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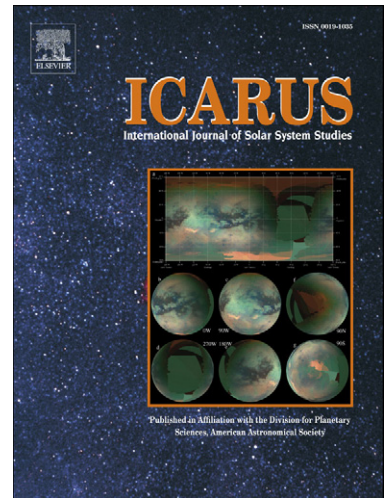
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**The sodium exosphere of Mercury: Comparison between observations during
Mercury's transit and model results**

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Key Words: Mercury transit, sodium exosphere, surface release processes, chemical sputtering

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3 ABSTRACT-

4 In this study we compare the sodium exosphere observations made by Schleicher et
5 al.(2004) with the result of a detailed numerical simulation. The observations, made
6 during the transit of Mercury across the solar disk on 7 May 2003, show a maximum of
7 sodium emission near the polar regions, with north prevalence, and the presence of a
8 dawn-dusk asymmetry. We interpret this distribution as the resulting effect of two
9 combined processes: the solar wind proton precipitation causing chemical alteration of
10 the surface, freeing the sodium atoms from their bounds in the crystalline structure on the
11 surface, and the subsequent photon-stimulated and thermal desorption of the sodium
12 atoms. While we find that the velocity distribution of photon desorbed sodium can
13 explain the observed exosphere population, thermal desorption seems to play a minor role
14 only causing a smearing at the locations where Na atoms are released on the dayside. The
15 observed and simulated distributions agree very well with this hypothesis and indicate
16 that the combination of the proposed processes is able to explain the observed features.

17 **1 Introduction**

18 In 1974, the UVE experiment on board Mariner 10 (Broadfoot et al., 1976) observed
19 a tiny exosphere around Mercury, made of hydrogen, helium, and, probably, oxygen.
20 Starting from 1985 (Potter and Morgan, 1985), many ground-based observations have
21 identified the presence of sodium in Mercury's exosphere. Most of these observations
22 indicate either north-south or dawn-dusk asymmetries (see Killen et al., 2007, for a recent
23 review on observations). Several processes, such as ion sputtering (IS), thermal
24 desorption (TD), photon-stimulated desorption (PSD), and micro-meteoroid vaporization,
25 have been proposed for being responsible for the formation of the sodium exosphere
26 (e.g., McGrath et al., 1986; Hunten et al., 1988; Potter and Morgan, 1997; Madey et al.,
27 1998; Yakshinskiy and Madey, 1999; Killen et al., 1999, 2001, 2004, 2007; Leblanc and
28 Johnson, 2003; Wurz and Lammer, 2003). In fact, Leblanc and Johnson (2003) concluded
29 in their study that the sodium surface density distribution becomes significantly non-
30 uniform from the day to the night side, and from low to high latitudes as well as from the
31 morning to the afternoon due to the rapid depletion of Na atoms in the surfaces of grains
32 mainly driven by thermal depletion. Killen et al. (2004) suggested that ion precipitation
33 increases the diffusion from the interior.

34 Recently, Schleicher et al. (2004) published sodium tangential column densities,
35 derived from observation of Mercury transit of May 2003. These column densities show a
36 strong dawn-dusk asymmetry, an enhancement near the poles, and a moderate north-
37 south asymmetry. Also, the reported scale heights are several 100's of km, which is
38 difficult to reconcile with thermal desorption using realistic temperatures. The aim of the
39 present study is to investigate the possibility that these features may be the result of two
40 combined processes:

41 1) space weathering of the surface by precipitating solar wind protons, which cause
42 chemical liberation of sodium atoms at the surface, and

43 2) photon-stimulated desorption of the liberated sodium from the surface into the
44 exosphere.

45 For this purpose we have developed a numerical model that is able to reproduce the
46 proposed processes and which allows the comparison of the simulated data with the

47 observations. Already in earlier observations Na and K were sometimes found in
48 localized enhancements at elevated latitudes, which was associated with solar wind entry
49 through the magnetospheric cusps. Also dawn-dusk asymmetries were observed earlier,
50 with pronounced Na and K dawn enhancements. A possible explanation for these features
51 was by recycling of Na and K, which become ionized in the exosphere, enter the
52 magnetospheric system, and with some probability are implanted on the surface again
53 (Sprague, 1992; Hunten and Sprague, 1997). Diffusion will bring these atoms back to the
54 surface where they will thermally desorb. Diffusion of Na and K from locations in the
55 regolith to the surface has been studied in detail (e.g., Sprague 1992; Killen et al., 2004).
56 Since diffusion and desorption are both thermally driven processes, they will not occur on
57 the night side and implanted Na and K will accumulate there until Sun rises.
58 Accumulation of Na and K on the night side explains in a natural way the dawn-dusk
59 asymmetry and the enhancements at high latitudes, the latter because of the regions of ion
60 precipitation on Mercury's surface.

61 In Section 2 we give a brief outline of the observations; in Section 3 the numerical
62 model used to simulate the data is described. A discussion of the results is given in
63 Section 4, followed by a summary and conclusion in Section 5.

64

65 **2 Observations**

66 On May 7, 2003, a transit of Mercury across the solar disk occurred. On the occasion of
67 this optimal observation configuration, Schleicher et al. (2004) obtained a series of 2D
68 spectra of the solar sodium resonance line at 589.0 nm (D2), with Mercury being
69 positioned near the field-of-view during the ~2 hours of observation (UT 8:27 to 10:25).
70 At each location h above the limb and at azimuth φ , the column density *along the line of*
71 *sight* $n(h, \varphi)$ has been derived from the observed equivalent widths $W_\lambda(h, \varphi)$ from the
72 curve-of-growth relation for an absorption tube. For the Doppler-width of the absorption
73 profile the value measured from the observed averaged profile of the excess absorption
74 was used. The equations are given in the appendix section. The derived tangential column
75 densities are displayed in figure 1.

76 These observations show a maximum Na density at the planetary limb, exponentially
77 decreasing with altitude. The density around the limb, however, is not uniform: two
78 maxima can be found near the polar regions, with a prevalence of the northern one.
79 There, the Na column density along the line of sight (in the following referred as
80 "tangential column density") is up to $8 \times 10^{10} \text{ cm}^2$, and the estimated volume density at the
81 surface is $2.6 \times 10^3 \text{ cm}^3$ (Schleicher et al., 2004); the presence of sodium is noticeable up
82 to more than 700 km above the surface. Between the two peaks, along the dawn limb, a
83 density excess can be seen. If we integrate the tangential column density over the entire
84 field of view, we obtain a total Na content in the exosphere of 4×10^{27} atoms. From the
85 Doppler width of the line profile of the excess absorption, Schleicher et al. (2004)
86 estimated that the parallel component of the velocity distribution was 1.6 km s^{-1} , which
87 may corresponds to a very high temperature ($\sim 3500 \text{ K}$) if we assume a Maxwellian
88 distribution of the particles.

89

90 [Figure 1]

91

92 **3 Model Description**

93 The general concept, underlying our simulations is that the surface abundance of
94 sodium is depleted by thermal and photon-stimulated desorption, and refueled by the
95 solar wind precipitation. In our study, we assume that for each solar wind proton
96 precipitating onto the surface, with some probability a sodium atom will eventually be
97 available at the surface, as the result of chemical alteration of the mineral grain
98 (described below). Hence, we first evaluated the solar wind proton flux onto Mercury's
99 surface corresponding to the solar activity conditions during the transit observations.
100 Then we simulated the sodium surface composition, which was finally used as an input
101 for our 3D exosphere model.

102 At the time of the considered observations of Mercury exosphere, the planet was 0.45
103 AU away from the Sun, at an anomaly angle of about 150° . The real physical conditions
104 in the solar wind (in particular speed, density, IMF, etc.) and the solar irradiative

105 background near Mercury during the transit are of critical importance for interpretation of
106 its exosphere observations and verification of the applied models. According to the
107 GOES satellite synoptic data, the Sun was relatively quiet during the whole transit of
108 Mercury on May 7, 2003, with just 3 X-ray events of C-class registered, of which only
109 one in the northern hemisphere (N15E88, C2.2 from 10:17 till 10:27) took place during
110 the performed observations, near the end of the transit. From these data it is justified that
111 we use as an input the average quiet Sun radiation flux in our model.

112 Because of the absence of *in-situ* measurements of the solar wind plasma parameters
113 near Mercury at the time of the transit, we used for their estimation the solar wind data
114 measured by the ACE satellite which is located downstream of Mercury at the Lagrange
115 point L1 at 1.5×10^6 km from the Earth. The fact that Mercury's transit was observed from
116 the Earth, and the ACE spacecraft is also located close to the Sun-Earth line, it makes it
117 possible to assume that the solar wind flow measured by ACE within the next 1 to 2 days
118 after the Mercury transit belongs to the same stream of the solar wind that passed near
119 Mercury.

120 Figure 2 shows the ACE data, measured components of magnetic field, solar wind
121 proton speed and density, as well as the distance from the spacecraft to Earth, during the
122 Mercury transit on May 7, 2003 (day of year 127) and two days after the transit
123 (<http://www.srl.caltech.edu/ACE/ASC/level2/index.html>). As it can be seen, a relatively
124 fast interplanetary CME passed ACE with a velocity ~ 890 km s⁻¹) on May 9, 2003.

125

126 [Figure 2]

127

128 However, taking into account the speed of this CME and mutual location of Mercury
129 and the ACE spacecraft, one can calculate that the CME passed Mercury after the transit.
130 Similar treatment of other parts of the solar wind speed curve measured by ACE makes it
131 possible to conclude that the solar wind portion with the speed ~ 780 km s⁻¹, registered by
132 ACE on May 8, 2003, was very likely passing Mercury on May 7, 2003 during the transit
133 observations. Taking into account the decrease of the solar wind speed with distance from

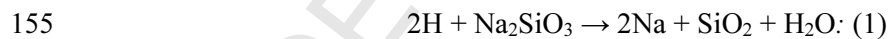
134 the Sun, we extrapolate ACE values down to the Sun and estimate the solar wind speed
135 near Mercury during the transit on May 7, 2003 as $\sim 800 \text{ km s}^{-1}$. Using ACE magnetic
136 field measurements (see Figure 2) and taking into account the decrease of magnetic field
137 with distance ($\sim 1/r^2$), as well as solar wind motion, the components of the IMF at
138 Mercury during the transit on May 7, 2003 can be estimated as (-20, 10, -10) nT.

139 The proton precipitation flux, which is needed for the exosphere modeling, was
140 obtained by using a single- particle model (Delcourt et al., 2003, Mura et al., 2005). The
141 original magnetic field model (Luhmann and Friesen 1979, Delcourt et al., 2003) was
142 adapted to the specific conditions at Mercury by adding the IMF field. The resulting
143 proton flux onto the surface has the general shape similar to that presented in Mura et al.
144 (2005). The total flux in the northern hemisphere is about $4 \times 10^{25} \text{ s}^{-1}$, while the negative
145 IMF x -component introduces a flux enhancement in the southern hemisphere similar to
146 the results in Sarantos et al. (2001).

147

148 **3.1 Chemical alteration of the surface composition**

149 The impact of energetic ions (solar wind or magnetospheric ions) on the surface
150 affects the topmost layer of the regolith. The induced processes are ion implantation,
151 sputtering of surface material, and chemical alteration, where the latter allows the
152 breaking of existing and creation of new chemical compounds. Production of sodium and
153 water by proton sputtering of sodium-bearing silicates was considered by the following
154 mechanism (Potter, 1995)



156 The free energy of this reaction is -4.7 kcal/mole, therefore it will proceed
157 spontaneously; however, the activation energy is unknown. Together with the liberated
158 Na, water is produced, with the supply rate of water molecules being half the supply rate
159 of Na by this process. The solar wind protons are implanted into the regolith grains and
160 are neutralized there. The proton fluxes onto the surface are high and saturation of the
161 regolith grains with hydrogen can be safely assumed, which assures the availability of
162 hydrogen for the chemical reaction given above. In summary, hydrogen reacts with the

163 sodium bearing rock, the Na atoms are liberated from their chemical bounds in the
164 crystal. Since the ion implantation is close to the surface, the atomic Na is produced near
165 the surface and will diffuse thermally to the surface. Atomic Na at the surface can be
166 easily released into the exosphere either by TD or by PSD (Yakshinskiy and Madey,
167 1999; 2004; Yakshinskiy et al., 2000). The process described in equation 1 causes also
168 the production of water. The global source rate for H_2O should be roughly half of that of
169 Na, even if the total exosphere content can be different because of different lifetimes. It is
170 worth noting that, recently, FIPS instrument on board MESSENGER has discovered
171 water group ions (Zurbuchen et al., 2008).

172

173 **3.2 Surface composition model**

174 The planetary surface was divided into 24×48 (latitude, longitude) surface elements.
175 Each surface element had a variable value for the sodium relative composition, $C(t)$,
176 which gives the numerical fraction of free sodium in the elementary surface with respect
177 to the total surface density. The time resolution of the simulation was 10 minutes; the
178 simulation lasted for a full Mercury's day (176 days). For each surface element, we
179 calculated the temporal evolution of $C(t)$, taking into account:

- 180 i) the planetary rotation and orbit;
- 181 ii) the solar wind proton precipitation;
- 182 iii) the photon-stimulated desorption;
- 183 iv) the thermal desorption;
- 184 v) the photoionization of sodium.

185 At each step, we first calculated the position of each surface element with respect to
186 the Sun, taking into account the planetary rotation and orbital speed. The apparent
187 angular velocity of the Sun is assumed constant. In fact, we were far from the perihelion
188 where the apparent angular velocity has large variability (where it is retrograde for few
189 days).

190 Then, for each surface element we calculated the photon-stimulated desorption rate:

191
$$\Phi_{PSD}(t) = N C(t) \Phi_{\gamma} \sigma \cos(\alpha) = A C(t), (2)$$

192 where Φ_{PSD} is the PSD neutral flux, Φ_{γ} is the relevant photon flux ($3 \times 10^{15} \text{ cm}^{-2} \text{ s}^{-1}$ at 1
193 AU; the flux is scaled as $1/r^2$), σ is the PSD cross-section ($2 \times 10^{-20} \text{ cm}^2$, Yakshinskiy and
194 Madey, 1999), N is the surface density ($7.5 \times 10^{14} \text{ cm}^{-2}$, Killen *et al.*, 2001), α is the
195 instantaneous angle from the sub-solar point (for $\alpha > 90^\circ$, Φ_{psd} is obviously zero).

196 To calculate the value of C at the equilibrium, we set $C(0) = 0$ and calculate the value
197 of $C(t)$ at the next integration step, by solving the following differential equation:

198
$$N \frac{dC(t)}{dt} = k \Phi_{PREC} - \Phi_{PSD}(t) = k \Phi_{PREC} - A C(t), (3)$$

199 where A is defined in Eq. 2; Φ_{PREC} is the flux of precipitating protons, and k is the
200 product of the overall process yield and the probability for the proton to interact with a
201 Na atom in the surface; by considering the fraction of Na bearing minerals (Feldspars) in
202 the regolith (Wurz *et al.*, 2008), here we have assumed that k is about 5%.

203 When a surface element is on the dayside, $C(t)$ raises or decreases exponentially, until
204 it reaches the equilibrium:

205
$$\Phi_{PSD} = k \Phi_{PREC}; (4)$$

206 the time-scale for the equilibrium is:

207
$$T_{SC} = (\Phi_{\gamma} \sigma)^{-1} (5)$$

208 which is of the order of one hour. When a surface element is on the night side, $C(t)$
209 increases if $\Phi_{prec} > 0$ (i.e., magnetospheric protons precipitate onto the surface) until this
210 surface element reaches the dawn terminator. Then, $C(t)$ is rapidly decreased by PSD
211 following Eq. 3. This leads to a maximum of concentration close to the dawn terminator,
212 and hence to a dawn-dusk asymmetry of C .

213 Note that the total amount of sputtered sodium particles has to be proportional (see
214 Eq. 4) to the total flux of proton precipitating onto the surface. Hence, the parameters Φ_{γ} ,
215 and σ influence only on time scales of the simulated density, but they have very small
216 impact on the results at the equilibrium.

217 Concerning thermal desorption, we find that particles released by TD always fall
 218 down onto the surface because their velocities are much lower than the escape velocity.
 219 Hence, TD does not contribute to the net flux from the surface. However, as outlined
 220 below, the Na atoms fall back within an area of radius <300 km (about 100 km on
 221 average, in our simulation). Thus, thermal desorption will cause a smearing of the places
 222 of Na release on the dayside. To include this effect in our simulation, we first estimated
 223 the TD rate:

$$224 \quad \Phi_{TD}(t) = \nu N C(t) e^{-\frac{U_{TD}}{k_B T}}, \quad (6)$$

225 where Φ_{TD} is the neutral flux, ν is the vibration frequency of the adsorbed atoms (10^{13} s^{-1} ,
 226 Hunten et al., 1988), N is again the regolith surface density, and U_{TD} is the binding
 227 energy. This last parameter has a big influence on the desorption rate, and has to be
 228 evaluated carefully (Yakshinskiy et al., 2000). Yakshinskiy et al. (2000) determined an
 229 energy range for U_{TD} between 1.4 to 2.7 eV. In this study, however, we used an average
 230 value for $U_{TD} = 1.85 \text{ eV}$, like Leblanc and Johnson (2003). The local temperature of the
 231 surface was assumed to vary according to (Leblanc and Johnson, 2003; Wurz and
 232 Lammer, 2003):

$$233 \quad T(\alpha) = T_n + (T_d - T_n) [\cos(\alpha)]^{1/4} \quad (7)$$

234 where the sub-solar point temperature (T_d) is scaled between 590 K and 725 K (Vilas,
 235 1988) according to the planetary distance from the Sun. The night side temperature was
 236 always 110 K.

237 Then, for each surface element, we distributed the flux Φ_{TD} to a large number of test-
 238 particles. We simulated their ballistic trajectories, starting with a Maxwell-Boltzmann
 239 surface velocity distribution with the proper surface temperature. We then evaluated the
 240 precipitation position and the lifetime of each test particle, and we redistributed the flux
 241 Φ_{TD} accordingly (decreased by photoionization, with lifetime 10^4 s). This latter flux can
 242 be considered as an additional source in Eq. 3, while Φ_{TD} can be added to Φ_{PSD} in the
 243 sink section of Eq. 3. Hence (as far as photoionization is negligible), the net effect is just
 244 a time and spatial blurring of the solution of Eq. 3.

245 Our simulation lasted one complete Mercury day. However, if we take C in a
 246 reference frame fixed with respect to the Sun (i.e., MLT, Mercury Local Time), then C
 247 reaches a stable equilibrium after about half a rotation or less (i.e. tens of days). In Figure
 248 3 we show intermediate steps of the temporal evolution of parameter C at different times.
 249 After one hour, the dayside configuration is more or less stable. In Figure 4a we show the
 250 values of Φ_{PSD} at the equilibrium, in a MLT vs. latitude map, and, for comparison, the
 251 proton precipitation flux (panel b). Since the flux in the dayside is basically proportional
 252 to the proton flux (Eq. 4), the two panels are similar in that area. The dawn-dusk
 253 asymmetry of the composition is responsible of the enhancement of Φ_{PSD} close to the
 254 dawn terminator ($\sim 6:00$ MLT).

255 [Figures 3, 4]

256

257 3.3 Exosphere model

258 To simulate the Na tangential column density in the exosphere of Mercury, we used a
 259 Monte-Carlo model. The energy distribution of the emitted Na atoms was extrapolated
 260 (Johnson *et al.*, 2002) by laboratory measurements of electron-stimulated desorption
 261 (ESD) of adsorbed Na from amorphous ice. It was assumed that the electron energy has
 262 little impact on the emitted neutral energy, and that PSD and ESD cause desorption of
 263 atoms via similar electronic processes. Johnson *et al.* (2002) have found a good analytical
 264 description of the energy spectrum using the following function:

$$265 \quad f(E) = \beta(1 + \beta) \frac{EU^\beta}{(E + U)^{2+\beta}}, \quad (8)$$

266 where β is the shape parameter (0.7 for Na) and U is the characteristic energy, which is of
 267 the order of 0.05 eV, for Na. Since the maximum ejection energy should be lower than
 268 the photon energy, we used a cut-off function (at about 10 eV) to eliminate the high-
 269 energy tail of the function, which we consider unphysical. To evaluate the effect of the
 270 source distribution function on the simulated exospheric density, we have also used a
 271 different source function:

272
$$f(E) = \frac{E}{(k_B T)^2} e^{(-E/k_B T)} \quad (9),$$

273 since other authors (Yakshinskiy and Madey, 1999, Leblanc and Johnson, 2003)
 274 suggested that the energy spectrum has a Maxwellian Boltzmann flux distribution, with T
 275 of the order of 1000 to 1500 K.

276 A large number ($>10^6$) of test particle trajectories were simulated; a weight w was
 277 associated to each test particle to reproduce the flux in Eq. 2 (see details in Mura *et al.*,
 278 2007). The trajectories were calculated using the classical equations of motion, including
 279 gravity and radiation pressure acceleration. The radiation pressure acceleration, for Na,
 280 can be up to 54% of the surface gravity, ranging between 20 and 200 cm s^{-2} , being
 281 function of the photon flux and of the amount of Doppler shift out of the Fraunhofer
 282 features (Smyth and Marconi, 1995; Potter *et al.*, 2002). Here we calculate this
 283 acceleration as in Leblanc and Johnson, (2003), i.e. we calculate the Doppler shift as a
 284 function of each particle's velocity, and then we calculate the acceleration; on average, at
 285 0.45 AU, this is 60 cm/s^2 , in the anti-sunward direction.

286 We defined a 3D cubic accumulation grid extending between $-12 R_M \leq x \leq 3 R_M$ (30
 287 steps) and $-2 R_M \leq y, z \leq 2 R_M$ (60 steps), with $R_M=2439$ km being the radius of Mercury
 288 and x pointing towards the Sun, z pointing towards north pole (MSE reference frame).
 289 The grid has wider x boundaries to enclose all the Sodium (see, for example, Potter *et al.*,
 290 2002). The Na density inside one grid cell was calculated taking into account the number
 291 of test particles, the weight w and the lifetime inside the cell. Finally, we integrated the
 292 simulated Na density along the x direction to obtain the tangential column density, to be
 293 compared directly with the observations.

294

295 **4 Results and discussion**

296 **4.1 Model results**

297 To reproduce the observed tangential column density, we need to assume some values
 298 for the simulation parameters. As already mentioned, TD causes just a temporal and
 299 spatial smearing of the signal, so the related physical parameters have a small impact on

300 the simulations. Leblanc and Johnson (2003) arrived at the same conclusion when they
301 compared the residence time of sodium atoms related to TD, PSD and sputtering in
302 Mercury's upper surface versus the solar zenith angle. It was found that TD is the most
303 efficient desorption process at low zenith angles but at higher zenith angles PSD and
304 sputtering become more efficient.

305 One of the most important parameters to be considered is the energy U (in Eq. 8),
306 which controls the energy distribution of the emitted sodium atoms. A best fit between
307 data and simulations to find the optimum value for U is not easy; however, we found that
308 a good agreement between observations and simulation can be obtained by taking $U =$
309 0.086 eV. In Figure 5a the result of the simulated sodium tangential column density is
310 given. As it can be seen, the simulated data show the same features as the observed ones
311 (Figure 1), which are the dawn-dusk and the north-south asymmetry. In the simulation we
312 find that the maximum tangential column density is located at the limb in the north-dawn
313 region and has a value of about $6 \times 10^{10} \text{ cm}^{-2}$.

314

315 [Figure 5]

316

317 Moreover, the apparent scale-height is similar to that in the observations (Figure 1).
318 This parameter results from the chosen energy distribution for the release of the particles:
319 a more energetic source distribution produces higher scale-heights. To evaluate how
320 sensitive our model is to the chosen energy distribution, we produced a similar
321 simulation, using Eq. 9 instead of Eq. 8, with $T=1000$ K. This energy distribution is
322 somewhat less energetic than the previous one (Mura *et al.*, 2007); the result of the
323 simulation is shown in Figure 5b. There is a substantial resemblance between the two
324 simulations, and it is difficult to tell just by visual inspection which fits better with the
325 observations. However, apparently the scale height of the first energy distribution (Eq. 8)
326 fits better with the observations.

327 More information on the energy distribution of the source can be obtained from the
328 observed velocity distribution. To study the velocity distribution of Na in the x direction,

329 a fourth dimension of the accumulation grid, consisting of 100 velocity steps from -10 to
330 +10 km/s, was included. In this way we were able to estimate the velocity distribution
331 shown in Figure 6. According to Schleicher et al. (2004), the observed velocity
332 distribution can be reproduced by a Gaussian function with a width $v_{th} = 1.6$ km/s. As
333 shown in Figure 6, the simulation is able to reproduce this feature reasonably well using
334 the energy distribution of Eq. 8. The small secondary peak, visible at about 2 km/s in the
335 figure, is probably due to the radiation pressure acceleration, which originates in the tail
336 up to few R_M behind the planet. In fact, this is the value that can be obtained by simple
337 calculations assuming an acceleration of -60 cm/s² and a tail size of about 3 R_M as
338 reported by Potter et al. (2002). For comparison, the velocity distribution obtained using
339 Eq. 9 (dashed line in Figure 6) substantially differs from the previous two. We concluded
340 that the source energy distribution is likely to be more energetic than a Gaussian at 1000
341 K.

342 The effect of the radiation pressure acceleration on the observed column densities is
343 negligible; in fact, since this force acts parallel to the line of sight, the first order effect is
344 null. To evaluate the effect of the radiation pressure, we removed this force from the
345 model: the simulated tangential column densities were very similar, almost identical, to
346 those shown in Figure 5a; however, the fraction of escaping Na particles dropped down
347 by a factor 2. We concluded that the radiation pressure acceleration, in the present
348 configuration, is responsible of about 50% of the Na escape rate.

349 [Figure 6]

350 Table 1 gives a summary of the observed and simulated physical quantities. The
351 tangential column densities are very close. However, the typical scale height in the model
352 calculations is higher than in the observations and therefore the total amount of Na in the
353 simulation is higher than that in the observations.

354 [Table 1]

355 The gardening rate at Mercury is estimated to cause a grain lifetime on the surface of
356 the order of $10^4 - 10^5$ years (Horz *et al.*, 1991); a complete discussion about how this
357 lifetime implies diffusion-limited supply rates in the exosphere of Mercury can be found
358 in Killen *et al.* (2004). These authors found that a supply rate up to 10^7 cm⁻² s⁻¹ is

359 consistent with a diffusion limited supply of Na. For comparison, in our study, the
 360 average PSD flux on the surface was found to be of the order of $10^7 \text{ cm}^{-2} \text{ s}^{-1}$, but the local
 361 PSD rate (see Figure 4) was higher in the areas of intense proton precipitation. This is
 362 consistent with the results of Killen *et al.*, (2004) when saying that higher supply rates
 363 can be the result of ion-enhanced diffusion.

364

365 **4.2 Ion sputtering**

366 The presence of the two maxima observed at high latitude is a hint for the presence of
 367 a space weathering process, such as ion sputtering. Hence, we simulated the Na
 368 exospheric density resulting from this process. We assumed that the proton precipitation
 369 flux was the same as shown in Figure 4b. Each impinging proton has some probability
 370 (yield, Y) to extract a neutral sodium atom from the surface; this probability is related to
 371 the proton energy (Lammer *et al.*, 2003); we have assumed an averaged value of 10% for
 372 simplicity. Other solar wind components, like α particles or high-charge-state particles,
 373 produce a comparable amount of ion sputtering (Johnson and Baragiola, 1991).
 374 Assuming that their precipitation patterns are similar to that of protons, we assumed a
 375 weighted yield of 20% as an upper limit for sputtering. The resulting Na flux is hence:

$$376 \quad \Phi_{IS} = Y c \Phi_{PREC} \quad (10)$$

377 where c is the surface abundance of sodium in the surface. While thermal and photon-
 378 stimulated desorption act on the extreme surface (a few monolayers, where the
 379 concentration of Na should be calculated as in Section 3.2), ion-sputtering extracts
 380 sodium from deeper and in a stoichiometric way. Hence, we assumed c uniform all over
 381 the surface and equal to 0.5% (Goettel, 1988).

382 The energy distribution of the ejecta can be simulated using the following function
 383 (Siegmond, 1961; Betz and Wien, 1994):

$$384 \quad f_s(E_e) \propto \frac{E_e}{(E_e + E_b)^3} \left[1 - \left(\frac{E_e + E_b}{E_i} \frac{(m_H + m_{Na})^2}{4 m_H m_{Na}} \right)^{\frac{1}{2}} \right], \quad (11)$$

385 where E_e is the ejection energy, E_i is the proton energy, E_b is the binding energy (here 2
 386 eV, as in Lammer *et al.*, 2003). We used this as an input for the exospheric model, then
 387 we integrated the result to obtain the tangential column densities to be compared with the
 388 observations. The result is shown in Figure 7a. There are at least three discrepancies
 389 between this simulation and the observations:

- 390 • the tangential column densities are about two orders of magnitude lower than those
 391 observed; in fact, for each proton, only 0.05% of Na is sputtered, i.e. released into the
 392 exosphere (Y times c).
- 393 • the simulated scale-heights are considerably larger than those observed; in fact the
 394 energy distribution in Eq. (11) is more energetic than that in Eq. (8);
- 395 • there is no evident dawn-dusk asymmetry.

396 In summary, ion sputtering, alone, is not able to explain the observed features.
 397 Moreover, since the contribution to the total column densities is only about 1% of the
 398 observed values, which is consistent with the results from Wurz *et al.* (2007), it is
 399 possible to neglect its contribution in the particular configuration of the present study. On
 400 the other hand, since the process is more energetic, most of sputtered Na are either
 401 photoionized (due to longer ballistic time) or lost (due to Jeans escape). Hence, this
 402 process must be taken into account while simulating the Na tail, as in section 4.4.

403 **4.3 Meteoritic and micrometeoritic impact vaporization**

404 Mercury is exposed to the constant precipitation of particles of small sizes ($<100 \mu\text{m}$),
 405 impacting the surface at a mean velocity of 20 km/s (Cintala, 1992), churning the regolith
 406 and vaporizing the surface. Larger objects impact the surface as well, causing local
 407 enhancement of the sodium exospheric density (Mangano *et al.*, 2007), but the
 408 contribution by these meteorites to the global Hermean exosphere is considered to be
 409 negligible (Killen *et al.*, 2007). Morgan *et al.* (1988) reported an average value of 2×10^5
 410 ($\text{cm}^{-2} \text{s}^{-1}$) released Na at aphelion, a factor 2 higher than the value reported by Cintala
 411 (1992) (see Killen *et al.*, 2007 for a detailed discussion). The first value, which we have
 412 used here as a worst case, is a factor 100 lower than our averaged PSD flux. If we assume
 413 that the ejecta have a thermal velocity distribution at about 2500 K (Killen *et al.*, 2007),

414 and that the precipitating particles are uniformly distributed over the surface, we obtain
415 the simulated Na tangential column densities of Figure 7b. Obviously, the precipitation
416 flux could be not uniform on the surface and so our estimation of the density due to
417 impact vaporization is probably locally inaccurate to a factor of two (Killen et al., 2004);
418 however, this simulation shows that, at a first order of approximation, we can discard
419 impact vaporization as a main Na source in this particular observing configuration.

420 **4.4 The sodium tail**

421 The presence of a sodium tail, extending in the anti-sunward direction, has been first
422 observed by Potter *et al.* (2002). Since this is an important feature of the sodium
423 exosphere, it should be taken into account by any model. In this section we discuss the
424 formation of the Na tail within our present model. The sodium tail is formed by those Na
425 atom whose ejection energy is higher than the gravitational escape energy (2.07 eV), or
426 by that atoms that can overcome the gravitational field thanks to a partial contribution of
427 the radiation pressure acceleration. These particles are accelerated by the radiation
428 pressure in the anti-sunward direction. In addition, photoionized Na can be picked-up by
429 the solar wind. The radiation pressure acceleration during the observation time, at 150°
430 anomaly angle, was about 60 cm s⁻², well below the maximum (200 cm s⁻¹), which occurs
431 at about 60° and 300° anomaly angle (Smyth and Marconi, 1995; Potter *et al.*, 2002). The
432 relation between the solar radiation pressure and the tail formation has been recently
433 investigated by Potter and Killen (2008). According to these authors, the tail is not
434 detectable from Earth with a radiation pressure below about 100 cm s⁻². In our case, the
435 acceleration was lower (60 cm s⁻²), but the proton precipitation was very intense, due to
436 the extreme solar wind conditions (see section 3). Hence, in our case we should obtain a
437 very faint tail. To simulate it, we used all the four processes described previously as a
438 source for our exospheric model; the PSD source function is that given in Eq. 8. The
439 result is shown in Figure 8. Such a tail is very faint and probably hard to observe from
440 Earth; in fact, in the nightside, the densities are 2 to 4 orders of magnitude lower than
441 those in the dayside. The contribution of thermal desorption is negligible, since only 3%
442 of the desorbed particles do not re-impact onto the surface, and only due to
443 photoionization. Also impact vaporization does not contribute significantly, since only
444 10% of the ejected particles are able to escape, mostly due to photoionization. The

445 fraction of particles desorbed due to photon-stimulation that escape was found to be
446 between 1% and 10%, depending on the source function we used, while 50% of the ion-
447 sputtered particles are able to escape. However, since surface flux for PSD is higher, both
448 these two processes contribute significantly to the formation of the sodium tail. A
449 summary of these values can be found in table 2. We conclude that, in general, our model
450 is consistent with the existence of a sodium tail.

451 [Table 2]

452 Recently, the sodium tail has been observed during the first MESSENGER flyby
453 (McClintock *et al.*, 2008). These authors have found that, at $2 R_M$ down the tail, the
454 traverse column density was $\sim 3.4 \times 10^9$ atoms cm^{-2} . In our simulation, we found, for the
455 same quantity, a value slightly less than 10^9 cm^{-2} . Even if a detailed comparison is
456 beyond the scope of this study, we note that there is no contradiction between these
457 values. In fact, during those MESSENGER observations, the radiation pressure was close
458 to its maximum, i.e. three times higher than that assumed in this study.

459 **5 Model limitations**

460 A critical hypothesis in our model is to assume that the proton precipitation flux (on
461 the night side) is constant over a very long time-scale (\sim weeks), which is clearly a major
462 simplification. However, as discussed in Section 3.2, the time-scale for the equilibrium
463 between proton fluxes and PSD fluxes is very short on the dayside (about one hour).
464 Therefore, we propose the following explanation. The north-south asymmetry is due to
465 the proton precipitation on the dayside, which rapidly results in an enhancement of the
466 Na density in the high latitude regions (by means of the combined mechanism described
467 in Section 3.1). The dawn-dusk asymmetry, on the other hand, is caused by the planetary
468 rotation, which is always in the same direction (except a few days of apparent retrograde
469 Sun motion), and by the presence of some magnetospheric proton precipitation on the
470 night side; such a precipitation is predicted for most of the IMF conditions (see, for
471 example, Kallio *et al.*, 2003, or Mura *et al.*, 2005). Hence, in this first study we did not
472 perform a detailed estimation of the proton circulation and precipitation; moreover, the
473 TD effect causes a smearing of the surface composition, so that a detailed map of the
474 proton precipitation is not needed.

475

476 **6 Summary and Conclusions**

477 We presented a model for the formation of Mercury's sodium exosphere as it was
478 observed during the Mercury transit on May 7, 2003, involving two steps for the release
479 of Na atoms from the surface. The first step is the liberation of Na from the chemical
480 environment of the mineral by implantation of energetic hydrogen and subsequent
481 chemical reaction. The second step is photon-stimulated desorption of Na into the
482 exosphere. Thermal desorption only smears the location where the Na atoms are released.
483 For the simulation of this two-step process, a 3D exospheric model was adapted
484 accordingly.

485 Comparison of our model results with measurements by Schleicher et al. (2004) show
486 good qualitative agreement in the structure of Mercury's sodium exosphere. Our model
487 reproduces the high latitude features, and the asymmetries in the north-south and in the
488 dawn-dusk direction. Concerning the quantitative comparison, the simulated Na total
489 amount is of the same order of magnitude as that derived from observation. There are,
490 however, at least 3 parameters that control this value:

491 1) *The scale height.* The parameter U in Eq. 8 controls the energy distribution of the
492 PDS emitted Na, and hence the scale-height of the simulated exosphere. A larger scale-
493 height in the model causes the dayside population (which is the most relevant one) in the
494 simulations to rise above the planetary limb and therefore to become more visible from
495 the night side. Hence, the value of U is also related to the overall Na amount. Since the
496 scale-height of the simulation is higher than that of the observation, this may suggest that
497 a lower value for U should be used. We have also performed some simulations, using a
498 simple Gaussian distribution function (with temperature of 1000 K), instead of Eq. 8.
499 Even if the simulated densities (Figure 5b) and scale-heights were very similar to the
500 observed ones, such energy distribution failed to explain the measured velocity spread.

501 2) *The proton flux.* The simulated densities are proportional to the total precipitation
502 rate, and the shape depends on that of the proton flux onto the surface. In particular, the
503 proton precipitation onto the nightside, thanks to the rotation of the planet, is responsible
504 for the formation of the dawn dusk asymmetry. In addition to proton precipitation other

505 magnetospheric ions will precipitate as well. For example, Na^+ precipitation occur
506 nightside (see Delcourt *et al.*, 2003), which will increase the surface weathering effects.
507 In fact, according to Potter (1995), in the case of chemical sputtering caused by Na^+ , the
508 yield should be higher. In any case, the inclusion of any other precipitation or
509 replenishing process occurring on the nightside, which we have neglected in this first
510 simulation, will cause an enhancement of the simulated dawn-dusk asymmetry, and, in
511 fact, the dawn-dusk asymmetry is a somewhat more evident in the observations than in
512 the model. The effect of other ion precipitation on the nightside, as well as impact
513 vaporization, not included in the present simulation, can be estimated using the model. In
514 fact, adding an hypothetical, uniform value of Sodium $2 \times 10^6 \text{ cm}^{-2} \text{ s}^{-1}$ lead to a tangential
515 column density of $4 \times 10^{10} \text{ cm}^{-2}$, which is what is observed close to the dawn terminator.
516 In this way, it is possible to estimate the upper limit of the Na replenishment process that
517 can occur in the nightside as $2 \times 10^6 \text{ cm}^{-2} \text{ s}^{-1}$.

518 3) *The process yield.* Here, we have assumed that the averaged process yield is 5%,
519 and the simulated densities scale linearly with this parameter. Recently, Sarantos *et al.*,
520 (2008) have studied the influence of ion-enhanced PSD at the Moon, following the
521 mechanism proposed by Potter (2000); the mechanism is somewhat different from that
522 proposed here, but the global result is the same. These authors observed that the ion flux
523 increased to $3 \times 10^7 \text{ cm}^{-2} \text{ s}^{-1}$ during the passage of the Moon in the Earth's magnetotail,
524 and as a result, the PSD rate was higher then expected, and of the order of $2 \times 10^5 \text{ cm}^{-2} \text{ s}^{-1}$.
525 This would result in an averaged yield of the order of 1%, which is in good agreement
526 with our assumption, also because one could expect that the yield of the process may
527 depend on the ion energy ranges, that may differ from the Moon to Mercury.

528 Since the PSD release Na flux is proportional to the proton precipitation, one could
529 expect that, on the dayside (which is not visible in the observation) the Na exospheric
530 densities should resemble the proton flux in Figure 4b. As shown in Figure 8, however,
531 this is not the case. In fact, on the dayside also the Na population from thermal desorption
532 is present. Moreover, in the case of a non-uniform surface source, Mura *et al.*, (2007)
533 have estimated that the characteristic horizontal scale lengths of the exosphere are about a
534 factor 2 longer than that of the source, due to the ballistic trajectories of the particles.

535 Another effect, not yet included in this model, can be the Na release due to thermal
 536 diffusion, that should be maximal in the sub-solar point region, between our two
 537 precipitation maxima (Killen *et al.*, 2004).

538 The Na density in the tail predicted by our model is also in substantial agreement with
 539 that observed during the first MESSENGER flyby (McClintock *et al.*, 2008). Moreover,
 540 chemical sputtering of Na by protons causes also the production of water, and it is worth
 541 noting that the FIPS instrument on board MESSENGER has discovered such water group
 542 ions in the exosphere of Mercury (Zurbuchen *et al.*, 2008).

543 In a separate simulation run we have tried to simulate the Na density in a different
 544 way, by assuming that the proton precipitation causes only direct ion-sputtering of
 545 surface sodium. However, the simulated scale-heights were larger and the tangential
 546 column densities were about 100 times lower than those observed, because ion-sputtering
 547 has a lower yield (5%) and a more energetic velocity distribution. On the other hand, it is
 548 difficult to explain North-South asymmetries without including plasma precipitation
 549 effects. We also simulated the Na exospheric density arising from impact vaporization;
 550 also in this case, the tangential column densities were lower by a factor 100. Presently, it
 551 is therefore not possible to explain these observations without including a process that
 552 combines ion-precipitation and PSD via the chemical alteration of the surface induced by
 553 ion impact.

554

555 Appendix

556 From the detected excess absorption, densities of the sodium atoms in Mercury's
 557 exosphere could be derived using the following equations:

$$558 \quad W_{\lambda}(h, \varphi) = \int_{-\infty}^{+\infty} \frac{\Delta I_{\lambda}(h, \varphi)}{I_{\lambda}} \quad (\text{A1})$$

$$559 \quad \frac{\Delta I_{\lambda}(h, \varphi)}{I_{\lambda}} = 1 - \exp(-\tau_{\lambda}) \quad (\text{A2})$$

$$560 \quad \tau_{\lambda} = \kappa_{\lambda}^{(A)} n(h, \varphi) \quad (\text{A3})$$

$$561 \quad \kappa_{\lambda}^{(A)} = \kappa_0^{(A)} \frac{1}{\sqrt{\pi} \Delta \lambda_D} \exp\left(-\frac{\lambda}{\Delta \lambda_D}\right)^2 \quad (\text{A4})$$

562 Here, $W_\lambda(h, \varphi)$ is the equivalent width of the absorption excess ΔI_λ , observed at
563 location h above the limb at azimuth φ . I_λ is the solar background intensity (that is the
564 undisturbed solar D₂ line profile). $\kappa_0^{(A)}$ is the atomic absorption coefficient at line center of
565 the resonance line, $\Delta\lambda_D$ the Doppler width of the excess absorption. By inserting Eq. A2-
566 A4 into Eq. A1 one gets the relation between equivalent width and n , the column density
567 *along the line of sight*, which is nearly linear, because the excess absorption is nearly
568 optically thin. Using this relation, the *tangential column densities* displayed in Figure 1
569 have been derived from the observed equivalent widths; for the Doppler width the value
570 measured from the observed averaged profile of the excess absorption were used.

571

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577

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672

673

Table 1. Summary of observed and simulated physical quantities

Parameter	Observations	Simulation
Tan. col. dens. (max)	$7 \times 10^{10} \text{ cm}^{-2}$	$5 \cdot 10^{10} \text{ cm}^{-2}$
Total amount	4×10^{27}	5×10^{27}
Scale height	200 to 500 km	~ 1000 km

Table 2. Loss rates

Parameter	Jeans escape (%)	Photoionization (%)
Photon Stimulated Desorption	5%	25%
Thermal Desorption	<1%	3%
Impact Vaporization	2%	10%
Ion Sputtering	45%	45%

Figure captions

Fig. 1: Observed Na tangential column density during the Mercury transit of May 7, 2003. Data are from Schleicher et al. (2004). y and z axes are orientated according to the MSE frame (see text), i.e., z is positive towards north and y is positive towards dusk.

Fig. 2: Measured by ACE, during May 7-9, 2003, distance from spacecraft to Earth, components of magnetic field, solar wind proton speed and density (<http://www.srl.caltech.edu/ACE/ASC/level2/index.html>).

Fig. 3: Simulated temporal evolution of parameter $C(t)$. The pink line is a meridian line, fixed on the surface.

Fig. 4: Panel a: Simulated Sodium flux due to PSD. The flux in the dayside (8:00 to 16:00 MLT) is basically equal to the H^+ flux (see Eq. 4). The flux close to the dawn terminator (6:00) is enhanced because the Na composition in the night side is enriched by the proton precipitation. Panel b: H^+ precipitation flux.

Fig. 5. Panel a: Simulated Na tangential column density. Panel b: idem, but using the source distribution function in Eq. 9.

Fig. 6. Parallel (x) velocity distribution of the simulated particles (dotted line). The observed velocity distribution can be reproduced by a Gaussian function with $v_{th} = 1.6$ km/s (solid line). The dashed line shows the simulated velocity distribution using Eq. 9. The small secondary peaks visible at about 2 km/s are due to radiation pressure acceleration.

Fig. 7. Panel a: Simulated Na tangential column density, for Ion sputtering. Panel b: idem, but for impact vaporization.

Fig. 8. Simulated Na density in the xz plane. Sun is to the right.

