Extraterrestrial Exosphere and Surface Simulations

*Lunar Water Exosphere*

Alexander Smolka

*Lunar and Planetary Exploration*
*Technical University of Munich*
Alexander Smolka

Researcher, Technical University of Munich, Lunar and Planetary Exploration

Research Topic: Modelling of the Lunar Water Exosphere and its Interaction with the Surface

Methodology: Numerical simulations using our specially developed high-performance Julia code base.
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Prof. Dr.-Ing. Philipp Reiss
Lunar and Planetary Exploration

- better understanding of volatiles and space resources
- instrumentation to enable their in-situ characterization
- extract and utilise resources
The Lunar Exosphere
The Lunar Exosphere

Surface-bounded Exosphere

"[...] atmosphere-like volume surrounding a planet [...] where molecules are gravitationally bound to that body, but where the density is so low that the molecules are essentially collision-less."

(Image credit: NASA)
The Lunar Exosphere

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The Lunar Exosphere

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Densities are highly dependent on the position (equatorial/polar) and time (day/night)!

Comparison with Earth’s atmosphere: $2.687 \times 10^{19} \text{ cm}^{-3}$

We can simulate them individually!
The Lunar Exosphere

We cannot simulate all of them!

We can simulate them individually!

Surface-bounded Exosphere

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The Lunar Exosphere

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Monte Carlo simulation

We can simulate them individually!

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The Lunar Exosphere

Sources & Sinks

- Solar wind
- Micrometeoroid Impact
- Micrometeoroid Impact Vaporization
- Sputtering

- Gravitational Escape
- Photolysis
- Sputtering
- Permanent Cold Trapping

(Image credit: NASA)
The Lunar Exosphere

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Ions: 
\[ \approx 96\%: \text{p}^+ \]
\[ \approx 4\%: \text{He}^+ \]
Lunar Exosphere Simulation

Monte Carlo simulation

mostly noble gases

custom model

Lunar Exosphere Simulation
Modeling and Simulation of our Moon’s Surface-Bounded Exosphere
RT-MA 2022/03
Lunar Exosphere Simulation

Assumptions:

- 2D landing position calculation instead of 3D ODE trajectory solver
- Only neutral gases
  - Only gravity
- Steady-state conditions without Earth's influence
- ...
Lunar Exosphere Simulation

My model predictions

Grava et al., 2019
Grava et al., 2015
Sarantos et al.
Lunar Exosphere Simulation

Grava et al., 2019
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My model predictions
Lunar Exosphere Simulation

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Modeling and Simulation of our Moon’s Surface-Bounded Exosphere

RT-MA 2022/03
Velocity distributions

Maxwell-Boltzmann Velocity Distribution

Maxwell-Boltzmann Flux Velocity Distribution
Velocity distributions

Maxwell-Boltzmann Velocity Distribution

2D/3D Trajectories
Velocity distributions

Maxwell-Boltzmann Velocity Distribution

Temperature Distributions

Maxwell-Boltzmann Flux Velocity Distribution

Temperature Distributions

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Temperature Distributions
Velocity distributions

Maxwell-Boltzmann Velocity Distribution

Temperature Distributions

Discretization
Lunar Exosphere Simulation

The Julia Programming Language

Julia in a Nutshell

Fast
Julia was designed from the beginning for high performance. Julia programs compile to efficient native code for multiple platforms via LLVM.

Dynamic
Julia is dynamically typed, feels like a scripting language, and has good support for interactive use.

Reproducible
Reproducible environments make it possible to recreate the same Julia environment every time, across platforms, with pre-built binaries.

Composable
Julia uses multiple dispatch as a paradigm, making it easy to express many object-oriented and functional programming patterns. The talk on the Unreasonable Effectiveness of Multiple Dispatch explains why it works so well.

General
Julia provides asynchronous I/O, metaprogramming, debugging, logging, profiling, a package manager, and more. One can build entire Applications and Microservices in Julia.

Open source
Julia is an open source project with over 1,000 contributors. It is made available under the MIT license. The source code is available on GitHub.

https://julialang.org/

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Lunar Water Exosphere Simulation

Conversion Reactions

Diagram showing the reactions involving H, H₂, OH, and H₂O.
## Lunar Water Exosphere Simulation

### Conversion Reactions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Quiet Sun Photoreaction Rate in $10^{-7}$ s$^{-1}$</th>
<th>Active Sun Photoreaction Rate in $10^{-7}$ s$^{-1}$</th>
</tr>
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<tbody>
<tr>
<td>1 $\text{H} + \nu \rightarrow \text{H}^+ + e^-$</td>
<td>0.726</td>
<td>1.720</td>
</tr>
<tr>
<td>2 $\text{H}_2 + \nu \rightarrow \text{H}(1s) + \text{H}(1s)$</td>
<td>0.480</td>
<td>1.090</td>
</tr>
<tr>
<td>$\text{H}_2 + \nu \rightarrow \text{H}(1s) + \text{H}(2s \text{ or } 2p)$</td>
<td>0.344</td>
<td>0.821</td>
</tr>
<tr>
<td>$\text{H}_2 + \nu \rightarrow \text{H}_2^+ + e^-$</td>
<td>0.541</td>
<td>1.150</td>
</tr>
<tr>
<td>$\text{H}_2 + \nu \rightarrow \text{H}^+ + \text{H}^+ + e^-$</td>
<td>0.095</td>
<td>0.279</td>
</tr>
<tr>
<td>17 $\text{OH} + \nu \rightarrow \text{O}(3p) + \text{H}$</td>
<td>(120.00) 65.400</td>
<td>(138.00) 71.700</td>
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<tr>
<td>$\text{OH} + \nu \rightarrow \text{O}(1d) + \text{H}$</td>
<td>(70.10) 6.350</td>
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<td>14.800</td>
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<td>8.280</td>
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*Huebner et al., 1992*
Lunar Water Exosphere Simulation

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Table 1. Fractions of Incident Protons Entering Each Branch After Surface Interaction

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<th>Backscatter H</th>
<th>Sputtered H</th>
<th>Desorbing H</th>
<th>Convert to H$_2$</th>
<th>Convert to OH</th>
<th>Convert to H$_2$O</th>
</tr>
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<tr>
<td>.01</td>
<td>.0001</td>
<td>.27</td>
<td>.6</td>
<td>.1</td>
<td>.02</td>
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Crider and Vondrak, 2002
Subsolar Longitude

\[ LT = \frac{(\Theta + \pi)}{\pi} \cdot 12\text{hr} \]
Subsolar Longitude

\[ \theta = -\pi \text{: MIDNIGHT} \]
\[ \frac{\pi}{2} \leq \theta < -\frac{\pi}{2} \text{: SUNRISE} \]
\[ \theta = 0 \text{: NOON} \]
\[ -\frac{\pi}{2} \leq \theta < \frac{\pi}{2} \text{: SUNSET} \]

\[ LT = \frac{(\theta + \pi)}{\pi} \cdot 12 \text{hr} \]

\[ n_0 / [\text{cm}^{-3}] \]

\[ n_0 / [\text{cm}^{-3}] \]

\[ \cdot 10^5 \]

\[ \cdot 10^4 \]

\[ \cdot 10^3 \]

\[ \cdot 10^2 \]

\[ \cdot 10^1 \]

\[ \cdot 10^0 \]

\[ \cdot 10^{-1} \]

\[ \cdot 10^{-2} \]

\[ \cdot 10^{-3} \]

\[ \cdot 10^{-4} \]

\[ \cdot 10^{-5} \]
DON'T MIND THESE EXACT VALUES!

\[ LT = \frac{\theta + \pi}{\pi} \cdot 12 \text{ hr} \]
Almost no surface reactivity
A lot of surface reactivity
A lot of surface reactivity
Lunar Water Exosphere Simulation

Conversion Reactions

\[ \begin{align*}
H & \leftrightarrow H_2 \\
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Lunar Water Exosphere Simulation

Conversion Reactions
Lunar Water Exosphere Simulation

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Conversion Reactions

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Lunar Water Exosphere Simulation

Conversion Reactions

- **Irradiation**
  - bombardment with D+; dissociation upon impact

- **Characterisation of Irradiated Samples**
  - ToF-SIMS to measure water group molecule concentration
  - ERDA (Elastic Recoil Detection Analysis) to determine deuterium depth

- **Laser Pulses to Simulate MMI**
- **TPD Measurements**
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Generally: Improve the framework and explore the lunar water cycle