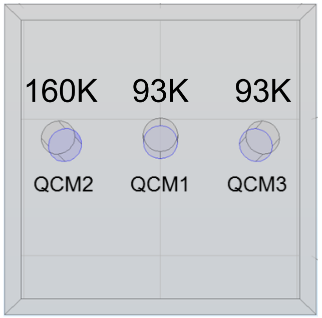
Side view of a gap



Composite and MLI were tested alone to determine the relative amount of moisture individually held

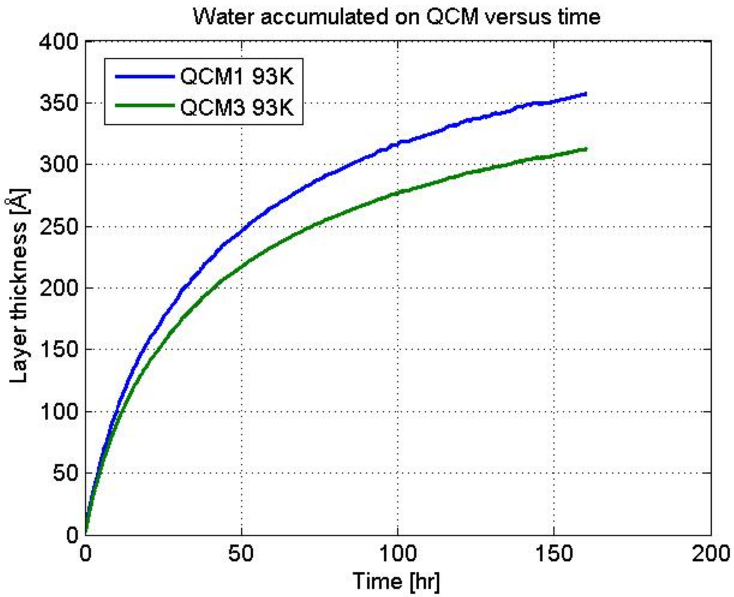
MLI and Composite Results

Accumulated water on 93K QCMs



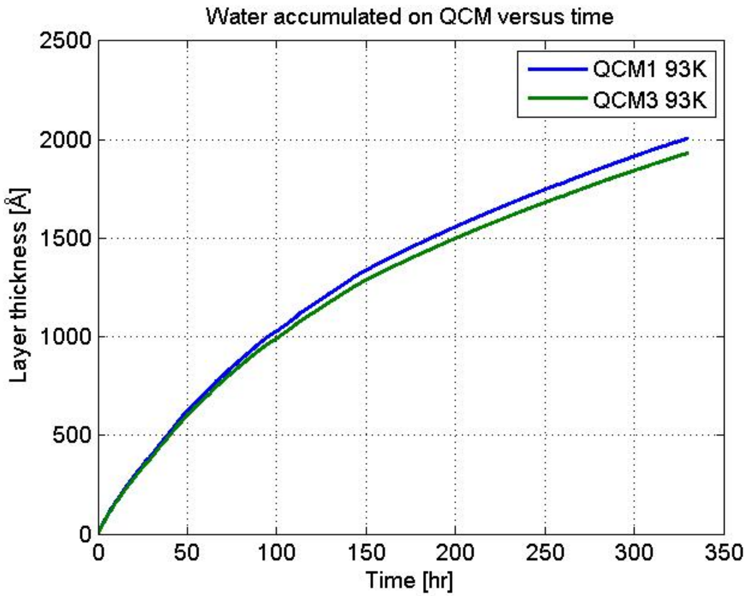
Looking
through the
test fixture

MLI blanket



Total Accumulated:
370 Å (QCM1)
312 Å (QCM3)

Composite panel



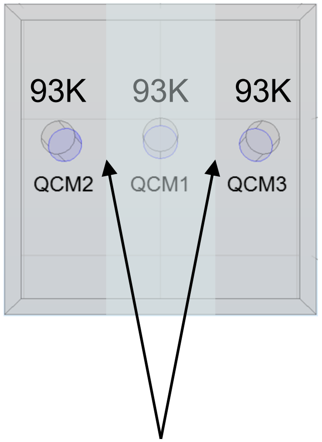
Total accumulated:
2000 Å (QCM1)
1930 Å (QCM3)

note: as expected that QCM3 should receive slightly less material since it is closer to the edge. This has been confirmed by simulation

MLI water outgassing was almost an order of magnitude lower than composite material

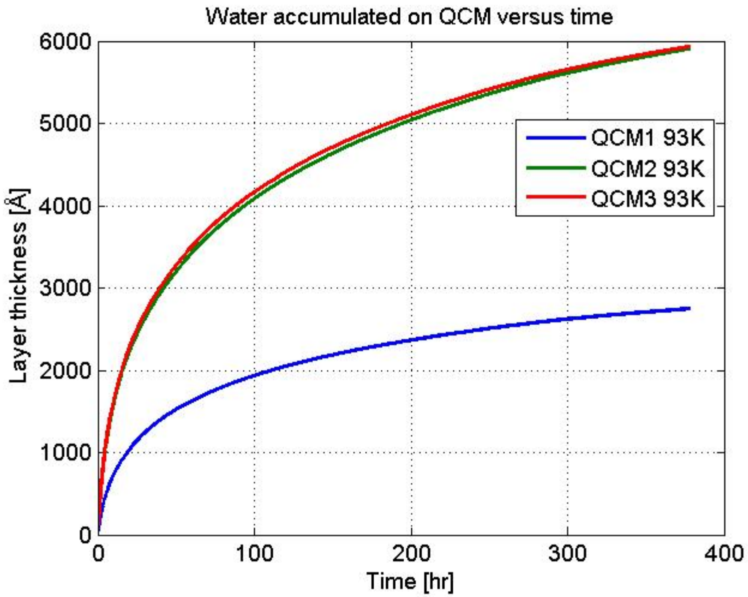
Composite wrapped in MLI panel results

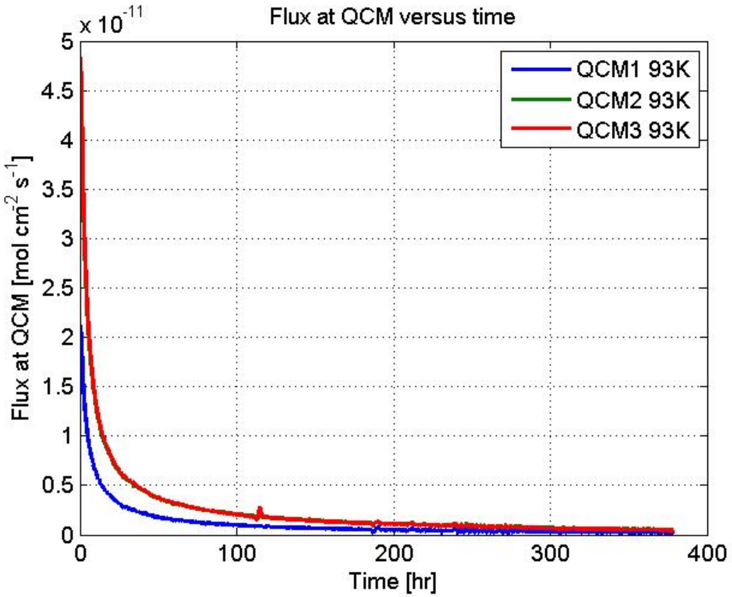
Molecular flux and accumulated water on 93K QCMs



gaps

Looking
through the
test fixture





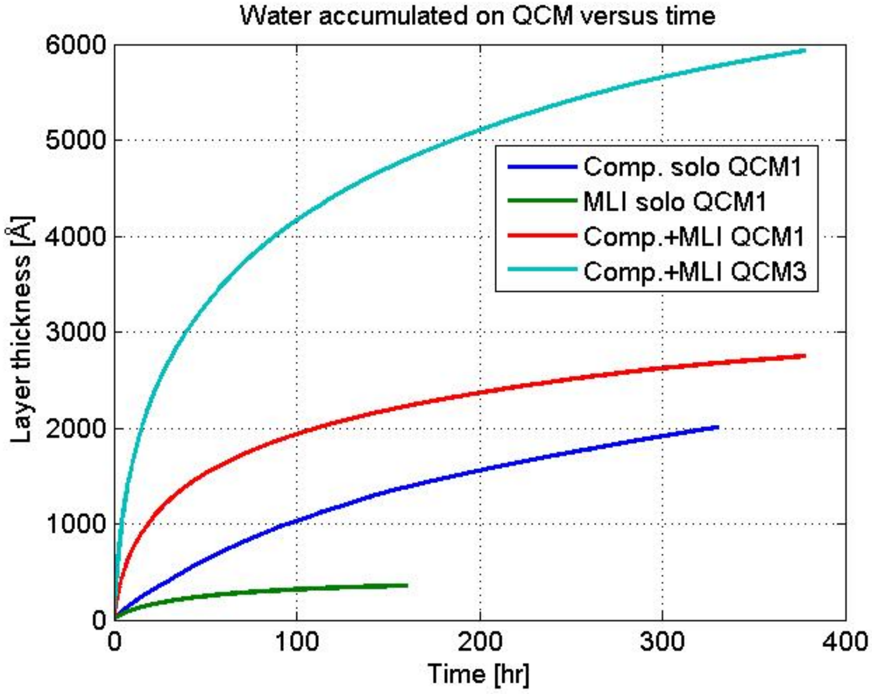
Total accumulated:
2750 Å (QCM1)
5900 Å (QCM2)
5930 Å (QCM3)

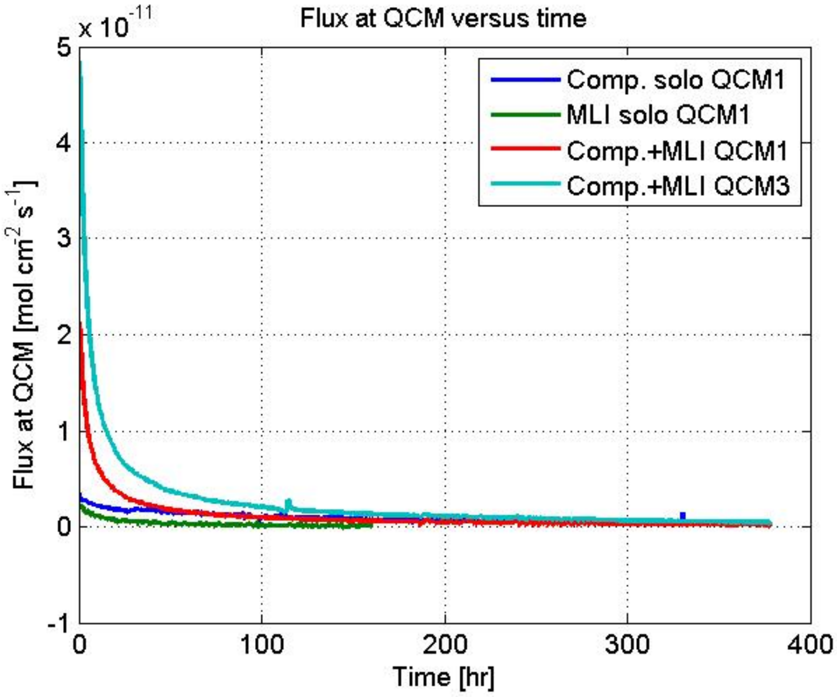
note: as expected that QCM2 and QCM3 should see more materials since they are closer to the gaps. Even when blocked with a piece of MLI, QCM1 still sees a large flux

QCM thermal gravimetric analysis confirmed material desorbed around 156K for water

Comparing molecular flux and accumulated water

Shows QCM1 data for solo composite and solo MLI





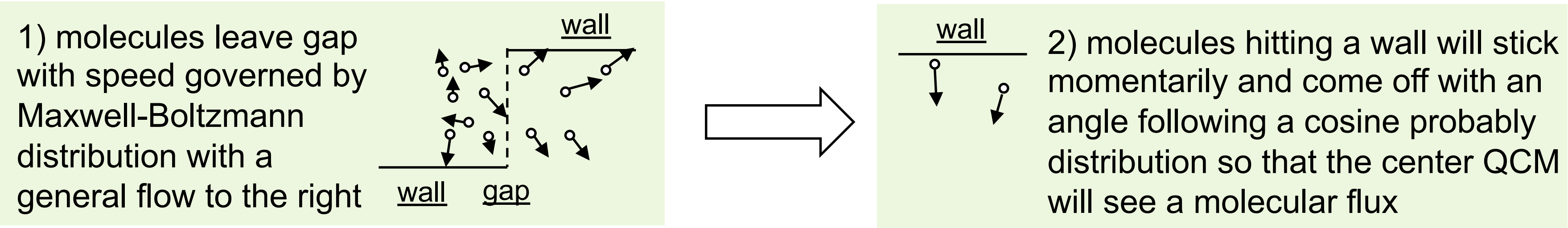
note: water collected from MLI solo plus composite solo cannot explain the higher accumulation when composite is wrapped in MLI blanket.

Composite wrapped in MLI blanket increases the flux on the QCMs significantly, likely due to a funneling effect

Observations

What we have learned so far from these experiments

- MLI blanket alone does not outgas as much water compared to the composite alone
- Another set of data (not in this package) showed that the interior aluminized Mylar holds very little water compared to the outer layers
- MLI wrapped around a composite material traps and redirects the water molecules toward gaps
- MLI blanket alone cannot explain the amount of water molecules accumulated on the center QCM in the MLI+composite test
  - *Even without direct line-of-sight to the gaps, the center QCM still saw a large molecular flux*
  - *The following illustrates what probably occurs when water molecules exit the gap*



1) molecules leave gap with speed governed by Maxwell-Boltzmann distribution with a general flow to the right

2) molecules hitting a wall will stick momentarily and come off with an angle following a cosine probably distribution so that the center QCM will see a molecular flux

Observed relatively small amount of water from MLI compared to the composite material

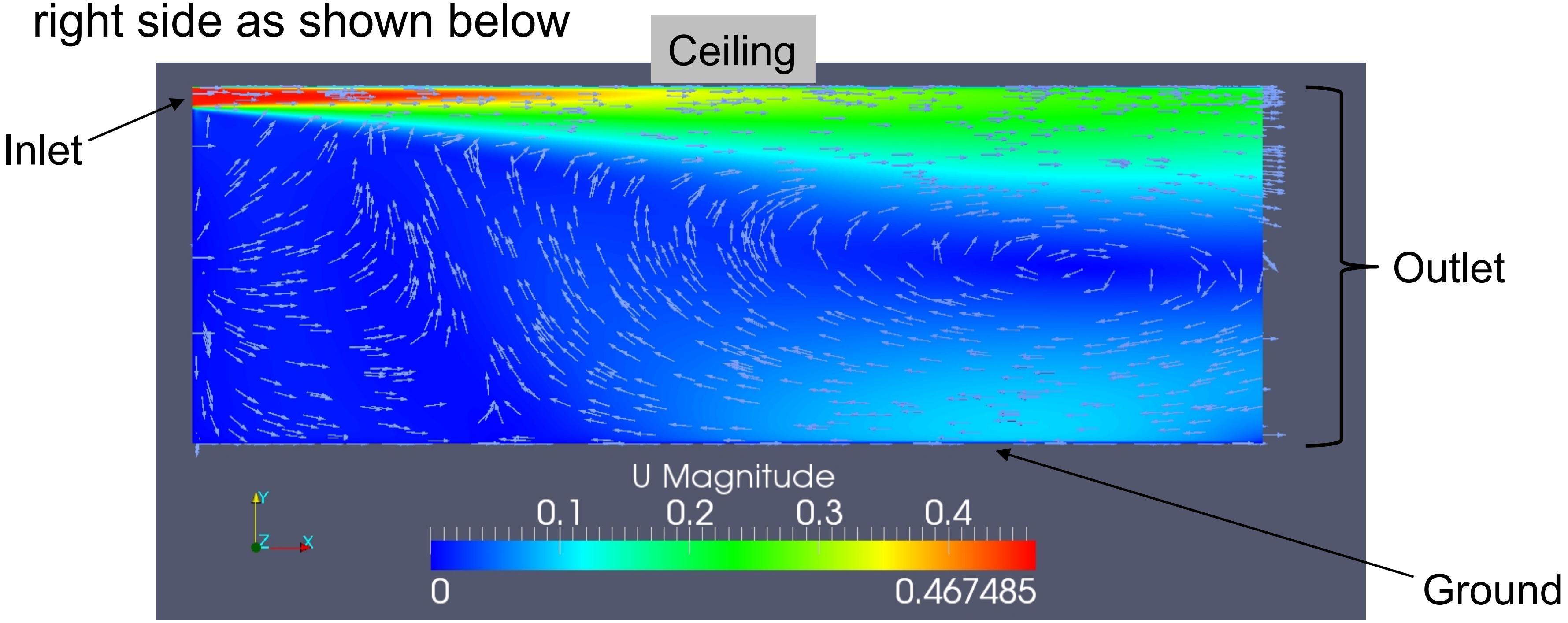
Misconception 3

Molecules are redirected by flow of other molecules

What we observe on the ground

Continuum flow

- On the ground, an airflow from inlet at the top of a room will only slightly disturb the flow close to the ground
- Assuming inlet at the top and on the right is empty space
- We expect the flow of air will more or less shoot directly out toward the right side as shown below

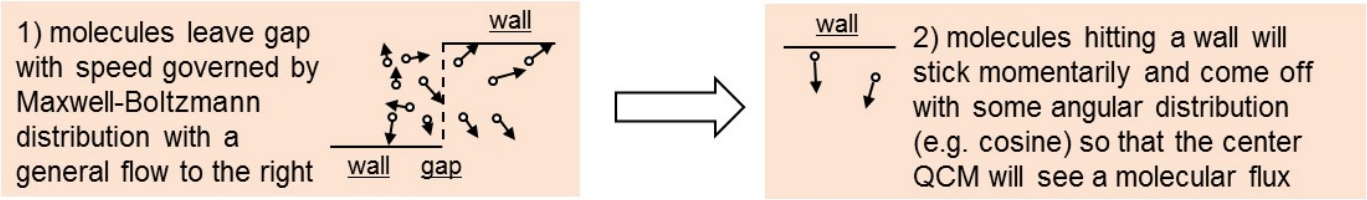


It has been suggested that materials from a gap will shoot toward the right

Contaminant distribution influence by nearby surfaces

Molecular flow

- Simulated transport of water molecules from an inlet gap bounded by a wall above that represents the bottom of the space vehicle
- Assumptions currently made
  - *Gap size of 1 cm*
  - *Inlet conditions: Maxwellian gas with a temperature of 200K and number density of 5x10^{17} m^{-3}*
  - *Diffused reflection at the bottom of the space vehicle*
    - When the molecules hit the bottom of the space vehicle (SV), its initial velocity is reset
    - The molecules come off the surface with a new velocity distribution that corresponds to the SV surface temperature
    - Molecules come off with a cosine probability distribution

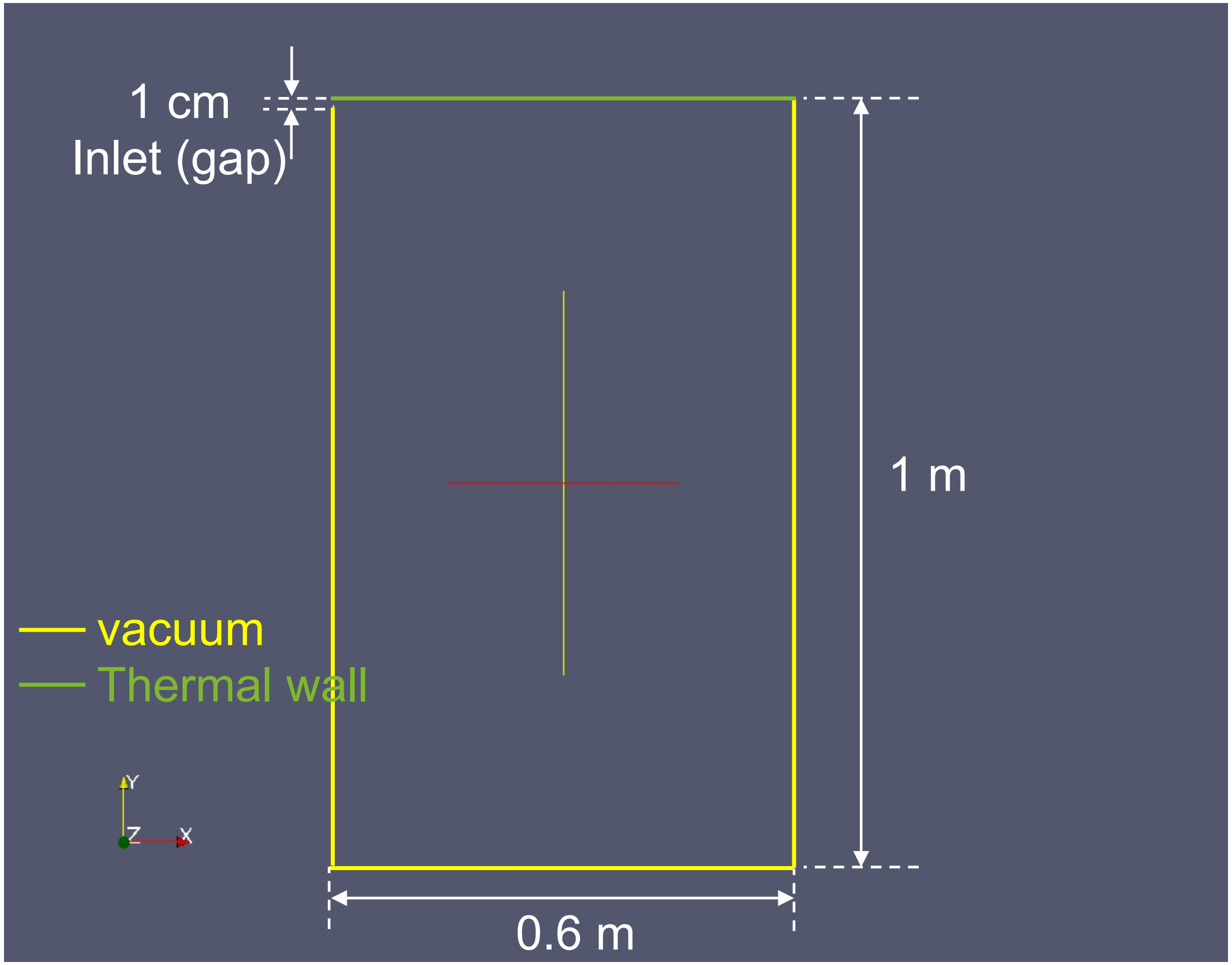


1) molecules leave gap with speed governed by Maxwell-Boltzmann distribution with a general flow to the right

2) molecules hitting a wall will stick momentarily and come off with some angular distribution (e.g. cosine) so that the center QCM will see a molecular flux

Geometry and boundary conditions

2D simulation performed to speed up the model



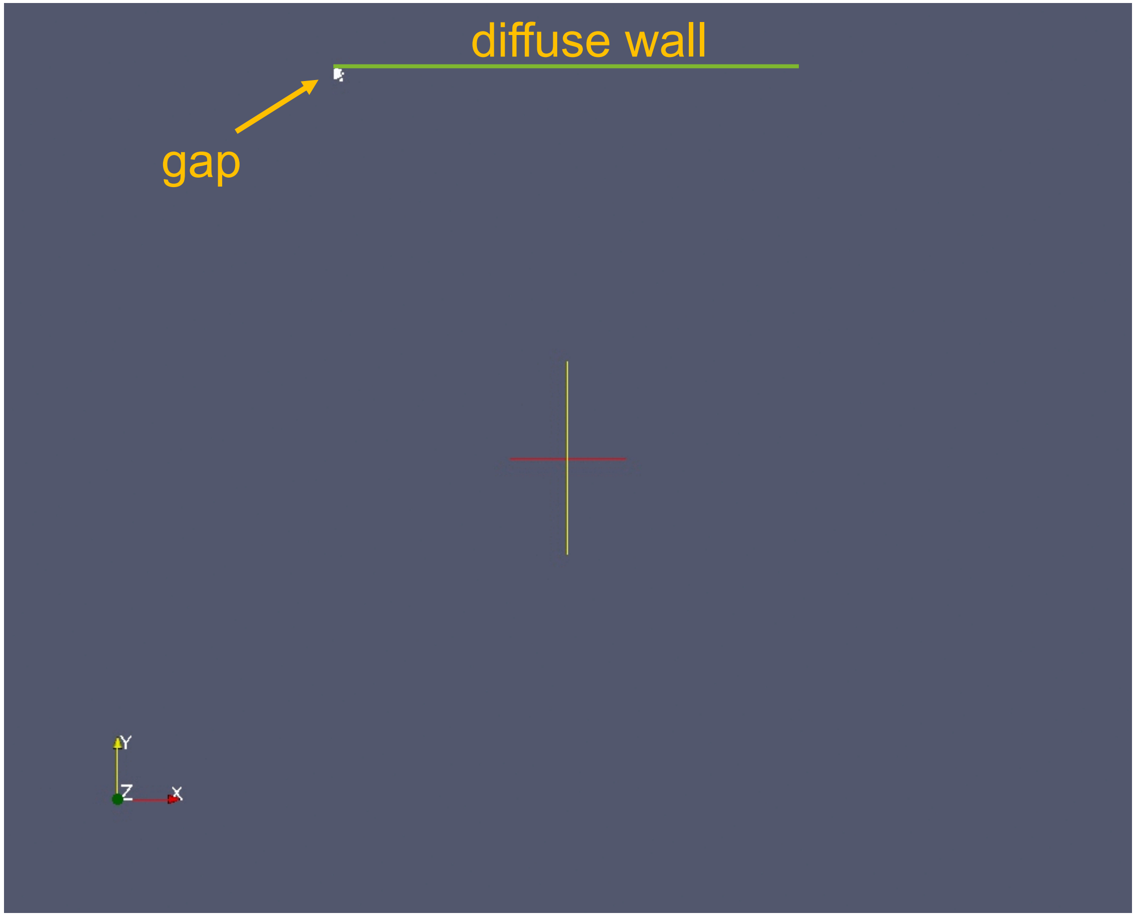
- Inlet modeled as gas with thermal velocity and no directed flow
- When a molecule hits the thermal wall
  1. initial velocity is reset
  2. velocity distribution changes due to colder thermal wall
  3. molecule comes off the surface with a cosine prob. distribution (diffused reflection)
- Molecules disappear at the vacuum boundaries

Geometry can be viewed as an infinite plane in the z-direction

Animation of molecules coming out of the gap

Model shows worst case spread of molecules from a 1 cm MLI gap

Animation in full display mode



Animation shows that molecules do not shoot straight out to right and can be directed downwards from the diffuse wall

Each frame corresponds to 10 microseconds

Summary

Molecular Contaminant Transport Phenomena

- 3 misconceptions of molecular transport that we often hear

  1) Molecules are impervious through tortuous paths

    - Performed experiment/model to show measurable pressure differential across a test structure with narrow L-shaped path
    - Thermal velocity is very fast and the Argon gas can move quickly through gaps

  2) Direct line-of-sight is needed for molecules to contaminate a surface

    - Performed experiments with water emitting from MLI gaps

  3) Molecules are redirected by flow of other molecules, related to #2

    - Performed Monte Carlo simulation to show how water can spread

- These misconceptions can be removed by keeping in mind the following:
  - *In space vacuum, molecular interactions are rare events and that interactions with walls are much more frequent*
  - *Walls can be treated as thermal walls where a molecule's direction and velocity are reset coming off the walls*
- Heavier and stickier molecules can still be transported depending on the temperature profile

Misconceptions can be removed by keeping in mind that molecular interactions are rare and that direction and velocity of a molecule are reset coming off the walls