Multi-Element Lunar Exosphere Simulation to Improve the Prediction of Ballistic Migration of Water.

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Introduction

- New **numerical model** of the lunar exosphere based on the Monte-Carlo method, simulates individual, weighted particles in thermal equilibrium with the Moon surface (Smolka, 2022; Tucker et al. 2019).
- Simultaneously simulates **H, H_2, OH, and H_2O**, connected through conversion reactions like **photo-dissociation** and **geochemical surface reactions.**

Method

- The model takes advantage of a nested-loop architecture that iteratively solves for the **surface number density** while calculating particle conversions to be applied as source rates in the following iteration.
- Assumes pseudo-stationary **surface-bounded exosphere** in thermal equilibrium with a **Maxwell-Boltzmann flux** distribution of energies and full thermal accommodation (Brinkmann, 1970; Smith et al., 1978).
- The **loss and source mechanisms** of all four species are connected through particle conversion, based on **dissociation rates** (Huebner et al., 1992) and surface **reaction probabilities** (Crider end Vondrak, 2002).
- Uncertain parameters are modelled with probability distributions (like in Tucker et al., 2018), allowing a statistical analysis of the **uncertainty propagation.**

Results

- Adsorption during the night and desorption at sunrise leads to **OH and H_2O accumulating at the morning-terminator**, exhibiting a "snowplow" effect stretching from pole to pole.
- While H does not ad- or desorb, its peak must originate from the **connection to OH and H_2O.**
- Conversions act as efficient recycling of particles, leading to **generally higher densities** compared to single-element studies.
- Confirms expected surface number densities of
  H_2: ~ 1200 ± 400 cm^{-3} (LAMP, Hurley et al., 2017)
  OH: ~ 10^4 cm^{-3} (Wang et al., 2015)
  but *cannot* reproduce expectations for
  H_2O: ~ 60cm^{-3} (Jones et al., 2018).

Hydrogen bearing species **require multi-element models** and **simultaneous simulations** to predict the ballistic transportation of water. For accurate description of OH/H_2O accumulations, a more sophisticated **geochemical lunar regolith model is needed**.

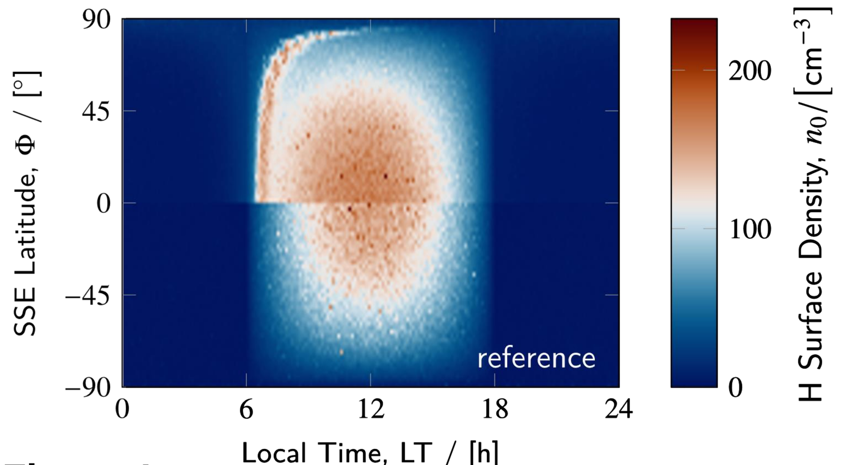

Figure 1
Comparison of exospheric atomic hydrogen predictions of the multi-element study with a reference single-element simulation.

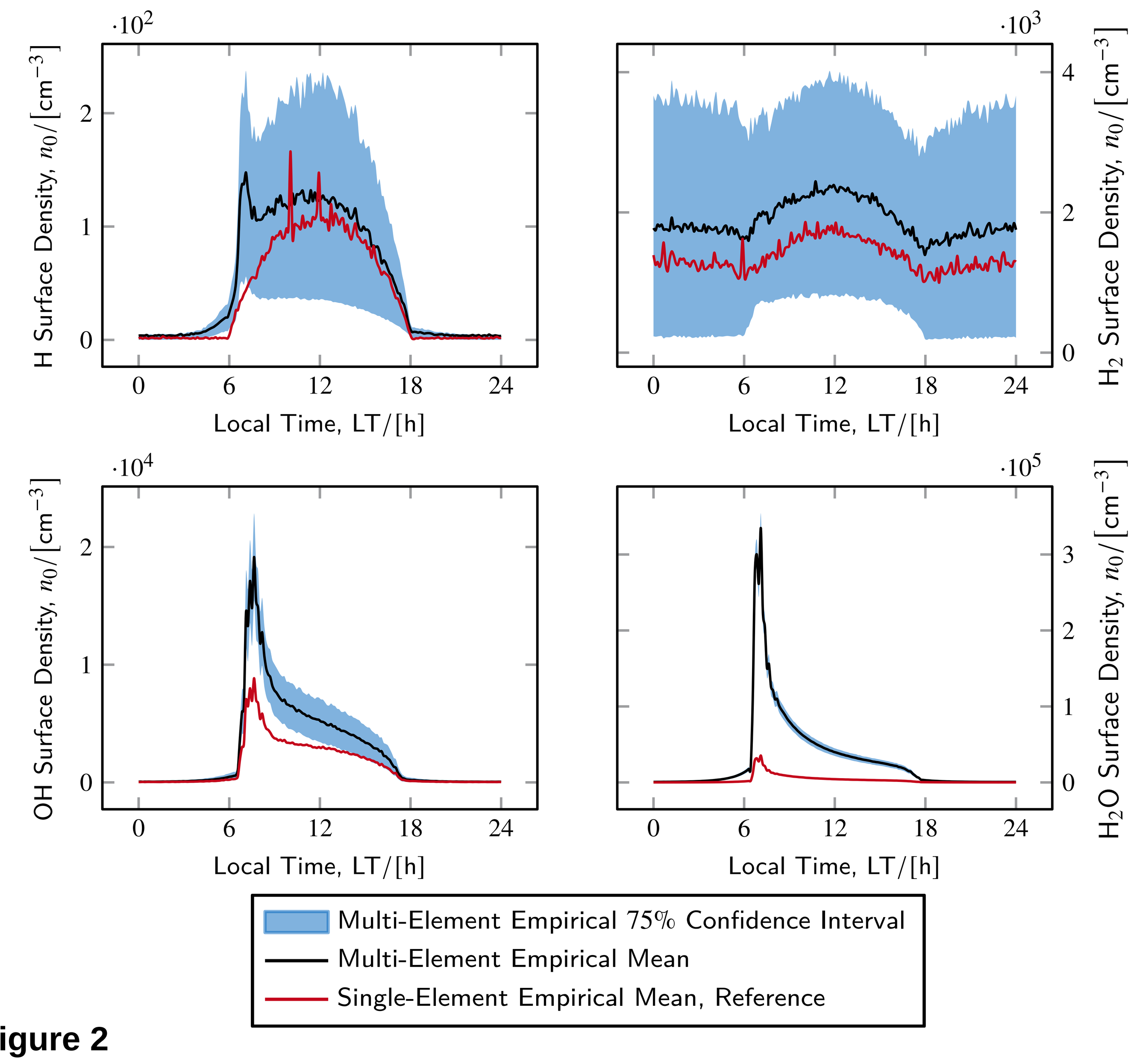

Figure 2
Surface number densities of H, H_2, OH, and H_2O of the multi-element study including its empirical 75% confidence interval, and a reference density as a result of a single-element study with the same parameter setup.

Conclusion

Clear changes in the surface number densities are visible once the species were connected in a multi-element model respecting particle conversions. Non-condensable species, like H, **develop a morning-terminator peak** due to heavy OH and H_2O desorption and dissociation. **Globally increased densities** suggest that conversion acts as a recycling mechanism.

Large uncertainty intervals and density increases strengthen the need for a **more sophisticated geochemical model** to better describe the **lunar water cycle**. Models of Jones et al. (2018), Tucker et al (2019), and Grumpe et al. (2019) will be used as guidelines in future iterations of the numerical model, especially focussing on **better descriptions of the OH/H_2O behavior.**

Supplemental Materials

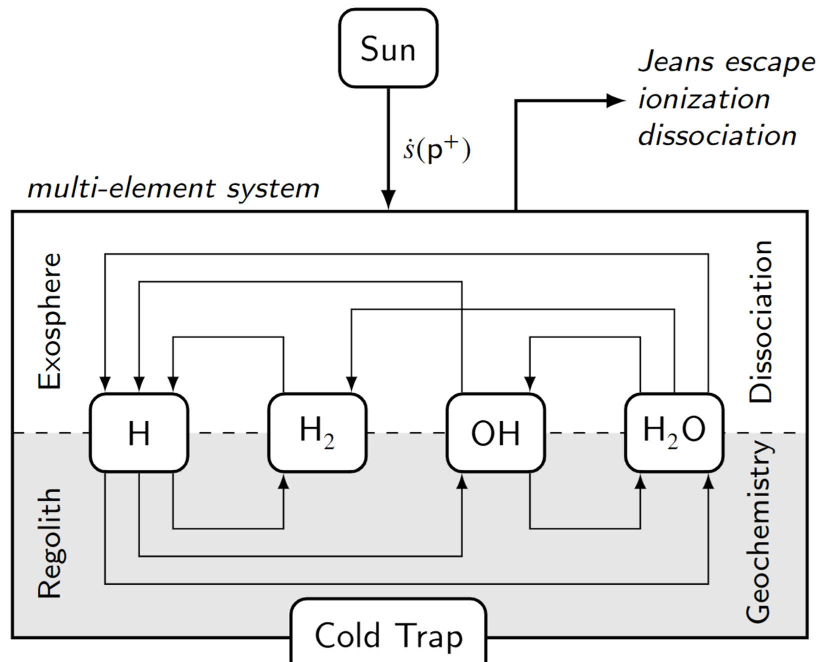

Figure 3
Schematic of the implemented conversion processes in both the exosphere and the lunar surface.

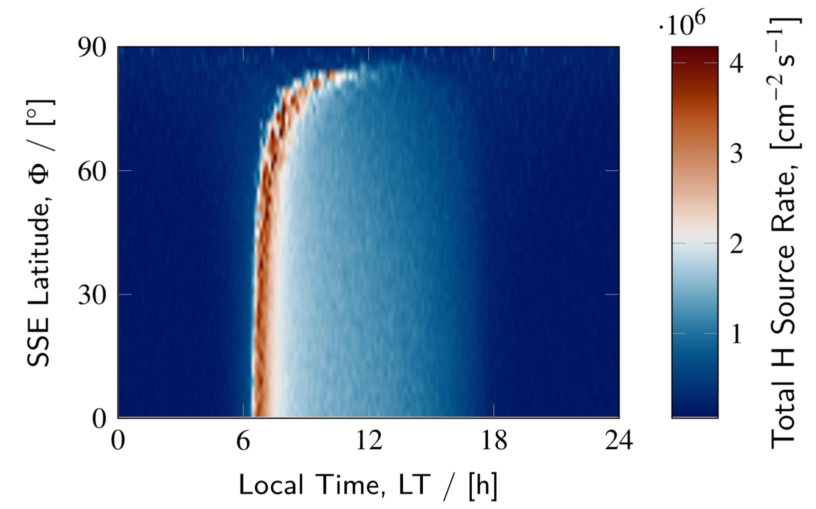

Figure 4
Total source for H particles based on conversions from H_2, OH, and H_2O through photo-dissociation.

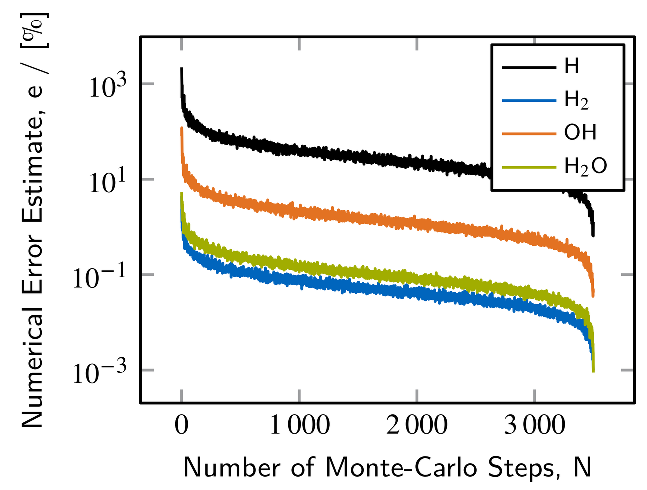

Figure 5
Numerical error estimation for all four constituents over the number of Monte-Carlo steps. Measured at a reference point on the day-side.

Brinkmann, R., 1970, Departures from jeans' escape rate for h and he in the earth's atmosphere. *Planetary and Space Science, Vol. 18.*
Crider, D., Vondrak, R., 2000, The solar wind as a possible source of lunar polar hydrogen deposits. *Journal of Geophysical Research, Vol. 105.*
Huebner, W. et al.,1992, Solar photo rates for planetary atmospheres and atmospheric pollutants. *Astrophysics and Space Science, Vol. 195.*
Hurley, D.M. et al., 2017, Contributions of solar wind and micrometeoroids to molecular hydrogen in the lunar exosphere. *Icarus, Vol. 283.*
Jones, B.M. et al. 2018, Solar wind-induced water cycle on the Moon. *Geophysical Research Letters, Vol. 45.*
Smith, G et al., 1978, Monte Carlo modeling of exospheric bodies: Mercury. *Journal of Geophysical Research, 83.*
Smolka, A., 2022, Lunar Exosphere Simulation: Modeling and Simulation of our Moon's Surface-Bounded Exosphere. *Thesis, Technical University of Munich.*
Tucker, O.J. et al., 2019, Solar wind implantation into the lunar regolith: Monte-Carlo simulations of H retention in a surface with defects and the H_2 exosphere. *Journal of Geophysical Research: Planets, Vol. 124.*
Wang, J. et al., 2015, An unprecedented constraint on water content in the sunlit lunar exosphere seen by Lunar-based Ultraviolet Telescope of Chang'e-3 mission. *Planetary and Space Science, Vol. 109-110.*

Data availability
For data and model access, please contact Alexander Smolka (alexander.smolka@tum.de).

Previous work: https://mediatum.ub.tum.de/node?id=1658109