Pressure and ion composition boundaries at Mars

Shaosui Xu,[1,2] Michael W. Liemohn,[2] Chuanfei Dong,[2,3] David L. Mitchell,[1]

Stephen W. Bougher,[2] and Yingjuan Ma[4]

Corresponding author: Shaosui Xu, Space Science Laboratory, University of California, Berkeley, California, USA. (shaosui.xu@ssl.berkeley.edu)

[1]Space Science Laboratory, University of California, Berkeley, California, USA.

[2]Department of Climate and Space Sciences and Engineering, University of Michigan, Ann Arbor, Michigan, USA.

[3]Princeton Plasma Physics Laboratory, Princeton University, Princeton, New Jersey, USA

[4]Institute of Geophysics and Planetary Physics, UCLA, Los Angeles, California, USA,

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Abstract.

This study analyzes results from a multifluid MHD simulation to investigate the shape and structure of the pressure and composition boundaries at Mars, which can provide physical insight for the observational analysis. These boundaries are examined via the unity contours and gradients of the plasma β, as well as β^*, which includes the dynamic pressure in the numerator, and the ion mass and number density ratios. It is found that unity contours are well aligned with the gradient extrema, indicating that the unity contour is a topological boundary. In addition, these two transitions of pressure and composition are of a thickness of $0.05-0.1$ R_M near the subsolar region to $1-1.5$ R_M in the tail. The comparison of the pressure and composition boundaries indicates that the two are very similar and that not only the plasma sheet but the full volume of the lobes are dominated by planetary ions. It suggests that the tail escape for ions not only concentrates in the central plasma sheet but also the magnetic lobes. It is also worthy pointing out that the ion number density ratio unity contour is found to be systematically smaller than other unity boundaries, which calls for attention when the ion number density is used to identify such boundaries. Finally, the comparison between the boundaries of this study and two analytical fittings is carried out. We found a good agreement with the Vignes fitting, with little flaring in the tail, in contrast to a larger flaring angle from the Trotignon fitting.

1. Introduction

₂₄   *Moore and Delcourt* [1995] came up with the concept of the geopause, which marks

₂₅   the boundary between solar and terrestrial dominance of near-Earth space. Multiple

₂₆   geopause boundaries exist, depending on the parameter used to define the boundary. The

₂₇   magnetopause is the arguably the most well known of these geopause boundaries, but

₂₈   *Moore and Delcourt* [1995] also discussed the existence of plasma pressure and density

₂₉   geopauses. At such interfaces, energy and particle interchange between the solar wind and

₃₀   the planetary ionospheric plasmas could occur, resulting in dynamics and perturbations

₃₁   that are essential for geostorm development. Such a concept can be applied to other

₃₂   planets, such as Mars, to provide insight into the physics of magnetic topology and ion

₃₃   escape, as one way for cold planetary ions to attain escape energy is through such a

₃₄   coupling with the solar wind plasma at this interface.

₃₅   Mars is usually classified as an unmagnetized planet in terms of the interaction with

₃₆   solar wind due to the absence of a significant global intrinsic magnetic field. This in-

₃₇   teraction results in several distinct regions, such as the magnetosheath, the magnetic

₃₈   pileup region, and the tail region [e.g. *Nagy et al.*, 2004; *Bertucci et al.*, 2012]. The

₃₉   existence of localized crustal fields [e.g. *Acuna et al.*, 1999] complicates this interaction

₄₀   [e.g *Brain et al.*, 2003, 2007; *Harnett and Winglee*, 2005; *Liemohn et al.*, 2006, 2007; *Ma*

₄₁   *et al.*, 2014; *Dong et al.*, 2015a; *Xu et al.*, 2014]. The transition between the magne-

₄₂   tosheath and the magnetic pileup region has several observational characteristics, which

₄₃   have been identified by different instruments on various spacecraft. One feature is a sharp

₄₄   increase in magnetic field strength coincident with a decrease in field fluctuations, which

was observed by Phobos-2 [e.g. *Riedler et al.*, 1989], the Mars Global Surveyor (MGS)

spacecraft [e.g. *Vignes et al.*, 2000; *Crider et al.*, 2002; *Bertucci et al.*, 2005] and also

the Mars Atmosphere and Volatile Evolution (MAVEN) spacecraft [e.g. *Jakosky et al.*,

2015a, b; *Connerney et al.*, 2015; *Halekas et al.*, 2015; *Matsunaga et al.*, 2015]. These

observations resulted in the names known as the magnetic pileup boundary (MPB) or the

induced magnetosphere boundary (IMB). Another feature of this transition is a switch

from solar wind ions to planetary heavy ions, which was observed by Phobos-2 [e.g. *Sauer

et al.*, 1992; *Trotignon et al.*, 1996], Mars Express [e.g. *Dubinin et al.*, 2006, 2008; *Fränz

et al.*, 2006] and MAVEN [e.g. *Ma et al.*, 2015; *Dong et al.*, 2015b; *Matsunaga et al.*,

2015]. This resulted in the names including the protonopause and the ion composition

boundary (ICB). These boundaries located at the inner side of the magnetosheath were

also identified and studied by plenty of simulation efforts [e.g. *Sauer et al.*, 1994; *Ma et al.*,

2002, 2004; *Boßwetter et al.*, 2004; *Brecht*, 1990, 1997; *Harnett and Winglee*, 2005; *Mod-

olo et al.*, 2006; *Kallio et al.*, 2006; *Simon et al.*, 2007; *Brain et al.*, 2010]. In particular,

Fang et al. [2015] showed the irregularity of MPB and how it varies with the crustal field

rotation.

The transition between the magnetosheath and magnetic pileup region at Mars gener-

ally resembles Earth's geopause, because of the sharp transitions between the solar wind

and planetary plasmas. In this study, we analyze the results from a BATS-R-US Mars

Multifluid MHD model to quantitatively study these boundaries by looking at plasma-

type (thermal and dynamic) and magnetic pressures. There are different ways to define

such boundaries, such as locations where the dominant contribution to the total pressure

changes or where the dominant ion species changes, or where sharp gradients in the pres-

sure terms or composition occur. Pressure and composition boundaries often appear sharp

on time series figures of spacecraft observations, particularly on the day side. Similarly,

boundaries identified in simulations are often displayed as lines and surfaces. However,

the thicknesses of these transitions are typically not considered, especially downstream

of the terminator. Transition thicknesses can be determined both observationally and

from simulations, which is useful for assessing the transition from solar wind to planetary

influence. In addition, due to limitation of instruments of many spacecraft, the relation

of MPB and ICB was not well understood. This study will also present a systematic

comparison between the two from a theoretical view.

2. BATS-R-US Mars Multifluid MHD Model Description

The University of Michigan 3-D Block-Adaptive Tree Solarwind Roe-type Upwind

Scheme (BATS-R-US) multifluid MHD (MF-MHD) model was initially developed for the

Earth environment [*Powell et al.*, 1999; *Glocer et al.*, 2009; *Tóth et al.*, 2012] and then

adapted to Mars [*Najib et al.*, 2011; *Dong et al.*, 2014]. The Mars MF-MHD model com-

putes a full set of continuity, momentum, and energy equations for four ion species, H^+,

O^+, O_2^+, and CO_2^+. Due to a much weaker magnetic environment at Mars, and thus a

much slower Alfven speed, the inner boundary of the Mars MF-MHD model is set at 100

km altitude. This altitude is below the ionospheric density peak, thus the model is able

to simulate the entire plasma environment around the planet.

The model includes detailed ionospheric chemistry, photoionization, charge exchange,

recombination, and electron impact ionization. The chemical reaction schemes are de-

scribed in *Ma et al.* [2004] and *Najib et al.* [2011]. Electron impact ionization rates are

given by *Cravens et al.* [1987] and collision frequencies between species are given by *Schunk*

90 *and Nagy* [2009]. At the inner boundary, O^+, O_2^+, and CO_2^+ are assumed to be in pho-

91 tochemical equilibrium and H^+ is set to be approximately 30% of the solar wind density,

92 to account for proton penetration into the ionosphere. Additionally, the velocity u is set

93 to be a reflective boundary condition. Furthermore, the ion and electron temperature

94 is set to be the same as the neutral temperature at the inner boundary, given frequent

95 collisions between neutral particles and plasma. The 60° harmonic expansion developed

96 by *Arkani-Hamed* [2001] is incorporated into the MF-MHD model to take into account

97 the crustal fields.

98   The simulation domain is within $-24R_M \leq X \leq 8R_M$; $-16R_M \leq Y, Z \leq 16R_M$, in

99 a nonuniform spherical grid structure with a radial resolution varying from 5 km near

100 the inner boundary to 1000 km near the outer boundary with an angular resolution of

101 $1.5° - 3.0°$. R_M is the Mars radius and the results of this study are shown in the Mars-

102 centered Solar Orbital (MSO) coordinates, with x axis pointing at the Sun, y axis opposite

103 to the Mars orbital direction, and z axis perpendicular to the Mars orbital plane. The

104 neutral atmosphere is adopted from the Mars Global Ionosphere Thermosphere Model

105 (M-GITM) [*Bougher et al.*, 2015] for the cold neutral component and from the Mars

106 exosphere Monte Carlo model Adaptive Mesh Particle Simulator (M-AMPS) [*Lee et al.*,

107 2014a, b, 2015] for the hot neutral corona.

108   For this study, we have chosen the solar maximum ($F_{10.7} = 200$ sfu), perihelion condi-

109 tions with the subsolar longitude set to 180°W (strong crustal field regions on the dayside)

110 to explore the boundaries. The solar wind inputs are specified as follows: a density of 4

111 cm^{-3}, a plasma temperature of 3.5×10^5 K, a velocity of 400 km/s, and the interplanetary

112 magnetic field (IMF) being 3 nT in a typical away-sector (IMF pointing away from the

113 Sun) Parker spiral pattern with an angle of 56°. These inputs correspond to Case 17 of

114 *Dong et al.* [2015a].

3. Pressure Boundary

115   In the Mars plasma environment, the total pressure consists of three terms: magnetic

116 pressure, dynamic pressure, and thermal pressure. These three pressures from the MF-

117 MHD run are shown in the three rows, respectively, in Figure 1 and the three columns

118 planar cuts Z=0, X=-1.5 R_M, and X=-3 R_M in MSO coordinates. Typical structures of

119 the interaction between an unmagnetized planet and the solar wind can be identified in the

120 Z=0 plane. The bow shock is located ~ 1.7 R_M at the subsolar point, upstream of which

121 the solar wind dynamic pressure dominates. After the bow shock, most (not all) of the

122 dynamic pressure is converted into thermal and magnetic pressure, with thermal pressure

123 prevailing near the subsolar region, and dynamic pressure progressively more important

124 in the flanks. Closer to the planet, magnetic pressure accounts for a larger fraction of the

125 total pressure because of mass loading effects and localized crustal fields. For $X < 0$, the

126 dynamic pressure dominates the magnetosheath once behind the obstacle. In the central

127 plasma sheet, the thermal pressure dominates the near Mars region $(-5 < X < 0)$ and

128 the dynamic pressure prevails in the distant tail $(X < -5)$. Complementing the plasma

129 pressure at $X < 0$, high magnetic pressures highlight two magnetic lobes, separated by

130 the central plasma sheet. The magnetic pressure differs significantly when comparing the

131 parallel and perpendicular regions (IMF parallel and perpendicular to the shock normal,

132 respectively) of the shock as shown in Figures 1a-1c: on the more perpendicular side of

133 the shock (+Y), there is a prominent increase in magnetic pressure, which is not present

134 on the more parallel side of the shock (-Y). Pressures are also shown in the two selected

135 cuts down tail, X=-1.5 R_M and X=-3.0 R_M, where two magnetic lobe structures can be

136 easily identified.

137   To help distinguish the different pressure regimes, we calculate the plasma beta ($\beta =$

138 p_{th}/p_B), i.e., the ratio of the plasma thermal pressure (p_{th}) and the magnetic pressure

139 (p_B), which is shown in Figures 2a-2c, at Z=0, X=-1.5 R_M, and X=-3 R_M, respectively.

140 However, the plasma dynamic pressure increases downstream of the planet, as seen in

141 Figures 1d-1f. Hence, we define $\beta^* = (p_{th} + p_{dyn})/p_B$, which is the sum of the plasma

142 thermal pressure (p_{th}) and dynamic pressure (p_{dyn}) divided by the magnetic pressure (p_B).

143 In other words, if $\beta^* > 1$, the region is dominated by the plasma-type pressures, or vice

144 versa. Figures 2d-f illustrate the distribution of β^* at the three cuts. The blue color

145 highlights regions dominated by the magnetic pressures while the red shading reveals

146 areas dominated by the plasma-type pressures, with the white showing parity. Overall, β

147 and β^* depict a similar pattern, with the magnetic pressure dominating the two lobes and

148 near the planet on the dayside, and plasma-type pressures prevail in the plasma sheet,

149 magnetosheath and beyond. The main difference is that, β^* defines a smaller magnetic

150 dominant region, as the numerator includes two pressure terms. To show this more clearly,

151 Figures 3a and 3b illustrate the contours of $\beta = 1$ and $\beta^* = 1$, respectively. The view

152 in both panels of Figure 3 is from above the ecliptic plane in the afternoon sector. The

153 green translucent surface shows the unity contour. For reference of scale, the inner, almost

154 spherical surface is in the ionosphere near the inner boundary of the simulation domain.

155 Both unity contours enclose the tail lobes but the β-unity contour has a larger extent and

156 extends more than 10 R_M downstream of the planet.

157 Another way to identify pressure boundaries is to compute the gradients of β and β^*.

158 Figure 4 shows the gradient of the logarithm of β (a-c) and β^* (d-f). The gradient is

159 calculated along the radial direction in each plane. For the two X cuts, it is appropriate

160 to assume small gradients along the X direction. For the Z=0 plane, however, such a

161 radial gradient ($r = \sqrt{X^2 + Y^2}$) is less suitable far down the tail because the gradient

162 should be primarily in the cylindrical radial direction, i.e. in the $|Y|$ direction for this

163 plane. Hence, we should focus more on the dayside for the gradients on the Z=0 plane.

164 Also note that the color bars are in different ranges for three planes. As we can see, the

165 strong gradient layers for betas are thin on the dayside, becoming increasingly thicker and

166 more subdued with distance downstream of the planet. The thickness of the boundary

167 layer in the tail is of $1 - 1.5$ R_M. In addition, the unity boundaries of both β and β^*

168 (black crosses) are coincident with the strong gradient layers (the dark red region where

169 the value is greater than one, indicating an order of magnitude change per R_M). On

170 the other hand, even though the unity contour extends to large distances down the tail

171 ($> 10R_M$), the transition becomes too gradual, as indicated by the large area colored

172 white in Figures 2a and 2d for $X < -4$ R_M, to be a meaningful boundary indicator. In

173 addition, the grid resolution is rather coarse in the far tail. Hence, we only select y-z

174 planar cuts as far as 3 R_M down tail.

4. Ion Composition Boundary

175 As mentioned above, four ion species, H^+, O^+, O_2^+, and CO_2^+, are included in the

176 simulation. Figure 5 shows the H^+ mass (also number) density, the heavy ion (CO_2^+, O^+,

177 and O_2^+) mass density, and the heavy ion number density from the MF-MHD model in the

178 three rows, respectively. The three columns again are for Z=0, X=-1.5 R_M, and X=-3

$_{179}$ R_M cuts. H$^+$ dominates the sheath and beyond (Figures 5a-5c), and high H$^+$ density is

$_{180}$ also seen near the planet (Figures 5a and 5b), of a planetary origin as the density is too

$_{181}$ high to be solar wind originated. High heavy ion density is seen near the planet as well

$_{182}$ as the central plasma sheet, as expected. Further down the tail, the heavy ion escape is

$_{183}$ more concentrated in the plasma central sheet, as seen by comparing Figures 5e and 5h

$_{184}$ with Figures 5f and 5i. The energetic loss plume due to pick up ions by the convective

$_{185}$ electric field carried by the solar wind ($\mathbf{E} = -\mathbf{U} \times \mathbf{B}$) is also seen in Figures 5e, 5f, 5h,

$_{186}$ and 5i, oriented in the +Z direction due to the +By component of the input IMF, but

$_{187}$ less prominent in the number density figures.

$_{188}$ To define a model-based ion composition boundary, we calculate the ratio of the H$^+$

$_{189}$ density and the heavy ion density, for both mass density and number density. The results

$_{190}$ for the aforementioned three cuts are shown in Figure 6, the first row for the mass density

$_{191}$ ratio and the second row for the number density ratio. An interesting finding is that the

$_{192}$ white color, indicating a ratio of 1, encloses both the plasma sheet and the magnetic lobes,

$_{193}$ indicating that both regions are dominated by planetary heavy ions. Again, for $X < -4$

$_{194}$ R_M, the transition from H$^+$ to heavy ions becomes less distinct with increasing distance

$_{195}$ down the tail.

$_{196}$ Figure 7 shows the unity contours for the mass density ratio (a) and the number density

$_{197}$ ratio (b). The view is from slightly above the ecliptic plane and slightly sunward of the

$_{198}$ dusk terminator. Both unity boundaries extend very far down the tail ($> 10R_M$) and

$_{199}$ also overlap with the magnetic lobes. The mass density unity contour is larger than the

$_{200}$ number density ratio unity contour because it has a mass multiplier. Also, the plume is

more prominent and extended for the mass density ratio unity contour but barely seen in the number density ratio unity contour.

In a similar fashion, the gradients of the logarithms of the density ratios are also calculated, shown in Figure 8, a-c for the mass density ratio and d-f for the number density ratio. The gradients are computed in the same way as the betas. Again, thin and sharp strong gradient layers are seen on the dayside (Figures 8a and 8d), and also coincide with the unity boundaries, marked by the black crosses. In the tail (Figures 8b, 8c, 8e, and 8f), the strong gradient layers, again, are of a thickness of $1 - 1.5 \ R_M$, similar to Figure 4, and become thicker further down tail, comparing Figure 8b with 8c and Figure 8e with 8f. Furthermore, the gradients are about the same for the mass density ratio and the number density ratio as the mass multiplier is mostly cancelled from the logarithmic gradient calculation. With that as a reference, the unity of the mass density ratio, naturally larger, marks the center of the strong gradient layer while the unity of the number density ratio is more closely aligned with the inner edge.

5. Comparisons

Now that we have defined model-based pressure and composition boundaries, resembling the observationally based magnetic pileup and ion composition boundaries, the next step is to compare these boundaries. Figure 9 shows the comparisons between the pressure boundary and the ion composition boundary via different methods. The three columns are for $Z = 0$ (Figures 9a, 9d, and 9g), $X = -1.5 \ R_M$ (Figures 9b, 9e, and 9h), and $X = -3$ R_M (Figures 9c, 9f, and 9i). The first row shows the unities of β, β^*, ion mass density ratio, and ion number density ratio, colored in black, blue, green, and red, respectively. For the equatorial plane, we have zoomed in to focus on the dayside. The unity contours

²²³ for these four quantities are basically on top of each other and exhibit asymmetry about

²²⁴ the X axis probably due to the effects of quasi-parallel and quasi-perpendicular shocks

²²⁵ (see Figure 1a). The two betas also have another inner unity curve, a balance between the

²²⁶ ionospheric plasma-type pressure and the magnetic pressure. For the tail cuts, the unities

²²⁷ of β, β^*, and ion mass density ratio mostly coincide on the outer edge at $X = -1.5$

²²⁸ R_M, while the ion number density ratio unity is systematically smaller. Further down

²²⁹ tail, at $X = -3R_M$ (Figure 9c), the β unity is the outmost, then slightly inward are the

²³⁰ overlapping β^* and ion mass density ratio unities, and ion number density ratio unity is

²³¹ located as the innermost curve.

²³² Upstream of the planet (X> 0) along the Mars-Sun line (Figure 9d, leftmost column),

²³³ transitions in the pressure and density ratios are apparent at the bow shock (X=1.75) and

²³⁴ near the MPB ($X = 1.2 - 1.3$). Downstream of the planet ($X < 0$), the unities begin to

²³⁵ separate along Y with distance down tail as the transition from plasma-type pressure and

²³⁶ H^+ dominance to magnetic pressure and heavy ions dominance becomes more gradual, as

²³⁷ shown in the right two columns of Figures 9. Each quantity has sharper transitions closer

²³⁸ to the planet.

²³⁹ To better compare the locations of unities with the locations of maximum gradient

²⁴⁰ in the various quantities, the bottom row shows the gradient of the logarithmic values

²⁴¹ along the Mars-Sun line (Figure 9g) and in the cross-tail Y direction at X= -1.5 and

²⁴² $X = -3$ (Figure 9h and 9i), with color-coded vertical dashed lines marking the innermost

²⁴³ and outermost unity locations. The maximum gradients of the four quantities are nearly

²⁴⁴ co-located. The tailward magnetosheath ($2.5 < |Y| < 4R_M$, and $-3 < |Y| < -1.5R_M$

²⁴⁵ approximately) is a region dominated by H^+ (density ratio $\gg 1$) and dynamic pressure

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246 ($\beta^* \gg \beta$). At the inner edge of this region ($|Y| \sim 2 - 2.5R_M$), the composition and all of

247 the pressure terms exhibit sharp gradients at nearly the same location (right two columns

248 of Fig. 9), suggesting that all mark the same physical transition. Third, gradient extrema

249 agree very well with the unities of β, β^*, and ion mass density ratio, while the ion number

250 density unity is located systematically inward of the gradient extrema (Figure 8 and

251 Figure 9). Thus, the unities in β, β^*, and mass density ratio provide convenient proxies

252 for the boundaries between distinct regions of the Mars plasma environment. This also

253 shows that the same physical boundary may be identified using different measurement

254 techniques.

255 Along the Mars-Sun line (Figure 9g), a strong gradient layer for all quantities is seen at

256 the bow shock (X$\sim$ 1.7 R_M) with a thickness of about 0.1 R_M ($300-400$ km). Downstream

257 of the bow shock, near 1.25 R_M, a positive gradient layer for β and β^* (nearly identical

258 due to a negligible dynamic pressure) is seen with a thickness of ~ 0.1 R_M. The behavior

259 of the ion density ratio near 1.25 R_M is slightly different. Both the mass and number

260 density ratio gradients are positive, primarily because the heavy ion density decreases

261 with altitude. However, the ion mass and number density unities are clearly offset from

262 the beta unity by $\sim 0.05R_M$ (Fig. 9d). To further examine this region, Figure 10 depicts

263 the heavy ion mass density (black), H$^+$ density (blue), and the ratio of the two (red)

264 along the Mars-Sun line (MSO X axis). Moving inward from the bow shock towards the

265 planet, the heavy ion mass density increases with decreasing altitude, slowly at first, then

266 more rapidly as the mass density unity is approached. Interior to the unity, the heavy

267 ion mass density rises steeply and soon dominates the total mass density. Meanwhile,

268 the proton density remains nearly constant until the unity is reached, and then drops

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269 gradually by a factor of ~ 3. The inflection in the heavy ion mass density from 1.2 to

270 1.35 R_M corresponds to the dips of the ion density ratio gradients (Figure 9g), which

271 are nearly co-located with strong beta gradients. This feature could be explained by an

272 increase in ion production due to the electron impact ionization and charge exchange near

273 the MPB [e.g. *Crider et al.*, 2000; *Jin et al.*, 2006] as well as the compression of planetary

274 plasma by the solar wind. If we take the ion composition boundary to be centered on the

275 mass density unity, then its thickness, as defined by the heavy ion mass density inflection,

276 would be $\sim 0.1 R_M$.

6. Discussion and Conclusions

277 This study quantitatively examined pressure and composition transitions in the Mars-

278 solar wind interaction region by calculating gradients and unities of plasma β and β^*,

279 as well as ion mass and number density ratios. We found that the unity contours are

280 nearly co-located with the gradient extrema, so that they may be conveniently used to

281 define physical boundaries in the system. Historically, these pressure and composition

282 transitions have mostly been simplified as sharp, cylindrically symmetric boundaries. In

283 this study, the unity contours and gradients of betas and ion density ratios have shown

284 that these boundaries are structured and have a finite thickness, ranging from $0.05 - 0.1$

285 R_M near the sub-solar region to $1 - 1.5 R_M$ in the tail. The unity contours enclose

286 magnetic lobes filled with planetary heavy ions to more than 10 R_M down tail. The

287 pressure and composition gradients get progressively weaker and broader with increasing

288 distance down the tail, presumably becoming indiscernible at large distances downstream.

289 With a comprehensive set of instruments to measure the near Martian space environment,

290 MAVEN data are being used to study these boundaries in detail [e.g *Matsunaga et al.*,

2015]. The boundary shape and structure presented here can provide physical insight for these observational studies.

We examined the relationship between pressure and composition boundaries (corresponding to the observationally based MPB and ICB, respectively) by comparing unities and gradients of two betas and two ion density ratios. The unities are nearly co-located (Figure 9), it is easy to see that the unities mostly match with each other, except for the ion number density ratio unity, which is systematically interior to other unity boundaries. In the tail, the locations of the pressure and composition boundaries are very similar, which means the planetary heavy ions dominate not only the central plasma sheet but also the magnetic lobes. Even though heavy ions are more concentrated near the plasma sheet, the magnetic lobes are devoid of H^+ so that heavy ions still prevail. This means that ion escape down the tail occurs in both the plasma sheet and across the much larger cross sectional area of the magnetic lobes. Downstream of the bow shock, Figure 10 shows that the decrease of solar wind proton density does not begin until the mass density ratio reaches unity. In addition, the model suggests that the ion composition boundary is structured, as revealed by an inflection in the heavy ion mass density gradient, which may be associated with enhanced electron impact ionization and charge exchange in this region.

While observationally, the MPB and ICB seem to occur close to one another, especially for $X > 0$, it has been unclear how these two boundaries are associated physically. In the tail region, the MF-MHD simulation exhibits a sharp outer edge to the lobes at the same location in both composition and beta. Magnetic field lines in the lobes are draped closely by Mars' upper atmosphere, and may in some cases be connected to planetary crustal fields. The ionosphere could then plausibly provide the source of planetary ions in

the lobes. The composition and pressure boundaries deviate from one another in the tail

near the $Y = 0$ plane for several reasons. First, there is a dense plasma sheet of planetary

ions that dominates the pressure between the lobes. Second, there is an energetic plume

of planetary ions in the $+Z$ direction that have very large gyroradii and move differently

than the magnetic field. Third, the convection electric field accelerates planetary ions

in the $-Z$ hemisphere back into the central tail region, which creates a small outward

extension of the composition boundary in that direction (seen in Figure 9b and 9c).

The comparison between the boundaries determined from a MF-MHD simulation with

the analytical fittings of MPB from *Vignes et al.* [2000] (based on MGS observations only)

and *Trotignon et al.* [2006] (the combination of Pbobos-2 and MGS observations) is shown

in Figures 4a, 4d, 8a, and 8d. The two fits are highlighted in green solid line and red

dashed line, respectively. In the tail, it is easy to see that the unity boundaries, except for

the ion number density ratio presented in this study, match with the Vignes fitting and

show little flaring, in contrast to a large flaring angle from the Trotignon fitting. The unity

contour of the ion number density ratio, in fact, moves inward (towards the X axis) with

distance down the tail, so the shape of this boundary depends on how it is defined. On

the dayside, unity boundaries in this study are mostly located outside both fits, especially

at higher solar zenith angle, and also exhibit a dawn-dusk asymmetry, probably due to

the different in shock geometries (quasi-parallel vs. quasi-perpendicular) at the dawn and

dusk sides. Existing data show a large spread of MPB locations at the tail [*Vignes et al.*,

2000], which can be attributed to many factors, such as the different upstream conditions

and different locations of strong crustal magnetic fields with respect to the sub-solar point.

However, it might also be partially due to the structure and asymmetry of this boundary, which have so far not been considered in observational studies.

Finally, this study focuses on the three dimensional shape and structure of the pressure and composition boundaries, which can be used as theoretical guidance for observational analyses. In particular, MAVEN data is now being used to study these boundaries in details [e.g. *Matsunaga et al.*, 2015]. Future work with a suite of MF-MHD models will investigate how the upstream conditions, strong crustal field locations, neutral atmosphere and ionosphere affect these boundaries.

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Figure 1.   The three rows, from top to bottom, show the magnetic pressure (Pa), the dynamic pressure (Pa), and the thermal pressure (Pa), and the three columns, from left to right, are for Z=0, X=-1.5 R_M, and X=-3 R_M in MSO coordinates. The values are logarithmic scale. The two vertical dashed lines in the first column mark the positions of the two X slices in the second and third columns.

Figure 2.   Plasma beta (β), i.e., the ratio of the plasma thermal pressure and the magnetic pressure, is shown in a-c, at Z=0, X=-1.5 R_M, and X=-3 R_M, respectively, while β^*, which is the sum of the plasma thermal pressure and dynamic pressure divided by the magnetic pressure, shown in d-f, at Z=0, X=-1.5 R_M, and X=-3 R_M, respectively. The values are logarithmic scale. The two vertical dashed lines in the first column mark the positions of the two X slices in the second and third columns.

Figure 3.   The contours of $\beta = 1$ (a) and $\beta^* = 1$ (b).

Figure 4.   The gradient of the logarithm of β (a-c) and β^* (d-f). From left to right, the three columns are for three cuts, Z=0, X=-1.5 R_M, and X=-3 R_M in MSO coordinates. The black crosses highlight the unities of β and β^*, as extracted from Figure 2. The green solid line and red dashed line in a and d represent the MPB fitting from *Vignes et al.* [2000] and *Trotignon et al.* [1996], respectively.

Figure 5.   The three rows, from top to bottom, show the mass density of H$^+$ (amu/cm^3), the mass density (amu/cm^3) of heavy ions (CO$_2^+$, O$^+$, and O$_2^+$), and the number density (cm^{-3}) of heavy ions, and the three columns, from left to right, are for Z=0, X=-1.5 R_M, and X=-3 R_M in MSO coordinates. The values are logarithmic scale. The two vertical dashed lines in the first column mark the positions of the two X slices in the second and third columns.

Figure 6. The ratio of the mass density of H^+ and heavy ions is shown in a-c, at Z=0, X=-1.5 R_M, and X=-3 R_M, respectively, while the ratio of the number density of H^+ and heavy ions is shown in d-f, at Z=0, X=-1.5 R_M, and X=-3 R_M, respectively. The values are logarithmic scale. The two vertical dashed lines in the first column mark the positions of the two X slices in the second and third columns.
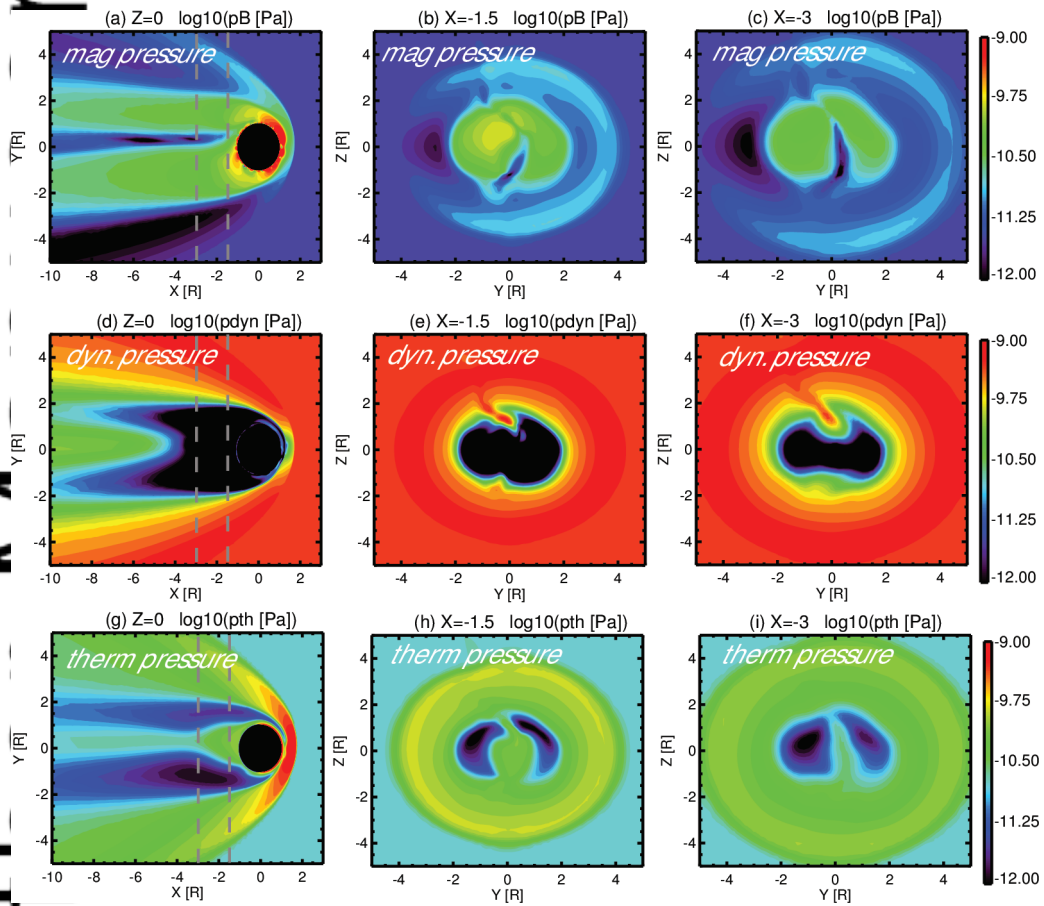
Figure 7. The contours of the ion mass density ratio = 1 (a) and the ion number density ratio = 1 (b).

Figure 8. The gradient of the logarithm of the ion mass density ratio (a-c) and the ion number density ratio (d-f). From left to right, the three columns are for three cuts, Z=0, X=-1.5 R_M, and X=-3 R_M in MSO coordinates. The black crosses highlight the unities of the ratios, as extracted from Figure 6. The green solid line and red dashed line in a and d represent the MPB fitting from [*Vignes et al.*, 2000] and *Trotignon et al.* [2006], respectively.

Figure 9. Comparison of unities and gradients at Z=0 (a, d, g), X=-1.5 R_M (b, e, h) and X=-3 R_M (c, f, i). The first row (a-c) shows the unities of β, β^*, ion mass density ratio, and ion number density ratio, colored in black, blue, green, and red, respectively. The second row shows the line plots of the logarithmic values of the same four quantities along the subsolar line for the equatorial plane (d) and against the Y axis at Z=0 for the two X cuts (e and f). The bottom row shows the gradient of the logarithmic values of the four quantities along the subsolar line for the equatorial plane (g) and against the Y axis at Z=0 for the two X cuts (h and i). The dash vertical lines in g-i mark the unity locations for two quantities with the innermost and outmost positions, color coded the same as the solid lines.

Figure 10. Heavy ion mass density (black), H$^+$ density (blue), and the ratio of H$^+$ density and heavy ions (red) against X axis. The unit for mass density is amu cm^{-3}, where amu is the atomic mass unit.

(a) Z=0   log10(pB [Pa])   (b) X=-1.5   log10(pB [Pa])   (c) X=-3   log10(pB [Pa])

mag pressure   mag pressure   mag pressure

(d) Z=0   log10(pdyn [Pa])   (e) X=-1.5   log10(pdyn [Pa])   (f) X=-3   log10(pdyn [Pa])

dyn. pressure   dyn. pressure   dyn. pressure

(g) Z=0   log10(pth [Pa])   (h) X=-1.5   log10(pth [Pa])   (i) X=-3   log10(pth [Pa])

therm pressure   therm pressure   therm pressure

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(a) Z=0   log10(beta)   (b) X=-1.5   log10(beta)   (c) X=-3   log10(beta)
(d) Z=0   log10(beta_str)   (e) X=-1.5   log10(beta_str)   (f) X=-3   log10(beta_str)

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(a) beta

[z [R]]

X [R]

Y [R]

-20

-15

-10

-5

0

(b) beta*

[z [R]]

X [R]

Y [R]

-20

-15

-10

-5

0

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(a) Z=0 grad. of log10(beta)
(b)X=-1.5 grad. of log10(beta)
(c) X=-3 grad. of log10(beta)
(d)Z=0 grad. of log10(beta_str)
(e)X=-1.5 grad. of log10(beta_str)
(f) X=-3 grad. of log10(beta_str)

Green solid: Vignes fitting
Red dashed: Trotignon fitting

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(a) Z=0 log10(rho_H [amu/cm^3]) (b) X=-1.5 log10(rho_H [amu/cm^3]) (c) X=-3 log10(rho_H [amu/cm^3])

rho_H

(d) Z=0 log10(rho_hvy [amu/cm^3]) (e) X=-1.5 log10(rho_hvy [amu/cm^3]) (f) X=-3 log10(rho_hvy [amu/cm^3])

mass dens. for hvy ions

(g) Z=0 log10(n_hvy [cm^-3]) (h) X=-1.5 log10(n_hvy [cm^-3]) (i) X=-3 log10(n_hvy [cm^-3])

num dens. for hvy ions

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(a) Z=0 log10(mass dens. ratio)   **(b) X=-1.5 log10(mass dens. ratio)**   **(c) X=-3 log10(mass dens. ratio)**

mass dens. ratio

(d) Z=0 log10(num dens. ratio)   **(e) X=-1.5 log10(num dens. ratio)**   **(f) X=-3 log10(num dens. ratio)**

num dens. ratio

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(a) mass density ratio

(b) num. density ratio

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(a) Z=0 grad of log10(mass dens. ratio)
Green solid: Vignes fitting
Red dashed: Trotignon fitting

(b) X=-1.5 grad of log10(mass dens. ratio)

(c) X=-3 grad of log10(mass dens. ratio)

(d) Z=0 grad of log10(num dens. ratio)
Green solid: Vignes fitting
Red dashed: Trotignon fitting

(e) X=-1.5 grad of log10(num dens. ratio)

(f) X=-3 grad of log10(num dens. ratio)

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(a) Unity comparison at Z=0
(b) Unity comparison at X=-1.5
(c) Unity comparison at X=-3
(d) Log10(var) comparison at Z=0
(e) Log10(var) comparison at X=-1.5
(f) Log10(var) comparison at X=-3
(g) Grad of log10(var) comp. at Z=0
(h) Grad of log10(var) comp. at X=-1.5
(i) Grad of log10(var) comp. at X=-3

Beta
Beta*
Ion mass dens. ratio
Ion num dens. ratio

<- Unities

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black: heavy ion mass density
blue: H+ mass density
red: H+/heavy ion

Mass density & H+/Hvy ion

X (Rm)

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