

NUMERICAL MODELLING OF SUBLIMATION LOSSES DURING SAMPLE HANDLING WITHIN THE LIGHT WAVE LUNAR WATER PROSPECTING INSTRUMENT. J. R. Michel¹

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Introduction: NASA's focus of exploring the Moon's south pole under the Artemis program has placed new emphasis on characterizing the quantity and distribution of water ice and other volatiles present within the Moon's permanently shadowed regions (PSRs), first measured during the 2009 LCROSS mission. NASA's VIPER rover is the first of a series of prospecting missions to characterize this water ice resource. NASA's Johnson Space Center (JSC) has developed the Light Water Analysis and Volatiles Extraction (Light WAVE) instrument shown in Figure 1 for a follow-on prospecting mission, designed to be a rover payload for water ice prospecting at various depths and locations within PSRs.

A key source of error for lunar water prospecting instruments, including Light WAVE, is the loss of water in an icy regolith sample to the lunar vacuum via sublimation due to heating above its ice-stable temperature. This abstract and conference presentation discuss a sublimation model for Light WAVE's sample crucible using COMSOL Multiphysics to assess the sublimation losses that would occur between sample collection from an external drill and sealing the sample within Light WAVE's boiler.

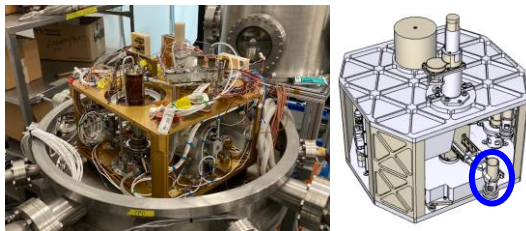


Figure 1. Light WAVE Instrument Engineering Test Unit (ETU) and Sample Crucible (Circled)

Model Detail: The results of this model have two primary uses: 1) assessing the need of an active crucible chilling system to keep sublimation losses below the instrument's measurement accuracy requirement, and 2) using flight data during the instrument's lunar surface operation to estimate sublimation losses and thereby refine water content measurements during the prospecting mission.

Geometry and Mesh. The Light WAVE sample container holds approximately 12 cm³ of icy regolith taken from an external drill. The sample geometry is cylindrical with a 0.889 cm radius and 4.8 cm depth. The sample was modelled asymmetrically in COMSOL and meshed with refinement at the top, bottom, and side surfaces to capture small length scale increased heating and sublimation rate in these regions. The meshed geometry is shown in Figure 2 below.

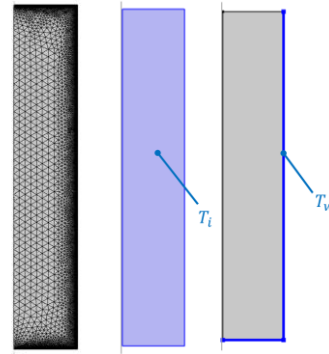


Figure 2. Meshed Axisymmetric COMSOL Geometry of Light WAVE Regolith Sample with Initial and Boundary Conditions

Heat Transfer. Heat transfer through the icy regolith sample is governed using the transient conduction heat equation implemented in COMSOL's Heat Transfer in Solids module. The equation is modified with a heat sink term that accounts for the latent heat of water ice sublimation, following the approach used by Formisano et al. for sublimation modelling of icy regolith.¹ The heat sink term differs from the Formisano et al. implementation by removing the diffusion flux term, which is instead accounted for in the Darcy's Law implementation discussed in the *Mass Transfer* section.

The regolith sample initial temperature T_i is assumed uniform throughout the domain, and fixed-temperature boundary conditions T_w are applied to the side and bottom surfaces of the sample, simulating a sample transferred into a crucible that is relatively warm. The crucible wall temperature is conservatively assumed fixed over time. The crucible walls being cooled by the sample and re-heated by ambient radiation from inside the rover are considered secondary effects and not included in the model.

The icy regolith sample's bulk thermal conductivity, specific heat capacity, and density were computed external to the COMSOL model in a set of MATLAB scripts created by Lisa Erickson at JSC for icy regolith thermal analysis.^{2,3,4} The resulting temperature-dependent bulk thermal conductivity, specific heat capacity, and density were imported into COMSOL's materials library for the environmental conditions and water ice content scenarios modelled.

Mass Transfer. Mass transfer of water vapor through the regolith sample is modelled using the one-dimension integrated form of Darcy's Law to account for the regolith's resistance to water vapor flow. The pressure at each node is calculated assuming the sample is at saturation conditions for the local

temperature, allowing computation of the nodal pressure from nodal temperature along water ice's sublimation curve, again following the approach used by Formisano et al.¹ The node's depth within the sample and the ambient vacuum pressure are then used to compute the one-dimensional pressure gradient driving water vapor out of the sample at the node

The effect of regolith head pressure on sublimation rate was also included in the model. For each time step at each node, the nodal pressure was computed by adding the ambient vacuum pressure to the static head pressure acting on the node at its depth within the sample. If this total pressure exceeded the sublimation pressure of the node at its current temperature during the given time step, the node's sublimation rate was set to zero. The nodal Darcy's Law sublimation rate calculation including the head pressure logic is shown in Figure 3 below:

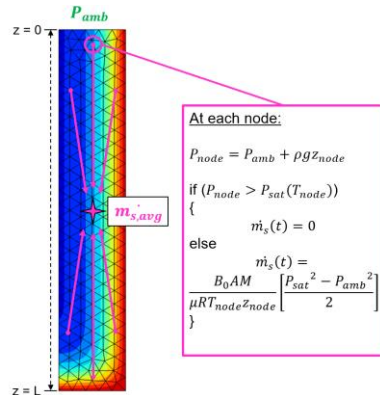


Figure 3: Nodal Darcy's Law Sublimation Rate Calculation Implementation

Literature review found no experimental values for Darcy's permeability constant of lunar regolith or lunar regolith simulants at medium- and high-vacuum pressures, so the Darcy's permeability constant was instead used as a tuning parameter to match the model's total sublimated water mass with the results from JSC's three Light WAVE sample crucibles sublimation tests in 2017, shown in Table 1.

Table 1: JSC Light WAVE Sublimation Test Conditions and Tuned Darcy's Constants from Model

Test Number	T_w [K]	T_i [K]	P_{amb} [Pa]	Tuned B_0 [log cm ²]
7.1.1	295.3	244.6	133.3	-8.03
7.1.3	290.8	207.3	173.3	-7.89
7.1.5	287.5	206.7	105.3	-7.34

Model Validation: The only experimental dataset found during literature review to validate the tuned Darcy's constants from the three JSC sublimation tests was from Toutanji et al.⁵ The published Darcy's constant values were for mean pressures between 10,000 and 50,000 Pa, significantly above the ~100 Pa pressures measured during JSC's Light WAVE sample sublimation testing, and using different lunar regolith

simulants and gas species. Nonetheless, this dataset provides an initial basis of comparison for the model. The tuned Darcy's constants followed the exponential pressure-dependent trend from the Toutanji et al. dataset, shown in Figure 4. Future model validation work will include additional Light WAVE sample sublimation testing and dedicated Darcy's permeability constant testing at these lower pressures with water vapor for direct comparison with this model.

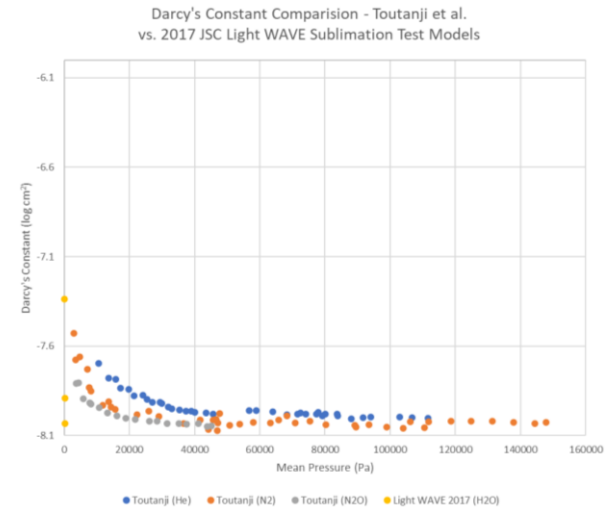


Figure 4. Tuned Darcy's Permeability Constants from Light WAVE Sublimation Tests vs. Toutanji et al. Dataset

Conclusion: The tuned model was applied to lunar PSR temperature, pressure, and gravity conditions and showed a crucible chiller is unnecessary to keep sublimation losses during sample handling within the instrument's accuracy requirement. The physics-based framework of the model can also be applied to more complex geometries for other in-situ resource utilization water processing equipment, such as modelling sublimation from icy regolith feedstock hoppers for Moon or Mars water processing plants.

Acknowledgments: This modelling effort would not have been possible without the support of the JSC Light WAVE engineering team, especially the project's manager Aaron Paz. The work of Lisa Erickson consolidating icy regolith thermal property models into MATLAB scripts was also key to this model's development.

References: [1] Formisano, M. et al. (2019) *Planetary and Space Science* 169, 8–14. [2] R. Robinson, M. A. Siegler, and D. A. Paige (2019), *Journal of Geophysical Research: Planets*, vol. 124, no. 7, pp. 1989–2011. [3] The International Association for the Properties of Water and Steam (2009), *IAPWS R10-06*. [4] Reiss (2018). *Technical University of Munich*. [5] Toutanji, H. et al., 2012. *Advances in Space Research* 49, 1271–1276.