

Numerical models of volatiles loss during Lunar Resource Prospector Mission

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Introduction: Here we report on our latest effort to model the volatiles transport in lunar regolith. This research has been performed in the context of the NASA's Resource Prospector (RP). The main aim 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: *i*) The Neutron Spectrometer System (NSS) will search for high hydrogen concentrations and in turn select optimum drilling locations; *ii*) The Near Infrared Volatile Spectrometer System (NIRVSS) will characterize the nature of the surficial and subsurface water ice; *iii*) The Drill Subsystem will extract samples from the top meter of the lunar surface for examination by NIRVSS and deliver them to the Oxygen and Volatile Extraction Node (OVEN); *iv*) The OVEN will heat up the sample and extract the volatiles therein, that will be *v*) 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. H₂O, OH, CO₂, N₂, 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, and a *v*) post-test water distribution within the lunar simulant.

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. 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 track 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*: $\tau_K \propto \exp[-Q/(KT)] * T^{1/2}$, where K and Q are the Boltzmann's constant and sublimation enthalpy. 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 $\tau_K(\mathbf{r}, t)$ within the simulation volume, where \mathbf{r} and t denote position and t , 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 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. A grain that presents less than fifty monolayers on its surface is considered dry and molecules are not allowed to leave.

Conclusions: We present the numerical results of large scale molecular simulations of water molecules during Resource Prospector sample acquisition. The current model 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 denote the experimental points, *ii*) grey region represents the numerical models in which a fraction of 0.01 departed from the surface in average, while *iii*) cyan line denotes the old model in which only a few monolayers were allowed to leave the surface.

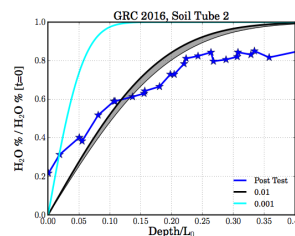


Figure 1. Final water distribution profile. Dark blue denotes the experimental measurement, the grey regions represent the latest model, and the cyan line shows the model presented at LEAG 2016.