# Molecular Diffusion of $H_2O$ in Lunar Regolith During Lunar Resource Prospector Mission Sample Acquisition

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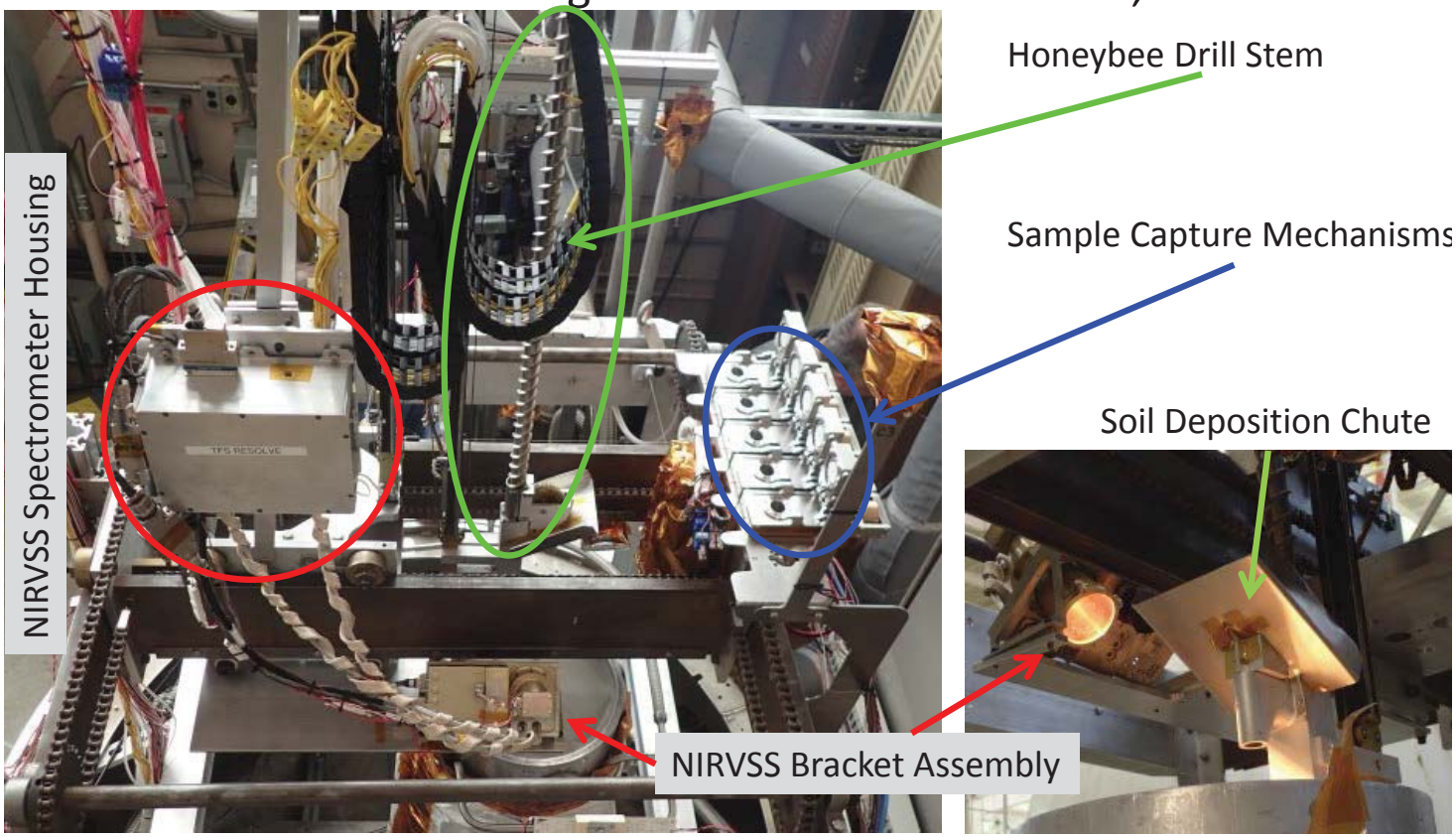
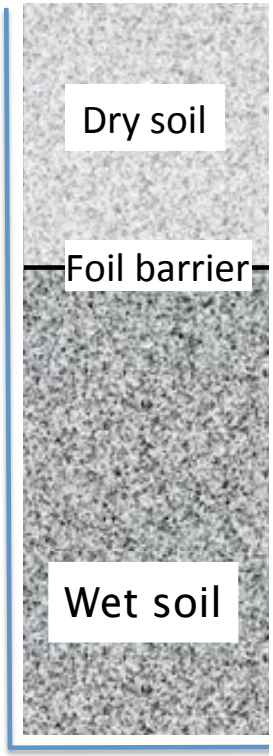
# Experimental Apparatus I

March 2015 NIRVSS + Honeybee Robotics Drill in GRC vacuum chamber to observe drilling into frozen lunar simulant, T ≈173° K




Credit: Ted Roush and Julie Kleinhenz

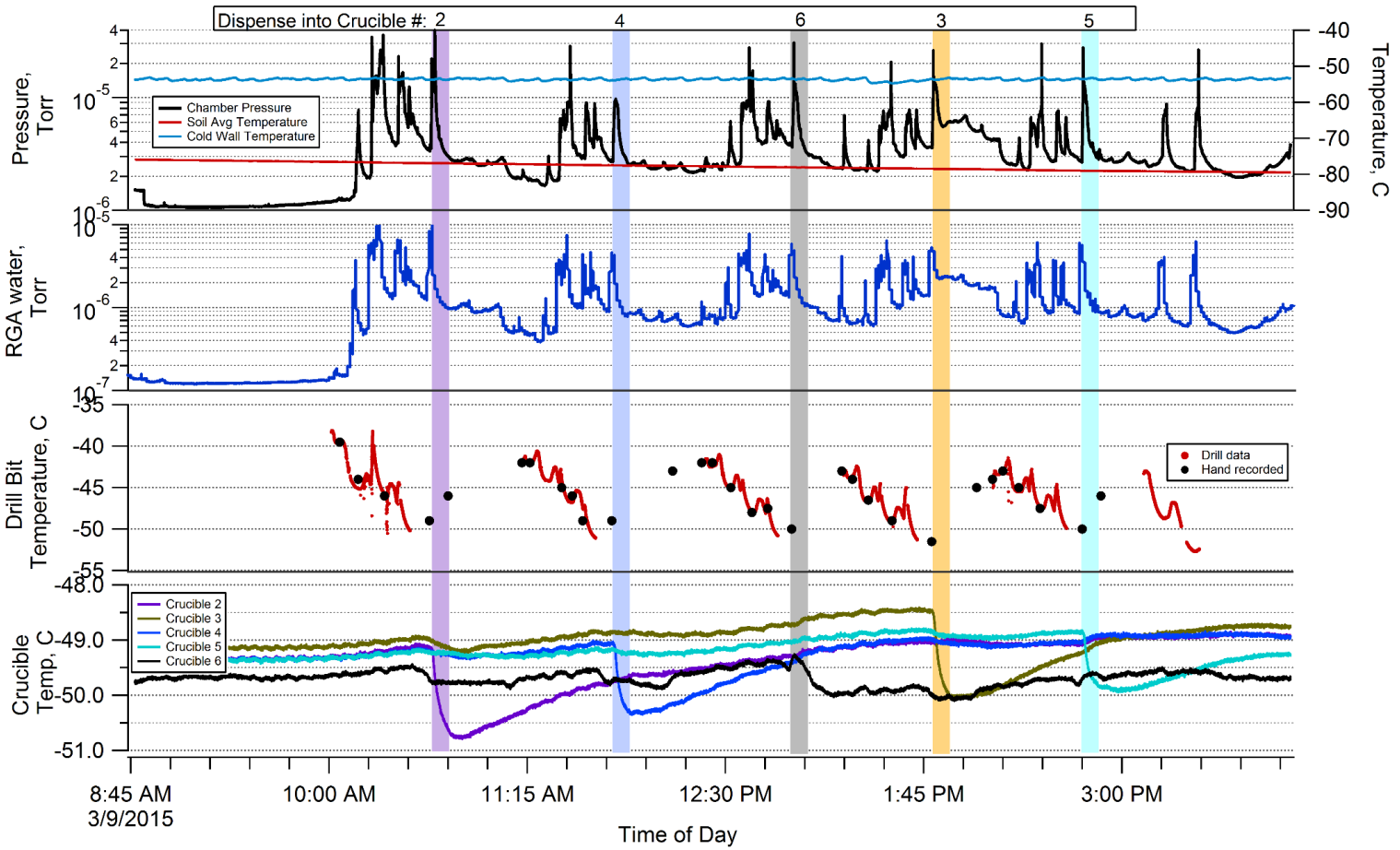
# Experimental Apparatus II



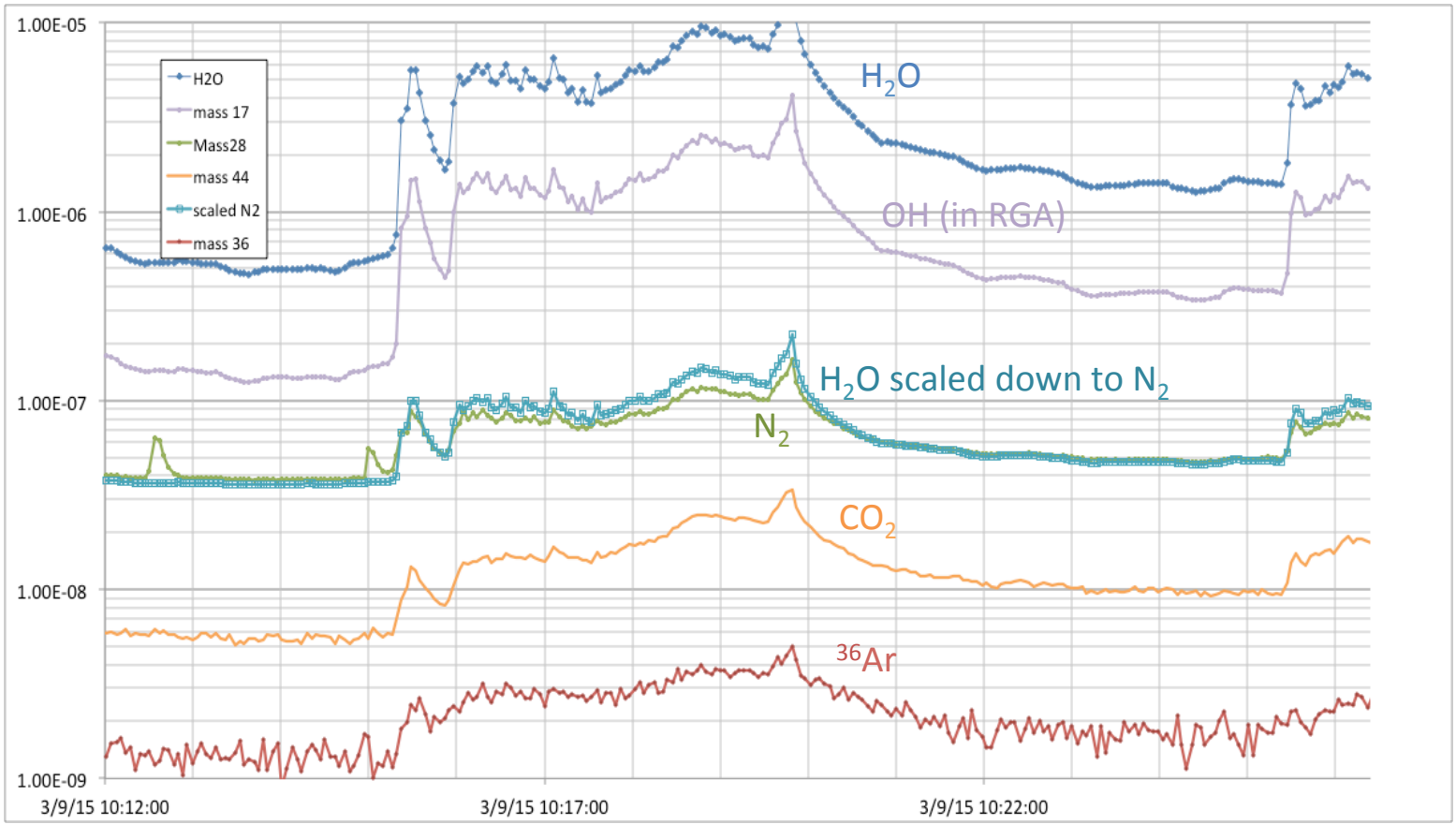



Kleinhenz, Paulsen and Zacny, 2015, AIAA SciTech, 8th Symposium on Space Resource Utilization

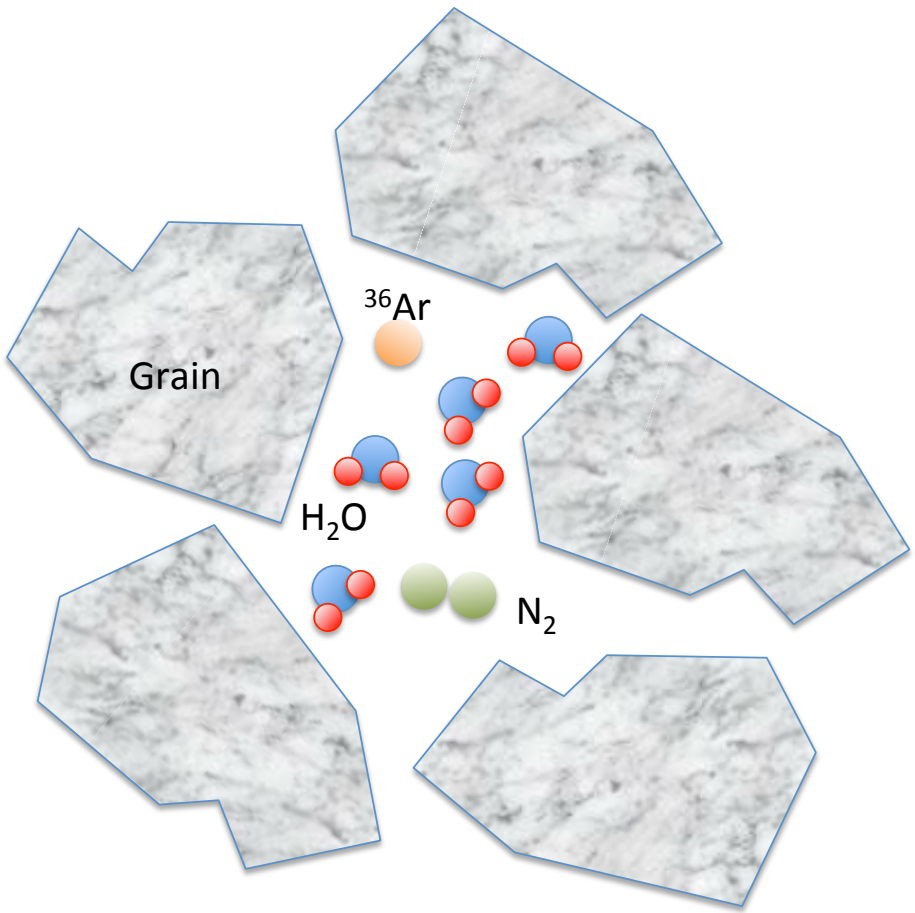
# Characterist RGA signatures during drilling/sampling; Test # 1



# Gas Release from drilling and soil deposition

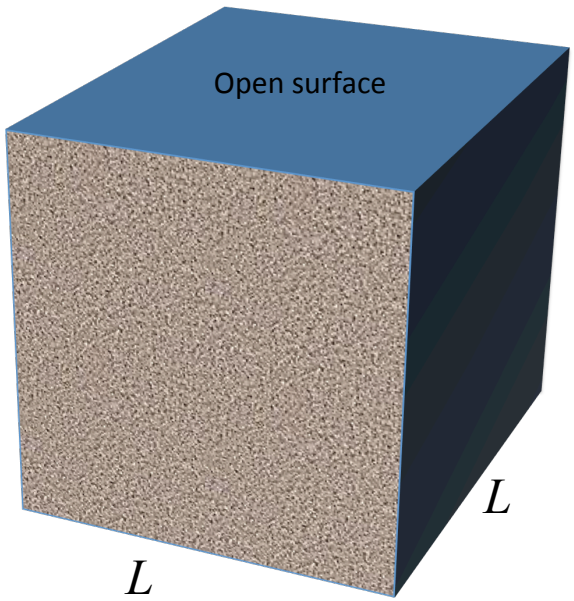


# At the grain/pore level




- Vapor is in the pore spaces between grains
- $H_2O$ assumed in quasi-equilibrium with solid ice-surfaces - at saturation vapor pressure for soil temperature
- $N_2$ and Ar are residual from atmosphere prior to pump down
- Pore and grain are similar

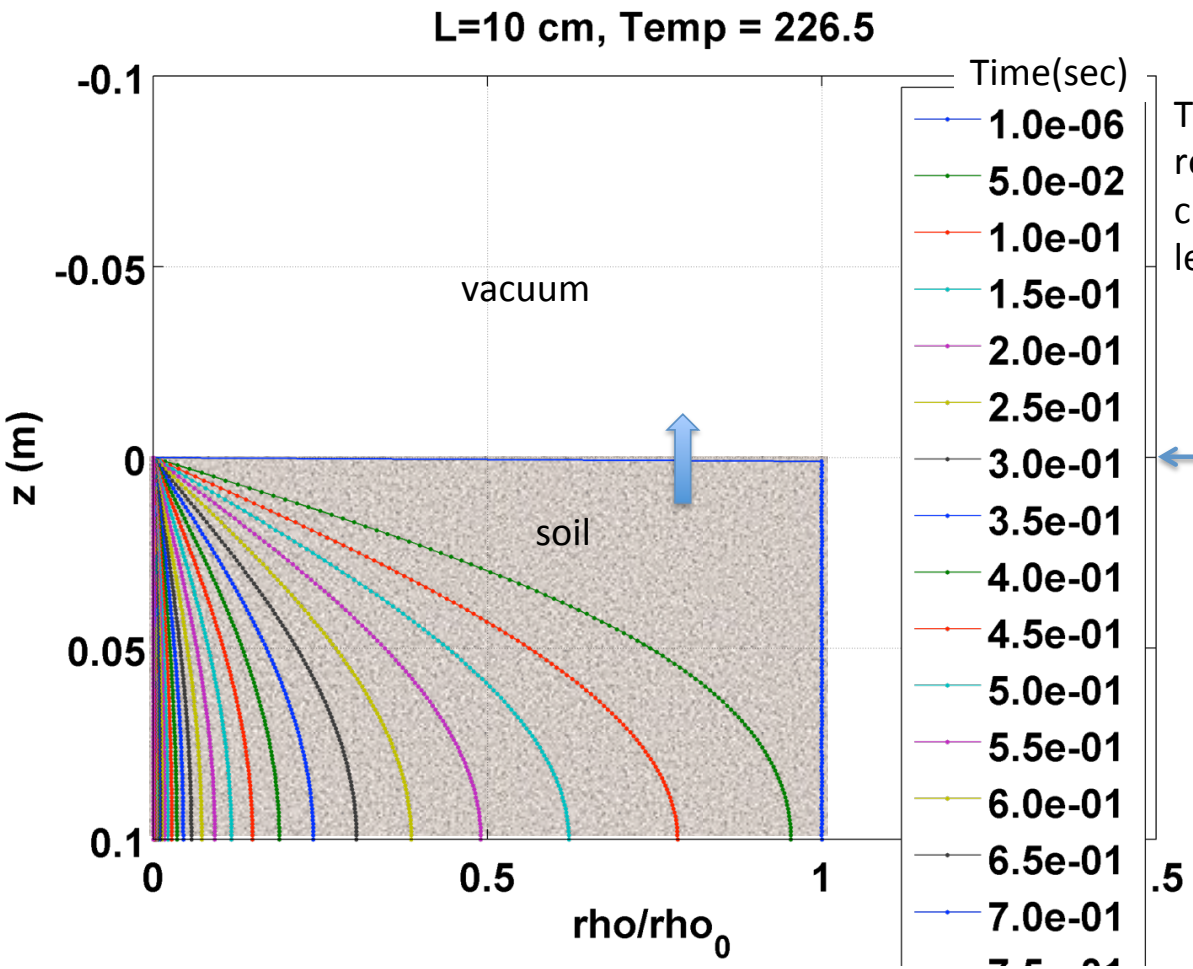
# Simple Model for Gas Loss from a Slug of Soil




- Assume a cube, with only the top open to vacuum
- Porosity is such that pore size and grain size equal - assume 75 $\mu$m pores
- We model the gas diffusion out of this volume
- Assume each side of cube is 10 cm in length

$$\rho(t,z) = \frac{2^2\rho_0}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\exp\left[-Dt\left(n+\frac{1}{2}\right)^2\frac{\pi^2}{L^2}\right]\sin\left[\left(n+\frac{1}{2}\right)\frac{\pi z}{L}\right]$$

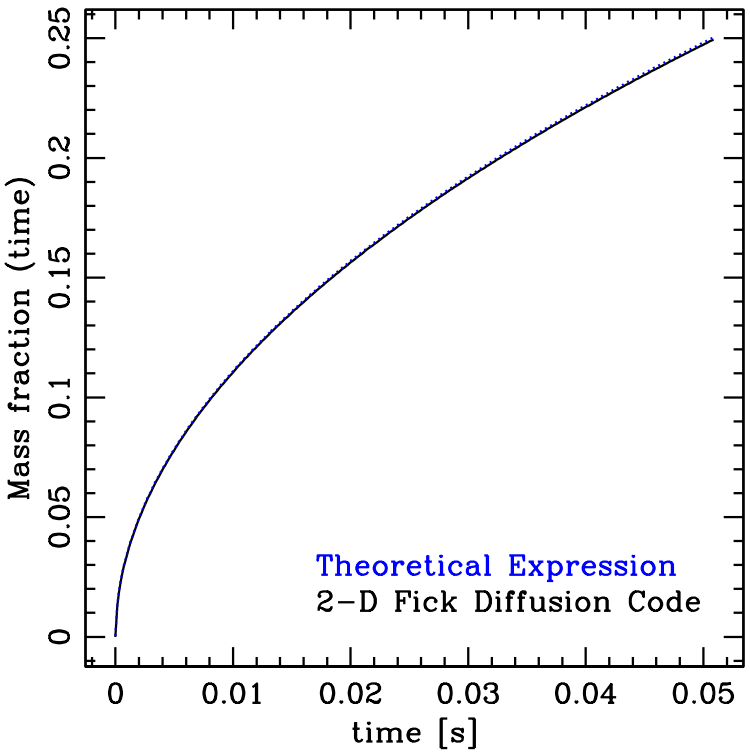
# Density profile of Vapor Density vs Depth and Time




The time scale for release of gas to the chamber is seconds, or less.

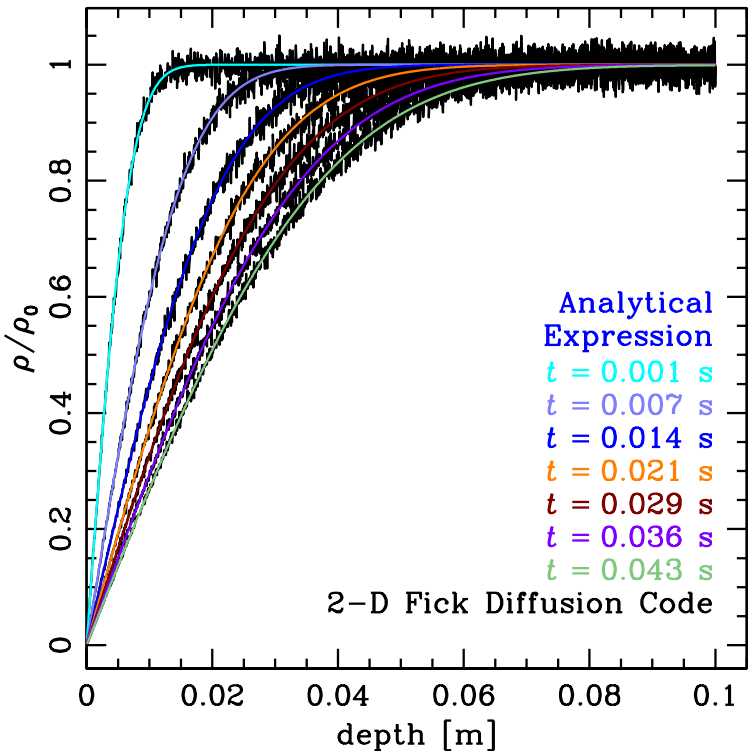
Soil surface at z=0

# 2-D particle simulation of degassing: Mass fraction lost



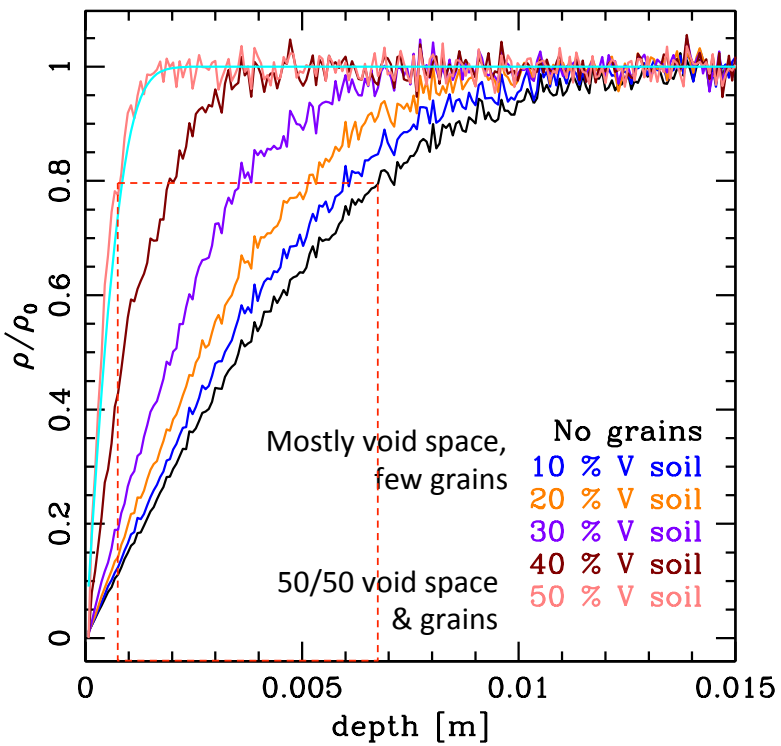

- We have developed 2-D and 3-D (parallel, f95+mpi) gas diffusion codes
- Used here with same temperature, pore size, etc. as analytic solution
- **Numerical and analytical solutions agree well**
- Therefore these codes can be used for more realistic shapes, configurations, etc.

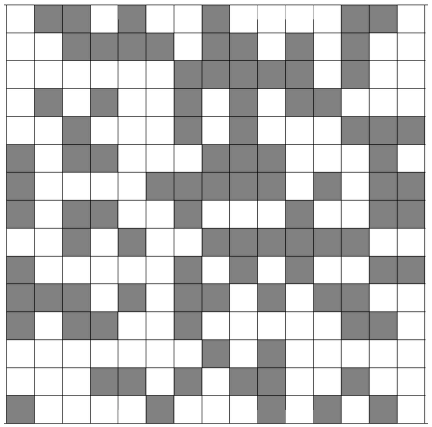
# 2-D Molecular Simulation of Vapor Profiles in Soils




- This simulation contains 5000 molecular per pore space to start with
- As time goes by, molecules diffuse stochastically out of the soil volume
- The simulation zooms in on evolution over the first 0.04 sec, and 10 cm of soil
- Solid lines denote the analytical solution for this isothermal problem

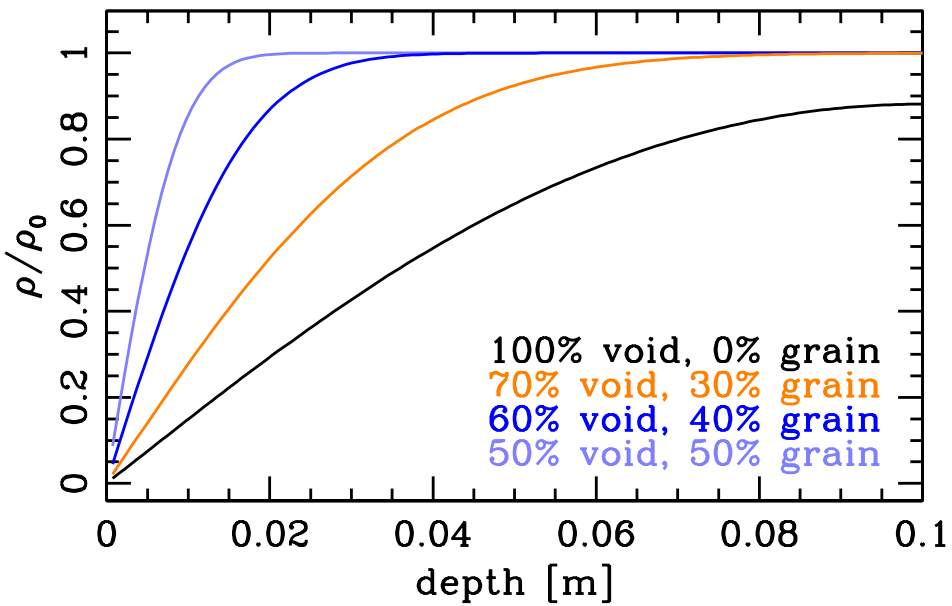
# A More Realistic simulation should include regolith grain "occlusions"



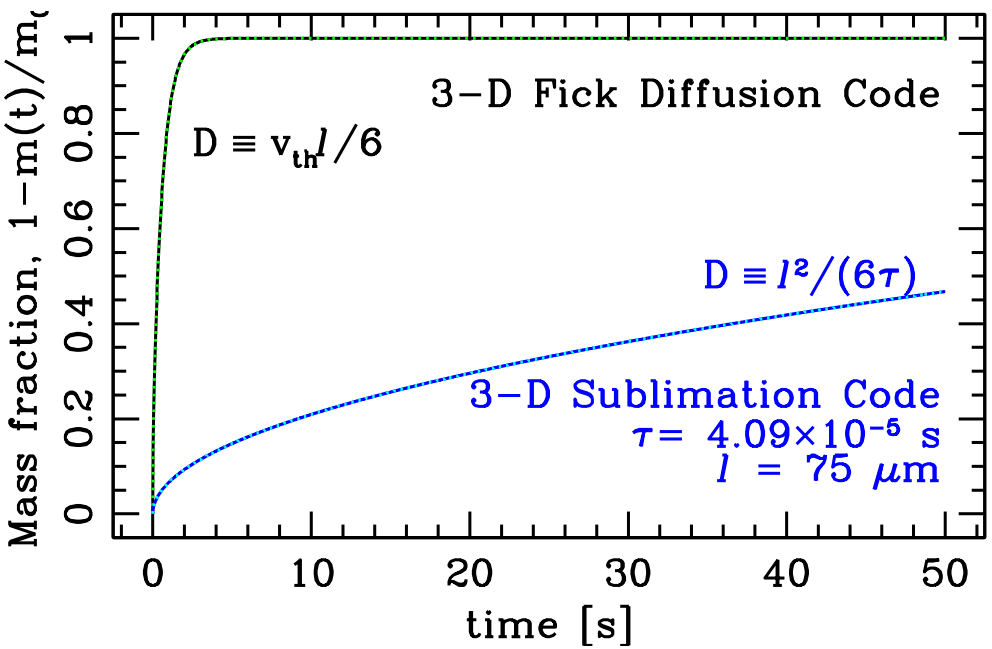
- Soil profiles at same time step
- Different amounts of soil gran volume - 50% is realistic
- **De-gassing is much slower in this more realistic case**

# 3-D Modelling



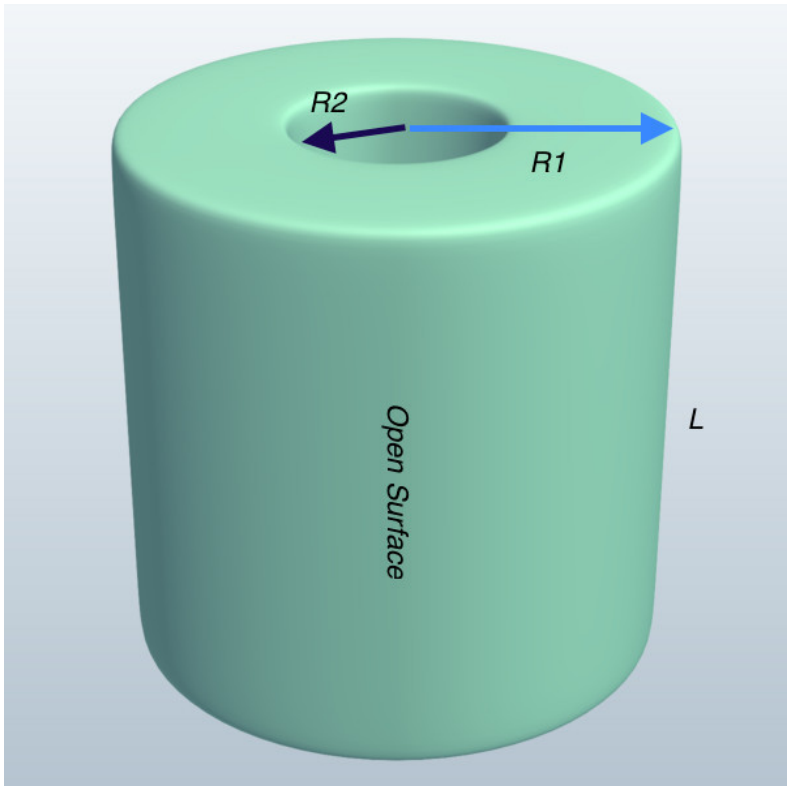

- $1336^3$ cubical mesh
- Four weeks per simulation on 200 processors
- Grain "occlusions" are generated randomly and fixed throughout the simulation

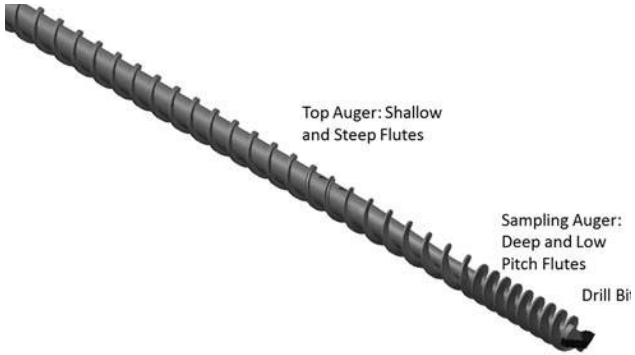
# Sublimation/Diffusion




- This is like the "no obstacles" gas calculation, but controlled by residence time of water molecular on grain surfaces
- Two residence times: more than 10 monolayers given by ice-ice (Schoerghofer & Taylor 2007), otherwise 10 times larger
- De-gassing is much faster than the $H_2O$ sublimation/diffusion process
- Only the top monolayer is available at each time step
- $1336^3$ cubical mesh, on 200 processors has taken $\sim$ five weeks

# Simple Model for Gas Loss from a Slug of Soil in the drill



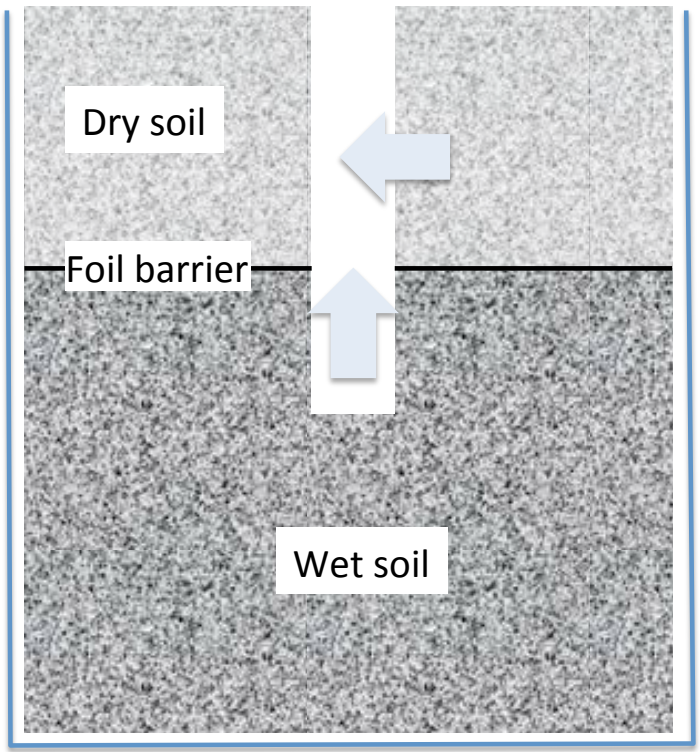




- cubical 3-D mesh, $300^2 \times 1300$
- Outer surface is free, no flux in the Inner surface, upper and lower surfaces are periodical
- There is an analytical model

## Future work

- **Realistic distribution of regolith sizes** currently we are assuming 75$\mu$m [Fick and Sublimation]
- **More Realistic distribution of velocities** So far we are only considering one single speed: $v_{thermal}$ [Fick]
- **More realistic geometries** [Fick and Sublimation]
- **No homogenous temperature field** [Fick and Sublimation]

# Even more realistic cases: Drill hole process




- More complex geometries can be simulated
- Gas diffusion following foil breach
- Ongoing sublimation out of wet soil
- Predict $H_2$ loss and compare with Glenn's repost $H_2O$ distributions.

# Conclusions

- We have implemented parallel (f95+mpi) 3-D Fick's Diffusion and Sublimation codes
- We are currently increasing the geometrical complexity of the modeling
- At the temperature considered (T= 226.45 K) **the Fick's flow is much faster than the Sublimation/diffusion**
- **Tortuosity** slows the flow considerably
- This research has considerable implications in the understanding of volatile's transport in the lunar subsurface.

# Acknowledgements

## Thank You!

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