EPSC Abstracts
Vol. 19, EPSC2026-662, 2026, updated on 15 Nov 2026
https://doi.org/10.5194/epsc2026-662
Europlanet Science Congress 2026
© Author(s) 2026. This work is distributed under
the Creative Commons Attribution 4.0 License.

Particle-Resolved Kinetic Modeling of Solar-Wind Hydrogen Release from Lunar Regolith

Alexander Peschel[1], Jurij Simčič[2], and Philipp Reiss[1]
[1]Technical University of Munich, Lunar and Planetary Exploration, TUM School of Engineering and Design, Ottobrunn, Germany (a.peschel@tum.de)
[2]Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

Solar-wind protons implanted into the upper nanometers of lunar regolith are an important source of hydrogen-bearing species on the Moon. These particles may diffuse through mineral grains, bind to oxygen sites, form OH, recombine to H_2, or contribute to H_2O production and release. Which pathway dominates depends on temperature, binding energies, surface coverage, and the availability of reactive sites (Jones et al., 2021, 2024). These microscopic processes control how much implanted hydrogen is retained in the regolith and how much is released into the surface-bounded exosphere. However, global lunar exosphere models usually cannot directly resolve this subsurface chemistry. We address this scale gap with a particle-resolved time-stepping Monte Carlo model that links solar-wind proton implantation, regolith chemistry, and volatile release.

The model tracks individual H-bearing particles diffusing in a one-dimensional depth grid representing the near-surface (400nm) region of a regolith grain (Nagai et al., 2020; Hansen et al., 2013). Solar-wind proton implantation is implemented using a SRIM/TRIM-informed Gaussian depth distribution centered at 20–25 nm (Farrell et al., 2015). Diffusion and release are controlled by temperature- and coverage-dependent activation energies. Previous versions of the activation energy model assumed infinite diffusion efficiency (Schörghofer, 2023, 2025), leading particles to always choose the deepest available binding site. We extended the model by adding a finite-diffusion efficiency term that allows implanted particles to sample binding sites across a broader local activation-energy distribution, rather than imposing a sharp transition between filled and empty sites.

Using this framework, we are performing a parameter study of the activation energies. We vary the OH binding-energy distribution, recombinative desorption barriers, the probability of H_2 formation, and additional physical parameters. Preliminary results show that the parameters of the OH energy distribution have the strongest influence on the partitioning between retained OH, released H_2, and recombined H_2O. They show distinct dayside desorption patterns controlled by the imposed diurnal temperature and solar-wind flux profiles. These results indicate that the hydrogen release ratios are sensitive to the assumed activation-energy distribution and must be constrained before they can be used as robust source terms in global exosphere simulations.

An example output of the release rates is shown in the **Figure,** displaying how much of the implanted solar wind protons (SWP) is released at each surface location over one lunation. These rates represent only outgassing from previously implanted protons; they do not include deposition or re-implantation of particles returning from the exosphere. The resulting pattern shows a strong temperature dependence in the outgassing, with enhanced release in warmer regions near the subsolar point.

To couple the micro-scale model with global-scale investigations, the H_2 release is used as a source term in a lunar exosphere simulation and tested against reported densities from LAMP and CHACE measurements (Stern et al., 2013; Cook et al., 2013; Hurley et al., 2017; Thampi et al., 2015). Preliminary comparisons indicate that 40–60% of the implanted solar-wind proton flux must be released as H_2 to reproduce the observed exospheric densities. This constraint provides an initial benchmark for the activation-energy parameter study: parameter combinations that retain too much hydrogen as OH, or release too little H_2, are unlikely to reproduce the observed lunar H_2 exosphere.

The model results will be constrained by ongoing laboratory work at the Jozef Stefan Institute (Simčič et al., 2025), where Nuclear Reaction Analysis (NRA) is used to measure implanted-particle depth profiles and retention behavior. These experiments will provide independent constraints on diffusion and desorption parameters. Together, the particle-tracking model, the H_2 exosphere comparison, and the laboratory measurements will provide a consistent framework for linking solar-wind implantation, regolith-scale physical chemistry, and volatile release from the lunar surface.

References

Cook et al. (2013), *Icarus*, *225*(1), 681–687. 10.1016/j.icarus.2013.04.010

Farrell et al. (2015), *Icarus*, *255*, 116–126. 10.1016/j.icarus.2014.09.014

Hansen and McDonald (2013), *Theory of Simple Liquids*. 10.1016/b978-0-12-387032-2.00007-6

Hurley et al. (2017), *Icarus*, *283*, 31–37. 10.1016/j.icarus.2016.04.019

Jones et al. (2021), *Earth and Planetary Science Letters*, *571*, 117107. 10.1016/j.epsl.2021.117107

Jones et al. (2024), *The Planetary Science Journal*, *5*(8), 171. 10.3847/PSJ/ad5542

Nagai et al. (2020), *Journal of Chemical Theory and Computation*, *16*(12), 7239–7254. 10.1021/acs.jctc.0c00448

Schörghofer (2023), *The Planetary Science Journal*, *4*(9), 164. 10.3847/PSJ/acf19b

Schörghofer (2025), *The Planetary Science Journal*, *6*(7), 164. 10.3847/psj/ade5b2

Simčič et al. (2025), *European Lunar Symposium*. 10.5281/ZENODO.15470820

Stern et al. (2013), *Icarus*, *226*(2), 1210–1213. 10.1016/j.icarus.2013.07.011

Thampi et al. (2015), *Planetary and Space Science*, *106*, 142–147. 10.1016/j.pss.2014.12.018