MODELING OF VOLATILES LOSS DURING LUNAR RESOURCE PROSPECTOR MISSION SAMPLE ACQUISITION Luís F. A. Teodoro[1], R. C. Elphic[2], A. Colaprete[2], T. Roush[2], J. E. Kleinhenz[3], J. Smith[4], A. Cook[5], C. Zacny,[6] [1]BAER Inst., NASA Ames Research Center, Moffett Field, CA 94035-1000, USA; luis.f.teodoro@nasa.gov; [2]NASA Ames Research Center, Moffett Field, CA 94035-1000, USA; [3]NASA Glenn Research Center, Cleveland, OH 44135, USA; [4] NASA Kennedy Space Center, Titusville, FL 32899, USA; [5] Millenium Eng., NASA Ames Research Center, Moffett Field, CA 94035-1000, USA; [6]Honeybee Robotics Pasadena, Pasadena, CA 91103

Introduction: Here we report on our current effort to model the volatiles transport in lunar regolith. This research has been carried out in the context of the NASA's Resource Prospector (RP) [1]. The main objective of this NASA mission to the high latitudes and permanently shadowed regions of the Moon is the identification and extraction of volatile species in the top meter of the lunar regolith layer. Briefly, RP consists of five elements [1]:

a) The Neutron Spectrometer System (NSS) will search for high hydrogen concentrations and in turn select optimum drilling locations;
b) The Near Infrared Volatile Spectrometer System (NIRVSS) will characterize the nature of the surficial water ice;
c) The Drill sub-system will extract samples from the top meter of the lunar surface and deliver them to the Oxygen and Volatile Extraction Node (OVEN);
d) The OVEN will heat up the sample and extract the volatiles therein, that will be
f) transferred to the Lunar Advanced Volatiles Analysis (LAVA) instrument.

Over the last few years a series of vacuum experiments have been taking place at NASA's Glenn Research Center with the aim of quantifying volatile loss during the RP drilling/sample acquisition phase and sample delivery to the crucibles steps. Outputs of these experiments include:

i) Pressure measurements of several chemical species (e.g. H_2O, OH, CO_2, N_2, Ar);
ii) Temperature measurements within and on the surface of the lunar simulant using thermocouples;
iii) Surficial temperature NIRVSS measurements;
iv) Temperature measurements at the tip of the drill;
v) "Post test" water distribution within the lunar simulant.

In May 2016, two different aluminum tubes (ST1 and ST2) were prepared with lunar highlands simulant (NU-LHT-3M) containing ∼5 wt.% water. The two STs were placed in the Glenn vacuum chamber on different dates, ST1 was deployed on 17 May 2016 and ST2 on the 26th of the same month. Once each tube was placed in the vacuum chamber, a thermal shroud was used to surround all components, the chamber was sealed and evacuated for ∼48 hours. During evacuation liquid nitrogen flowed through coils wrapping the STs with the aim of cooling the soils. The thermal shroud was maintained at 223 K and 93 K for ST1 and ST2, respectively. Once all the operations ended, the vacuum chamber was open and measurements of the water distribution within each ST were taken.

We report on the numerical modeling we have been carrying out to understand the physics underpinning these experiments. Given the measured temperature field and the low volatile density our modeling employs the Knudsen's (sublimation of volatile molecules at the grain surface) law [2]. Furthermore, we also mimic the soil porosity in randomly allocating 75 micron particles. To model the molecular diffusion of volatiles we have implemented a 3-D numerical code that tracks one 1 billion macro-particles (each macro-particle represents a large number of water molecules) within the computational volume. At each instant, we compute a time-step that takes into account the relevant local time scale. The Knudsen's law has the following time scale which depends strongly on temperature: Knudsen's law residence time [3]:

$$\tau_K \sim \exp\left[-\frac{Q}{K_B T}\right] \times \sqrt{T}, \qquad (1)$$

where K_B and Q are the Boltzmann's constant and sublimation enthalpy, respectively. As the temperature field is not uniform throughout the simulation volume and changes during the duration of the experiment, one chooses the time-step, δt, at a given instant in time, t, as the largest of the $\tau_K(r,t)$ within the simulation volume, where r and t denote position and time, respectively. The initial conditions of each numerical model is a constant 5 wt% water ice concentration throughout the simulation domain. This corresponds to ∼3000 water ice monolayers are on the surface of each grain. At each time step, the number of particles leaving is proportional to the number of particles present at the grain surface with a "half-time" given by the local residence time. The fraction of molecules going in one given direction is drawn using a Monte Carlo procedure in assuming an exponential distribution with a given mean value λ. A grain that has less than fifty monolayers on its surface is considered dry and molecules are not allow to leave.

Here we report on our space parameter search to study ST2. This parameter space is spanned by the following parameters:

1. Fraction of monolayers on the grain surface that leave at each time step, this is parametrized via λ (the mean number of monolayers leaving);
2. The mean density of water molecules (ρ_0) at the free surface of the ST.

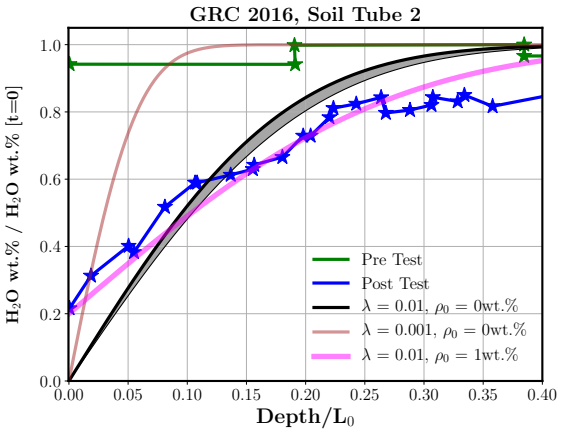

Figure 1: Final water distribution profile. Dark blue and green lines denote the "Post Test" and "Pre Test" experimental measurements, respectively. The grey region and magenta lines represent the model with parameters ($\lambda = 0.01$, $\rho_0 = 0$ wt.%) and ($\lambda = 0.01$, $\rho_0 = 1.00$ wt.%), respectively. The brown line shows the model presented at LEAG 2016, its parameters are ($\lambda = 0.001$, $\rho_0 = 0$ wt.%).

Conclusions: We present the numerical results of large scale molecular simulations of water molecules during Resource Prospector sample acquisition. The current model (grey and magenta lines) when compared to the "Post Test" results show a better agreement than previous models. Figure 1 presents the final water distribution profile: *i)* dark blue denotes the experimental points, *ii)* grey region represents the numerical models in which λ =0.01 and $\rho_0 = 0$ wt.%, while *iii)* brown line denotes the old model in which only a few monolayers were allow to leave the surface and *iv)* magenta line represents a model with a fixed mean water density of 1wt.% and λ =0.001.

References: [1] D. R. Andrews, et al. (2014) *Introducing the Resource Prospector (RP) Mission* American Institute of Aeronautics and Astronautics doi. [2] F. Reif (1965) *Fundamentals of Statistical and Thermal Physics* Waveland Press. [3] N. Schörghofer, et al. (2007) *Journal of Geophysical Research (Planets)* 112(E11):2010 doi.