Contamination Analysis Tools

Lubos Brieda
Particle In Cell Consulting LLC

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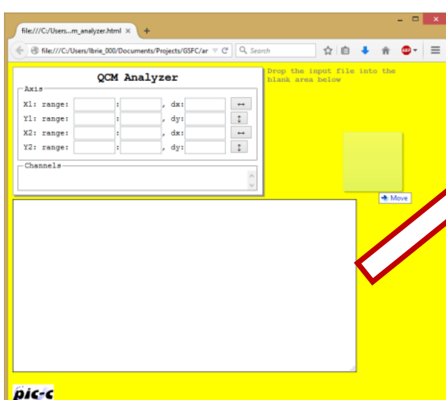
Introduction

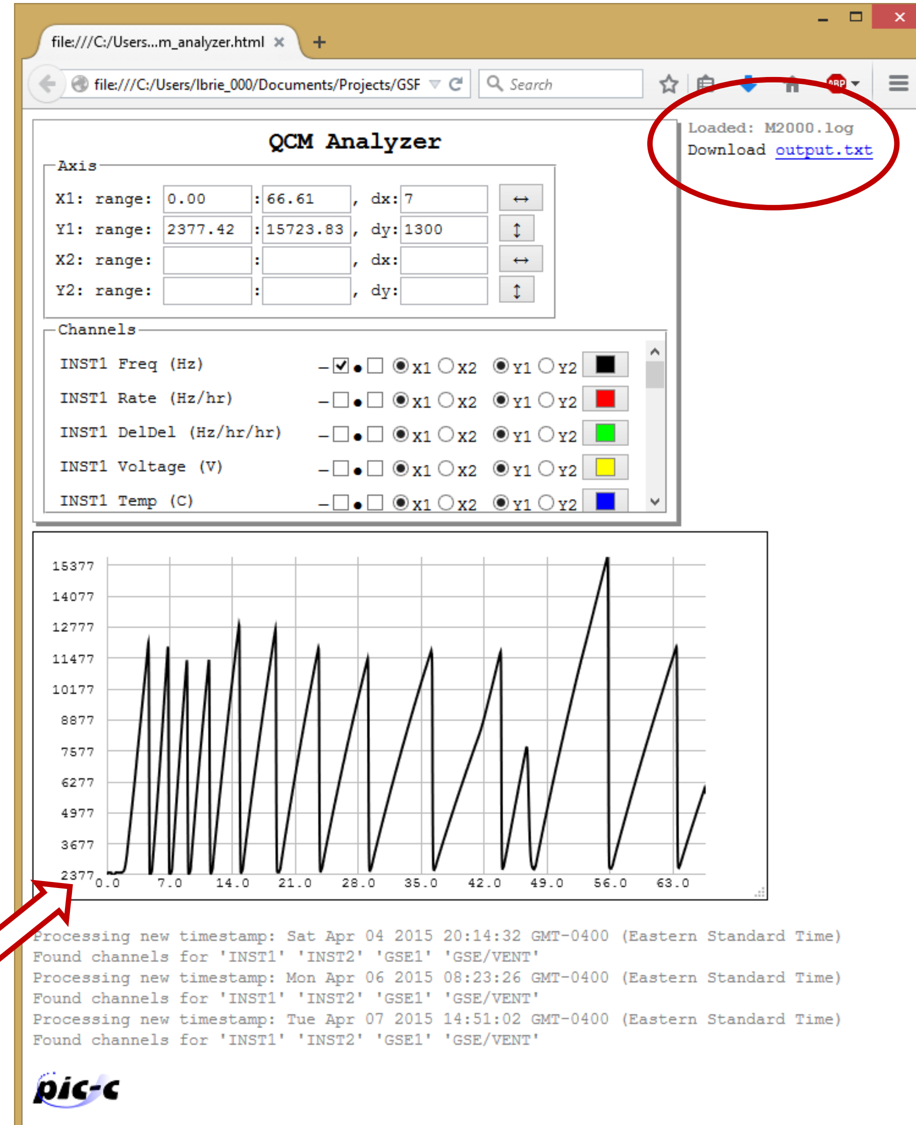
- This talk presents 3 different tools developed recently for contamination analysis:
  1. **HTML QCM analyzer:** runs in a web browser, and allows for data analysis of QCM log files
  2. **Java RGA extractor:** can load in multiple SRS .ana files and extract pressure vs. time data
  3. **C++ Contamination Simulation code:** 3D particle tracing code for modeling transport of dust particulates and molecules. Uses residence time to determine if molecules stick. Particulates can be sampled from IEST-STD-1246 and be accelerated by aerodynamic forces.

HTML TQCM ANALYZER

Overview

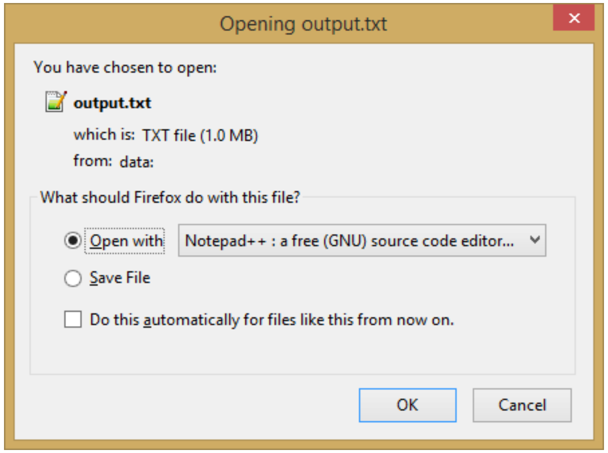
- Issue: QCM Research log files comments added to a new line – confuses Excel
- Also, post-processing required to compute delta-deltas or TGA
  - Time consuming
- Developed a Javascript/HTML program to simplify QCM analysis
  - Why Javascript? Every computer contains a web browser – no need to install a compiler
  - Websites are also by design interactive





Data Output

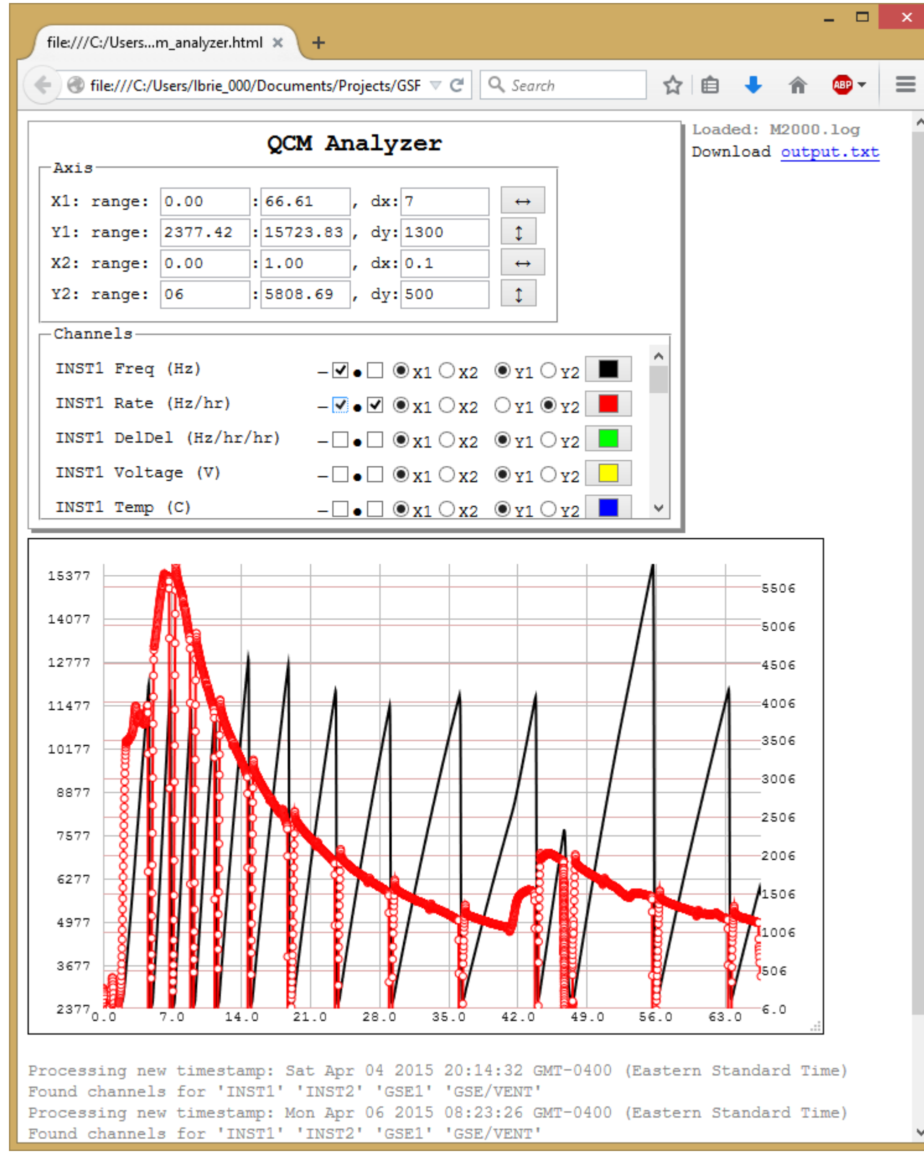
- Drag and drop log file
  - Supports QCM Research and CrystalTek
- Right click on "output.txt" to save it
- The resulting text file can be opened with Excel
  - Comments moved to a new column, can now easily generate x-y plots

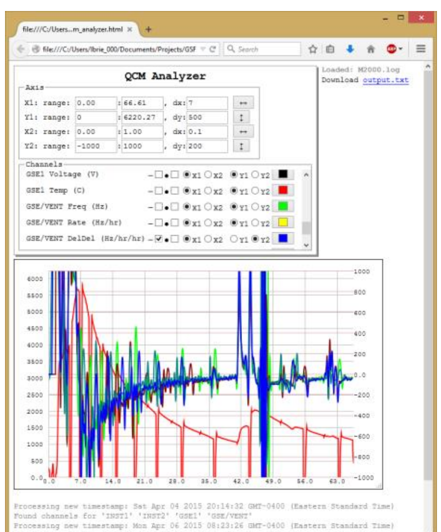


	A	B	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF
1			GSE/VENT											
2	TimeStamp	Minutes	Temperat	Voltage	Frequency	RawRate	SmoothRa	DeltaDelta						
93	4/4/2015 21:48	94	20	0	2418.53	0.04	41.96	2939.82						
94	4/4/2015 21:49	95	20	0	2418.6	0.12	51.02	2943.03						
95	4/4/2015 21:50	96	20	0	2418.67	0.48	59.04	2944.24						
96	4/4/2015 21:51	97	20.01	0	2418.83	0.45	67.83	2943.47						
97	4/4/2015 21:52	98	19.58	0	2424.36	10.63	78.36	2940.71						
98	4/4/2015 21:53	99	18.59	0	2425.36	0.06	89.82	2935.97						
99	4/4/2015 21:54	100	17.56	0	2427.1	4.07	103.45	2929.23						
100	4/4/2015 21:55	101	16.55	0	2428.38	1.22	121.07	2920.5						
101	4/4/2015 21:56	102	15.56	0	2429.83	0.62	141.93	2909.78						
102	4/4/2015 21:57	103	14.55	0	2431.56	1.68	154.92	2897.08						
103	4/4/2015 21:58	104	13.55	0	2433.68	2.21	171.96	2882.38						
104	4/4/2015 21:59	105	12.55	0	2435.84	-2.26	205.72	2865.7						
105	4/4/2015 22:00	106	11.54	0	2439.04	5.86	248.75	2847.03						
106	4/4/2015 22:01	107	10.55	0	2442.84	4.41	300.86	2826.37						
107	4/4/2015 22:02	108	9.55	0	2447.44	4.88	363.64	2803.72	6370.2 Change shroud temp to 60C, MGSE to 20C, TQCM to -20					
108	4/4/2015 22:03	109	8.53	0	2453.32	8.73	435.49	2779.08						
109	4/4/2015 22:04	110	7.54	0	2460	6.4	516.36	2752.45						
110	4/4/2015 22:05	111	6.54	0	2468.49	9.74	607.32	2723.83						
111	4/4/2015 22:06	112	5.54	0	2478.86	18.25	705.81	2693.22						
112	4/4/2015 22:07	113	4.56	0	2490.37	13.23	813.26	2660.62						
113	4/4/2015 22:08	114	3.57	0	2505.13	20.41	927.62	2626.04						
114	4/4/2015 22:09	115	2.56	0	2520.57	19.69	1049.46	2589.46						
115	4/4/2015 22:10	116	1.56	0	2539.02	21.18	1176.88	2550.9						
116	4/4/2015 22:11	117	0.57	0	2559.25	21.5	1306.59	2510.34						

Plotting

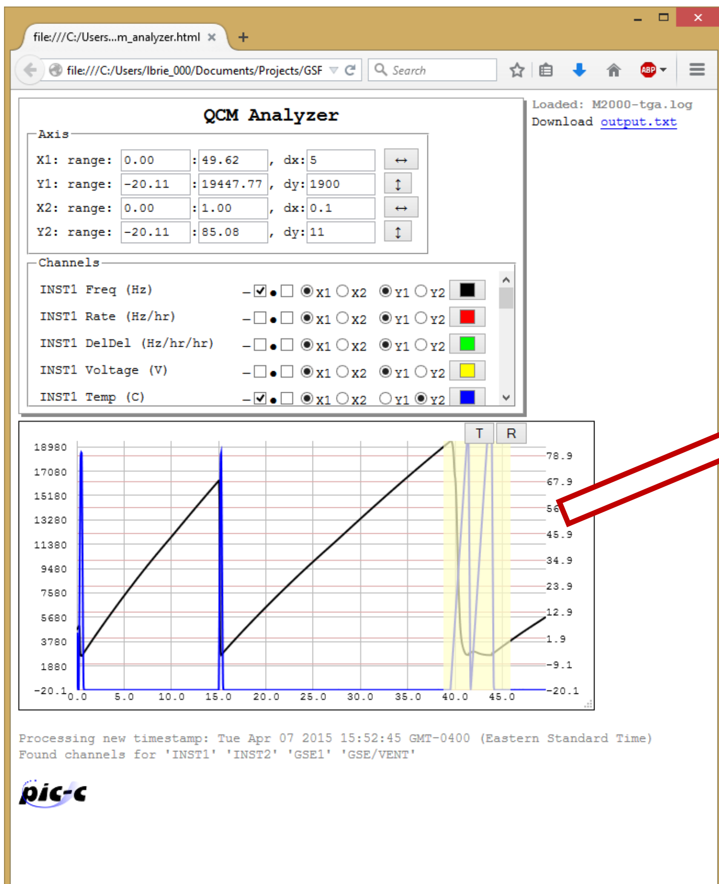
- The analyzer also contains a built-in plotter
  - Useful if Excel not available
  - Can plot frequency, frequency rate, crystal temperature, delta-delta, and voltage for each channel
- Data can be plotted using lines and/or markers, and can be plotted on one of two axis

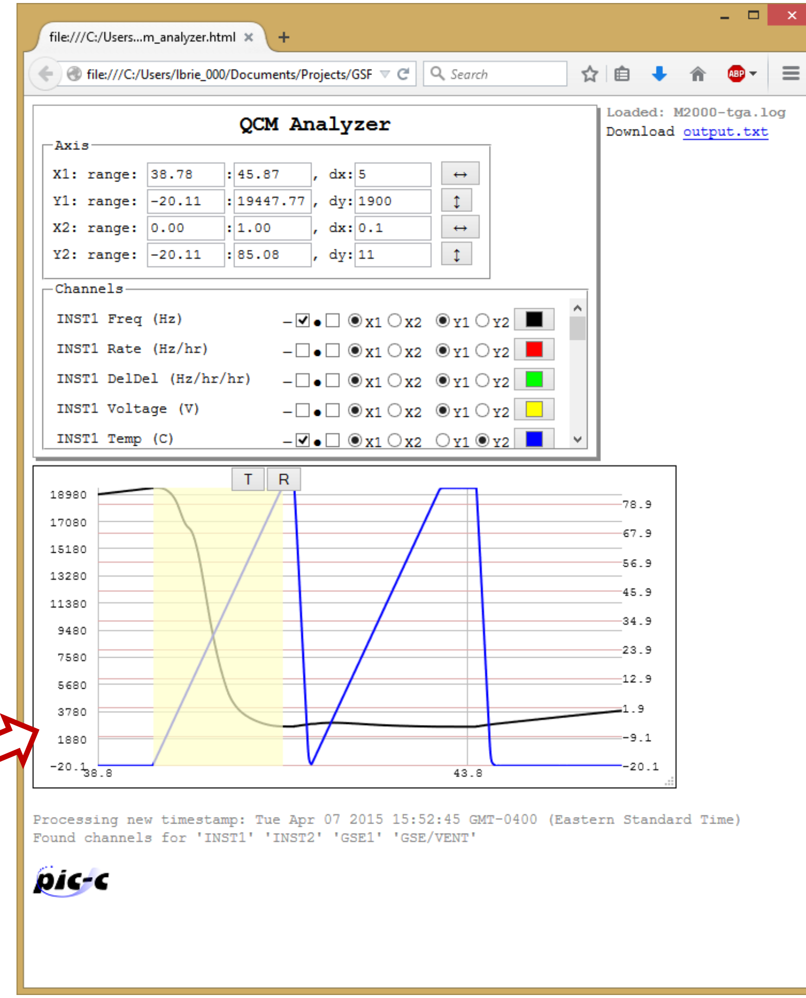




User Interface

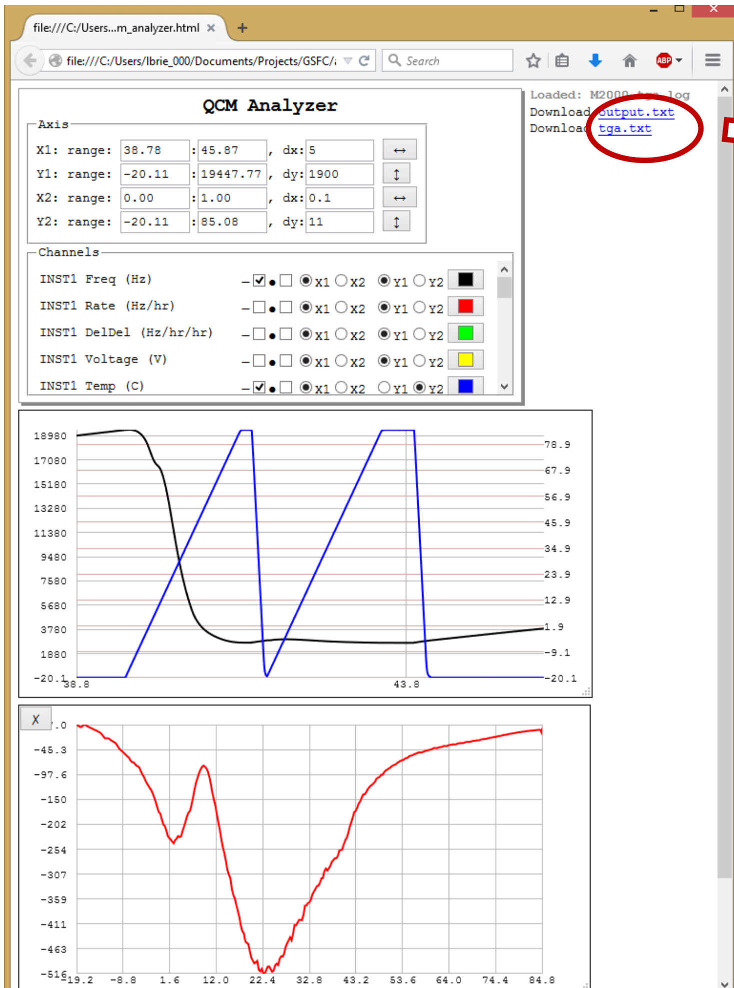
- Data ranges set using input fields
- Or: zoom-in by highlighting a region and double-clicking

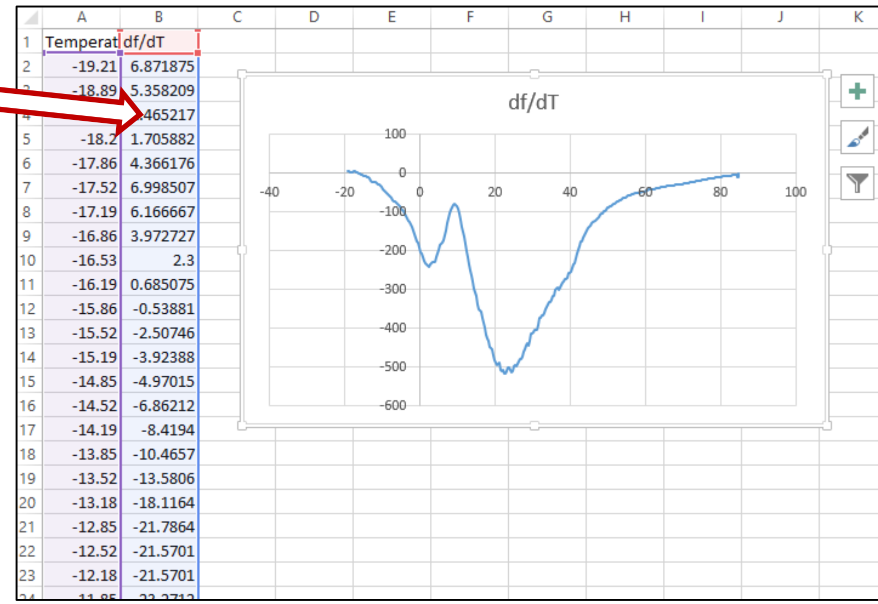




TGA

- Highlighting a region and pressing the “T” button results in TGA being computed
  - Uses the active frequency and temperature data set
  - Can export as text file for plotting in Excel

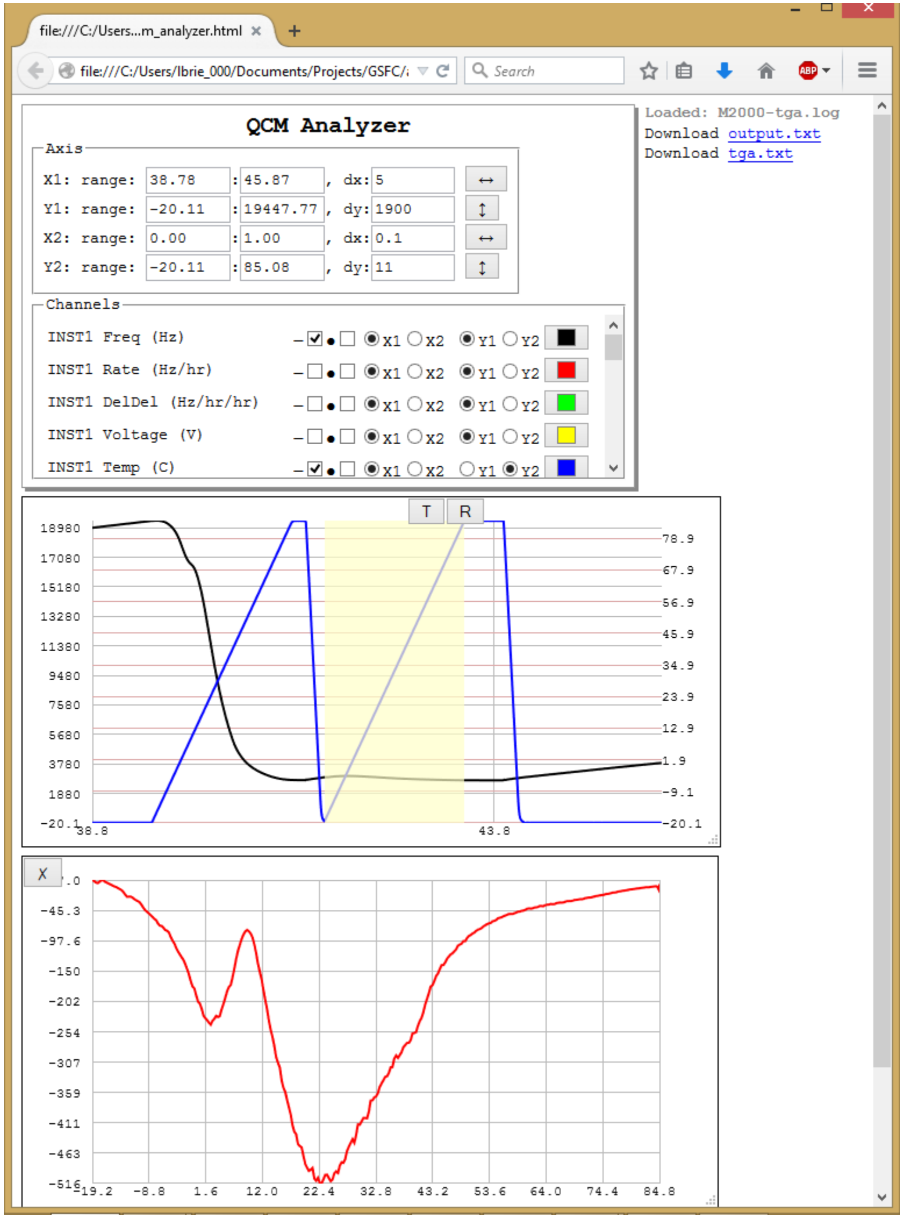




	A	B
1	Temperat	df/dT
2	-19.21	6.871875
3	-18.89	5.358209
4	[illegible]	[illegible]465217
5	-18.2	1.705882
6	-17.86	4.366176
7	-17.52	6.998507
8	-17.19	6.166667
9	-16.86	3.972727
10	-16.53	2.3
11	-16.19	0.685075
12	-15.86	-0.53881
13	-15.52	-2.50746
14	-15.19	-3.92388
15	-14.85	-4.97015
16	-14.52	-6.86212
17	-14.19	-8.4194
18	-13.85	-10.4657
19	-13.52	-13.5806
20	-13.18	-18.1164
21	-12.85	-21.7864
22	-12.52	-21.5701
23	-12.18	-21.5701

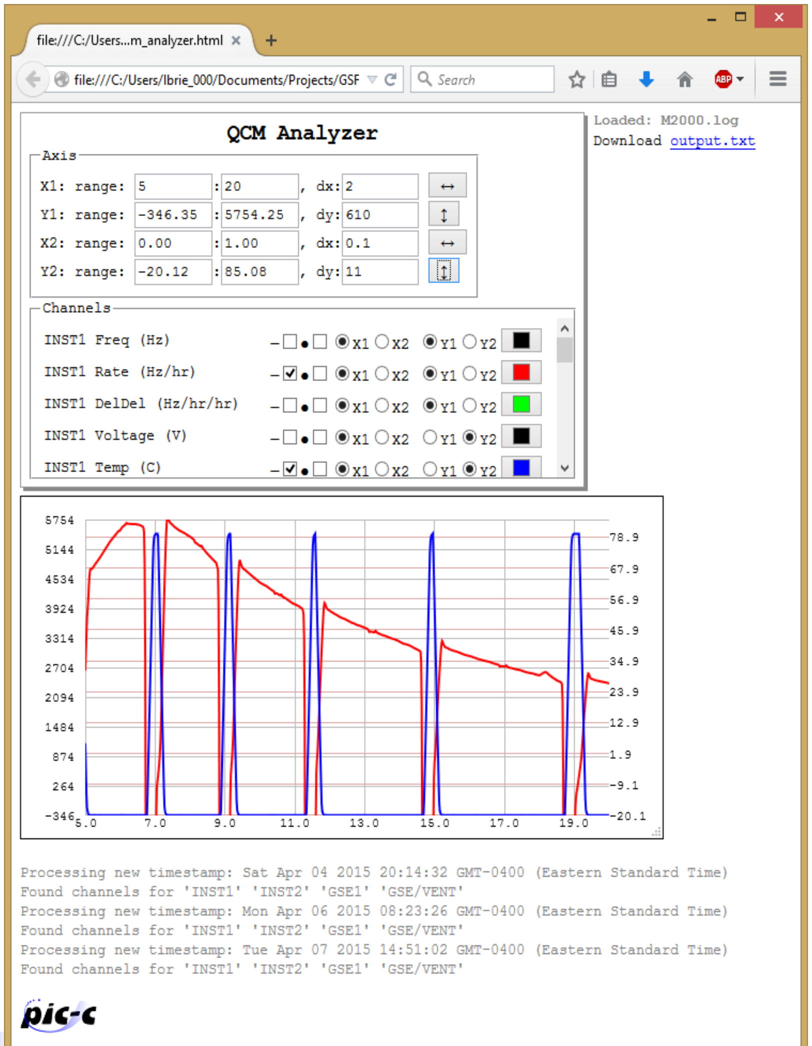
TGA Reference Curve

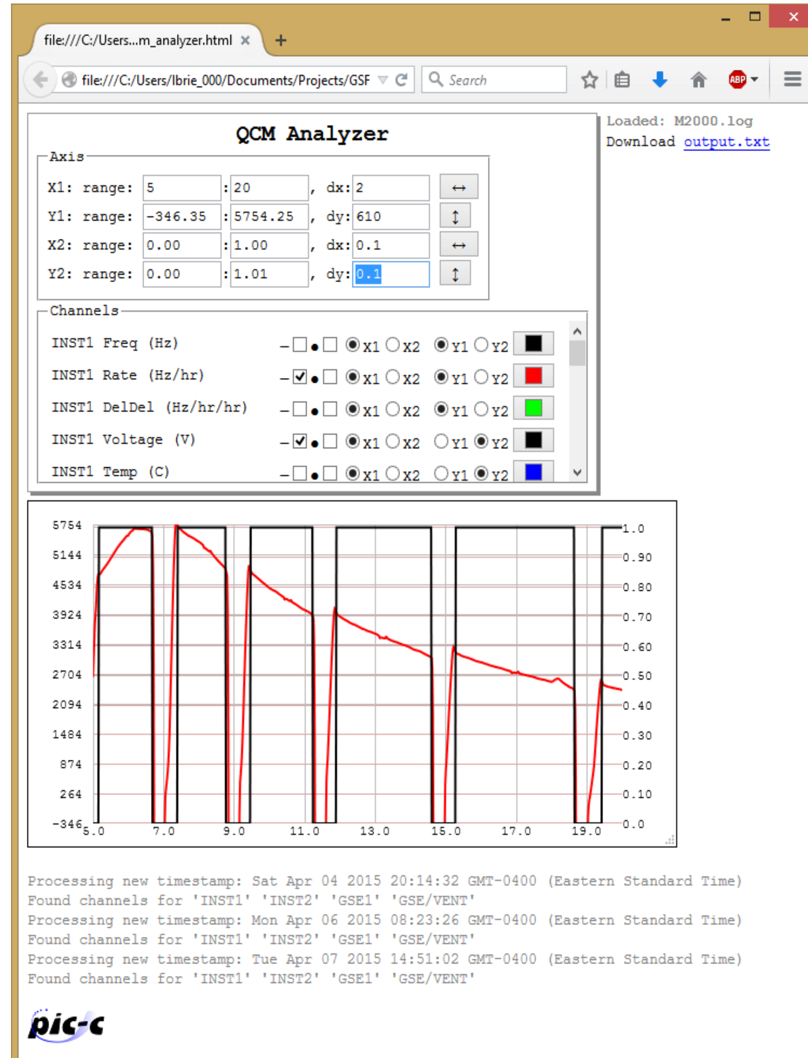
- The “R” button can be used to subtract reference TGA curve



Delta-Delta

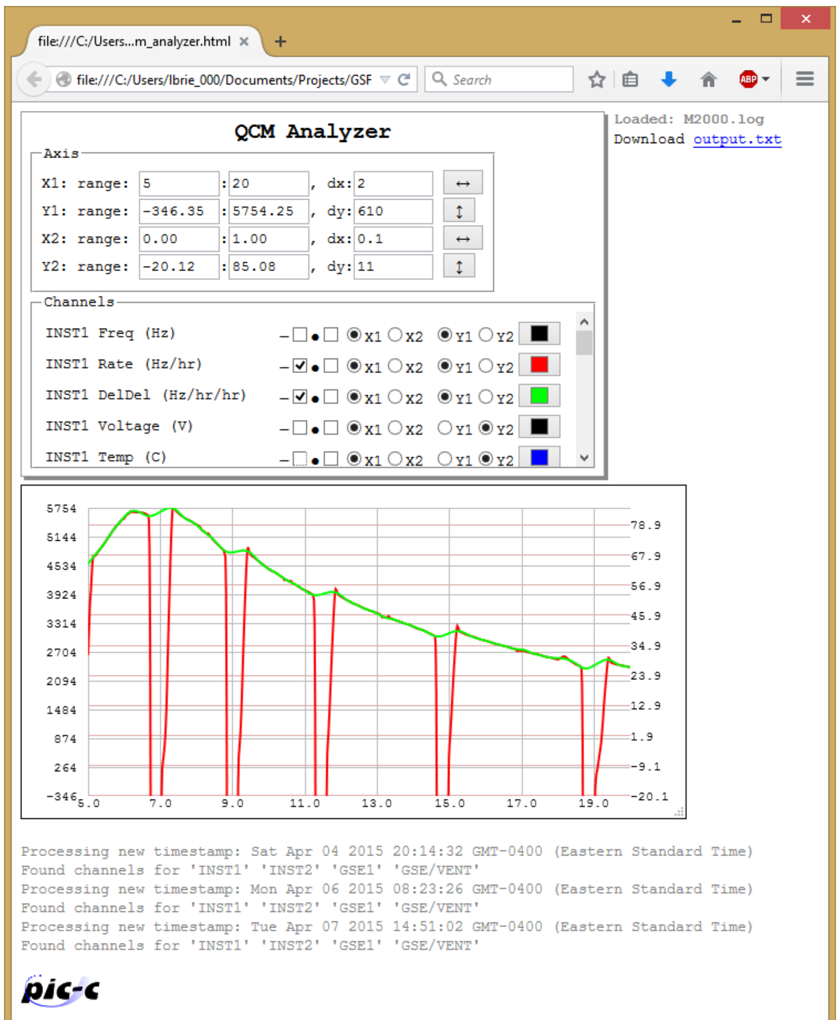
- The analyzer also computes delta-deltas
  - Uses temperature rate change to automatically discard crystal bakeoffs

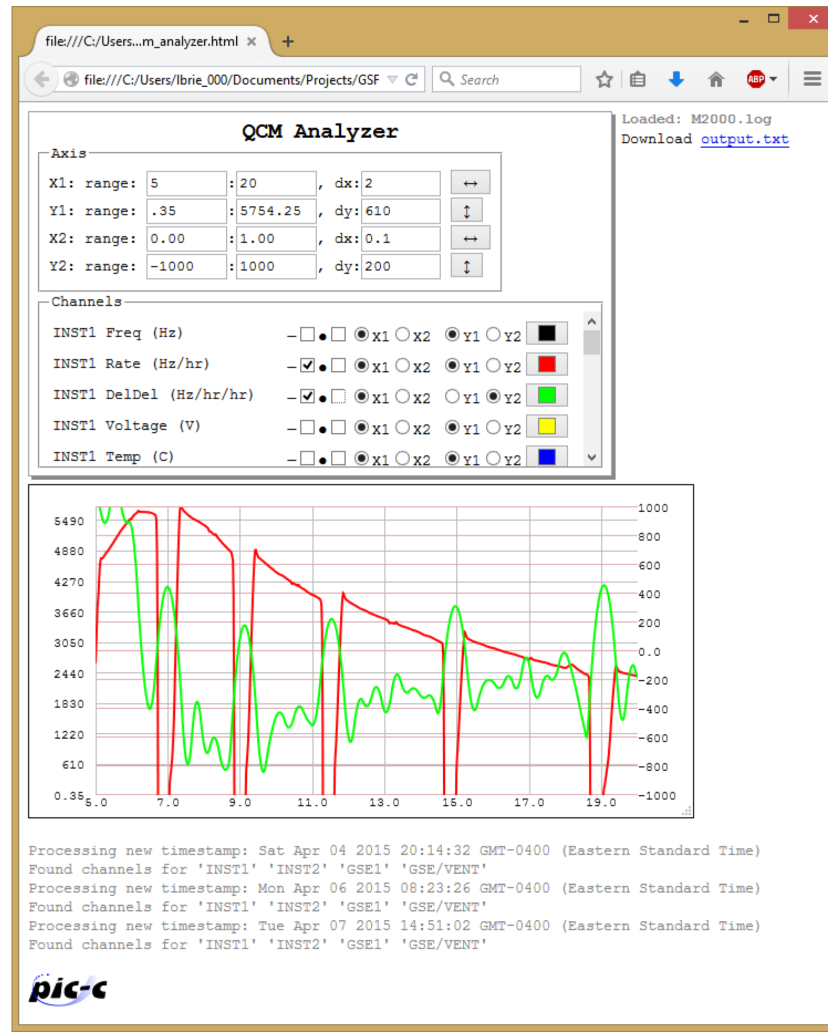




Delta-Delta

- The analyzer then fits a cubic spline to the remaining data
- Delta-Delta is the first derivative of the cubic spline





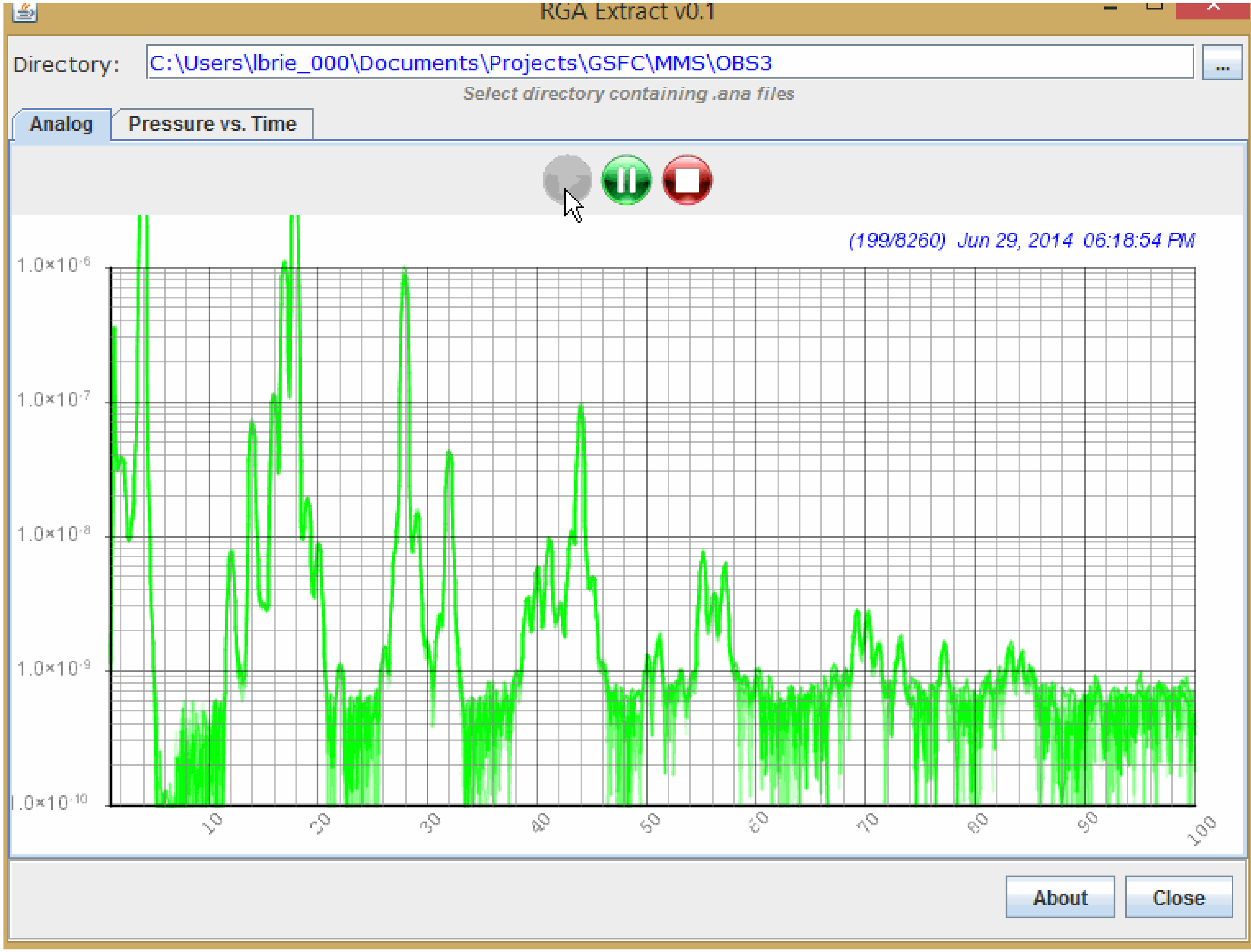
RGA EXTRACT

Overview

- After a long TVAC campaign, we ended up with multiple .ana scan logs from SRS RGA
  - New file was generated whenever scanning restarted due to changing scan parameters, computer restarts, etc..
- We were interested in pressure vs. time of selected species over the entire TVAC
  - SRS RGA program can load a single .ana file for post-processing, it was not clear how to load multiple files
- Developed a Java RGA analyzer
  - Loads **all** .ana files from a selected directory, sorts entries by date
  - Analog scans can be animated
  - Can also extract pressure vs. time for all data

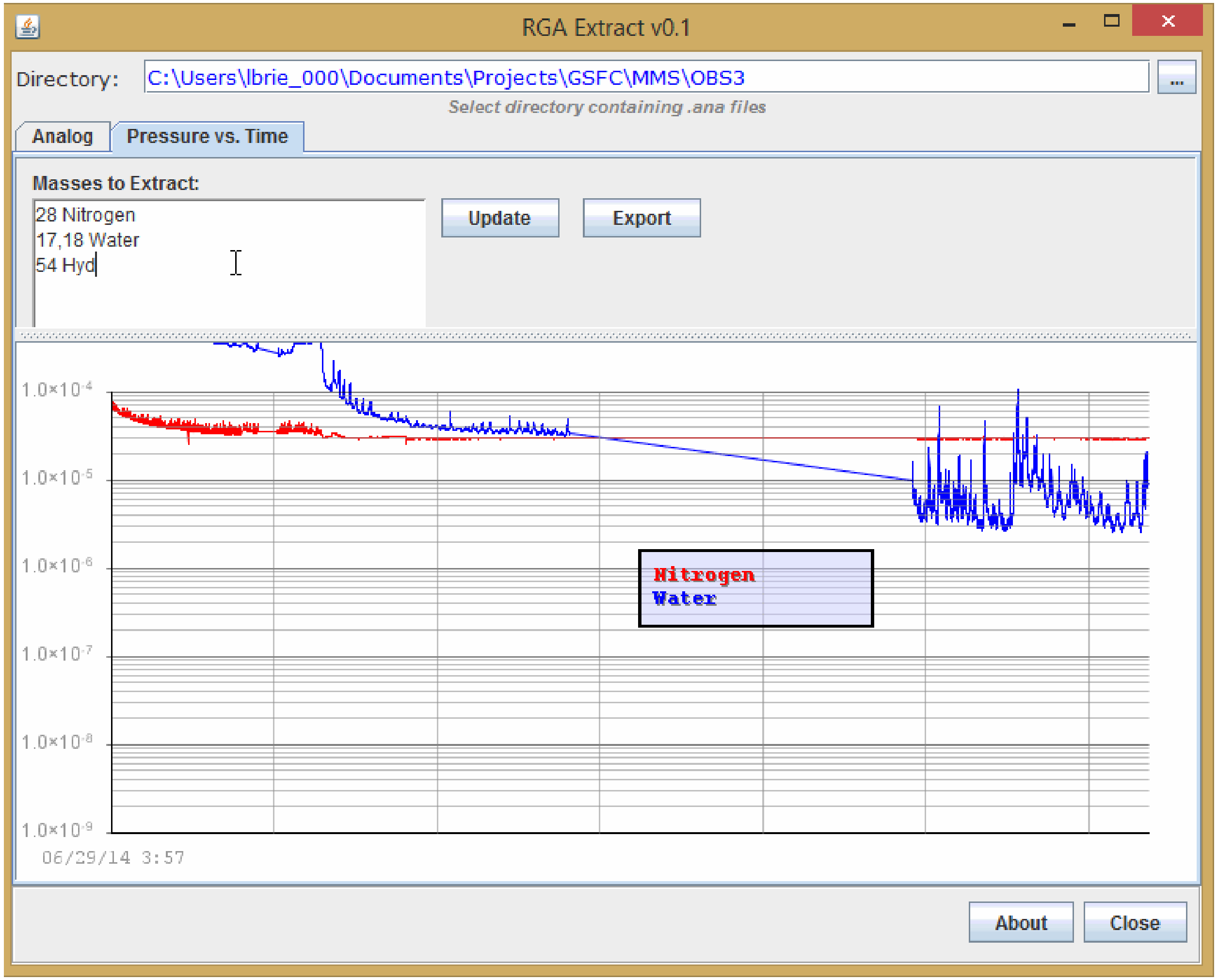
Analog Plot

- Start by selecting a directory
- Analog data can be animated
  - For now, x-y limits are hardcoded



Pressure vs. Time

- Can also easily generate and export pressure vs. time data
- Partial pressures can be computed over ranges of masses or multiple unique values:
  - 17, 18
  - 54:200



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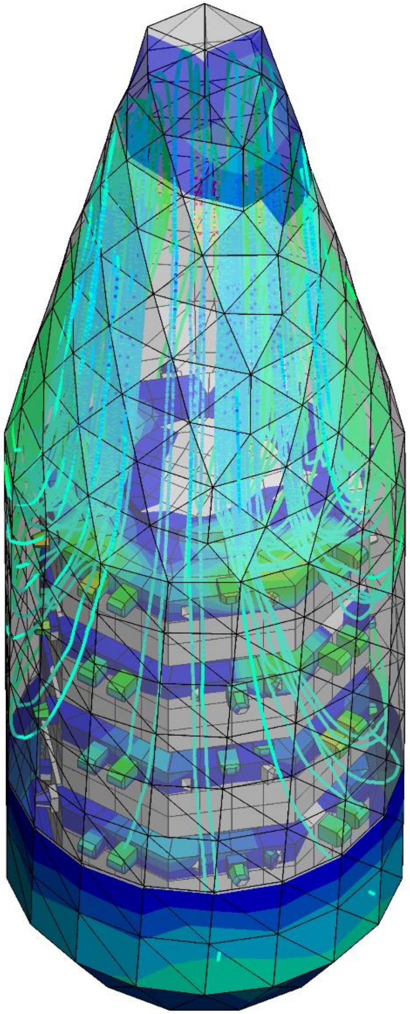
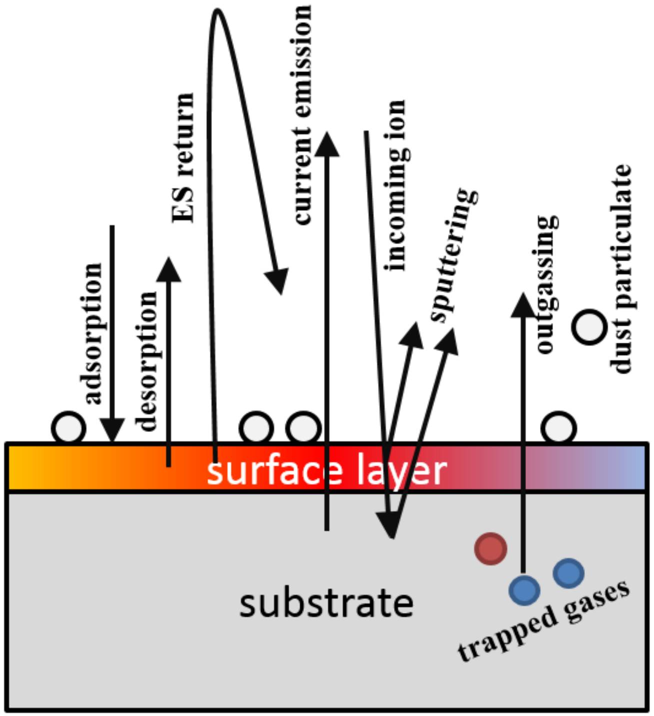
CONTAMINATION TRANSPORT SIMULATION PROGRAM

Particle Push

- Simultaneously pushes multiple particles
  - Similar to DSMC or PIC, but collisions or electrostatic effects not considered
  - Different from ray tracing codes such as Thermal Desktop which trace a ray from start to finish and only consider surface flux
  - Particle positions updated from $x^{k+1} = x^k + v^{k+0.5}\Delta t$
  - Supports finite-sized particulates sampled from IEST-STD-1246 or free molecular flow
- Particle positions can be used to obtain gas density
  - Scatter particle positions to a volume mesh
- Octree used to store surface elements, retrieves elements to check for surface impact during particle push
- Another octree can be used to store point cloud data for a force field:
  - Examples: flow velocity for dust particulate transport, electric field for electrostatic return



Surface Model



- Also developed a new surface model
- Objects exposed to vacuum assumed to be composed of a base substrate containing trapped gases, and a surface layer with multiple adsorbed materials
- Instead of using predefined sticking coefficient, residence time for an impacting particle is computed from

$$\tau_r = \tau_0 \exp\left(-\frac{E_a}{RT}\right)$$

- If $\tau_r > \Delta t$, the particle is adsorbed into the surface layer
  – Contains counts for all flying materials
- First-order desorption used to determine number of molecules to inject into gas phase: $\frac{dN}{dt} = \frac{1}{\tau_r} N$
- Outgassing mass from $\frac{dm}{dt} = Cm \frac{\exp(-E_a/RT)}{\sqrt{t}}$

Surface Model Algorithm

- Pseudo code of the surface model is below:

```
load material data (density, molecular radius, TML, ...)
load component data (temperature, total mass, cleanliness level, ...)
initialize surface data structures

for each timestep:
   %particle push
   for each particle:
      if surface impact:
         compute residence time
                  if greater than time step:
                     deposit to surface layer
                  else:
                     re-emit following cosine law

   %outgassing model
   for each component:
      compute mass outgassing mass loss
      add to surface layer

   %desorption
   for each surface element:
      compute desorption loss
      inject particles with cosine distribution
      deplete surface layer
```

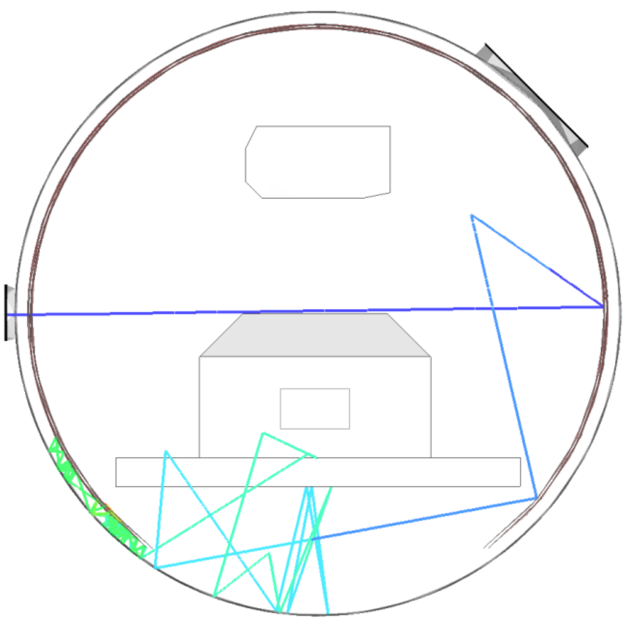
CTSP Input File

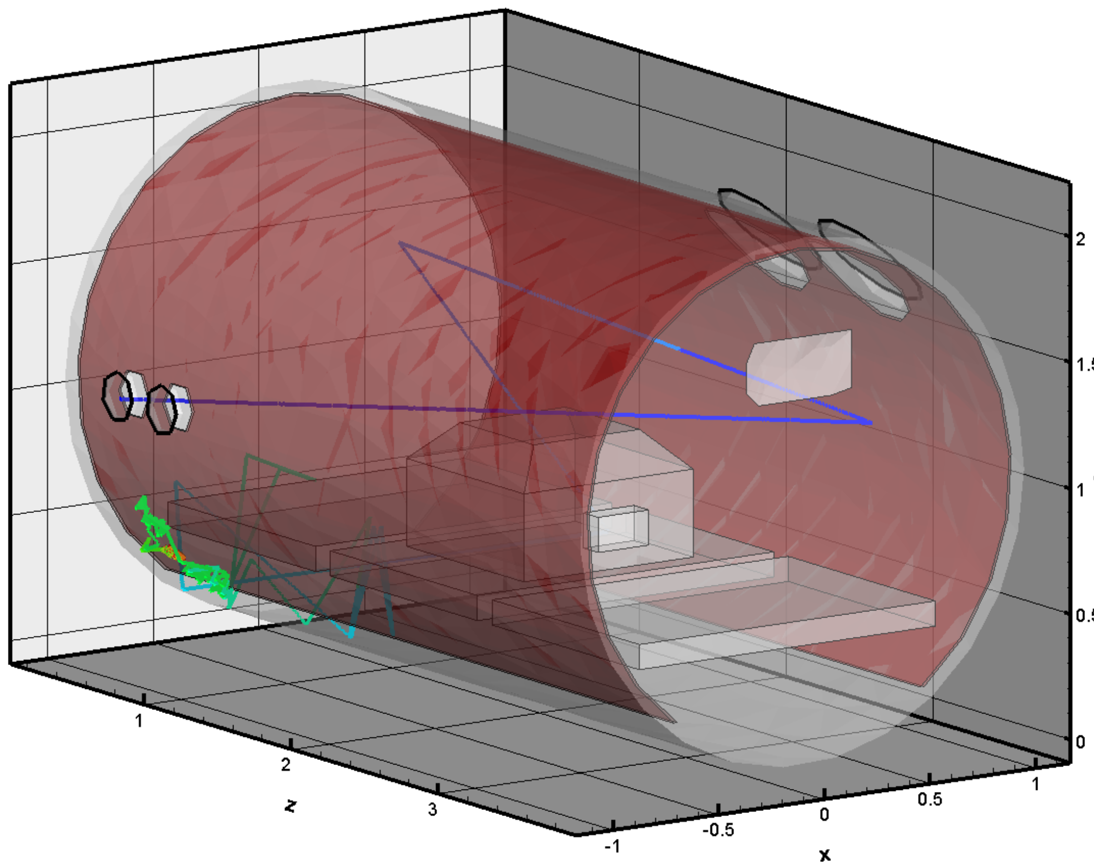
- CTSP uses a JSON-like syntax:

```
#load surface
surface_load_stl{file_name:"chamber.stl"}

#define volume mesh, before materials are loaded
volume_mesh{dx:0.05,dy:0.05,dz:0.05}

#materials
solid_mat{name:black_paint, mass: 100}
gas_mat{name:hc1, mass: 94, spwt: 1e10, Ea:12, C:10}

#define components
comp{name:ebox, mat:al, trapped_mass:1e-3, trapped_mat:[0.005*n2, 0.05*water, 0.75*hc1],
          surf_h:1e-10, surf_mat:water, temp:350}

#enable outgassing
source_outgassing{}

#surface source
source_maxwellian{comp:port1, Q:1e-9, mats:[0.75*n2, 0.25*o2], temp:300, v_drift:100}

#attach probes
probe{comp:port1,type:qcm}

#specify output
surface_save_vtk{skip:10000,file_name:"surf"}
volume_save_vtk{skip:10000,file_name:"field",vars:[pressure,nd-ave.n2,nd-ave.water]}

#run simulation
ctsp{dt:1e-6,nt:60000,diag_start:1,diag_skip:20}
```

Particle Trace

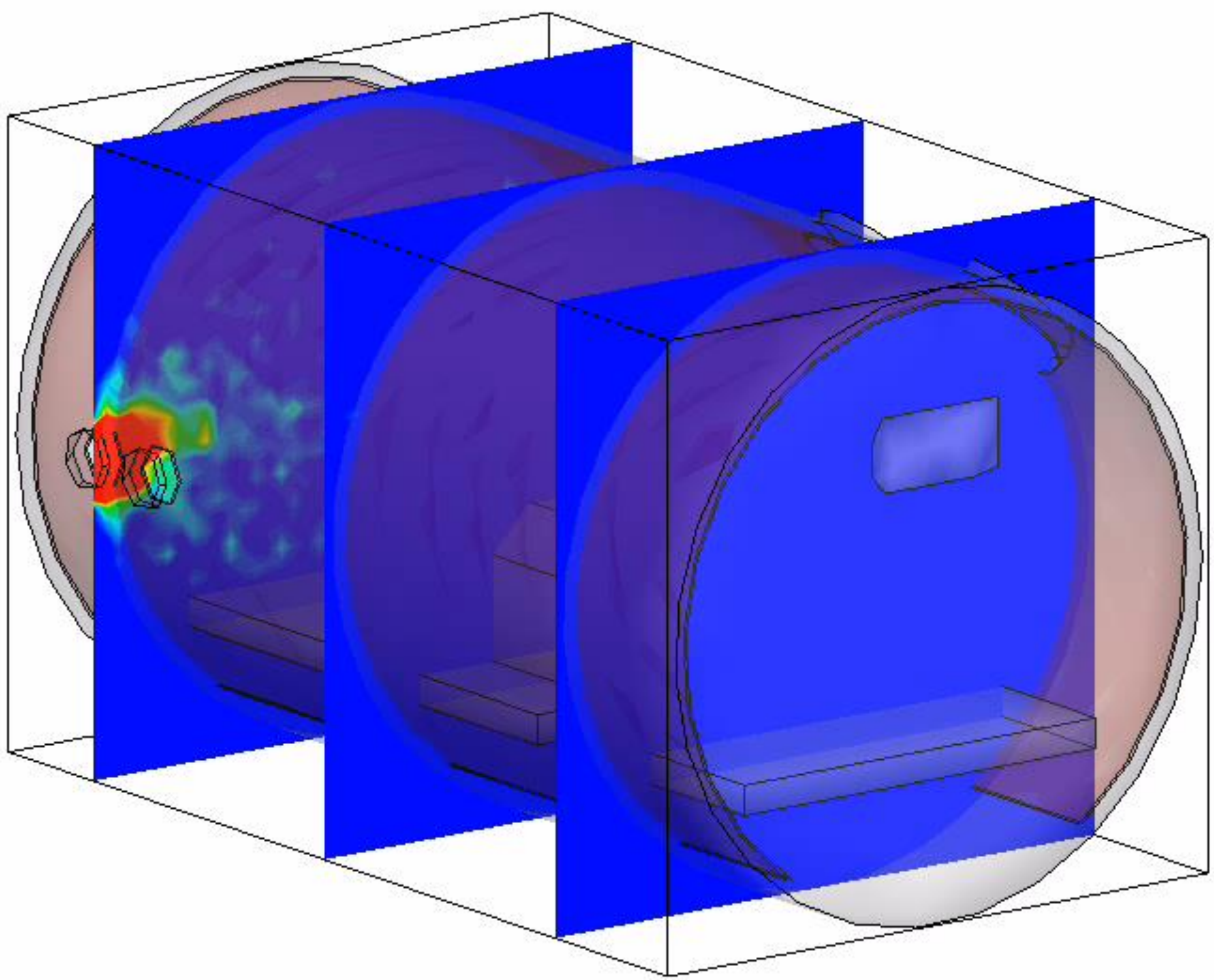
- Plot shows a trace of a single particle bouncing around a vacuum chamber
  - Particle introduced at a port, after multiple impacts ends up between chamber wall and the thermal shroud
  - If the simulation ran for a longer time, the particle would eventually be collected by the cryopump





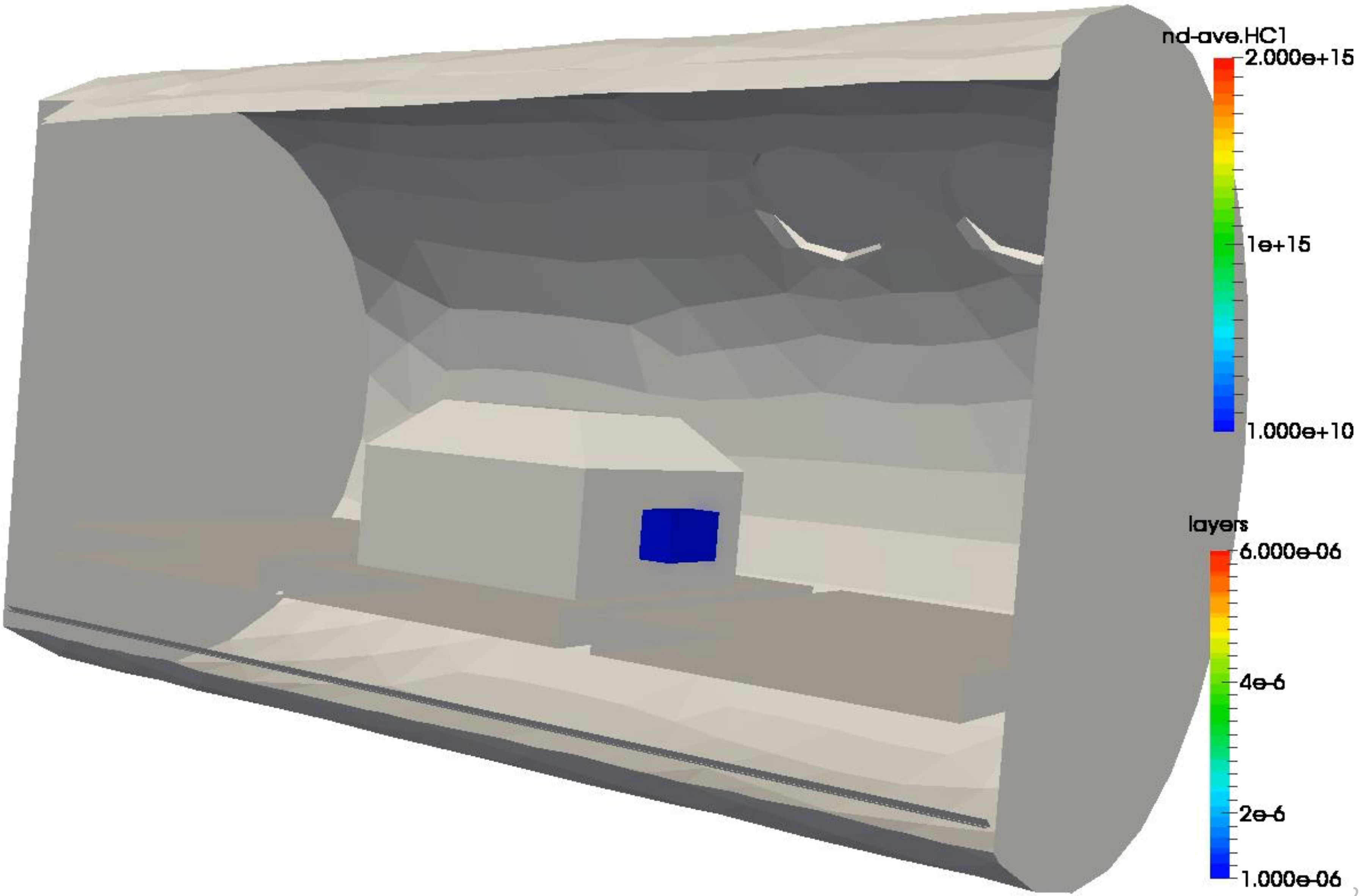
Chamber repress

Example of chamber repress (gas injection). Because of thermal spread, some molecules strike the back side of the shroud and remain in the narrow region between chamber wall and thermal shroud



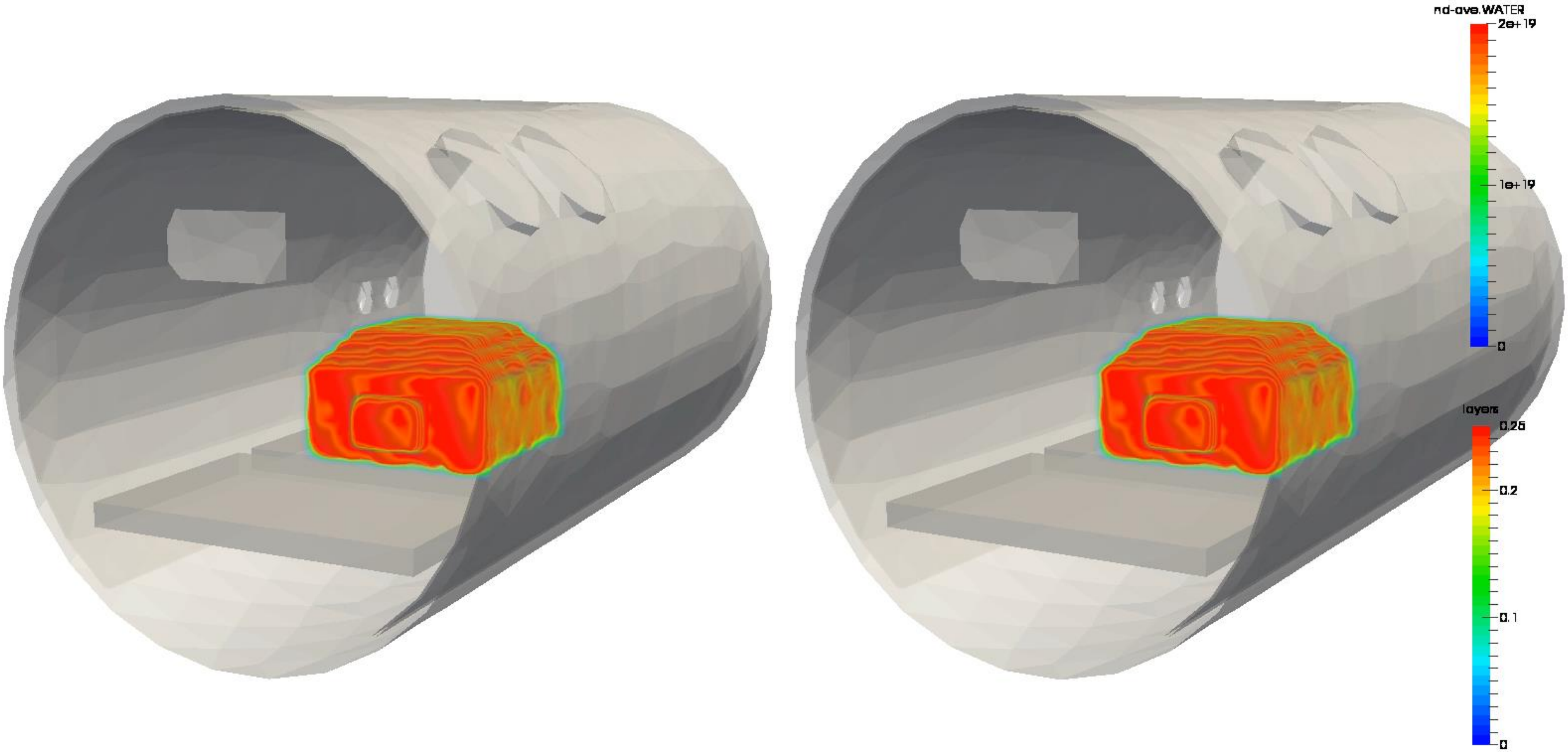
Hydrocarbon Outgassing

Hydrocarbon outgassing from an electronics box and depositing on walls



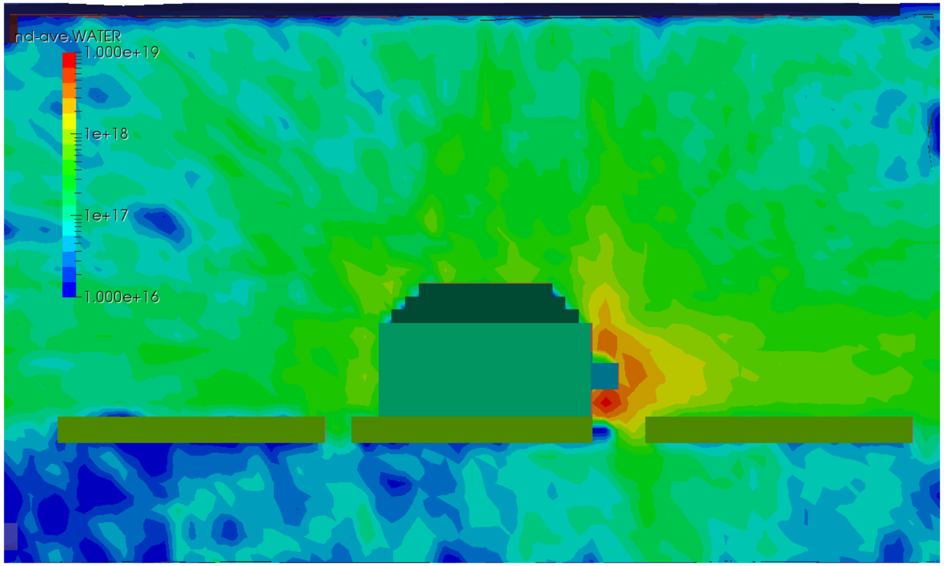
Impact of Shroud Temperature

Water flashing off and outgassing from a test article. Case on left is with 300K walls, while case on right is with 100K walls. The test article also contained trapped nitrogen, and the e-box was outgassing a hydrocarbon (shown on next slide)

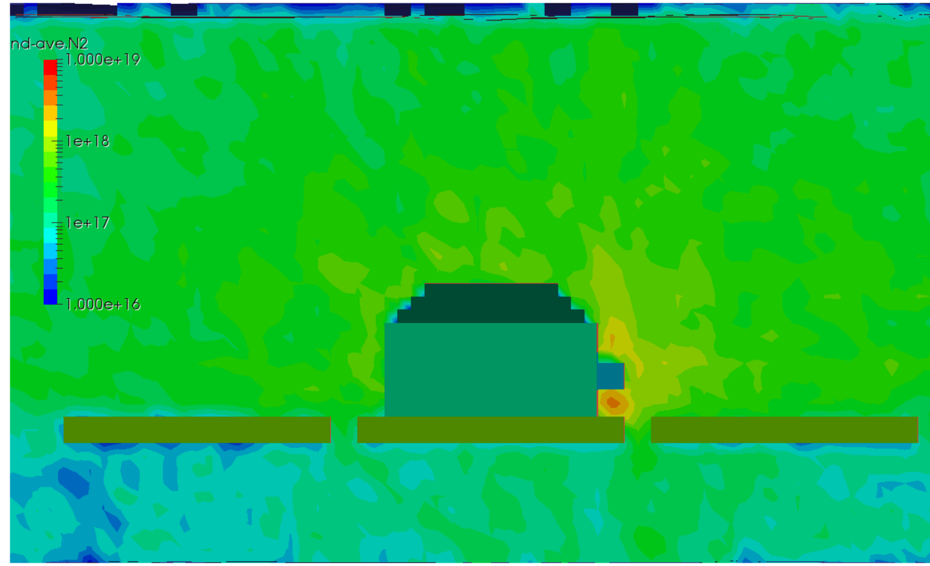


Species Partial Pressures

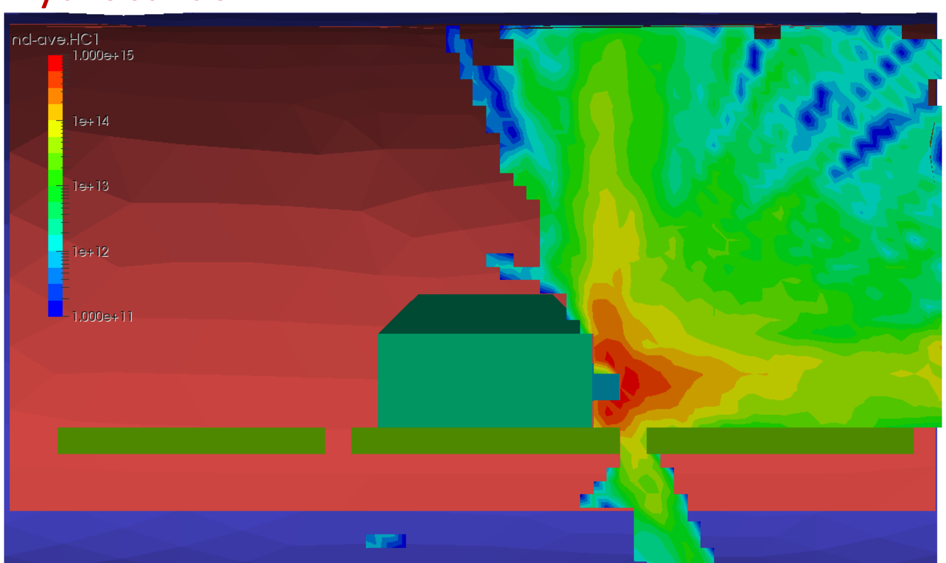
water



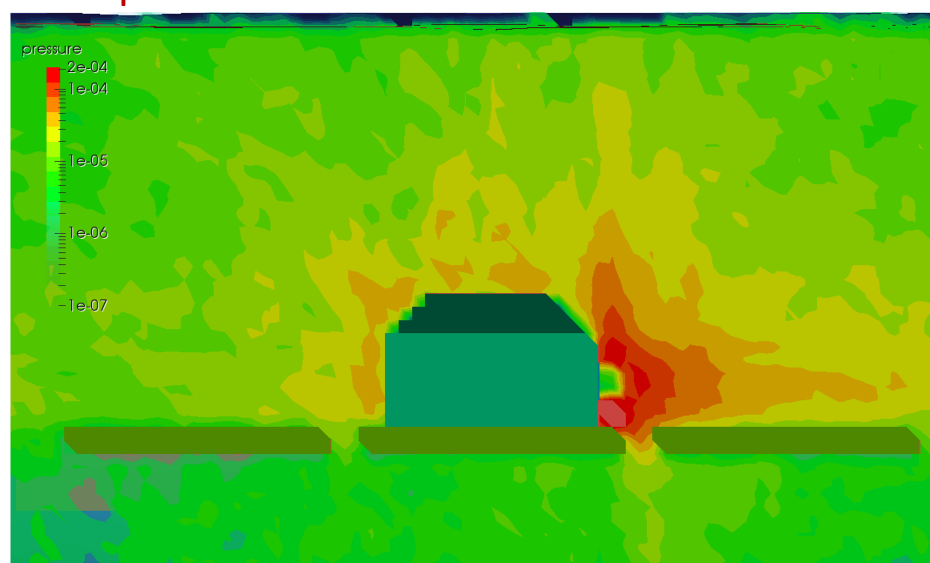
nitrogen



hydrocarbon

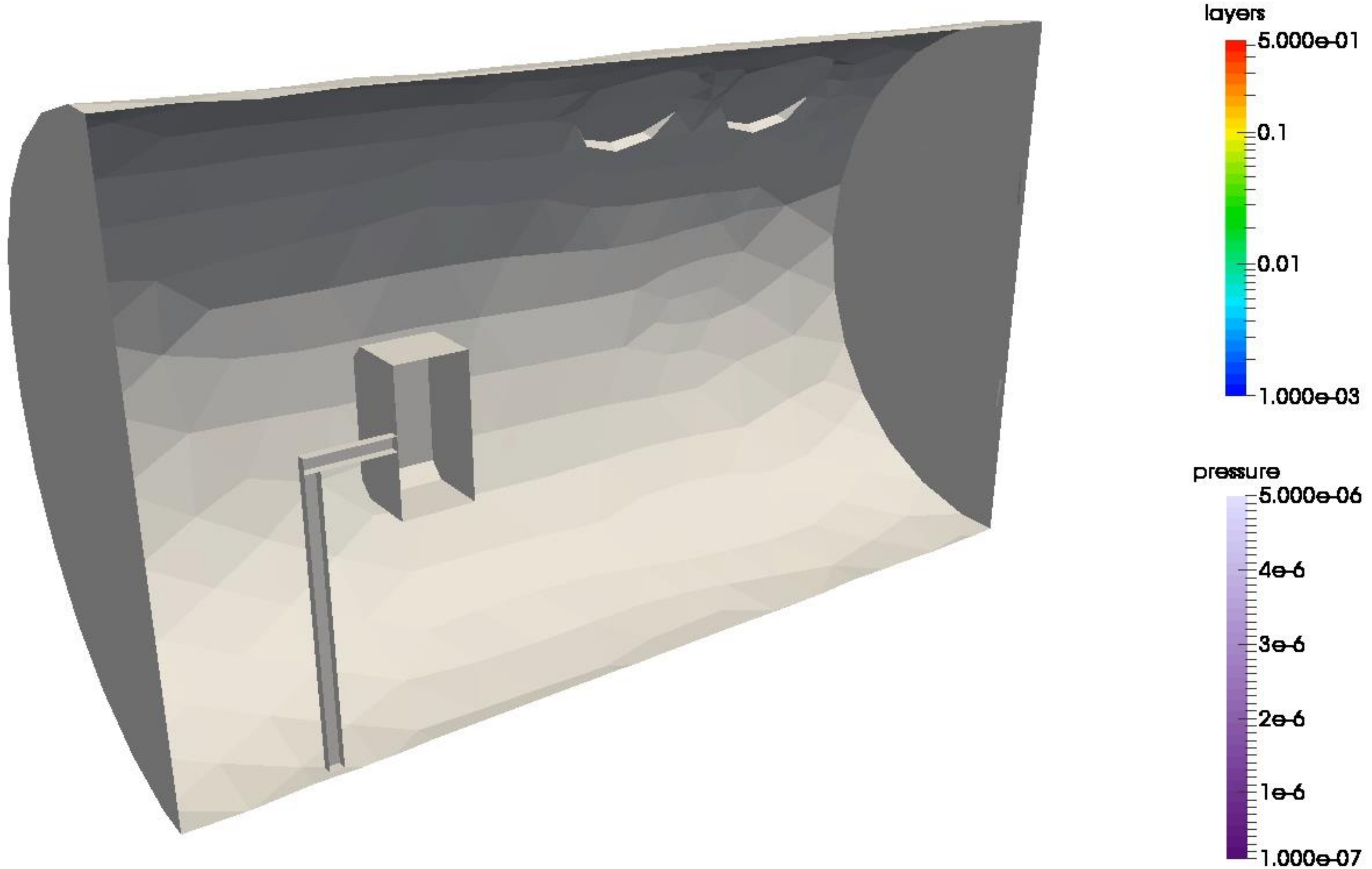


total pressure



Electric Propulsion Study

Plasma thruster firing at a beam dump initially cold enough to condense the propellant. Later, gas injected through the port for facility effects study. Next, beam dump is warmed up, resulting in flash off of the collected material.



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Summary

- Three new contamination analysis tools were presented:
  1. **QCM Analyzer:** HTML/Javascript in-browser program that simplifies post-processing of QCM log files. Automatically computes delta deltas and TGA.
  2. **RGA Extractor:** Java program for loading multiple SRS RGA scan log files and exporting pressure vs. time data over all of them. Partial pressures can be computed over a range of values.
  3. **Contamination Transport Simulation Program:** C++ code for modeling transport of dust particulates and molecules. Particulates can be sampled from IEST-STD-1246 distribution and can be accelerated by aerodynamic forces. Detailed surface model supporting outgassing and desorption is used instead of sticking coefficients for free molecular flow. Allows to resolve temporal effects such as warming up of surfaces.

Questions?

Contact: lubos.brieda@particleincell.com