MODELLING THE LUNAR WATER CYCLE THROUGH COUPLED MONTE-CARLO SIMULATIONS OF THE MOON'S SURFACE AND EXOSPHERE. A. Smolka[1], [1]Technical University of Munich, Lise-Meitner-Str. 9, 85521 Ottobrunn, Germany, alexander.smolka@tum.de.

Introduction: Over the past decades, our understanding of water on the Moon has developed significantly. Before the Apollo mission, some theories featured a "wet" Moon, which was undermined by the lack of volatiles found in the collected samples [1]. While Urey (1958) [2] already noted that the lunar topography and low obliquity would create permanently shadowed regions (PSRs) near the poles, which would act as cold traps for any volatile species of the Moon's exosphere, it took several more years to reignite the discussion about the lunar water cycle through the discovery of hydrogen in pyroclastic glasses [3].

Previous studies by the author presented a coupled numerical model of the lunar H, H_2, OH, and H_2O exosphere, including photo-induced conversions above the surface and geochemical conversion reactions in the regolith. The main limitation of the model proved to be the crude approximation of the surface, which is the focus of this work.

Firstly, the need for a more sophisticated lunar regolith model, including a wide variety of geochemical reactions and conversion between the four species named above, is highlighted. Secondly, the complex model of the lunar water cycle is presented.

The Numerical Model: A coupled Monte-Carlo (MC) model was created, which is simulating individual weighted particles during their "life" in the lunar water cycle, ending either through their atmospheric escape,

Table 1. List of relevant photo-processes for H, H_2, OH, and H_2O, including their rates at varying Sun conditions [4].

Reaction		Rate Coefficient, k $[10^{-8}s^{-1}]$	
		Quiet Sun	Active Sun
$H + \nu \rightarrow$	$H^+ + e^-$	7.3	17.2
$H_2 + \nu \rightarrow$	$H + H$	8.2	19.1
	$H_2^+ + e^-$	5.4	11.5
	$H + H^+ + e^-$	1.0	2.8
$OH + \nu \rightarrow$	$O + H$	724.0	884.0
	$OH^+ + e^-$	24.7	65.2
$H_2O + \nu \rightarrow$	$OH + H$	1030.0	1760.0
	$H_2 + O$	59.7	148.0
	$H + H + O$	75.5	191.0
	$H_2O^+ + e^-$	33.1	82.8
	$H + OH^+ + e^-$	5.5	15.1
	$H_2 + O^+ + e^-$	0.6	2.2
	$OH + H^+ + e^-$	1.3	4.1

permanent trapping in PSRs or through conversions into other particles.

The simulation assumes an idealized spherical Moon, subsolar-stationary temperature conditions, Maxwell-Boltzmann flux distributed particle energies, and full thermal accommodation. For the geochemical reactions, the activation energies are all uniformly distributed, out of convenience and due to their simplicity.

Conversion Rates: The new model aims to capture a more complete overview of the lunar water cycle by combining all known conversion reactions between the hydrogens, hydroxyl and water, both in the exosphere as well as in the lunar regolith. With the assumption of no particle collisions, the only reactions taking place in the former are photoionization and photodissociation. **Table 1** lists the rates for these reactions for quiet and active Sun conditions, respectively [4].

The surface-bound particles are also subject to photo-processes though with rates additionally depending on their positioning in the lunar regolith. Furthermore, several physical and chemical reactions can occur, that either change the state of the current particle or even convert it into one of the other three. The following lists a set of reactions included in the model, with $M - O$ representing an active site on a generic metal oxide in the chemical equations: solar wind backscattering $(p^+ \rightarrow p^+; p^+ \rightarrow H)$; proton implantation $(M - O + p^+ \rightarrow M - OH)$ and hydrogen diffusion $(M - O + H \rightarrow M - OH)$; molecular hydrogen recombination $(H + H \rightarrow H_2)$ and recombinative desorbtion $(M - OH + M - OH \rightarrow M - O - O - M + H_2)$; second-order desorption and dissociative adsorption $(M - OH + M - OH \leftrightarrow M - O - M + H_2O)$. [5,6]

Discussion: With the current model being unable to predict the water cycle densities accurately, a more complex model is presented, which includes both the previous numerical model, as well as the conversion rates listed above. The result is a more complete overview of the lunar water cycle, which will act as a new starting point for the numerical investigation of the Moon.

References: [1] Lucey P. G. et al. (2021) *Chem. Erde* 82, 3. [2] Urey H. C. (1958) *Z. physik. Chem.* 16. [3] Saal A.E. (2008) *Nature* 454. [4] Huebner et al. (1992), *Astrophys. Space Sci* 195. [5] Hurley D.M. et al. (2017) *Icarus* 283. [6] Jones B.M. et al. (2018) *Geophys. Res. Lett.* 45.