

THE EFFECT OF ISOTOPIC COMPOSITION AND SURFACE RESIDENCE TIMES ON LUNAR VOLATILE TRANSPORT. C. Alfaro^{1,3}, A. Tran^{2,3}, K. A. Carr^{1,3}, O. Azubuiké^{1,3}, C. Carreira^{2,3}, P. Prem³, G. Dominguez⁴, B. T. Greenhagen³, D. M. Hurley³, A. M. Stickle³, G. W. Patterson³, J. T. S. Cahill³, ¹University of Maryland, Baltimore County, Baltimore, MD (c204@umbc.edu). ²Johns Hopkins University, Baltimore, MD. ³Johns Hopkins University Applied Physics Laboratory, Laurel, MD (parvathy.prem@jhuapl.edu). ⁴California State University, San Marcos, San Marcos, CA.

Introduction: Permanently shadowed regions near the lunar poles may act as cold-traps for volatiles, including water ice, over geological timescales [1], preserving a unique record of the delivery of water to the inner solar system. In the quest to better understand the origins of polar volatiles on the Moon, it is important to have a thorough understanding of if and how the isotopic composition of these volatiles may change from the time of delivery to the time of cold-trapping. Isotopic composition reflects the history and origins of volatiles, and can affect factors such as the length and duration of ballistic hops through the exosphere [2], the rate of thermal escape, and interactions with the lunar surface. We aim to understand, through numerical modeling, the influence of isotopic composition and variable surface residence times in the transport, loss and deposition of lunar volatiles, particularly water and eventually carbon dioxide. This abstract focuses on H₂O and HDO.

Currently, there are a variety of theories about the origins of water on the lunar surface, including deposition by asteroid or comet impacts, outgassing from the lunar interior, or formation as the result of solar wind interacting with the lunar surface [3]. The D/H ratio of water can yield important information about its origins [4]. Thus far, it is unclear if transport processes yield an enrichment [2] or depletion [5] in the D/H ratio

of cold-trapped species. Other topics that have not been studied in detail are the influence of different isotopologue surface residence times on isotopic fractionation, and the fractionation of other potential lunar volatiles, such as carbon dioxide [6].

Method: We model volatile transport using a Direct Simulation Monte Carlo (DSMC) code called PLANET. PLANET simulates gas behavior by modeling the motion of a large number of representative molecules and the exchange of energy between molecules during collisions. In the simulations presented here, exospheric density is sufficiently low that PLANET behaves as a collisionless Monte Carlo code. We run the same simulation with adjustments to the code for each volatile of interest and compare differences in behavior. We plan to incorporate LRO/Diviner bolometric temperature maps to accurately model lunar surface temperature, but currently estimate the surface temperature in PLANET using an analytical expression derived from observational data [7]. When the simulation begins, PLANET initializes 1×10^7 simulated molecules, uniformly distributed across the lunar surface. The molecules then ballistically travel across the surface; as they move, they are subject to various environmental effects, such as photodestruction when exposed to sunlight, capture by cold-traps in the polar regions, or escape from the gravitational domain of the

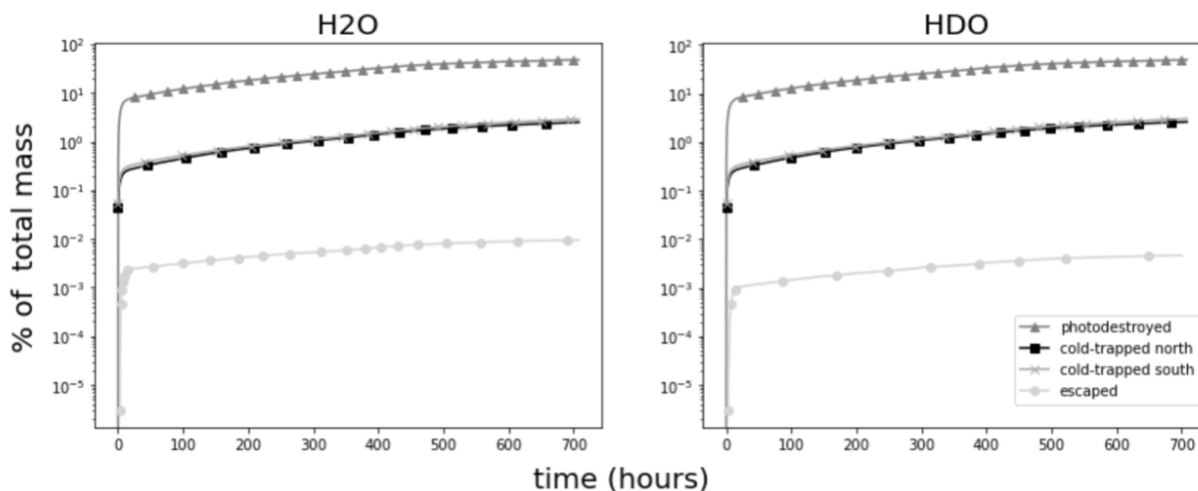


Figure 1: The fraction of H₂O (left) and HDO (right) molecules that are cold-trapped near the north and south poles, photodestroyed, and that thermally escape over the course of one lunar day.

Moon. The model also assumes a specific value for surface residence time, which affects the time between ballistic hops. The mean surface residence time is calculated as $t_{res} = (1/\nu)\exp(-E_a/k_B T)$, where ν is a characteristic frequency of 10^{13} s^{-1} , E_a is desorption activation energy, k_B is the Boltzmann constant, and T is local surface temperature. The baseline results presented here use a value of $E_a = 0.7 \text{ eV}$ [8,9] for both H₂O and HDO, but subsequent simulations will account for instantaneous, mass-dependent fractionation during desorption.

Results and Discussion: The results shown in Figure 1 highlight differences in the transport of H₂O and HDO over the course of one lunar day (~709 hours). The only difference between how these two cases are simulated is molecular mass ($29.9 \times 10^{-24} \text{ g}$ for H₂O vs. $31.6 \times 10^{-24} \text{ g}$ for HDO).

Although the behavior of H₂O and HDO is broadly similar, there are some noticeable differences between the two isotopologues. Figure 1 shows $9.5 \times 10^{-3} \%$ of the mass escapes for H₂O, compared to $4.7 \times 10^{-3} \%$ for HDO. This is attributable to the lower thermal velocity of heavier molecules, and is consistent with previous work [2]. However, 47.7% of the initial H₂O released is photodestroyed, compared to 49.3% for HDO. We attribute this to the fact that heavier molecules are likely to require more time to traverse the same distance, and thus spend more time in sunlight during migration to polar cold-traps. Finally, 0.13% (averaged between the north and south polar regions) more of the initial mass of HDO is cold-trapped in comparison to H₂O.

Conclusions and Future Work: The results discussed above show that HDO's heavier molecular mass contributes to less thermal escape, but more cold-trapping and photodestruction during the simulation. These results would therefore predict an enrichment in the D/H ratio of cold-trapped water. The baseline simulations described above will be run for a period of three lunar days, in order to more clearly identify how molecular mass affects volatile transport and loss rates. We will then account for differences in the activation energies required for desorption of the two isotopologues, which we anticipate will slow the transport of HDO, and potentially affect exospheric structure [11]. We also plan to build on previous investigations [12] by modeling the exospheric transport and fractionation of carbon dioxide, which is more volatile and less readily photodestroyed than water [13,14].

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