

Free Molecular Simulations of Vapor Dynamics Following a Lunar Impact

D. B. Goldstein¹, S. A. Stern², D. H. Crider³, G. R. Gladstone⁴, D.D. Durda², E. Asphaug⁵, B. Larignon¹, P. L. Varghese¹, L. M. Trafton¹

¹ U. Texas at Austin, TX, ² SWRI, Boulder, CO, ³ Catholic U., ⁴ SWRI, San Antonio, ⁵UC Santa Cruz

Abstract. We examine by free-molecular simulation both the short- and long-time evolution of an H₂O and OH atmosphere on the moon following an intentional spacecraft impact. In one case a spacecraft is to strike a polar cold trap in an attempt to liberate a visible plume of water vapor from ice trapped in the cold soil. We find that, depending on assumed initial conditions, a plume may be observable if O(10-50kg) of vapor is produced. In second type of experiment, 2400kg of water is purposely deposited on the moon to create a transient vapor atmosphere that could be monitored as water molecules migrate to the cold traps. In this case, it is found that though the atmosphere could be observed for days-to-months, it is unclear how such observation could be directly related to the efficiency of transport to the permanent polar cold traps.

Keywords: Collisionless atmosphere, exosphere, lunar atmosphere, lunar impact.

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Introduction: For nearly 50 years it has been thought that it may be possible for water ice to persist in permanently shadowed lunar polar craters. Such craters are deep enough and the inclination of the sunlight at these latitudes low enough that portions of the crater bottom remain dark at all times (Watson, Murry, & Brown 1961; Arnold 1969). The resulting surface temperature would be low enough (perhaps < 90K) that ice loss due to sublimation would be minimal over geologic time. There are other loss mechanisms possible as well, but we neglect them herein. While such ice has not been definitively detected on the moon, it has been found on the similar airless poles of the planet Mercury. More detailed references to such issues appear in our earlier papers on this subject (Goldstein et al. 1999, 2001, Goldstein 2003, Stern 1999, Crider & Vondrak, 2000).

If ice is there, it may have accumulated gradually - one molecule at a time - or may have arrived in episodic bursts as a comet struck the moon and released a tremendous amount of water. The transport processes associated with slow versus impulsive releases are different. For a slow gas release, the molecules would interact with pristine surface materials (regolith) and would also be exposed to intense sunlight. After a large impulsive release, the regolith can easily be coated with a monolayer or more of volatile species (it takes $\sim 6 \times 10^{14}$ g water to coat the lunar surface to a depth of 5cm with a monolayer) and the temporary volatile atmosphere can be appreciably opaque to ionizing and dissociating sunlight (Vondrak 1974). A key parameter to be described in either of these scenarios is the efficiency of transport of volatile material from its source to a permanent cold trap. Unfortunately, the gas migration processes associated with either form of gas release has not been well observed. An exception was the study of the artificial atmosphere created by the vehicles and astronauts during the Apollo landings (Vondrak, 1974). In that case, water deposited during daytime landing and departure was apparently detected by the SIDE detector during a single following sunrise as water molecules sublimated off the warming ground (Freeman & Hills, 1991).

In the present work, we briefly examine simulations of proposed lunar impact experiments meant to shed light both on (1) whether or not ice does exist in cold traps and, separately, on (2) how water molecules migrate about the moon following a cometary impact event.

In the first case, the Lunar Reconnaissance Orbiter (LRO) was recently moved to the Evolved Expendable Launch Vehicle but there was 1000kg of extra payload available that NASA made available to do an exploration mission to

the lunar poles. At least three groups proposed to use this opportunity to repeat - in a much-improved way - the 1999 Lunar Prospector (LP) Impact Experiment. At the end of the LP active mission, the depleted spacecraft was in a polar orbit. A controlled impact was performed into a south polar crater (now called Shoemaker crater) in an unsuccessful attempt to vaporize enough trapped ice to make a plume that could be telescopically detected from Earth. With the new “LCROSS” or similar proposed LRO tag-along missions, one could have a higher impact angle, greater impact mass, improved targeting, and observation platforms in lunar orbit and attempt to provide more definite evidence of the presence or absence of water ice in the target regolith.

In the second case a dedicated Discovery-class mission was studied by a group led by one of us (Stern) to create and study a synthetic lunar atmosphere (the Synthetic Lunar Atmosphere Mission, SLAM). His idea was to simply deposit a large quantity of well characterized water on the moon via impact and observe the subsequent evolution of the gas as it makes its way to the cold traps or is lost. In this case, using an Atlas V class launch vehicle and the controls of its Centaur upper stage, a simple and cheap payload of about 2400kg could be delivered with fairly good targeting and no specific spacecraft development would be required. LRO, SELENE or Chandrayaan-1 and ground or Earth-orbiting spacecraft could make observations.

In both cases the main issue the present simulations address is the potential visibility of the volatile atmosphere, either water vapor itself or its photodissociation product OH. The limiting physics in the two cases differ, however. In the cold trap impactor experiment (1), we have a limited knowledge of the physics of the impact: the detailed velocity, mass, and vapor content distribution of the material immediately arising from the several meter wide impact crater. In the SLAM experiment (2), since we know how much water is being deposited, that is not of interest. It is the long-term evolution of the atmosphere that is crucial, so the understanding of the gas-surface interaction is what limits our ability to simulate the event. We first present the common physics of the simulations and then the results for the individual scenarios.

Methods: Away from the immediate vicinity of the deposition region, the gas density is so low that the motion is free molecular so that intermolecular collisions are ignored. Molecules are thus tracked as they individually move on ballistic (elliptical) trajectories having lengths of several tens of kilometers. Molecules hop between sites on the surface. They are emitted with a velocity based on the local surface temperature which varies with the time of day and is given by $T = (T_{ss} - T_{mid}) \cos^{1/4}(\theta) + T_{mid}$ where T_{ss} is the subsolar surface temperature (=370K), T_{mid} is the midnight or dark side temperature (=120K) and θ is the sub-solar angle as is suitable for the slowly rotating moon in radiative equilibrium. ($T = 120K$ at night.) Inside several discrete polar craters the surface temperature is assumed very cold (90K). Molecules, including the free radical OH, touching the surface have a residence time assumed to be given by $T_{reside} = (1/\nu)e^{\Delta H/kT}$ where (for H_2O) $\Delta H/k = 4815K$ and $\nu = 2 \times 10^{12} \text{ sec}^{-1}$ (Sandford & Allamandola, 1990). At each time step, a random number is drawn to determine if stuck molecules are released. Diffusion into and out of the pores of the regolith is not otherwise modeled. Effectively, nearly all molecules stick on the night side with a residence time of days-to-years while on the warm dayside, nearly all molecules are released within seconds. As the moon rotates, stuck molecules tend to be released at sunrise as the ground warms. We acknowledge that the assumptions about the OH surface interactions are questionable at best.

The time step is usually ~1sec so ballistic trajectories are made up of many steps. At each step, those molecules in sunlight are subject to photodissociation and photoionization. The time scales for these damaging events during solar minimum (suitable for the 2008 launch time frame) are $t_{dissoc} = 8.3 \times 10^4 \text{ sec}$ and $t_{ionize} = 2.45 \times 10^6 \text{ sec}$

(Huebner et al. 1992). Hence, at each step, a pair of random numbers is tested against $e^{-\Delta t/t_{damage}}$ to determine if the water molecule is photodamaged. Photodissociation products are predominantly OH and H. The subsequent H is ignored but the OH is tracked. The OH interaction with the regolith is treated just as is the original H_2O as we have no other residence time numbers available. It is possible that the OH recombines with H (of solar wind origin) on the surface to re-form H_2O . In the present work we ignore recombination as a conservative approximation. Ions created through photoionization (H_2O^+ and OH^+) are assumed to be immediately scoured away by the solar wind and lost. This too is a conservative assumption because perhaps 50% of ions would be driven back to the surface and neutralized.

The observable quantities are presumed to be column-integrated H₂O and OH densities as well as surface accumulations of water ice. OH fluoresces in sunlight at 3085 Å and could be visible from space or from telescopes on Earth using narrow band filters. Water may be visible from space (perhaps via the ODIN spacecraft that detected Deep Impact water or once on the surface via the LRO LAMP instrument). From Earth, telluric water vapor would swamp any lunar water signal. Thus, for the SLAM project it was anticipated that heavy water, D₂O, would be used in the impactor to provide a signal that would be spectrally distinct when seen through Earth's atmosphere. Finally, during the Deep Impact mission, it appears that much of the water vapor signal came from secondary sublimation of the debris raised into the sunlight. We do not model this process but instead assume all H₂O is released in prompt emission upon impact.

Re-doing the LP Impact Experiment: We first describe the modeling of the impact of a spacecraft into a south polar cold trap in an effort to make a detectable plume of water or OH vapor. We assume:

- 1) There was a single impact at 88S, -45W eight days past full moon.
- 2) The impact made a small crater perhaps tens of meters in size (smaller than a pixel size) that spread warm dirt (see 4) around in a similarly small area. "Small" means that we model the source as a point source.
- 3) The dirt was spread quickly (<100sec) and did not rise high enough above the crater rim to itself be visible. "Quickly" is important so that crater formation time is small compared to plume evolution time. That the dirt did not rise high means it will not scatter light and any ice crystals traveling with the dirt will not rise into sunlight and evaporate. Also, the dirt did not have much time to radiatively cool during flight.
- 4) The dirt was 400K. This 400K is a big IF; it is based on a rough conservation of energy estimate of a 300K temperature rise for impact-heated soil for the LP spacecraft impact (Goldstein, et al 1999). This temperature basically governs how large the plume will get and, hence, how observations should be made. If the dirt is too cool, say much below 273K, little ice will sublimate and separate out of the dirt and then almost certainly nothing much could be seen. For an impact at 2-3km/s it is hard to believe much dirt will be heated much warmer than 400K. If any dirt is, we can expect water molecules from that region of very hot dirt to move much more quickly and form a very rarefied plume. Hence, we treat the 400K estimate as an arguable free parameter pending future experimental evidence.
- 5) The dirt was spread around over a fairly flat area. We ignore any gas dynamic focusing effects arising from the bowl-shape of the crater or other effects from there being a mean ground tilt or the presence of high crater walls around the cold trap.
- 6) We examine, in effect, two different surface areas for the origin of the vapor. In the first case we assume the dirt patch is small enough that the molecules collide among themselves in the near field and then expand into a collisionless plume. Earlier DSMC simulations had shown that the molecules then tend to approach the ultimate speed of an isentropic expansion (Goldstein et al., 1999) and have a mass flux distribution approximated well by a cosine² of the angle from the surface normal. Hence, all molecules are assigned speed $V_{ultimate}$ (=1215m/s) and their directions are chosen from a cosine² distribution. In a second case we assume that the gas origin was large enough that the molecules escaping the warm disk of dirt are collisionless. The molecules thus have a thermal range of speeds and a cosine directional distribution.

Assuming a near-normal impact of the spacecraft, the ejecta plume of debris should be nearly axisymmetric and produce a disk shaped debris fan. The important unknowns are the fraction of the target regolith that is water ice (presumably < 10%) and the velocities and temperatures of the initial debris. Because the amount of water released is poorly constrained, we present results on a per-kilogram-released basis.

We present shaded contour results for the water column density (in #/m²) and for the OH brightness at 3085Å (in Rayleighs). Black lines indicate the local surface temperature. In figure 1, we see the evolution of the slant water column density over the first 5000 sec from an Earth view. The color bar varies logarithmically from 10¹⁰ to 10¹⁴. One sees the rise and collapse of the initial plume. After the collapse, a subsequent sublimation atmosphere develops on the sunlit (right) side of the moon. This atmosphere begins to fade after about an hour as the water molecules diffuse in every direction but particularly north (up) and over to the night side where they stick to the surface. The highest column densities of O(10¹⁴) are predicted to occur in the leading edge of the rising and falling plume front. However, since this front moves rapidly, it may be difficult to detect these column densities because observation times of tens of seconds may be necessary, and the best chance at detection would be from the later more steady dayside sublimation atmosphere. The OH brightness of figure 2 largely tracks the water column density and shows a

peak in OH brightness of $\sim 1\text{R}$ per kg of water released – a small number both because of OH losses and because little dissociation has occurred by this time. We note that the minimum detectable OH signal over the dark limb of the planet is $\sim 10\text{--}20\text{R}$. The single inset figures are the results from a similar simulation at a time of 1000sec, in which the molecular velocities were simply assumed to be thermal at 400K. That is, we assume that the impact site or source region is large enough so that the vapor over the impact site is non-collisional and thus does not equilibrate and reach V_{ultimate} in the process of expanding. The main difference is that the plume front is diffuse and no longer distinct and the peak water or OH signal instead occurs later near the day side surface.

Figures 3 and 4 show the corresponding view as seen from directly over the South Pole. This view may be suitable for a polar-orbiting spacecraft. One sees the same general features of the rise and fall of the plume and the subsequent sublimation atmosphere mostly over the day lit side. From this point of view, however, one sees that the highest signal would be right over the impact point and would persist for perhaps 2000 seconds. By 5000sec in the last image, 35% of the water molecules remain airborne (65% are trapped on the dark side), 3.8% have dissociated and a negligible number are ionized. As the inset figures show, if the vapor were non-collisional all the way to the surface, the peak signal over the impact site would be diffused. The airborne, trapped and dissociated numbers would be then 25%, 75% and 2.5%, respectively, after 5000sec.

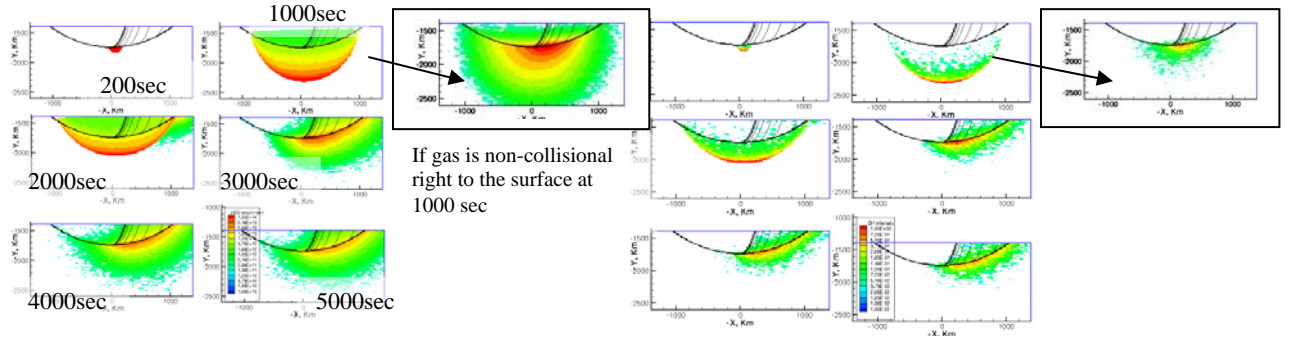
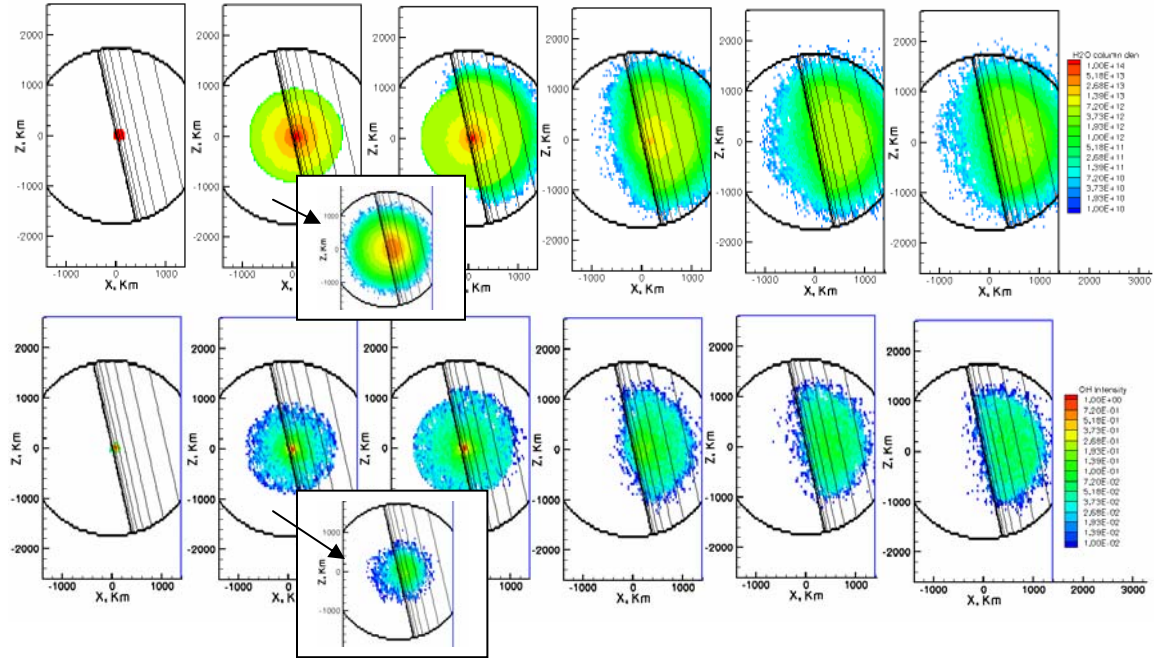


Figure 1 & 2. In fig. 1 (left) water molecule column density is shown in $\#/\text{m}^2$. Axes are in km. Black lines are lunar surface temperature – the Sun is on the right. Peak column is $\sim 10^{14}/\text{m}^2$ per kg released. Figure 2 (right) shows OH brightness at 3085\AA , in Rayleighs. As in fig. 1, times shown are 200, 1000, 2000, 3000, 4000 and 5000sec. Peak brightness is $\sim 1\text{R}$ per kg H_2O released.



Figures 3 and 4. Water column density and OH brightness as seen from over the South Pole. The color bars and times correspond to those of Figures 1 & 2. Inset figures show results at 1000sec if the vapor were diffusing out of the surface and were non-collisional.

SLAM: For the SLAM experiment, imaging the initial vapor plume was not the issue. Instead, monitoring the evolution of the vapor atmosphere as it migrated to the cold traps was of most interest. Thus, longer simulations were needed. Several impact scenarios were considered with the goal of obtaining the most understanding of the migration process to cold traps. We illustrate here the use of an ‘air-blast’ to distribute a fine spray of droplets over a few square km of surface. Alternatives included using a single lump of ice or canister of water or a canister containing ice pellets of different sizes. The concern, however, was whether more discrete impactors could bury substantial portions of the water under enough regolith such that its gradual release would be difficult to understand. Exploding a pressurized canister of water just before impact, however, would produce a spray of droplets and vapor that would then simply hit the surface with minimal penetration. We show the result of exploding a pair of canisters at an altitude of 17km with an assumed relative droplet velocity of about 100m/s as the canister is falling at 2000m/s. The 2400kg mass of water is split evenly between two canisters, one at 45N and the other at 60N. The impacts occur at 90W longitude, near noon, on the sunlit side of the moon. In fact, none of these numbers - except the total water mass and the longitude of impact - really matter much. The water mass scales linearly with the magnitude of the signal; the dayside impact causes immediate evaporation off the hot surface. Impacts on the dark side deposit the water onto the surface and the water remains there as ice until sunrise when it sublimates as the surface warms over a period of a few hours.

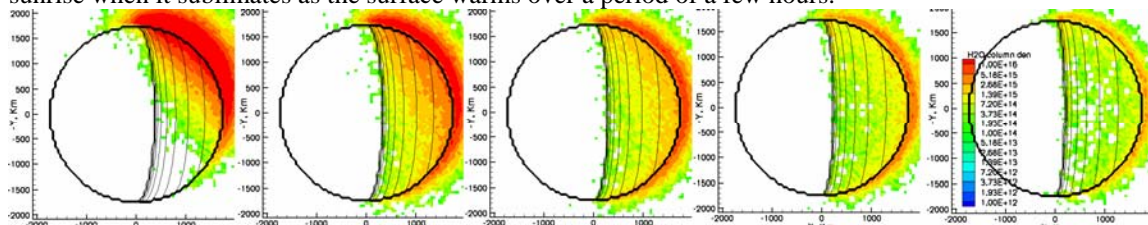


Figure 5. Water column density contours ($\#/\text{m}^3$) following SLAM impacts at 45N and 60N over the right hand sunlit limb at $t=5, 15, 25, 35$ and 45sec . Notice the slow motion of the terminator and the rapid progressive spread south of the atmosphere. The peak column density drops appreciably as molecules condense on the night side (85% after 50ksec) or dissociate (22%). One also sees the development of higher columns along the terminator as it advances toward the night side. Notice that the color bars are different from earlier figures. The water (or D2O) should be detectable in the radio at these times.

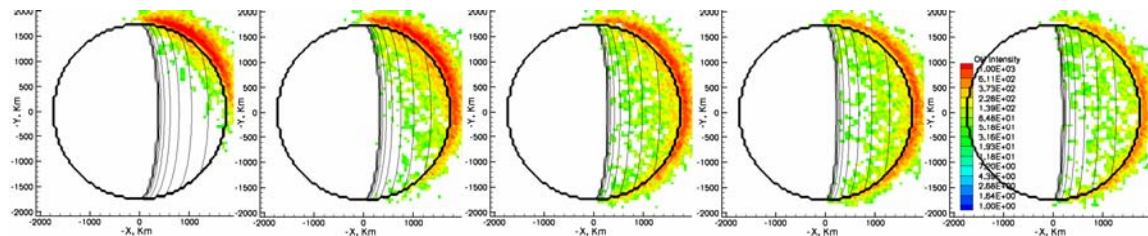


Figure 6. OH brightness corresponding to Figure 5 simulation. Note that the number of OH molecules increases in time due to water photo dissociation. Note too the lack of an OH signal along the terminator even after 50ksec.

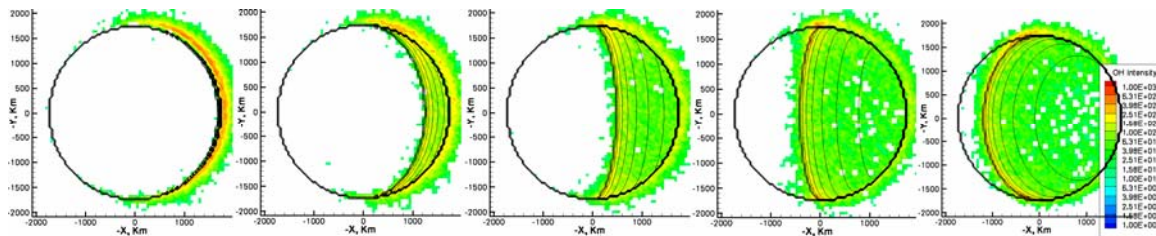


Figure 7. OH brightness, as in figure 6, but at later times (2100, 2300, 2500, 2700 and 2900ksec). The first image shows new moon with a bright OH signal over the right hand limb. 800,000 molecules were simulated. By 2900ksec, 94% were of remaining molecules (H_2O or OH) were stuck on the night side while 6% were aloft. 6% of the original inventory were ionized and not counted in the images. 73% of the particles remaining in the simulation were dissociated to OH.

Once the moon has rotated though about 1 lunar day, most of the molecules have been swept up onto the night side of the dawn (advancing daylight) terminator. This distribution of gas will persist for years as the molecules are slowly lost to ionization or to permanent cold traps. Figure 7 shows the OH atmosphere as it approaches its steady state but declining abundance as the moon rotates. The first image is at new moon and indicates that there would be appreciable

OH brightness over the dawn side. As the terminator advances, we see that OH moves with it and that there would be a declining OH signal over the day side on the right. The atmosphere is largely symmetric north-to-south: memory of the northern latitudes of the initial deposition is lost to diffusion. There is a slight enhancement of the signal over the poles due to the broader region of surface ice accumulation there where the terminator advance speed is slower. The H₂O images look essentially the same but are progressively dimming due to photoionization and photodissociation and the water vapor would be undetectable at these times. OH losses are more gradual due to the greater photoionization lifetime. OH, like H₂O, is subject to photodamage only when it is aloft and in sunlight.

Conclusions: Two types of simulation were done – an impact into a polar cold trap and a disbursement of water at lower latitude. The initial plumes and subsequent sublimation H₂O and OH atmospheres were modeled. For a cold trap impact we find that where to make observations in the initial plume will depend strongly on the velocity distribution of the molecules right near the source. If the gas near the source is collisional, the gas can equilibrate as it expands and it will form a distinct plume front. If, however, the gas is released slowly or is widely spread by the impact, it may be non-collisional and will only form a thin diffused front that may not be visible. The possibly observable signal is linearly proportional to the mass of gas released and 10-20kg appears necessary in order to have much hope of observing the photodissociation product OH. The water itself appears likely too dim to observe. Since the target craters are small compared to the present simulation resolution or to the Earth-based observation resolution, it does not matter much whether the impact occurs as a single event or via a “grape shot” approach with several distributed sub-impactors. Of course, if higher spatial resolution were possible (say, from a chase spacecraft), the distribution of impactors should be re-evaluated.

For a SLAM-type experiment, there would be a clearly visible water and OH plume immediately following the impact. One should be able to observe the latitudinal spread of the vapor at least over several hours. Later, though, photodissociation and condensation will deplete the water signal appreciably and only the OH atmosphere would likely be visible. One could hope to observe the OH over one or more lunations. The key issue here is the gas-surface interaction. If the reactivity, residence times, recombination probabilities, etc. of the water and OH differ much from those assumed above, the results could be greatly different. However, simply seeing the atmosphere slowly dim would not likely tell us much about how efficiently water was transported to permanent cold traps. However, if a lander with an instrument similar to the Apollo SIDE was present near the location of the impact, the gas-surface interactions could be much better understood; the mass flux obtained through simulations could be compared to the observation made by the lander and the gas-surface interaction thereby calibrated.

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