MOLECULAR DIFFUSION OF H$_2$O IN LUNAR REGOLITH DURING LUNAR RESOURCE PROSPEC-TOR MISSION SAMPLE ACQUISITION. Luís F. A. Teodoro[1], R. C. Elphic[2], A. Colaprete[2], T. Roush[2], J. E. Kleinhenz[3] [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; NASA Glenn Research Center, Cleveland, OH 44135, USA.

Introduction In the context of NASA's Resource Prospector (RP) mission to the lunar poles, we study 3-D models of volatile transport in lunar regolith. This transport is studied in terms of: *i)* Fick's law [1], and *ii)* Knudsen's flux [2]. The former is relevant to the behavior of any residual gaseous species trapped in the regolith, while the latter is central to the sublimation loss of exposed ice monolayers on the regolith grain surfaces.

The goal of the RP mission is to extract and identify volatile species in the top meter of the lunar regolith layer [3]. The RP payload 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 hydrocarbons, mineralogical context for the site, and the nature of the water ice; *iii)* The Drill Sub-system will extract samples from the top meter of the lunar sub-surface and deliver them to Oxygen and Volatile Extraction Node (OVEN); *iv)* The OVEN will heat up the sample and extract the volatiles therein, and, eventually, *v)* these will be transferred to the Lunar Advanced Volatiles Analysis (LAVA) subsystem.

Julie E. Kleinhenz and co-workers have been performing a series of experiments with the aim of quantifying the volatile losses during the drilling phase [4]. In Figure 1 we present the partial pressure measurements of five gas species over 14 min centered around 03/09/15 10:19:00 am from one such experiment. The species were measured by a residual gas analyzer (RGA), and are H$_2$O (blue), OH (violet, created from H$_2$O in the RGA), N$_2$ (light green), CO$_2$ (orange) and Ar (red). We also show a scaled version of the water curve (green); with this procedure we try to visualize any potential differences in the temporal behavior of the two species. Although different species have different measured partial pressures, all present a very similar overall temporal variation. At the temperatures used in the experiment, nitrogen and argon neither condense nor freeze on the surface of the regolith grain. Hence, the analogous temporal behavior indicates the same type of transport for all species and in particular does not reflect the sublimation of volatiles in the soil but rather the evacuation of gases trapped in the interstices of the porous regolith during the preparation of the experiment. (To prevent desiccation of a water-ice-bearing lower layer, an alu-
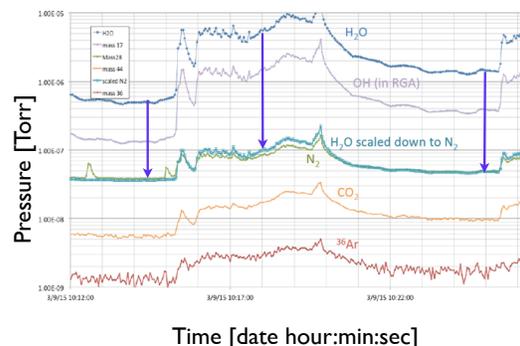

Figure 1: Temporal variations of five gaseous species partial pressures in the camera: H$_2$O (blue), OH (violet), N$_2$ (light green), CO$_2$ (orange) and Ar (red). In green we also present a scaled version of the water curve trying to match it with the nitrogen counterpart.

minum foil barrier was placed between the upper dry layer and the lower layer).

Fick's and Knudsen's transport in the lunar regolith
Knudsen's transport: Schörghofer and Taylor 2007 [2] investigated the migration of H$_2$O molecules in the lunar regolith by random hops within the pores. Central to their work are three main assumptions: *i)* water molecules migrate through interstices in a porous regolith and they do not interact with one another, moving in straight trajectories between points on the surface of grains; *ii)* molecules stay at the surface of such grains for a residence time which corresponds to the local saturation vapor pressure for ice at that temperature; and *iii)* when leaving the grain surface, molecules can move in any direction with a hop size given by the average grain size, ~75 μm [5]. In their work the modeling was one dimensional and there also was the implicit assumption that when a water molecule stays at the surface the only relevant vibration is the water ice. However, if a silicate grain is coated by a small number of water ice monolayers the vibration modes between water molecules and their silicate counterparts also come into play. This can change the residence time by orders of magnitude [6].

In our numerical implementation of the Knudsen's transport we use a 3-dimensional mesh: $1334^2 \times 133$ grid in which each mesh has a $(75\mu m)^3$ volume. All the boundaries are impermeable except for one of the 1334×133 sides where the molecules are allow to leave the volume. In all the simulations reported here we are using the same temperature throughout the entire volume: 226.45 K (-46.7° C). In each time step, only the

molecules comprising the top water ice monolayer at each location are allowed to move into the neighboring mesh volumes which share surfaces with the initial mesh. The remaining molecules, which occupy the remaining monolayers at the surface of a grain, do not move. The direction of motion for the liberated molecules is chosen using a Monte Carlo approach. The duration of each time step is set equal to the residence time. To take into account the aforementioned change in residence time due to the proximity of the silicate substrate we assume that once the number of monolayers is less than ten, sublimation does not take place. Finally, molecules that reach the impermeable surfaces are bounced back into the mesh volume where they were in the previous timestep. In Figure 2 we present the mass fraction lost ($\equiv$ 1-mass remaining within the volume after time t /initial mass) after 1,333,000 time steps, or 50 sec (blue). We also show the analytical solution for the diffusion equation (dotted cyan).
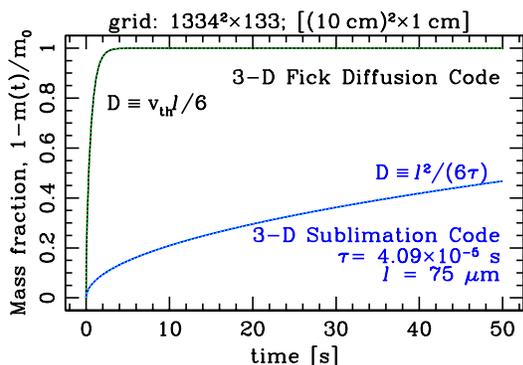

Figure 2: Comparison between change in time of the mass fraction for Knudsen's (blue) and Fick's (black) transport in lunar regolith with a typical grain size of 75 μm and an underlying temperature of 226.45 K (-46.7° C). m(t) and m_0 denote total mass at time t and t = 0, respectively. The number of time steps for the Knudsens and Ficks simulations are 1,333,000 and 9,045,000, respectively. The dotted -cyan and -green denote the analytical expressions for the Knudsen's and Fick's transport problems, respectively.

Fick's transport: Molecules also have a thermal ($\equiv$ random) motion in the interstices of the porous regolith. This is known as Fick's transport. To model it we will use the same grid and all molecules within the computational domain will move at each time. As in the previous case, at a location molecules only can access adjacent mesh cell volumes. The time step is given by the ratio between the mesh size l (=75 μm) and the thermal velocity v_{th} (= 516 m/s, at T = 226.45 K). In Figure 2, we present Ficks mass fraction over the first 9,045,000 time steps (black) as well as the analytical expression for the same problem (dotted-green). In this calculation, nearly half the initial water ice mass has been lost by 50 sec.
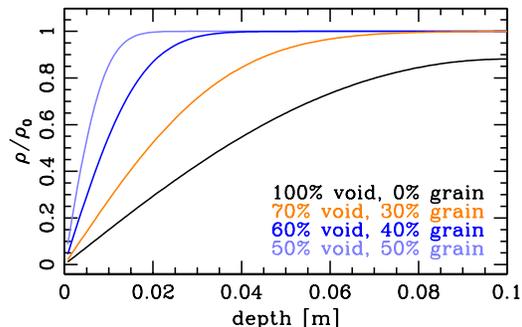

Figure 3: Density versus depth in the Fick's transport context after 1,000,000 time steps (=0.14 s) for simulations with 0%, 30%, 40% and 50% of the volume occupied by grains.

Tortuosity: Thus far, all space within the simulation domain can be accessed by the water molecules. In the lunar regolith, however, this is not case, as the volume occupied by the soil grain is off limits for molecule hopping. In order to mimic this we forbade the water molecules to access some locations chosen randomly at the beginning of the simulations. In Figure 3, the increase in tortuosity ($\equiv$ fraction of the volume in silicate grains) leads to a considerable slowing down of the diffusive process: the density profile without any forbidden regions (black) is roughly 80% of its initial value at a depth of 6.5 cm after 0.14 seconds while more realistic model of the lunar regolith with 50% of the simulation domain forbidden to the molecules (powder blue) shows the same fraction of the initial density at depth of 1cm at the same instant.

Conclusions We present the numerical results of five large scale molecular diffusion simulations of H_2O during lunar Resource Prospector sample acquisition. Although the geometry of our numerical experiment is not the most realistic, it allows us to demonstrate that the regolith tortuosity will play a major role in understanding the losses during sample acquisition.

References: [1] F. Reif (1965) *Fundamentals of Statistical and Thermal Physics* Waveland Press. [2] N. Schörghofer, et al. (2007) *Journal of Geophysical Research (Planets)* 112(E11):2010 `doi`. [3] D. R. Andrews, et al. (2014) *Introducing the Resource Prospector (RP) Mission* American Institute of Aeronautics and Astronautics `doi`. [4] J. E. Kleinhenz, et al. (2015) *Impact of Drilling Operations on Lunar Volatiles Capture: Thermal Vacuum Tests* American Institute of Aeronautics and Astronautics `doi`. [5] G. H. Heiken, et al. (1991) *Lunar sourcebook - A user's guide to the moon.* [6] A. W. Adamson *Physical Chemistry of Surfaces* Wiley-Interscience ISBN 13:9780471078777.