**MULTI-ELEMENT LUNAR EXOSPHERE SIMULATION TO IMPROVE THE PREDICTION OF BAL-LISTIC MIGRATION OF WATER.**

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Introduction: While many resources are required to sustain a human-based exploration campaign, water is one of the most important elements. It has been established that water accumulates inside permanently shadowed regions at the poles. With three main sources of lunar hydrogen, namely the solar wind, interior outgassing, and impactor contributions, the question remains of how the molecules are transported to the poles [1]. One mechanism is the ballistic travel of individual particles. Several models of this already exist, though almost all simulate only a single species of the lunar exosphere at a time, thus, lacking the capability to include multi-element effects.

Numerical Model: This new pseudo-2D stationary lunar exosphere model [2] utilizes the Monte-Carlo method [3] to simulate individual particles, which are assumed to be in thermal equilibrium with the surface of the Moon and exhibit a Maxwell-Boltzmann flux distribution of energies and velocities [1,4,5], based on surface temperatures derived from Diviner measurements [6]. It simulates photo-reactions, ion recycling, surface interactions including geochemical reactions, and cold-trapping. Figure 1 presents a schematic overview of the multi-element conversion sub-model, based on geochemical reactions [7] inside the lunar regolith and photo-dissociation in the exosphere [8].

Results & Discussion: To demonstrate the impact of geochemical and photo-dissociation based conversions, Figure 2 shows a direct comparison of the surface number densities of exospheric atomic hydrogen predicted by the multi-element model (top) and a reference single-element model (bottom), relative to a uniform solar wind influx of H^+ (typically in the order of $2\text{-}3\times10^8$ cm^{-2} s^{-1}). The main difference is the sharp peak at the morning-terminator region (6h, local time), which only the multi-element model can predict.

Such behavior follows the sudden release of surface-bonded particles after extensive night-time adsorption, though H does not adsorb into the regolith, even at the lowest lunar temperatures. The change in
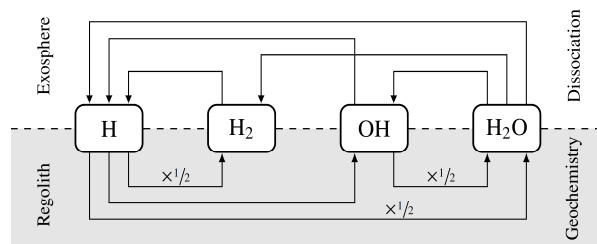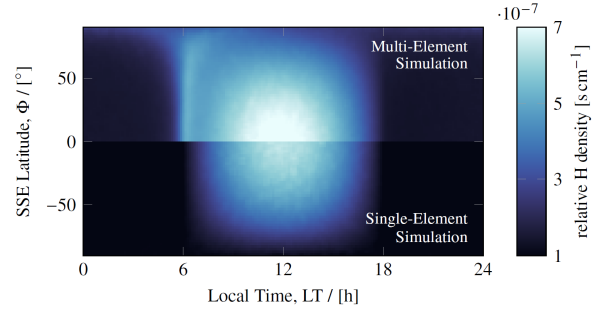
Figure 2: Comparison of atomic hydrogen relative exospheric surface number density.

the dynamics can only be explained through the connection to condensable species like OH and H_2O. It shows that single-element simulations are incapable of predicting relevant features of the lunar water cycle.

Conclusion: Understanding the lunar water cycle is key to identifying ice accumulations and informing future utilization of such resources in terms of their distribution and accessibility. Exospheric transport of water, as well as its constituents, is a crucial element in this cycle and enhanced numerical models will be able to help to improve our understanding of this.

The current model can be further improved in many ways (i.e., extension to three dimensions, adding transient simulations, lunar topography, and electromagnetic forces). However, the conversion mechanisms in the lunar regolith as well as in the exosphere are most important, as they are critical for a physically accurate description of the particle behavior. The currently used simplistic geochemical model assumes static conversion probabilities [7], regardless of the temperature and the composition of the local lunar surface material. Models that use Gaussian distributions for implantation depths and activation energies [9], as well as models that feature additional conversion pathways like 2nd order dissociative desorption [10], have already been published and can be taken as a reference during further development.

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Figure 1: Multi-element conversion setup.