DSMC SIMULATIONS OF LUNAR COMET IMPACTS AND THE DELIVERY OF WATER TO PERMANENTLY SHADOWED CRATERS

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1 Background & Objectives

Over the years, a number of missions have recorded observations that suggest the presence of water on the Moon, particularly in regions of permanent shadow near the lunar poles. Several mechanisms, such as liberation of primordial water from the lunar interior, the interaction of solar wind protons with surface minerals and the impact of volatile-rich meteorites and comets, could have delivered water (and other volatiles) to the lunar surface. Our focus is on this last source. Over the last four billion years, \( \sim 10^{17} \) kg of cometary material is estimated to have impacted the Moon \cite{1}. Water ice is thought to be the primary constituent of comet nuclei and, although, due to tremendous impact velocities (20-50 km/s), much of the water that comets deliver to the Moon might simply escape, analytical \cite{2, 3} and computational \cite{3, 4} models predict that a significant amount may remain gravitationally bound and migrate to permanently shadowed polar craters (‘cold traps’), where temperatures are low enough to trap water over geological time scales.

Our objective is to constrain the amount of water that comets could have contributed to the lunar volatile inventory, and to understand how impact parameters (such as speed and angle) influence volatile fallout, by modeling the transport processes that lead to deposition of cometary volatiles in cold traps. This is a complex problem: On impact, a comet vaporizes, giving rise to a high-temperature, high-velocity plume that expands unsteadily into essentially a vacuum background. The volatiles that do not immediately escape form a collisionally thick transient atmosphere that surrounds the Moon for days to months, during which some portion of the vapor condenses into cold traps. The range of spatial and temporal scales involved, together with the transition of the flow regime from continuum through to free molecular, make this a computationally demanding problem. Consequently, prior models of volatile retention after impact have largely been restricted to the short-term and near-field. Similarly, models of planetary-scale loss processes and migration of molecules have dealt primarily with the collisionless, free-molecular limit. Our approach \cite{4} includes and connects both these limits. Here, we present results of our simulations of lunar comet impacts and the associated accumulation of water in cold traps, and discuss the temporal evolution and gas dynamic characteristics of the transient atmosphere, with implications for polar ice deposits.

2 Computational Method

Our simulations take a hybrid approach, making combined use of the SOVA hydrocode \cite{5} and the Direct Simulation Monte Carlo (DSMC) method \cite{6}. The immediate physics of the impact are simulated using the SOVA hydrocode, which models the phase changes that occur in both the target and the projectile as a result of successive compression and rarefaction waves, and solves for the relatively dense, hydrodynamic flow of molten/vaporized target and projectile material. In the present simulations, the comet is modeled as a sphere of pure water ice, and the lunar surface is assigned the material properties of dunite. Subsequent evolution of the water vapor plume is tracked using a DSMC code designed to model rarefied planetary flows. DSMC is a statistical method that models molecular interactions by moving and colliding a representative number of simulated molecules within a gridded domain. Molecular properties can be sampled within cells to determine macroscopic characteristics.

Figure 1: Density contours in the plane of impact, 5 s after a 60°, 30 km/s impact. Within the red semi-circle (the interface between the codes) are SOVA contours for rock (green) and water (gray). The DSMC code models only water vapor.

Figure 1 illustrates the coupling between the SOVA/DSMC codes: Unsteady data from the SOVA solution (density, bulk velocity, temperature etc.) are output over a hemispherical shell of cells, 20 km in radius, centered at the point of impact. The SOVA output is then used to create representative molecules that are allowed to move into the planetary-scale DSMC domain. The present DSMC implementation \cite{4} is fully three-dimensional, and parallelized for computational speed. The code includes variable gravity, diurnally varying surface temperatures, temperature-dependent residence times for water molecules that land on the lunar surface and a photodestruction probability for molecules in sunlight. Seven cold traps (six at the South Pole and one at the North Pole) are modeled; any molecule that lands in a cold trap is assumed to be permanently captured, and remains frozen where it landed, for the duration of the simulation.

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3 Results & Discussion

We have previously run complete simulations of a 45°, 30 km/s impact [4]. To explore the influence of impact parameters on volatile retention, we are currently modeling two further impacts that differ from this baseline case in impact angle (60°) and speed (20 km/s). The results presented here are for a 60°, 30 km/s impact at the lunar North Pole. Figure 2 depicts the water vapor plume 30 s after impact. At this stage, vapor is still expanding radially outward from the point of impact—much of it traveling at speeds far higher than lunar escape velocity.

![Figure 2](image.png)

Figure 2: Radial velocity contours 30 s after impact; streamlines are superimposed.

At later times, slower moving vapor, which remains gravitationally bound, begins to fall back to the lunar surface. The concentric shells of increasing radial velocity seen in Figure 2 evolve under variable gravity to form the characteristic, near-spherical envelope of streamlines shown in Figure 3. Vapor outside this envelope continues to move away from the Moon, and vapor inside falls back along ballistic trajectories. Although the gas is still collisional, it is so cold that collisions barely modify trajectories from the ballistic. Faster moving vapor takes longer and travels further before it begins to fall back, and hence the fallback envelope grows in size as time progresses.

![Figure 3](image.png)

Figure 3: Number density contours 6 hours after an impact at the North Pole; streamlines are superimposed.

Vapor that falls back on the cold night side of the Moon largely remains frozen to the surface until local sunrise, whereas vapor that lands directly in cold traps is considered to remain frozen to the surface for the duration of our simulations. Meanwhile, vapor falling back on the warm day side has a much shorter residence time, which gives rise to a relatively dense, transient day side atmosphere. The vapor pressure over the day side results in the formation of a shock, as the cold, rarefied, high velocity vapor falling back encounters the denser region close to the surface. This surface shock turns the ballistic fallback into a low speed, surface-hugging flow, driven by global pressure gradients. For an impact at the North Pole, there is a north-south pressure gradient as well as a day-night one. Over time, more vapor diffuses from the day side to the night side, where it condenses on the cold night side surface. Another striking feature of the flow field shown in Figure 3 is the convergence of streamlines antipodal to the point of impact, resulting in the channeling of water to the surface at the antipode. This flow field, with its shocks and pressure driven winds, presents a picture of volatile transport that is qualitatively quite different from prior models of largely collisionless transport through ballistic hops. Figure 4 tracks the amount of water that is lost (to photodestruction or leaves the Moon’s Hill sphere), and the amount deposited at the north and south polar cold traps. Interestingly, for an impact at the North Pole, antipodal effects lead to thicker deposits at the South Pole.

![Figure 4](image.png)

Figure 4: Temporal evolution of cold trap deposits, over ~ 3 days.

The simulations are continued from hours to days and months, with the flow transitioning to the free molecular regime as water is lost to photodestruction and condensation on the night side and in the cold traps. As the transient atmosphere becomes more and more rarefied, the antipodal shock vanishes. Meanwhile, the sublimation of night side deposits at sunrise sustains a localized flow field at the dawn terminator [4]. Ultimately, all the water is either lost or captured.

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References