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Signal inversion for exospheric mass spectrometry: Mercury case study

Paul F. Miles *, Stefano A. Livi, Ben D. Teolis

Southwest Research Institute, P.O. Drawer 28510, San Antonio, TX 78228-0510, United States

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ABSTRACT

A new era of exosphere study is beginning with observations being conducted by orbiting neutral mass spectrometers. We have developed a new analysis framework to improve our ability to invert the detection signal of these instruments into local and near-surface densities. By leveraging Liouville's theorem we are able to rapidly reach a source solution that best matches exosphere filling processes to an observable signal. Two approaches are developed in this work, the Liouville Algorithm and a traditional Forward Monte Carlo model that acts as validation. The Liouville Algorithm can be applied to the interpretation of photometric observations but is especially powerful for *in situ* study. This type of analysis is motivated by the velocity dependence of mass spectrometers, which demands that the velocity space be fully resolved. Several examples are described to demonstrate the consistency of the two approaches and highlight the strengths of the new algorithm when used in conjunction with or in lieu of Monte Carlo. Our examples focus on Mercury and the BepiColombo instrument SERENA–Strofio, but these methods apply equally to other surface bounded exospheres like those of the Moon or other airless bodies.

1. Introduction

Mercury's exosphere will be measured *in situ* for the first time by an orbiting spacecraft in the upcoming BepiColombo mission (Benkhoff et al., 2010). BepiColombo will launch in early 2017 and consists of two orbiters: the Mercury Planet Orbiter (MPO) and the Mercury Magnetosphere Orbiter (MMO). Each spacecraft follows an inertial polar orbit with periapsis of 400 km. MPO maintains a lower altitude below 1500 km for detailed surface and exosphere study; MPO traverses much of the magnetosphere to an altitude of ~12,000 km to investigate solar wind and magnetospheric dynamics. Strofio, one of the four units of the MPO SERENA suite (Orsini et al., 2010), is a new generation, high sensitivity mass spectrometer that will detect neutral species of mass 2–100 Da that it encounters with ram velocity enhancement. Beyond identifying the species in the exosphere, Strofio aims to deduce from its measurements the exosphere filling processes active on the surface. All surface bounded exosphere (SBE) studies to date have been conducted remotely or briefly during discrete flyby encounters (i.e. Cassini-INMS). ROSETTA-ROSINA mass spectrometers sample commentary outgassing of predominantly radially flowing neutral particles including molecules (Balsiger et al., 2007). For gravitationally bound SBEs, LADEE-NMS and Strofio's extended observation and sampling capabilities open up new possibilities for surface study not possible with other observation platforms. This interpretation requires an inversion from the detection signal down to a source distribution, a process that requires a new kind of modeling.

An exosphere, by definition, has such a low density that particles travel on ballistic trajectories with low probability of ever interacting with another particle. On planets with conventionally understood atmospheres, the exosphere only exists above an elevation (called the exobase) where collision-free motion dominates. On Mercury and the Moon, as well as numerous other satellites, that exobase is the surface. While making detection difficult, the tenuous nature of surface bounded exospheres carries the advantage that deterministic trajectories can be traced to their origin at the surface. This property makes possible Strofio's top-level science goal of studying the surface via the exosphere.

Most of what we currently know about Mercury's exosphere comes from measurements that are able to detect faint resonantly scattered sunlight. Examples of this are ground based observation (Killen and Ip, 1999) and Messenger MASCS (McClintock and Lankton, 2007). Photometric methods integrate all scattered light in a column passing tangentially over the surface and can rapidly determine the global spatial distribution, flattened along the line of sight. This approach is non-stoichiometric, giving preference to certain atomic species (i.e. sodium, potassium, calcium, and magnesium) whose scattering efficiency, *g*-value, is high enough to permit detection at low densities. Modeling efforts to interpret

* Corresponding author.
E-mail addresses: pfmiles@gmail.com (P.F. Miles), slivi@swri.edu (S.A. Livi), ben.teolis@swri.org (B.D. Teolis).

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these data most often employ Forward Monte Carlo (FMC) techniques that initialize test particles at the surface and follow ballistic trajectories until affected by some loss process (Hodges, 1980). Particle loss for exospheres is dominated by return to the surface and sticking, Jean's escape, or photoionization. Surface conditions are initialized by ansatz with the resultant exosphere model ready for comparison to observation only after lengthy global simulations. When many locations are sampled with near-simultaneity as with remote scattered light measurements, this larger picture is needed so the computational volume is not committed in vein. *In situ* measurement, as will be employed in the upcoming BepiColombo mission, does not benefit from completeness of these simulated data. Concurrent measurements only sample a single point in position space, or in any case very few. Strofio's detection efficiency is also velocity dependent, making a fully populated phase space model key to interpretation of the data. However filling the three dimensions of velocity space at all points in position space in the vicinity of the planet by FMC is profoundly intensive. Such computational overhead makes exploration of parameter space difficult and a comprehensive inversion out of reach. Remote sensing by resonantly scattered light is much less sensitive to the particle velocities and so does not require statistically resolved velocity space populations at a given point. The Doppler shifting of the solar spectrum is key to the *g*-factor of many species observed by resonantly scattered light and is dominated by the planetary motion with a radial velocity up to 10 km/s. In contrast, mass spectrometer transmission functions in comoving velocity space tend to vary over a small fraction of the escape speed at Mercury, or on the order of 0.1 km/s. It is clear that effective simulation for exosphere detection by mass spectrometry is more demanding than for remote observation.

Mercury's surface bounded exosphere is so tenuous that the mean free path of particles in the exosphere is longer than a typical trajectory. The collisionless nature of the exosphere not only enables forward single particle tracing Monte Carlo simulations, it also permits backward particle tracing. Though we don't know the distribution at the point of detection because it is composed of particles from many different source distributions, we can sample at the trajectory's point of origin. This owes to Liouville's theorem stating that phase space density of a collisionless mechanical system is constant along its trajectories. In one respect the reversibility of ballistic trajectories is straightforward, but it requires a fully inverted simulation strategy. Rather than producing a population of test particles at an initial state in proportion to a pre-determined distribution function, a grid in phase space (at the points of detection) is weighted by a distribution function (at the point of origin). This method and its usefulness in inverting *in situ* exospheric measurements will be explored.

2. Simulation

2.1. Forward Monte Carlo algorithm

We developed two models with fundamentally different approaches to evaluate their correspondence and cover a wider range of simulation capabilities. The first is a traditional Forward Monte Carlo (FMC) model consistent with that described by past studies (Hodges, 1980; Wurz and Lammer, 2003; Leblanc and Johnson, 2010). Since FMC has a strong body of supporting work in the literature we adopt our version as the benchmark for evaluating the Liouville model's accuracy.

All particle tracking is recorded in a fixed, planetocentric coordinate system between Mercury's spherical surface ($R_M = 2439.7$ km) and a radius defining the region of interest at $4R_M$. Mercury's rotation period, 58.7 days, is so slow that it allows us to neglect the surface rotation velocity and non-inertial frame forces. This assumption is often adopted by authors (Wurz and Lammer, 2003) for Mercury (and the Moon) since the maximum tangential velocity change is 3 m/s and rotation angle in a characteristic particle flight time, $\tau = \sqrt{4\pi^2 R_M^3 / GM_M}$ is merely 0.3°. All particles are followed individually in 3D double precision. Forces acting on the particle include central gravity, averaged acceleration from radiation pressure, and solar gravity. The later two can often be ignored, with radiation pressure negligible for many species and circumstances and solar gravity typically 1% of Mercury's surface gravity (though as high as 15% at $4R_M$). Since inclusion of these forces comes at trivial cost in the FMC code they are maintained for completeness. An example morphology solution subject to non-central forces is presented in Fig. 1; details of the physical conditions are discussed in Section 3.2.

Particle generation, propagation, and loss evaluation are all conducted on uniform time steps Δt optimized between physical accuracy and computational efficiency. Particle state (position and velocity) is propagated using the conventional 4th order Runge–Kutta method. The time step must be small enough that trajectory errors are inconsequential and so that the model is insensitive to the order of operations. The particles are followed until loss by ionization or crossing the boundary $R_M < r < r_{ROI}$. This region of interest (ROI), typically a few R_M, is meant to constrain the computational volume to only locations relevant to our investigation. Particles that leave the ROI with positive total energy are discarded. When a particle crosses r_{ROI} with a velocity lower than the ROI escape speed, its inbound position and velocity, along with orbit advance time is calculated. Loss rate at all positions outside the ROI is calculated and the particle is retained with probability $e^{-t_{adv}/\tau_{loss}}$, where t_{adv} is the duration of the orbit outside r_{ROI} and τ_{loss} is the characteristic loss time.

Particles are initialized on the surface in accordance with production rate maps that can be modified to represent probable source conditions or parameterized to try to match exospheric

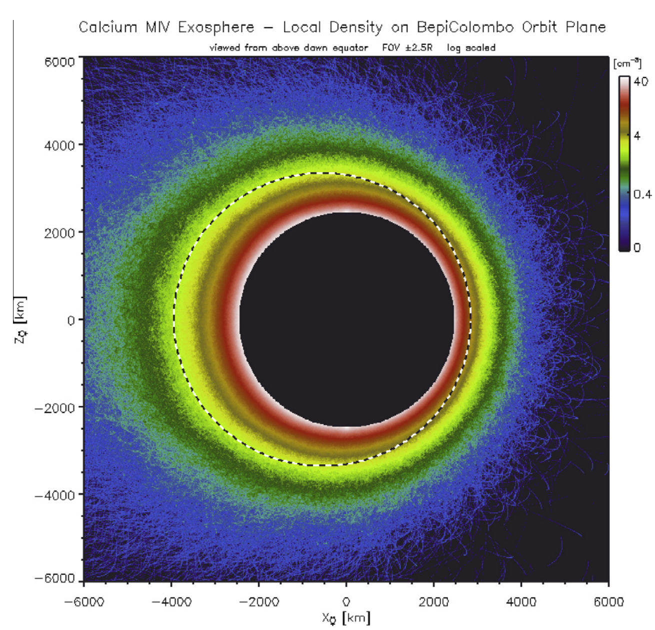

Fig. 1. Calcium exosphere from a uniform impact vaporization source. Local density is on the orbital plane ($y \pm 100$ km) and binned with 20 km spatial resolution. Source distribution is Maxwellian at 4000 K, collisionless trajectories are followed until impact with the surface or escape. Particles are also subject to radiation pressure and photoionization loss from the Sun (right in figure). The simulation tracks 10^5 computational particles simultaneously and recycles lost particles for a total of $2 \cdot 10^7$ trajectories. The BepiColombo orbit is superimposed.