Summary: Although still being debated, Lunar Prospector and Clementine data appear to support the contention that there are water ice reservoirs in the permanently shaded craters near the lunar poles. This project focuses on the process of atmospheric water vapor condensation into such cold traps following a comet impact that produced a temporary near-continuum atmosphere. We concentrate here on the complex gas flow produced by a comet impact.

Background: Clementine mission data [1] may indicate the presence of water ice in cold traps in the lunar South polar region. The interpretation of that data remains contentious, however [2-4]. In addition, the results from the Lunar Prospector (LP) mission appear to provide an even stronger case that there exists water near both poles [5, 6]. Water, if it exists there, presumably condensed in the traps directly from the vapor phase after being transported from elsewhere. A major presumed source for water is the episodic impact of large comets. Comets are thought to contain about 80% of water by mass with the average mass being 7×10^{16}g [7] and the average time between impacts on the Moon being 10 to 100 million years.

The atmospheric flow associated with a large comet impact is qualitatively different from that of steady water sources. The fraction of H_{2}O escaping the Moon depends on the specific conditions of each impact especially the impact velocity and angle. In particular, highly oblique impacts on low gravity bodies lacking an atmosphere lead to a small fraction of vapor retained [8, 9]. The H_{2}O which remained on the Moon would expand away from the impact site in a manner roughly described as a gas cloud or jet expanding into a vacuum. Cometary water vapor in contact with the surface will not condense on the sunlit side of the Moon (at 400K) but vapor which is on the dark side will condense quickly as the surface temperatures drop to perhaps 120K [10]. Hence, depending on which side of the Moon the comet hit, there could be dramatically different effects of condensation on the spreading of the vapor cloud.

Numerical Modeling: To model the immediate effects of a comet impact we use the three-dimensional Russian hydrocode SOVA [11], currently one of the impact codes involved in the benchmark and validation project for impact cratering models. We then simulate the low density atmospheric flow with the DSMC particle method [12]. In DSMC the motions and collisions of a relatively small number (O(10^{7})) of representative molecules are computed, from which the flow of the entire gas is statistically extrapolated. Mixtures of gas species having different numbers of rotational and vibrational degrees of freedom and exhibiting non-equilibrium radiation and chemistry effects can be modeled (Figure 1).

Results: A reasonable approximation of the initial state of the volatiles after an impact is crucial to understanding their subsequent evolution over the surface. One would want to know the velocities, densities and temperatures of the major species at several seconds after impact, as the flow transitions from a continuum gas-dynamic state to a low density, perhaps rarefied, state. To know those properties, one must solve the compressible hydrodynamic/Navier-Stokes equations for the impact fluid flow in which the temperatures and pressures are very high and the good representation of the impactor and target material via equations of state are most important. This is done by SOVA, which uses tabular equations of state developed from the thermodynamically consistent ANEOS code. We then use the flow field as the initial condition for the DSMC code and continue the simulation out to large times – all the

Figure 1. Physical domain used in the 3D DSMC simulations showing the grid, boundary conditions, and single processor domain. For parallel simulations each processor is assigned a "melon slice".

Figure 2. Illustration of a vertical impact and how the DSMC and SOVA codes are merged. At a fixed boundary macroscopic SOVA properties are sampled at selected time steps. Such properties are used to generate DSMC particles from an appropriate Maxwellian distribution via an acceptance/rejection technique. These particles are then drifted into the DSMC domain.

Figure 3. Diagram showing the physical domain, grid, boundary conditions, and single processor domain. For parallel simulations each processor is assigned a "melon slice".
way out to the free molecular regime. We have done computations of several kinds of transient lunar atmospheres following a comet impact [14, 15] (Figures 2 and 3).

We here summarize example results for a full 3D simulation of a 45° 30km/s oblique impact (the most probable angle of impact). The comet is 2km in diameter and has an initial density of 1.1g/cm³. In Figure 3 are density contours on the symmetry plane from the hybrid run in the near field 1s after impact. SOVA results from the inner domain are passed to DSMC. Within the r<20km red interface, the gray contours represent the impactor material, modeled by SOVA with the ANEOS ice equation of state, while the green is the target, modeled by SOVA with the ANEOS granite equation of state. Color shading represents changes in material density. X- and Y-axes represent downrange and height, respectively.

This SOVA simulation used a resolution of 20 cells per projectile radius, corresponding to cells sizes of 50m. Outputs for DSMC were recorded every 0.01 s in the early phases of impact, and progressively increased to 0.1 s. The material's thermodynamic evolution is recorded in terms of temperature, pressure, density, energy in each cell of the mesh, and it depends on the equation of state used. By the time the gas reaches r=20km it has sufficiently cooled that the vapor chemical species are frozen. The DSMC model of the water includes internal (vibrational and rotational) degrees of freedom and infrared radiative cooling. Molecules striking the surface reside there for a time that depends on the local surface temperature.

The direction and velocity of the expansion plume depends on the angle of impact. A five-domain DSMC simulation on 34 processors was run with a total of 5 million cells and 1.1 million molecules (Figure 4). The cell sizes and time steps vary as the plume expands. Figure 4 shows the water vapor that passes through the interface during the first second after impact at three later times. The smallest innermost square represents the field shown in Figure 3. After 37.4s, a large slug of vapor is lofted well above the lunar surface. The lunar surface is seen as blue and green temperature contours. Clearly, the vapor passing through the inner hemisphere in the early phases of the impact was moving rapidly at early times and nearly all of it will escape from the Moon.

We are currently using our hybrid simulations to generate DSMC particles and use them in a parametric study of various surface temperature distributions (temperature as a function of distance from the impact site) to simulate comets impacting on different locations over the day and night sides of the Moon.

References:

Figure 3. A slice of a hybrid 3D simulation of a 2km comet impact on the Moon at 30km/s at 45° is shown after 1 second. The flow inside the inner 20km radius circle was computed with the continuum code SOVA. DSMC particles are then created in the cells on the inner red circle and DSMC is used thereafter. The water portion of the SOVA output (seen in gray) is carried into the DSMC domain. Along the outer red circle, SOVA and DSMC data can be directly compared.

Figure 4. Where the first second’s water goes. DSMC results 1.4s, 5.4s and 37.4s after oblique impact. Very little water has actually returned to strike the surface indicating that the water that took less than 1s to pass through the interface will largely be blown off the Moon. Note that the outermost domain top boundary is 1000km above the lunar surface.