Using Finite Element to Model Molecular Transport in a Vacuum

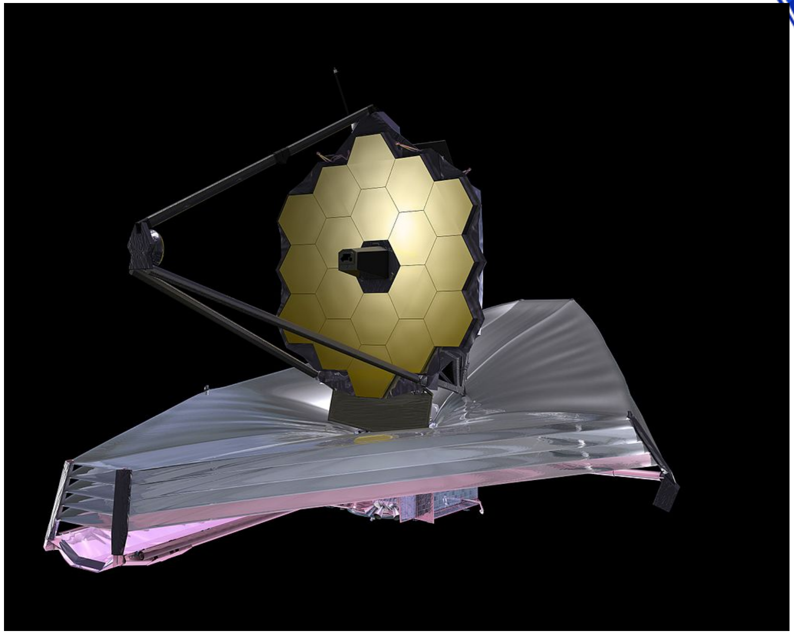
Andrew B. Robbins
Hagop Barsamian
De-Ling Liu

November 6-7, 2019
NASA CCMPP Workshop

Introduction

Why we model molecular contamination

- Molecular contaminants can originate from spacecraft materials
  - *Time and temperature dependent outgassing*
- Highly sensitive components have extremely stringent contamination requirements
- Contamination analysis is performed to assist developing mitigation plans



Credit: NASA

- Modelling of molecular transport can:
  - *Quantifiably estimate the extent of contamination on surfaces of interest*
  - *Handle any input/boundary conditions and complex geometry*
  - *Consider continuous phase to vacuum conditions*

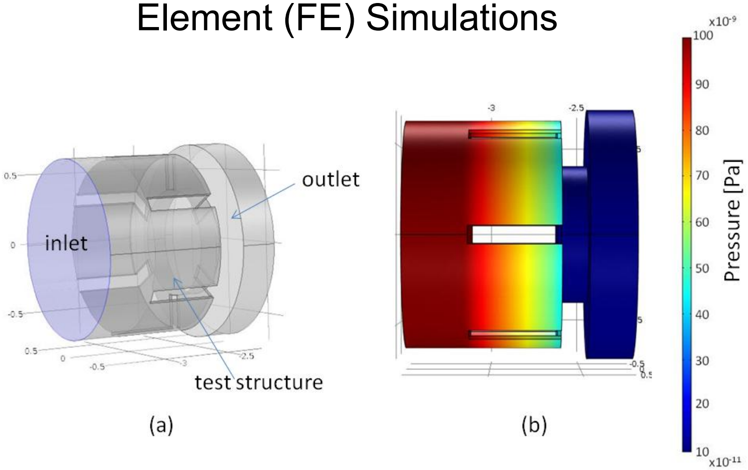
Proper modelling is necessary for reasonable predictions

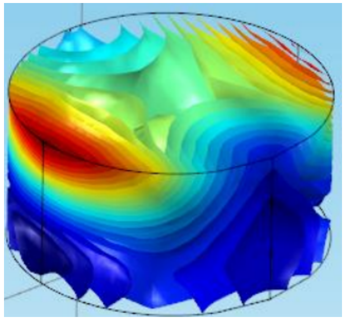
Background

Modelling molecular flow

- Analytical calculations can handle simple systems
  - *Molecular point source (e.g. Knudsen cell)*
  - *View factor between 2 surfaces*
- Challenges for real systems
  - *Irregular shapes and geometries*
  - *Time dependence*
  - *Temperature dependence*
  - *Chemical/physical surface interaction with contaminants*
  - *Space radiation*
- Numerical modelling using Finite Element (FE)
  - *With correct inputs, FE can be a useful tool to address the above challenges*

Examples of Finite Element (FE) Simulations





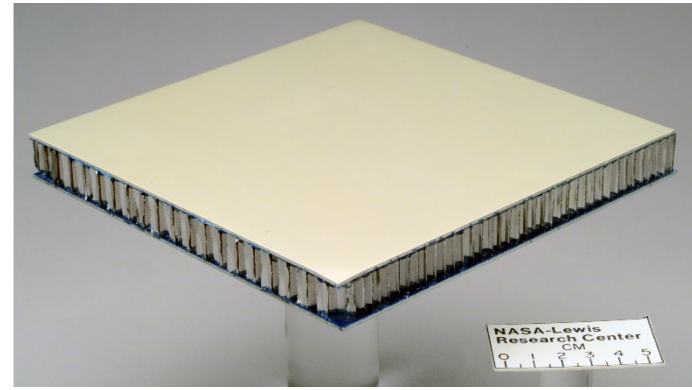
Ethridge, E., & Kaukler, W. AIAA Aerospace Sciences Meeting (2012). NASA Technical Reports Server, Document ID 20120004021.

Finite element modelling simplifies and expands simulation capabilities

Outline

Case studies

1) Model molecular spatial profiles from a venting honeycomb



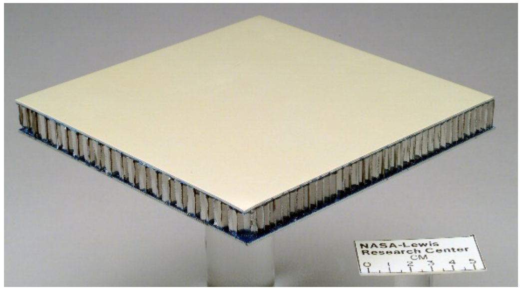
Credit: NASA

2) Molecular flux focusing in a vacuum chamber (per ASTM E1559 standard)

- *Verify and evaluate the model with experimental data*

Molecular Contamination Transport out of a Honeycomb

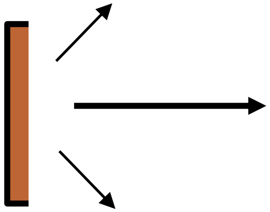
- Honeycomb/facesheets are a common structure for flight systems
  - *Vented for depressurization*
  - *Contamination sources available inside*



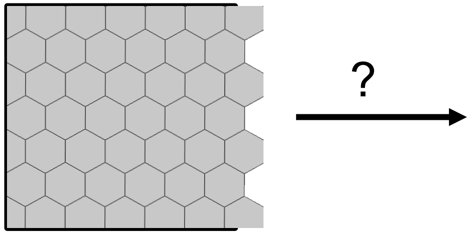
Credit: NASA

How to quantify molecular emission profile for arbitrary geometry?

- View factor from flat source is well known (cosθ)



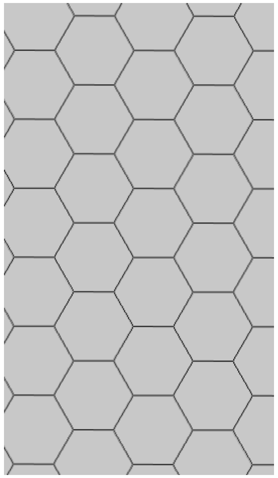
- What about structured surface with vent holes?

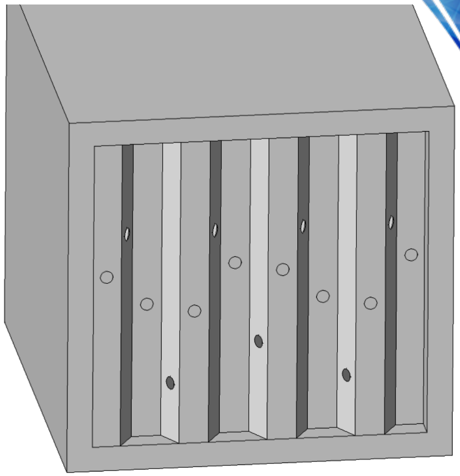


Finite element simulations help model complex structures

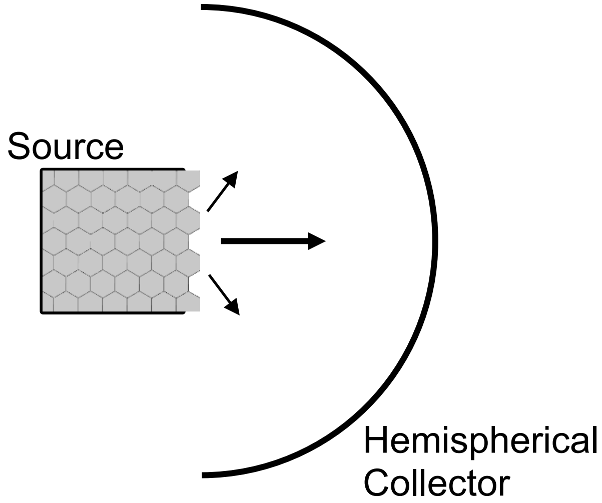
Setting up the Model

Using Finite Element to model honeycomb structure





- Governing Physics: **Free Molecular Flow**
  - *Molecules travel ballistically (no interaction)*
  - *Assumes MFP >> L*
    - MFP: molecule mean free path
    - L: length scale of structure
- The honeycomb structure is built in COMSOL
  - *Tessellated hexagonal prisms*
  - *Punctured with vent holes*
  - *Encapsulated on sides*
- Due to periodicity, a small representative unit is used for molecular transport simulations
- Boundary Conditions:
  - *Molecular source within structure*
  - *All walls are diffuse (molecules bounce off in random direction)*
  - *Molecules stick to hemispherical collector*

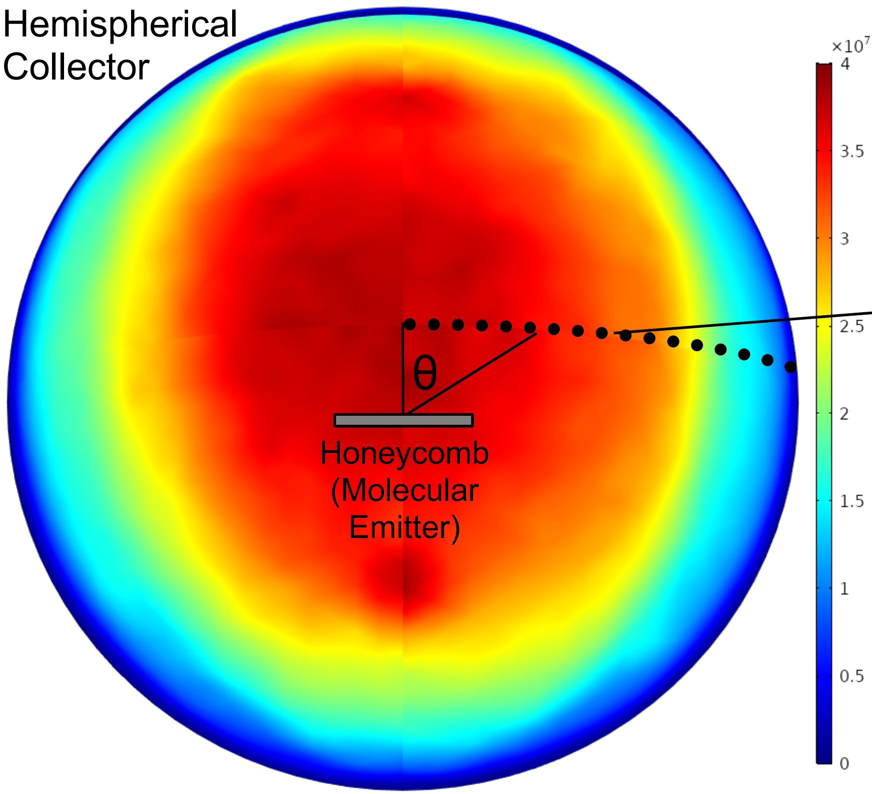


Structure can be customized to specific flight hardware

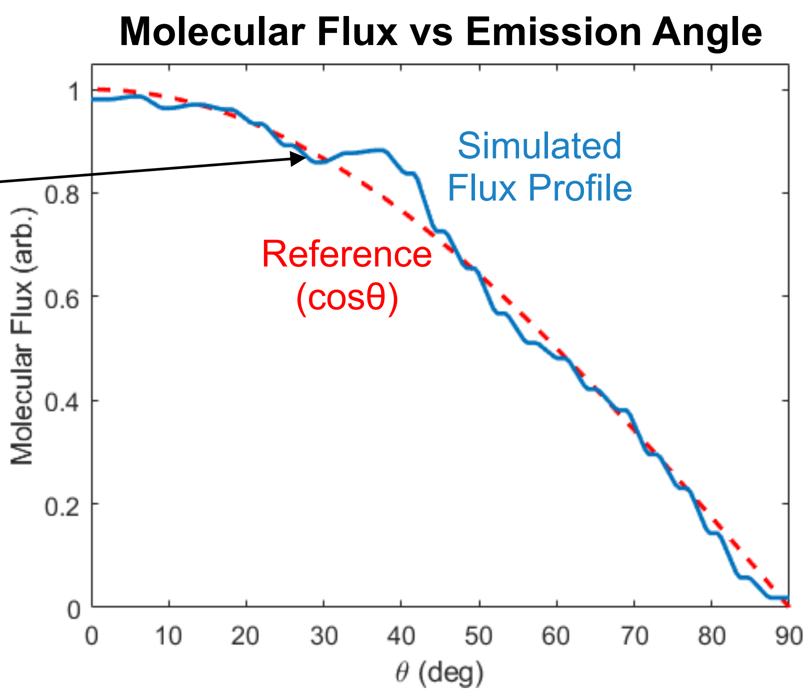
Results: Obtaining the Molecular Flux Distribution

FE predictions for molecular outflow from honeycomb

- Molecular flux is not focused



- Compare angular profile to ideal point source
  - *No significant difference*



Modelling is important to support or challenge assumptions about molecular transport

Outline

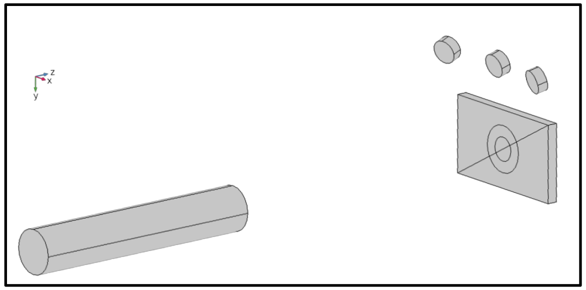
Case studies

1) Model molecular spatial profiles from a venting honeycomb

Credit: NASA

2) Molecular flux focusing in a vacuum chamber (per ASTM E1559 standard)

- *Verify and evaluate the model with experimental data*

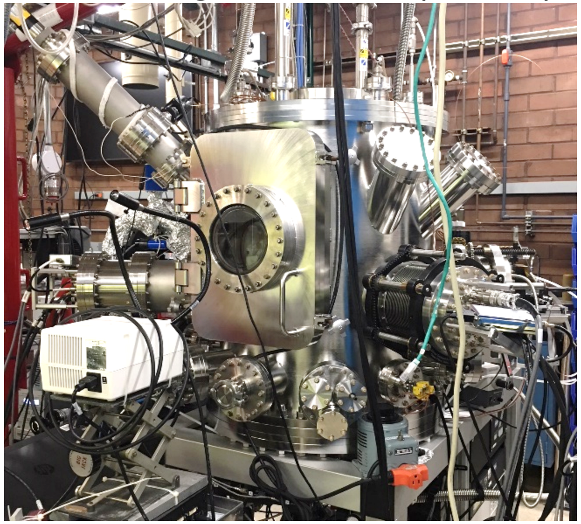


Flux Focusing

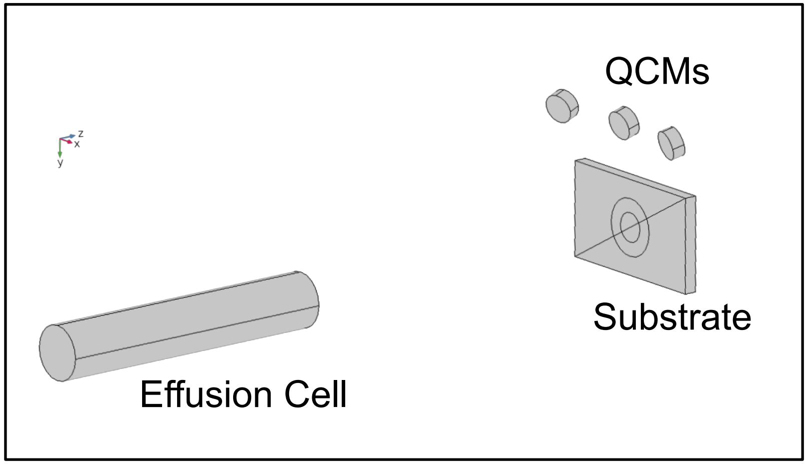
Accelerating Molecular Accumulation in Experimental Testing

- Test chamber often used to study molecular contamination on a substrate
  - *Requires deposition of enough contaminants*

Contamination Effect Research and Testing Chamber (CERT)



FE Model of CERT Chamber Testing



Problem: Low outgassing materials require many weeks of testing

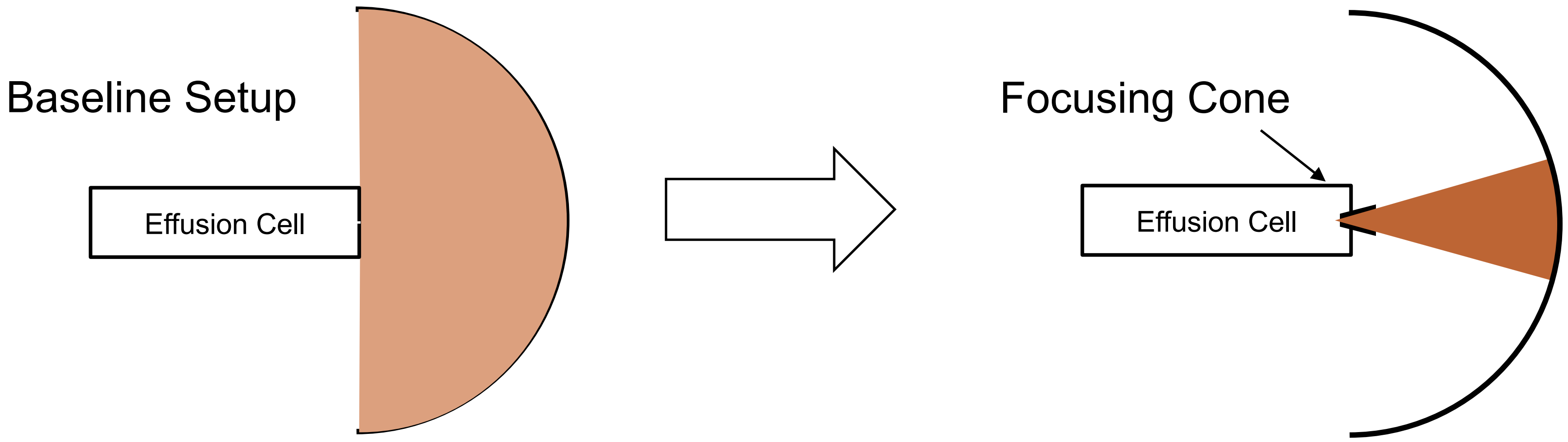
Proposed Solution: Focus molecular flux towards substrate

A focused molecular output can dramatically shorten test duration

How to Focus Molecular Flux

Testing hypothesis

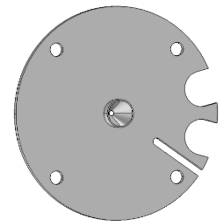
- Hypothesis: Fit effusion cell with focusing cone
  - *Redirect otherwise "wasted" flux to target*



Finite Element Simulations

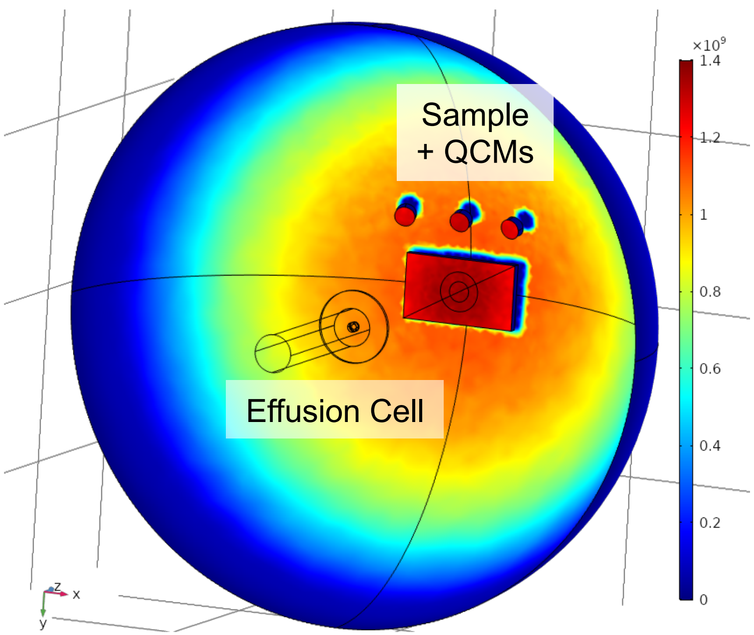
Model cone attachment and observe effect

- Measure flux profile emitted from effusion cell
- Compare **baseline** vs **cone**



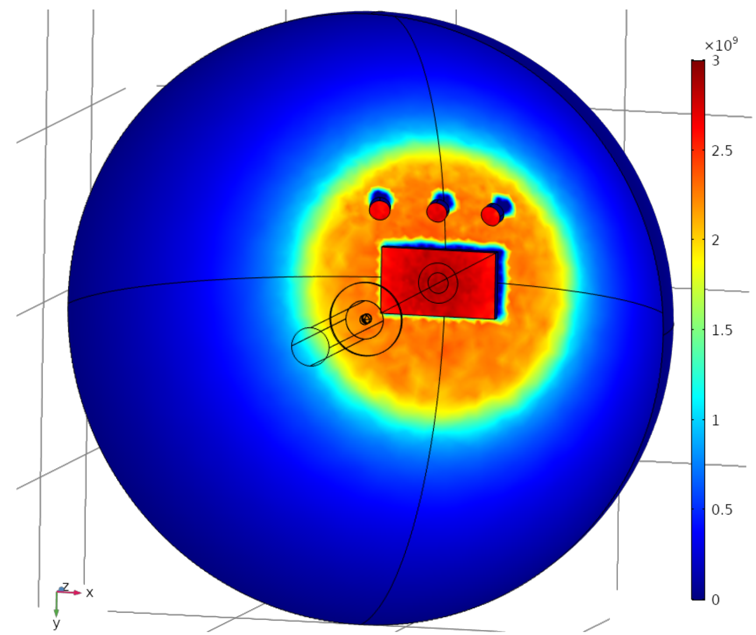
Attachment designed with 22° cone

Baseline Setup



Normalized Molecular Flux Profile

With Cone Attachment



Simulations show cone is able to focus molecular flux

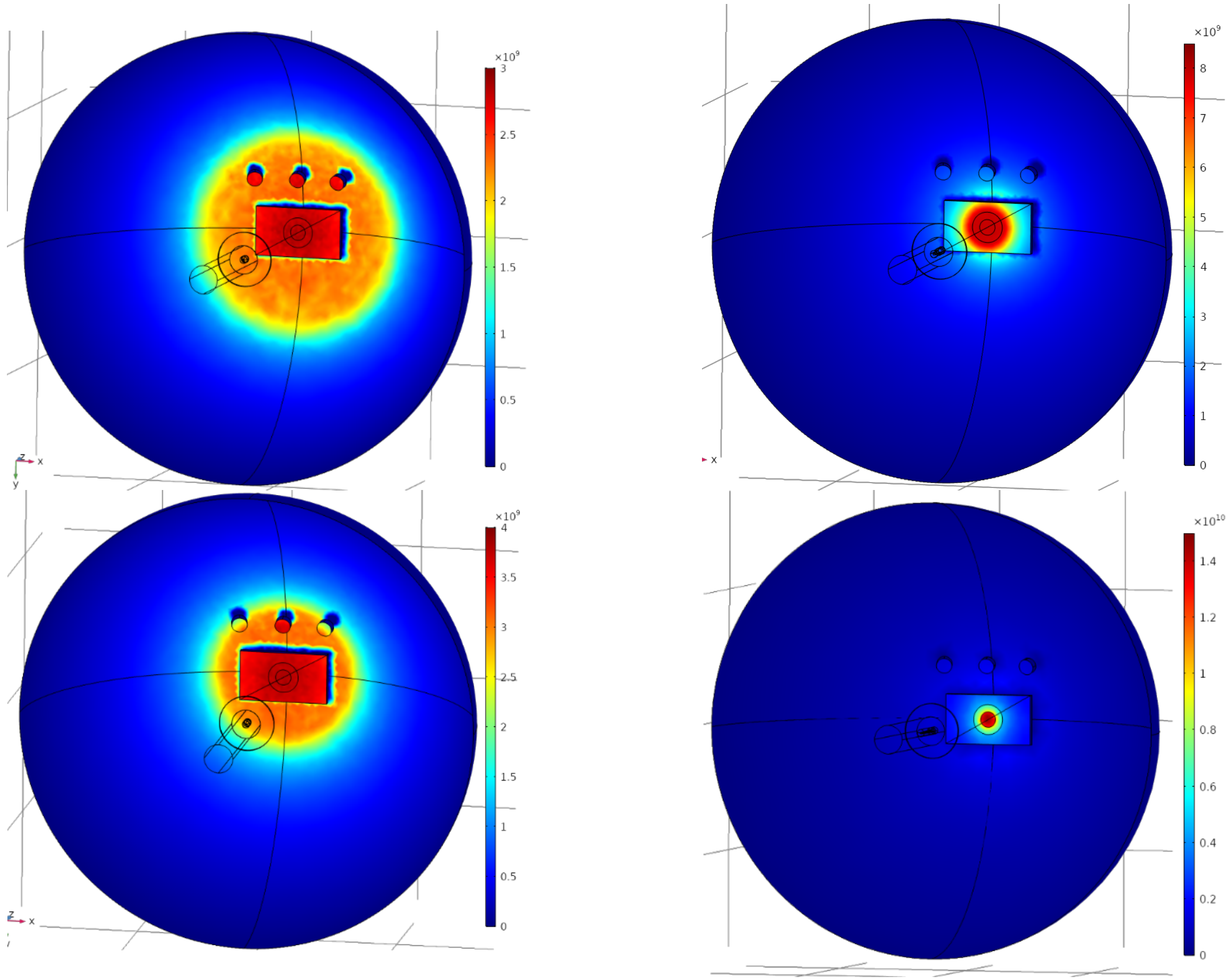
Designing Cone Attachments

Iterating Focusing Cone Designs

- Design cones of various angles and observe relative flux profiles

22° cone

4° cone



15° cone

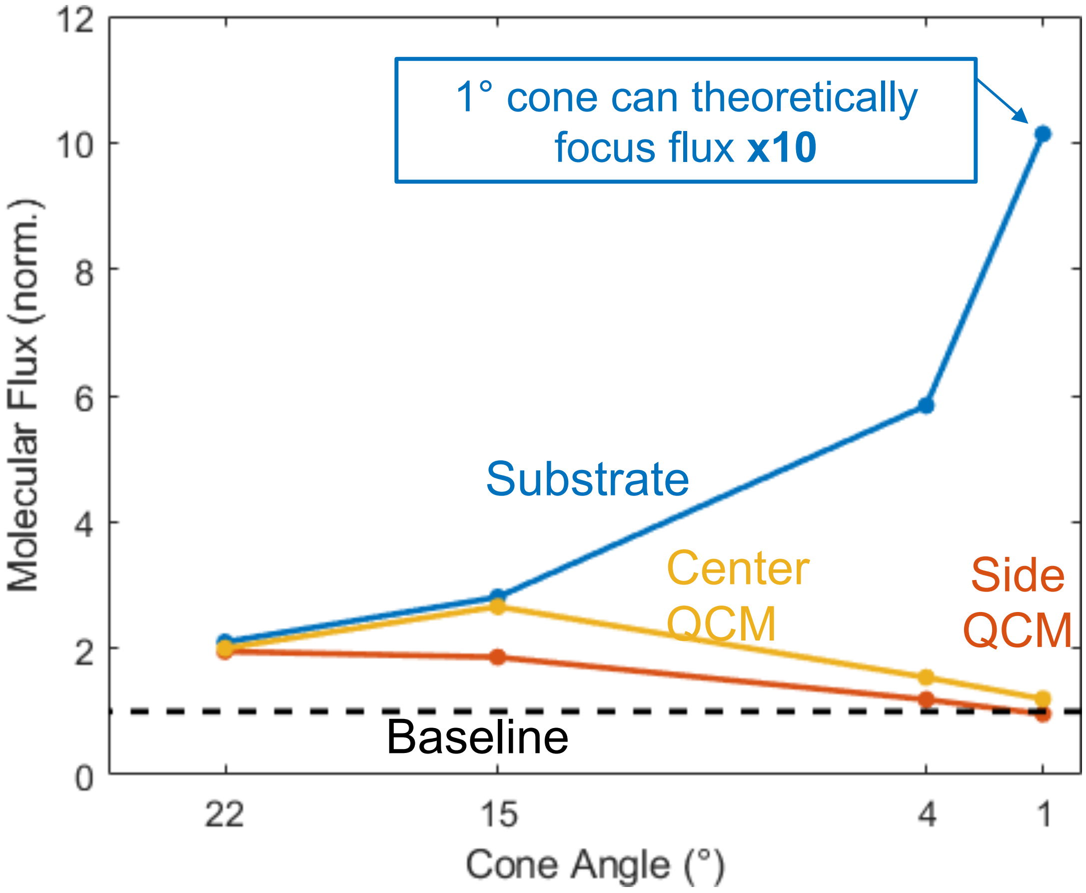
1° cone

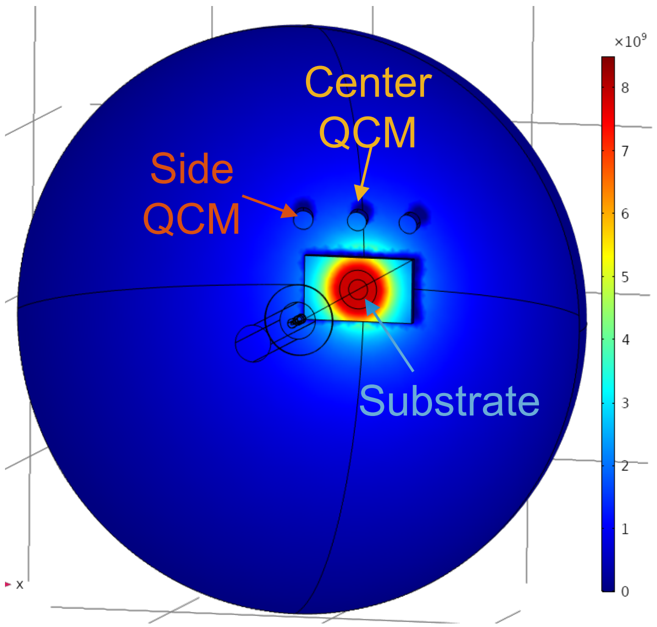
Simulations allow easy iteration and quantitative comparisons

Designing Cone Attachments

Iterating Focusing Cone Designs

- Compare QCM accumulation to baseline case to measure focusing power





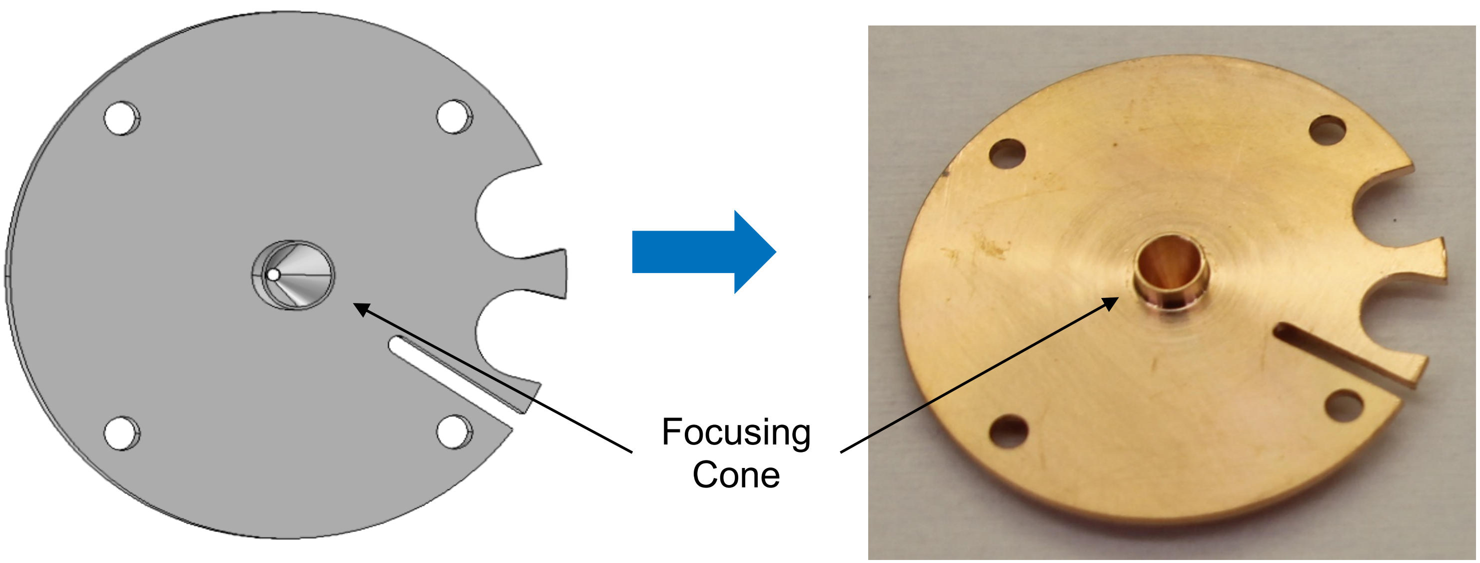
Simulations suggest large flux focusing potential

Experimental Validation

How do simulations compare to reality?

- Modelling enables design and approximate calculations
- But how accurate are simulations?

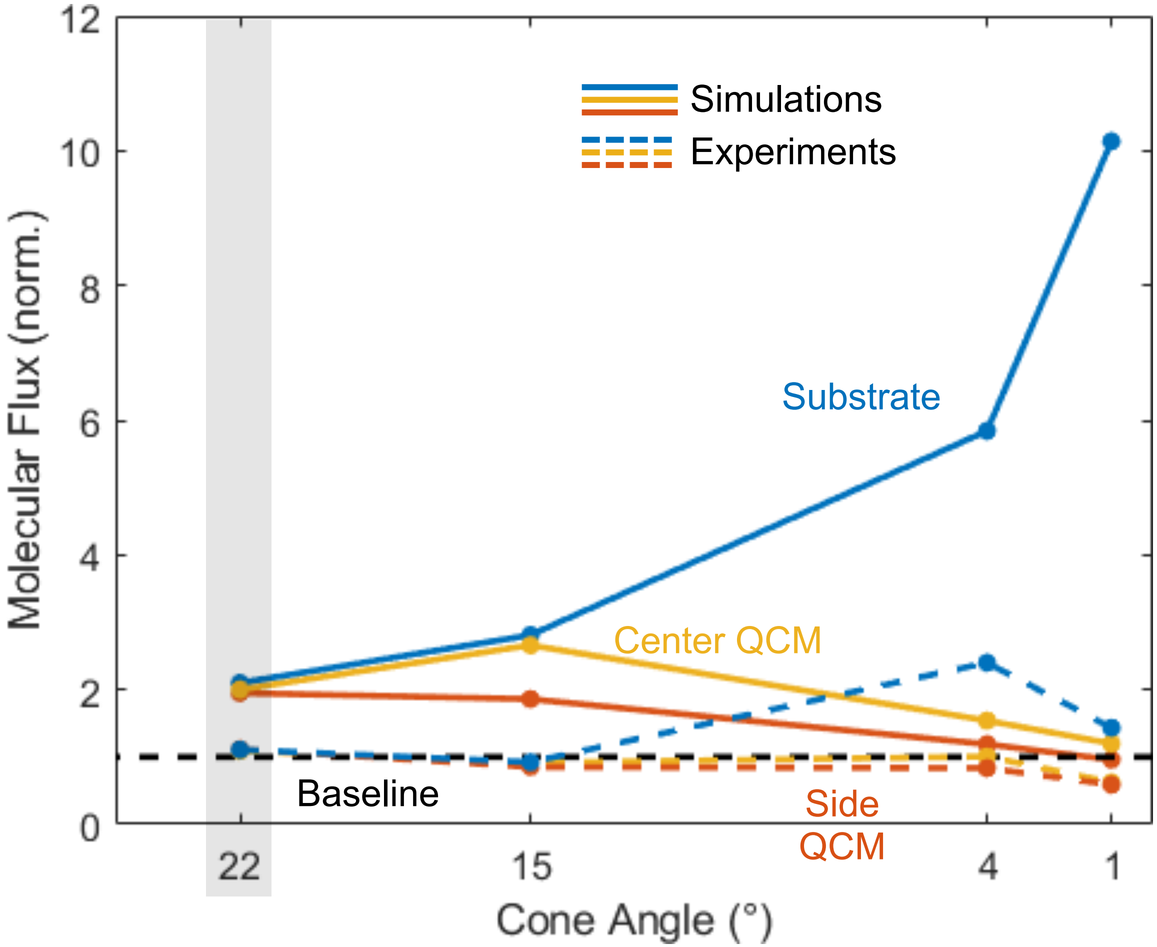
- Experimental overview
  - *Fabricate cone attachments*
  - *Measure molecular flux at different QCM positions*
  - *Compare with and without cone attachments*



*Experimental details available in backup

Experimental Results

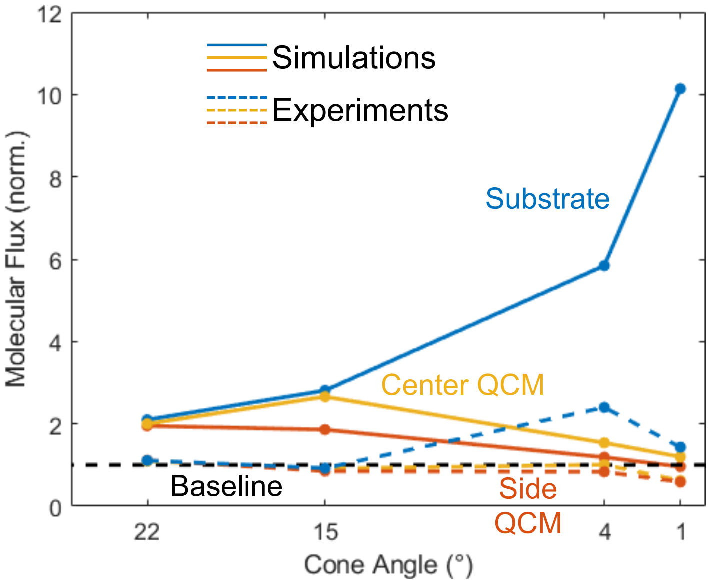
- Observations:
  - *No focusing effect for 22° and 15° cones*
  - *Focusing for 4° cone is ~40% of predicted (but still ~x2.5 focusing effect)*
  - *Focusing for 1° is minimal*
    - Highly sensitive to effusion cell alignment (likely not perfect, resulting in off-center flux)



Focusing effect experimentally observed at smaller magnitude

Flux Focusing Conclusions

- Modelling was used to successfully:
  - *Confirm flux focusing hypothesis*
  - *Iterate on designs before fabrication*
- Exact magnitude of effect reduced in experiments
  - *Non-idealities of molecular transport assumption with water*
    - Molecular flow requires P < ~10^{-3} torr
  - *Misalignment of effusion cell*
- Future work:
  - *Use lower outgassing rate materials to ensure free molecular flow regime*
  - *Account for effusion cell/cone angle alignment in testing*

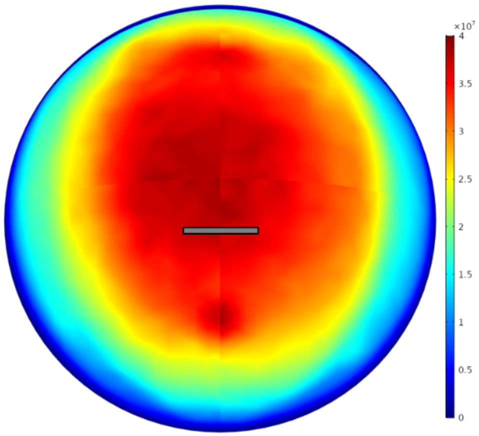


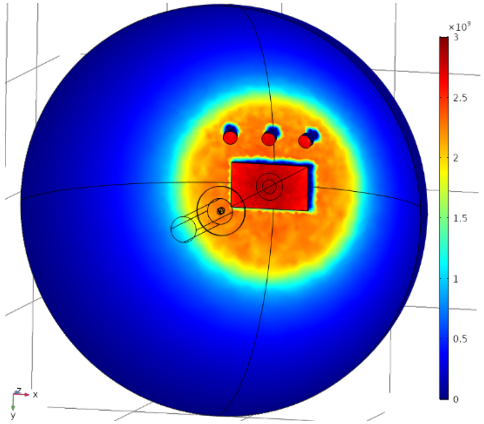
Flux focusing can accelerate experiments by more than a factor of 2

Conclusions

- Finite Element is a flexible tool to model complex geometries and quantitatively evaluate contaminant transport

- Due to non-idealities and unknowns, simulations may only be qualitative
  - *Always best to validate with experiments when possible*





Acknowledgements

Sustained Experimentation and Research for
Program Applications at The Aerospace Corporation

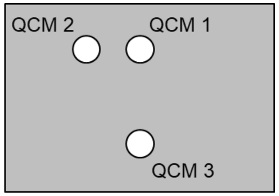
Questions?

Backup

Experimental Procedure Outline

Experiments performed September 26 – October 21, 2019

- Setup
  - *Prepare strips of composite in 90°C, 7% RH environment*
  - *Use 3 QCMs, with one in the sample position*

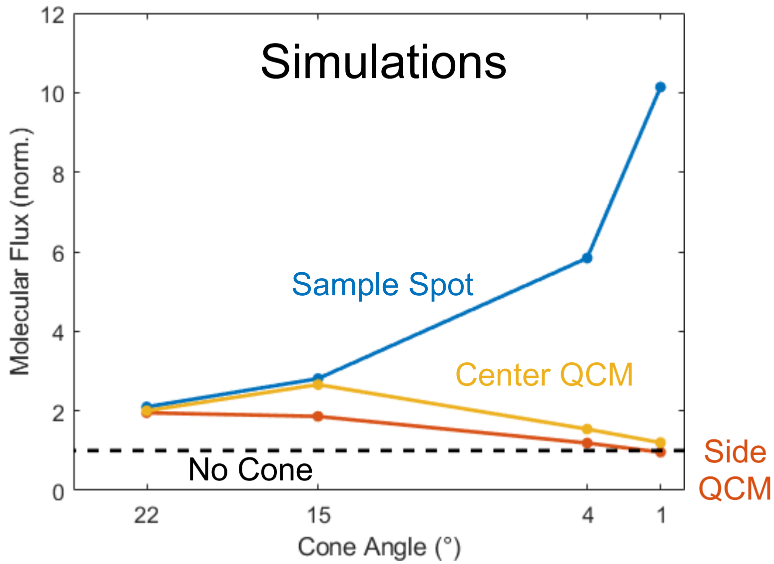


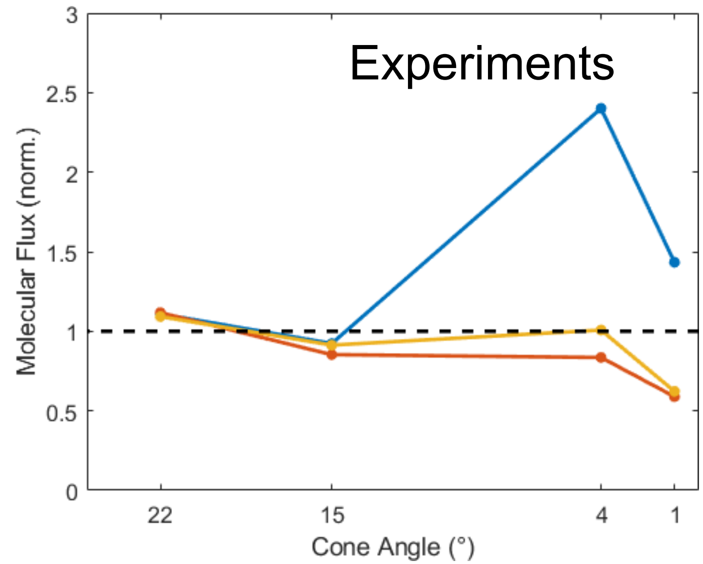
- Procedure
  1) *Set all QCMs to -173°C (100K)*
  2) *Heat composite samples in EC to 90°C*
  3) *Run for >10 hours*
  4) *Repeat*

- Notes:
  - *Multiple sets of composite strips were used, each within 1% of the same mass*
  - *Preconditioning and experiment runtimes were sufficient to nearly fully (de)saturate the composite source*
  - *Sample prep and experimental timing were standardized*

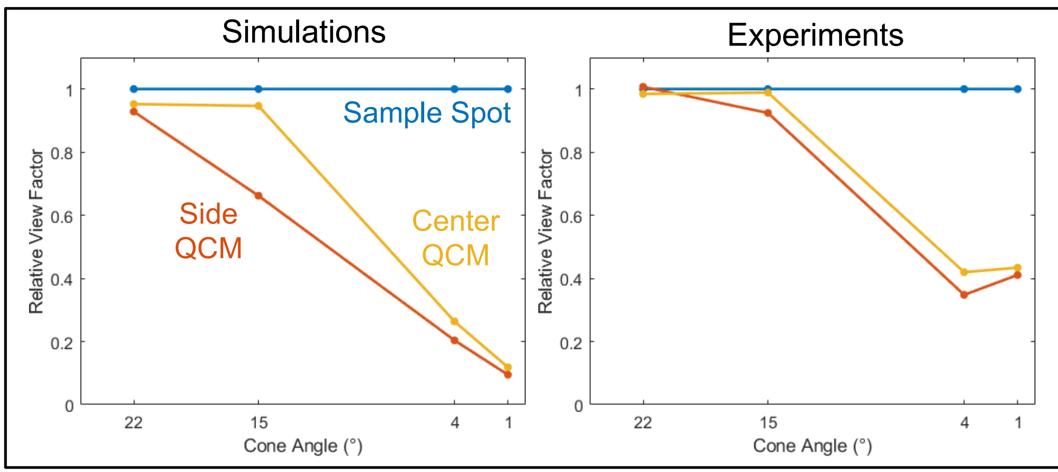
Experimental Results

Comparing Simulation vs Experiments





- *Experimental uncertainty not quantified, but is estimated to be >10%
- Plots of **View Factor** show somewhat better agreement
  - *Shows relative flux to each QCM for a single experiment*



Experiment shows focusing effect, but reduced magnitude