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2	AGU PUBLICATIONS
3	JGR: Space Physics
4	Supporting Information for
5 6	Advancing our Understanding of Martian Proton Aurora through a Coordinated Multi-Model Comparison Campaign
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37 Introduction

38 Herein we provide supplemental materials regarding the models used in the study, 39 cross sections used in the models, and additional information regarding the 40 locations of MAVEN and MAVEN/IUVS for observations taken during the orbit of 41 interest. In the Supplementary Text section, we present detailed descriptions of 42 each of the four proton/hydrogen precipitation models used in the study. 43 Descriptions are written by each modeling team and appropriate references are 44 given at the end of each section. In the Supplementary Figures section, we present 45 S1) maps showing the locations of the MAVEN spacecraft during the orbit used in 46 this study (including comparative locations of strong crustal fields), S2) ephemeris 47 data for the MAVEN/IUVS instrument while acquiring the periapsis limb scan data 48 used in this study, S3) relevant profiles used for the coronal thermal H background 49 subtraction method described in the text, and S4) preliminary results comparing the 50 assumption of monodirectional incident particle movement versus isotropic. Lastly, 51 we include a Supplementary Table with details regarding cross sections used by

- 52 each model and relevant references.
- 53

54 **Text S1.**

55 Kallio 3-D Monte Carlo Model Description

(i) General introduction: nature of the model, brief history of its development, and general references

The Kallio model is described in detail in *Kallio and Barabash*, 2000 and 2001. The model is a 3-D Monte Carlo (MC) model where the incident particle, either H⁺ or H, collides with neutral particles after which the velocity of the particle is changed. The model contains 6 elastic and 24 inelastic processes but, in this study, only the processes mentioned in the main text of this paper were used.

The model uses a Cartesian coordinate system both for the positions and velocities
 of the precipitating particles. In the coordinate system the x-axis points from the center of
 Mars toward the Sun.

66

67 (ii) Inputs, processes included (with relevant cross section references), and outputs

68 The model inputs are neutral atom densities, energy dependent total cross-sections

69 (CS), the differential scattering cross-sections (DSCS), the number of precipitating 70 particles ($N_{\rm H}$), and the initial positions ($r_{\rm particle}$ (t=0)) and velocities ($v_{\rm particle}$ (t=0)) of the 71 precipitating particles -- in the present case hydrogen atoms (H).

The total cross sections are given in *Kallio and Barabash, 2001* (Table 1 and Fig.

- 3) and the DSCS scattering angle distribution in *Kallio and Barabash*, 2000 (Fig. 1,
- ⁷⁴ "nominal") and 2001 (Fig. 2). Total cross sections give the probability that a collision

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75 occurs. Random numbers are used to model if a collision occurs, and which collision 76 process occurs. If a collision happens, then the DSCS determines the new velocity of the 77 incident particle after collision. The value of the scattering angle is obtained by using a 78 new random variable.

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80 (iii) Implementation and technical aspects: assumptions and constraints, domain of 81 applicability and grid description, spatial resolution and timesteps, number of particles, 82 overall performance, etc.

83 In the simulation, particles are injected into the upper atmosphere at the point [x, y]84 $z = [260 \text{ km} + R_{\text{Mars}}, 0, 0]$, where the radius of the Mars, R_{Mars} , was in the simulation 85 3393 km. The velocity of the particles in the analysis presented in this paper was a 86 constant $\mathbf{v} = [v_x, v_y, v_z] = [-400, 0,0]$ km/s, i.e., a beam of particles initially moving 87 exactly along the Sun-Mars line.

88 The model saves the position and the velocity of the particle if it has a Ly- α 89 collision process. The Ly- α volume production rate was derived from the saved positions of Ly- α processes by collecting the number of the Ly- α collision processes (d#_k^{hf}) at a 90 91 given altitude (h) range: $dh_k \equiv h_{k+1} - dh_k$. Then in Step 1 runs the Ly- α volume of the 92 emission was derived by using a 1-D approximation, i.e., assuming that the area of the 93 emission perpendicular to the x-axis (dA_{hf}) is equal to the initial area in the solar wind 94 (dA_{sw}) through which the precipitating particles initially came, $dA_{hf} = dA_{sw}$. Note that the 95 inaccuracy caused by the 1-D approximation, $dA_{hf} = dA_{sw}$, is small because the horizontal 96 movement of the colliding particles in the atmosphere is small compared with the radius 97 of the planet. Therefore, the volume (dV_k) from which the emission came within dh_k in 98 Step 1 runs was assumed to be $dV_k = dh_k \times dA_{sw}$. In Step 2 runs the volume dV_k was 99 derived without any approximations from the space angle and the altitude range.

The altitude dependent $Lv-\alpha$ volume emission rate

100 The altitude dependent Ly-
$$\alpha$$
 volume emission rate
101 $q_k^{\text{hf}} = d\#_k^{\text{hf}} / (dt \times dV_k) = d\#_k^{\text{hf}} / (dt \times dh_k \times dA_{\text{hf}}),$ (1)
102 which, as mentioned above, was in Step 1 runs derived by approximating $dA_{\text{hf}} = dA_{\text{sw}}$
103 $q_k^{\text{hf}} = d\#_k^{\text{hf}} / (dt \times dh_k \times dA_{\text{sw}}),$ (2)

is finally obtained from the particle flux of the precipitating H particles $(j_{\rm H})$, the number 104 105 of the particles used in the MC simulation $(N_{\rm H})$ and the time (dt) which takes $N_{\rm H}$ particles 106 to go through the area dA_{sw} : $N_{\rm H} = j_{\rm H} dt \times dA_{sw}$. This gives $dt \times dA_{sw} = N_{\rm H} / j_{\rm H}$ and Eq (2) 107 gets the form

 $q_{k}^{hf} = d\#_{k}^{hf} / (dt \times dV_{k}) = i_{H} [d\#_{k}^{hf} / (dh_{k} \times N_{H})].$ (3)

109 In the analyzed simulation $N_{\rm H}$ was 5000 and 100,000 in Step 1 and Step 2 runs, respectively. As can be seen in Eq. (3) the particle flux $i_{\rm H}$ is just a scaling factor and in 110 this paper, it was $10^7 \text{ cm}^{-3} \text{ s}^{-1}$. In the plots presented in this paper the Ly- α emission 111 altitude profiles were derived in 1 km altitude bins, i.e., $dh_k = 1$ km. This provided a 112 113 relatively good compromise between modest statistical fluctuations and the accurate 114 determination of the peak emission value and altitude.

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116 *(iv) Strengths and applications most suited for the model*

The largest uncertainty for the obtained Ly- α volume emission rate q_k^{hf} is related to 117 the uncertainty of the total cross-sections used and the differential scattering cross 118 119 sections between H and H^+ particles and CO₂ molecules. In the simulation many of these

120 H/H^+ collisions with CO₂ are modeled with H/H^+ collisions with O₂ and N₂ which was 121 published in the literature (see Kallio and Barabash, 2001, Table 1, for details). 122 As described in Kallio and Barabash, 2000 and 2001, functional forms of the 123 adopted DSCS are modeled following Noël and Prölss (1993). The used DSCS (see 124 Kallio and Barabash, 2000, Fig. 1a, the "nominal" DCSC and Kallio and Barabash, 125 2001, Fig. 2) is a fit to the data of $H - O_2$ collisions from Newmann et al., 1986, Table 4. 126 127 It is worth noting that although the statistical fluctuations in the derived emission 128 altitude profiles could be reduced by using a larger number of precipitating particles in 129 the 1 km altitude binning used, the statistical fluctuations are relatively modest already 130 for the number of particles used. 131 It is also worth noting that the MC model used can be automatically used in future 132 more complicated situations than done in this paper. In this study the precipitating 133 particles formed a monoenergetic beam. However, the velocity distribution function can 134 be more complicated; for example, a Maxwellian velocity distribution function, or the 135 velocities can be read from a file. Moreover, the atmospheric density profile, $n(\mathbf{r})$ can be 2-D, say $n(\mathbf{r}) = n(SZA, h)$. In such a case the MC model can be used to derive altitude 136 137 profiles at a given SZA (see Kallio and Barabash, 2001, for details). The atmospheric 138 density can also be 3-D, i.e., $n(\mathbf{r}) = n(x, y, z)$, which would result in the 3-D Ly- α 139 emission rates. In the simulation the particle flux and their velocity distribution can also 140 have latitude-longitude dependence (see Kallio and Janhunen, 2001, for details). 141 142 References: 143 Kallio, E., and S. Barabash, On the elastic and inelastic collisions between precipitating 144 energetic hydrogen atoms and Martian atmospheric neutrals J. Geophys. Res., 145 105, 24,973-24,996, 2000. 146 Kallio, E., and S. Barabash, Atmospheric effects of precipitating energetic hydrogen 147 atoms on the Martian atmosphere, J. Geophys. Res., 106, 165-178, 2001. 148 Kallio, E., and P. Janhunen, Atmospheric effects of proton precipitation in the Martian 149 atmosphere and its connection to the Mars-solar wind interaction, J. Geophys. 150 Res., 106, 5617-5634, 2001. 151 Newman, J. H., Y. S. Chen, K. A. Smith and R. F. Stebbings, Differential cross sections 152 for scattering of 0.5-, 1.5-, and 5.0-keV hydrogen atoms by He, H2, N2, and O2, 153 J. Geophys. Res., Volume 91, Issue A8, Pages 8947-8954,1986. 154 Noël, S. and G. W. Prölss, Heating and radiation production by neutralized ring current 155 particles. J. Geophys. Res., Volume 98, Issue A10, Pages 17317-17325,1993. 156 Rees, M. H., Physics and Chemistry of the Upper Atmosphere, Cambridge Univ. Press, 157 New York, 1989. Rudd, M. E., Kim, Y. K., Madison, D. H., & Gallagher, J. W., Electron production in 158 159 proton collisions: Total cross sections. Reviews of Modern Physics, 57, 965–994, 160 1985.

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- 166
- 167 **Text S2.**

168 Jolitz 3-D Monte Carlo Model Description (Name: "ASPEN")

169 ASPEN (Atmospheric Scattering of Protons, Electrons, and Neutrals) is a 3-D 170 Monte Carlo test particle simulation. This model was initially developed to predict 171 atmospheric ionization rates at Mars by solar energetic particles, which have higher 172 energies than the ENAs studied in this paper [Jolitz et al., 2017] and has since been used 173 to predict precipitating SEP electron fluxes at Mars [Jolitz et al., 2021]. The simulation 174 solves the Lorentz force equations for energetic particle motion and uses a Monte Carlo 175 approach to predict collisions and resulting energy loss in the atmosphere. Since 176 magnetic fields were set to zero for this study, the transport equations reduced to ballistic 177 motion.

The collisional energy degradation algorithm used in ASPEN was originally 178 179 developed and described in Lillis et al. [2008] for an electron precipitation model. It is 180 very similar to the Kallio model in approach. Stochastic collisions were modeled by 181 inverting the relation between intensity, density, and absorption cross-section for a 182 particle beam incident on a medium of scatterers (colloquially known as Beer's law) to 183 dynamically calculate a probability distribution function that is combined with a random 184 number to predict variable distances between collisions. This probability distribution 185 function is calculated for each individual particle and depends on the position, path, and 186 energy through the planetary atmosphere. Similarly, whenever a collision occurs, the type 187 of collision is predicted probabilistically using the relative cross-section of each possible collisional process and the particle energy is decremented by the corresponding energy 188 189 loss. As a particle loses energy, the relative cross-sections of each process change. For 190 example, a 2 keV proton colliding with a carbon dioxide molecule has a roughly 70% 191 likelihood of capturing an electron, but the likelihood for the same process when the 192 proton is 20 eV is only 20%.

193 This model is highly dependent on the choice of cross-sections. For the 194 application in this study, the selected cross-sections for hydrogen and proton impact on 195 carbon dioxide are described in Jolitz et al. [2017], with one exception. The cross-196 sections for proton- and hydrogen-impact excitation was replaced with Lyman-alpha 197 emission cross-sections. Unfortunately, experimental measurements of the Lyman-alpha 198 emission cross-section from proton and hydrogen atom impact on carbon dioxide is 199 limited. As of the time of this paper's writing, only one set of measurements exist for 200 1-25 keV protons and hydrogen atoms [Birely and McNeal, 1972]. The cross-section for 201 emission by protons and hydrogen atoms below 1 keV is unknown. In order to 202 approximate emission from particles at these energies, ASPEN uses a cross-section 203 calculated by scaling the corresponding emission cross-sections from impact on 204 molecular oxygen. ASPEN also accounts for the fact that proton-induced Lyman-alpha

205 emission can only occur in addition to a charge exchange collision, since Lyman-alpha206 can only be emitted by a hydrogen atom.

207 Since ASPEN is a 3-D Monte Carlo simulation, predicting an accurate emission 208 rate requires appropriate choice of initial conditions and a large volume of simulated 209 particles. For Step 1, we simulated 10,000 particles incident on the subsolar point from an 210 altitude of 600 km and calculated the emission rate by binning all Lyman-alpha emitting 211 collisions as a function of altitude and multiplying by the incident flux. For Step 2, we 212 simulated 10,000 particles uniformly distributed in space on a plane perpendicular to the 213 direction of solar wind flow. Each particle represents a fraction of the assumed incident 214 flux. The emission rate was then calculated by weighing the total number of emissions

- binned by altitude, solar zenith angle, and the fraction of flux associated with each
- simulated particle.
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255 256 257	Van Zyl, B., and H. Neumann (1988), Lyman α emission cross sections for low-energy H and H+ collisions with N2 and O2, J. Geophys. Res, 93(A2):1023-1027.

258 **Text S3.**

259 Bisikalo/Shematovich et al. 1-D Monte Carlo Model Description

260 The Bisikalo/Shematovich et al. model is a 1-D kinetic Monte Carlo model. The model considers three primary processes: 1) precipitation of high-energy hydrogen atoms 261 and protons that lose their kinetic energy in the elastic and inelastic collisions, 2) 262 263 ionization of target atmospheric molecules/atoms, and 3) charge transfer and electron capture collisions with the major atmospheric constituents (i.e., CO2, N2, and O). 264 Secondary fast hydrogen atoms and protons carry enough kinetic energy to cycle through 265 266 the collisional channels mentioned above and result in a growing set of translationally 267 and internally excited atmospheric atoms and/or molecules. 268 To study the precipitation of high-energy H/H^+ flux into the planetary atmosphere, we 269 solve the kinetic Boltzmann equations (Shematovich et al., 2011) for H⁺ and H, including

the collision term:

$$\mathbf{v}\frac{\partial}{\partial \mathbf{r}}f_{H/H+} + \left(\mathbf{g} + \frac{e}{m_{H+}}\mathbf{v} \times \mathbf{B}\right)\frac{\partial}{\partial \mathbf{v}}f_{H/H+} = Q_{H/H+}(\mathbf{v}) + \sum_{M=O,N_2,CO_2} J_{ml}(f_{H/H+}, f_M).$$
(1)

271 Equation (1) is written in the standard form for the velocity distribution functions

272 $f_{H/H+}(r,v)$, and $f_M(r,v)$ for hydrogen atoms and protons (Gérard *et al.*, 2000). The source

273 term $Q_{H/H+}$ describes the production rate of secondary H/H⁺ particles and the elastic 274 and inelastic collisional terms J_{mt} for H/H⁺ describe the energy and momentum transfer to 275 the ambient atmospheric gas which is characterized by local Maxwellian velocity 276 distribution functions. Our kinetic Monte Carlo model (Gérard et al., 2000; Shematovich 277 et al., 2011) is used to solve kinetic equation (1). The model is 1-D in geometric space 278 and 3-D in velocity space. Nevertheless, the 3-D trajectories of H/H⁺ are calculated in the 279 code with final projection on radial direction. In the current version of the MC model 280 (Shematovich *et al.*, 2019) an arbitrary structure of the induced magnetic field of Mars is 281 included; that is, all three components of the magnetic field $\mathbf{B} = \{Bx, By, Bz\}$, were taken 282 into account. The details of the model implementation and statistics control with the 283 variance below 10% can be found in (Shematovich et al., 2019).

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The essence of the kinetic Monte Carlo model is accounting of all possible collisions in the atmospheric region studied. Therefore, statistics for all collisional processes are accumulated during the numerical realization of the kinetic model of the proton aurora. It provides a good basis for the evaluation of the Ly- α source functions as keeping of all excitation processes and their spatial characteristics makes it possible to determine the statistical distribution of the emitted Ly- α photons.

291 The energy deposition rate of H/H+ flux is determined by the cross sections of the 292 collisions with the ambient gas. The energy lost by the H/H+ in a collision is determined 293 by the scattering angle γ

294 $\Delta E \sim E \times (1 - \cos \chi),$

295 where E is the initial energy of the impacting proton or hydrogen atom. It is apparent that 296 the energy loss for collisions in forward direction (for $\chi < 90^{\circ}$) at small scattering angles 297 χ is less than that for larger scattering angles. A key aspect of this kinetic MC model is 298 the probabilistic treatment of the scattering angle distribution, which influences both the 299 energy degradation rate and the angular redistribution of the precipitating protons and 300 hydrogen atoms (Bisikalo et al., 2018; Shematovich et al., 2019). The kinetic model 301 utilizes both total and differential cross sections when calculating the post-collision 302 velocities for high-energy precipitating H/H+ and atmospheric particles. In the model, the 303 most recent measurements or calculations of the required cross sections were adopted. 304 The cross sections and scattering angle distributions for H/H+ collisions with CO2 are 305 taken from Nakai et al. (1987) for charge exchange and stripping collisions, from Haider 306 et al. (2002) for ionization, Lyman alpha and Balmer alpha excitation, and from Lindsay 307 et al. (2005) for scattering angle distributions. The elastic and other inelastic collisions 308 cross sections for H/H+ collisions with CO2 are assumed to be the same as for O2 (see, 309 for details, Gérard et al. (2000)). The region under study is limited by the lower 310 boundary, which is placed at 80 km, where H/H⁺ particles are efficiently thermalized. The 311 upper boundary is set at 500 km, where measurements or calculations of the precipitating 312 fluxes of protons or hydrogen atoms are used as a boundary condition. Both table and/or 313 analytic (Maxwellian and/or kappa-distribution) functions representing the energy spectra 314 as well as the pitch-angle (monodirectional, isotropic, or limited by cone) distributions of 315 precipitating particles could be used at the upper boundary. Detailed description of all 316 modeled numerical aspects used for this kinetic MC model study could be found in recent 317 papers (Bisikalo et al., 2018; Shematovich et al., 2019).

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- 344

345 **Text S4**.

346 Gronoff et al. 1-D Kinetic Model Description (Name: "Aeroplanets")

347 A. Introduction

348 The Aeroplanets model (Gronoff et al., 2012a; Gronoff et al., 2012b; Simon 349 Wedlund *et al.* 2011) is a 1-D kinetic transport model computing the ionization and 350 excitation of atmospheric species by photon, electron, proton, and cosmic ray impacts, 351 including the effect of secondary particles (photoelectrons, secondary electrons and 352 protoelectrons). It is based on the Trans* model series, initially developed for the Earth 353 (Lilensten et al., 1999; Lummerzheim and Lilensten 1994; Simon et al., 2007 as Trans4), 354 and subsequently adapted to Venus (Gronoff et al., 2007, 2008), Mars (Witasse et al., 355 2002, 2003; Simon et al., 2009; Nicholson et al., 2009), Titan (Gronoff, Lilensten, and 356 Modolo 2009; Gronoff et al., 2009a, 2009b), etc., and including several other modules 357 such as a fluid model. Aeroplanets constitutes an improvement in modularity and 358 adaptability over Trans4, with every separate module having the option of being turned 359 off to study one specific aspect of particle precipitation in the atmosphere of planets.

The proton transport module is based on the work of Galand *et al.* (1997, 1998), Simon (2006) and Simon *et al.* (2007) for Earth, who solved semi-analytically the coupled proton-hydrogen dissipative kinetic transport equation for protons and hydrogen atoms charge-changing with neutral gas M:

 $\begin{array}{ll} 364 & H^+ + M \rightarrow H + M^+ Electron\ capture, \sigma_{10} & H + M \rightarrow H^+ + M + \\ 365 & e^- Electron\ loss/stripping, \sigma_{01}. \end{array}$

366 It naturally includes angular redistributions due to magnetic mirror effects and to
 367 collisions (Galand *et al.*, 1998)

- 368
- 369 B. Inputs and outputs

370 Inputs to the Aeroplanets model include cross sections, the vertical profile of atmosphere 371 composition (*i.e.*, composition at different altitudes), and the precipitating fluxes of particles such H and H⁺ at the top of the atmosphere. Outputs include the vertical profile 372 373 of H and H⁺ differential energy fluxes, and the vertical profile of the production rate of 374 excited and ionized species and electrons, including emissions. The produced 375 photoelectrons can be plugged into the main Aeroplanets electron model as an external 376 and additional source of ionization in the atmosphere. 377 Cross sections in Aeroplanets are taken from the latest version of the

378 ATMOCIAD cross section and reaction rate database compiled and developed by Simon

- Wedlund *et al.* (2011), Gronoff *et al.* (2012a) and Gronoff *et al.* (2020), and freely
- available in Gronoff et al. (2021) In ATMOCIAD, experimental and theoretical cross

- 381 sections as well as their uncertainties are collected. Many proton-hydrogen impact cross 382 sections have been discussed in the seminal works of Avakyan et al. (1998) and, in a 383 lesser degree, of Nakai et al. (1987); they contain a critical review of processes for 384 photons, e⁻, H, H⁺ colliding with various gases of aeronomic interest and have been fully 385 integrated into ATMOCIAD. 386 Specifically, the proton transport code uses the following energy-dependent cross 387 sections, process by process: 388 • Elastic. Parameterisations of Kozelov and Ivanov (1992) originally valid for (H⁺, 389 H) collisions with N₂, and assumed to be the same for CO₂ because of the lack of 390 any recent measurements. The parameters are available in their Tables 1 and 2. 391 **Ionization**. For H⁺, Rudd *et al.* (1983) for high energies, extended at E < 5 keV by ٠ 392 (Avakyan et al., 1998). For H atoms, cross sections are based on Basu et al. (1987) 393 for N_2 and on Avakyan *et al.* (1998) for the rescaling factor. 394 **Electron capture** ($\mathbf{H}^+ \rightarrow \mathbf{H}$). Kusakabe *et al.* (2000) for 0.2-4 keV protons, review • 395 by Avakyan et al. (1998) based on all other available data for higher energies 396 (Desesquelles, Do Cao, and Dufay 1966; Barnett and Gilbody 1968; Toburen, 397 Nakai, and Langley 1968; McNeal 1970; Rudd *et al.*, 1983 for 5 – 150 keV). Note 398 that recent sub-keV measurements have been made by Werbowy and Pranszke 399 (2016) for CO and CO_2 , although these are not yet implemented in the 400 ATMOCIAD. 401 **Electron loss** ($\mathbf{H} \rightarrow \mathbf{H}^+$). Smith *et al.*, (1976) between 0.25 – 5 keV, review by • 402 Avakyan *et al.*, (1998) using N₂ σ_{01} cross sections (Green and Peterson 1968) based 403 on all other available data for higher energies. Ly- α H(2p) and H(2s) states. For both H⁺ and H collisions, exciting state H(2p) 404 • 405 (Birely and McNeal 1972) corrected by factor 0.9 presumably because of 406 observation angle issues as per the recommendation of Avakyan et al. (1998). For 407 both impactors creating state H(2s), factor 1.35 on the measurements of (Birely and
- 408 McNeal 1972) is applied.

Although ATMOCIAD is an extensive collection of cross sections, there is still a rather
 poor characterization of cross sections at low energies (typically in the sub-keV range).

412 Regarding differential cross sections, Aeroplanets uses phase functions that are 413 convolved with the energy-dependent cross sections above. For the particular cases 414 computed for Step 1 of the present study, the following is used: for the two charge-415 transfer (10 and 01) and elastic cross sections, the screened Rutherford function is used, 416 equal to that of the electrons with a screening parameter ϵ of 10^{-3} (this is the same as in 417 Galand *et al.*, 1997, 1998 and Simon 2006, Simon *et al.*, 2007 for Earth's atmosphere):

418
$$\xi(\cos\vartheta) = \frac{4\epsilon(1+\epsilon)}{(1+2\epsilon-\cos\vartheta)^2}$$

419

420 with $\vartheta = \mu \mu' + \sqrt{1 - \mu'^2} \sqrt{1 - \mu^2} \cos(\phi - \phi')$. μ and μ' are the cosine of the pitch 421 angles before and after the collision, whereas ϕ and ϕ' are the azimuthal angles before 422 and after the collision. For ionization, forward scattering is assumed following Galand *et* 423 *al.*, (1998) for the Earth case.

424 Because of the seamless implementation of ATMOCIAD as input to Aeroplanets,
425 other available sets of cross sections may be used. It is possible to estimate the

426 uncertainties from the cross sections using a Monte-Carlo approach as described in

427 (Gronoff et al., 2012a; Gronoff et al., 2012b). The outputs of the proton-transport model

428 are the ionization and dissociation rates (including excited states productions), the

429 proton/H induced electron flux (which can be used in the electron model), and the

- 430 proton/H fluxes at the different altitudes.
- 431
- 432 C. Implementation

433 The solution of the dissipative coupled Boltzmann H/H⁺equation is based on the seminal work of Galand et al., (1997, 1998), later developed and adapted as a module into 434 435 Aeroplanets following Simon et al., (2007). It is based on the idea that dissipative forces 436 responsible for angular redistributions (due to elastic scattering) can be introduced in the 437 force term of the generalized Boltzmann equation (Galand et al., 1997). Rearranging the 438 energy/angle terms of the H^+/H coupled system of equations leads to a linear system of 439 equations parametrized by a large sparse square matrix A containing the energy 440 degradation without angular redistributions of the incoming particle, for each altitude zso that:

441

442

$$\frac{\partial \Phi}{\partial z} = A\Phi +$$

443 $\Phi = (\phi_{H^+} \phi_H)$ is the vector-flux of protons and hydrogen precipitating particles and B, 444 the angular degradation term, is thus the term coupling downward and upward fluxes. 445 Moreover, the mirror mode term can be switched on or off depending on the planet's 446 configuration. The equation can be solved by calculating the exponential of matrix A for 447 a typical grid of 100 energies and 10 angles, both of which can be increased by the user 448 for better resolution.

В

449 In order to achieve such a feat of simplification for a complex system of equations, the 450 following assumptions are made in the case of the Mars code: (i) plane parallel geometry, 451 with the atmosphere stratified horizontally, and the pitch angle of the particles can be 452 imposed, (ii) external forces neglected, (iii) steady-state fluxes, (iv) continuous slowing 453 down approximation assumed because of the low energetic losses by the precipitating 454 particles compared to the incident energy of the particles.

455

456 D. Strengths and applications

457 Aeroplanets is better qualified for the fast computation of the proton precipitation from a 458 measured spectra near the planet, and for the fast computation of the whole effect of that 459 precipitation thanks to its coupling with a secondary electron transport model. The 460 analytic computation approach and assumed geometry prevent the computation within 461 very complex magnetic topologies (which are best handled by Monte-Carlo models) but 462 is well suited for handling large sets of initial angles and energies.

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Figure S1. MAVEN spacecraft orbit information showing the locations of the
 spacecraft during Orbit 4235. The red/blue colors represent the magnitude and
 orientation of the crustal magnetic fields (see MAVEN PDS or Science Data Center
 website for more information). Note that the location of the periapsis is in the
 southern hemisphere and does not pass over any strong crustal magnetic fields.



Figure S2. MAVEN/IUVS information showing ephemeris data for the IUVS limb
scans during Orbit #4235 periapsis. Note that the location of periapsis is primarily
on the dayside of the planet (with the exception of a few limb scan observations
near the terminator) in the southern hemisphere and does not pass over any strong
crustal magnetic fields. Different limb scans are marked by different colors within
the orbit.

603





605 Figure S3. Altitude-intensity profiles and estimated heuristic thermal H background 606 used for the background subtraction method described in this study. Left: IUVS Ly-a 607 profiles for the orbit used in the data-model comparison (#4235), and a nearby orbit 608 with little/less proton aurora activity (#4229) used to create the best-fit heuristic 609 background coronal H profiles for each limb scan; peak profile SZAs for each scan in the two orbits are provided in the legend. Middle: Heuristic background thermal H 610 profiles estimated from orbit #4229 (black profiles) overlain on Ly-α profiles for 611 corresponding SZA limb scans in orbit #4235. **Right**: Final background-subtracted 612 613 profiles that represent the contribution from only H-ENAs in the IUVS proton aurora 614 observation in this orbit (i.e., removing the background contribution from coronal 615 thermal H). 616



618 619 Figure S4. Example comparison of assuming monodirectional movement of the incident particle population in the atmosphere versus isotropic (simulation results 620 from the Bisikalo/Shematovich et al. model). Left: Comparison proton aurora 621 622 profiles using each assumption; **Middle:** Simulated H energy flux in the downward and upward (zero in this case) directions using a monodirectional assumption; 623 **Right:** Simulated H energy flux in the downward and upward directions using an 624 625 isotropic assumption. The simulated proton aurora profile using the isotropic 626 assumption has a higher peak altitude and smaller VER due to the larger upward H population. The models in this study assume monodirectional particle movement, 627 which could in turn lead to some of the observed discrepancies between the data 628 629 and the models in Step 2 of the campaign. We note that neither of these two 630 extreme assumptions (i.e., purely monodirectional or purely isotropic incident particle movement) is a probable physical occurrence, and the actual particle 631 632 precipitation pattern is somewhere between these two limiting cases. 633

Cross Section (CS) Processes:	Elastic	Cha Excha e ⁻ Ca	arge ange/ pture	e [.] Stripping		Ionization		Lyman-α		Lyman-β &/or Lyman-γ		Balmer-α		Excitation of CO ₂		Differential Scattering Cross Sections (DSCS)			
	H-CO ₂ H ⁺ -CO ₂	H-CO ₂	H ⁺ -CO ₂	H-CO ₂	H ⁺ -CO ₂	H-CO ₂	H ⁺ -CO ₂	H-CO ₂	H ⁺ -CO ₂	H-CO ₂	H ⁺ -CO ₂	H-CO ₂	H ⁺ -CO ₂	H-CO ₂	H ⁺ -CO ₂	H-CO ₂ H ⁺ -CO ₂			
Jolitz:	Newman+ 1986 [for H/H ⁺ - N ₂]		Barnett+ 1977	Nakai+ 1987		Van Zyl+, 1978 [for H - O ₂] McNeal, 1970 [rescaling]	Rudd+ 1985	Van Zyl & Neumann [for H - O ₂] Birely & McNeal, 1971 [rescaling]	Avakyan+ 1998 [for H* - O ₂] Birely & McNeal, 1971 [rescaling]			x	x			Newman+ 1986 Noel and Prölss, 1993 [for H/H⁺ - O₂]			
Kallio:	Newman+ 1986 [for H/H ⁺ - N ₂]		Rees, 1989 [for H ⁺ - O ₂]	Van Zyl+, 1978 [for H - O ₂]		Van Zyl+, 1978 [for H - O ₂]	Rudd+ 1985	Van Zyl & Neumann, 1988 [for H/H⁺ - O₂]				x	x			Newn Noel and [for l	nan+ 1986 I Prölss, 1993 H/H ⁺ - O ₂]		
Bisikalo/ Shematovich <i>et al.</i> :	Porter+ 1976		Nakai+ 1987 [for H - O ₂ and rescaled]	Nakai+ 1987 [for H - O ₂ and rescaled]		Haider+ 2002 [for H - O ₂ and rescaled]		Haider+ 2002 [for H - O ₂ and rescaled]				x	x			Linds [for H/ re	say+ 2005 'H* - O ₂ and scaled]		
Gronoff <i>et al.</i> :	Kozelov & Ivanov, 1992 [for H/H⁺ - N₂]		Kusakabe+ 2000 Avakyan+ 1998	Smith+ 1976 Avakyan+ 1998 [for H - N ₂]		Basu+ 1987 [for H - N ₂] Avakyan+ 1998 [rescaling]	Rudd+ 1983 Avakyan+ 1998	Birely & McNeal, 1972 [rescaled as per Avakyan+ 1998]		Birely & McNeal, 1972 [rescaled as per Avakyan+ 1998]		x	x			x	x	Avaky Bas [Calculat angle usin type collis	yan+ 1998 u+ 1987 ed from pitch ng Rutherford- sion functions]

Table S1. List of cross sections (CS) that each model in this study may include. The five overlapping CS processes of each modeling team are shown in green, along with relevant references for those CS processes and Differential Scattering Cross Sections (DSCS). Bins marked with an "X" represent additional CS processes that can be included in models.