The roles of charge exchange and dissociation in spreading Saturn’s neutral clouds

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Abstract. Neutrals sourced directly from Enceladus’s plumes are initially confined to a dense neutral torus in Enceladus’s orbit around Saturn. This neutral torus is redistributed by charge exchange, impact/photodissociation, and neutral–neutral collisions to produce Saturn’s neutral clouds. Here we consider the former processes in greater detail than in previous studies. In the case of dissociation, models have assumed that OH is produced with a single speed of 1 km s$^{-1}$, whereas laboratory measurements suggest a range of speeds between 1 and 1.6 km s$^{-1}$. We show that the high-speed case increases dissociation’s range of influence from 9 to 15 $R_S$. For charge exchange, we present a new modeling approach, where the ions are followed within a neutral background, whereas neutral cloud models are conventionally constructed from the neutrals’ point of view. This approach allows us to comment on the significance of the ions’ gyrophase at the moment charge exchange occurs. Accounting for gyrophase: (1) has no consequence on the $H_2O$ cloud; (2) doubles the local density of OH at the orbit of Enceladus; and (3) decreases the oxygen densities at Enceladus’s orbit by less than 10%. Finally, we consider velocity-dependent, as well as species-dependent cross sections and find that the oxygen cloud produced from charge exchange is spread out more than $H_2O$, whereas the OH cloud is the most confined.
1. Introduction

The Enceladus plumes directly produce a dense H$_2$O torus centered on Enceladus’s orbit, within which charge exchange and dissociation subsequently produce neutrals that either feed Saturn’s extended neutral clouds, collide (absorb) with Saturn and its rings, or leave the system altogether on escape orbits. This paper is a report on the results of a sensitivity study of low-velocity charge exchange and dissociation within the neutral torus.

Several decades before Cassini arrived at Saturn and the Enceladus water plumes were discovered [Hansen et al., 2006], neutral hydrogen was observed in Saturn’s magnetosphere, both from Earth [Weiser et al., 1977] and from Voyagers 1 and 2 [Shemansky and Hall, 1992]. Hydroxyl was later discovered by Shemansky et al. [1993] with HST, and more recently, Esposito et al. [2005] detected atomic oxygen. These observations collectively hinted at the presence of a source of water, and models predicted its location to be near the orbit of Enceladus (c.f., Jurac et al. [2002]).

After identifying the Enceladus plumes as the dominant source of the water-group neutrals (O, OH, H$_2$O)—and indeed the co-rotating plasma itself via electron impact and photoionization [Young et al., 2005; Sittler et al., 2005, 2008]—researchers have been attempting to understand how neutrals are transported from Enceladus to 20 Saturn radii (R$_S = 6 \times 10^9$ cm) and beyond, as observed by Shemansky et al. [1993], Esposito et al. [2005], and most recently by Melin et al. [2009]. Early on, Jurac et al. [2002] mentioned the role of charge exchange in this inflation process. Johnson et al. [2006] later showed that if magnetospheric plasma is slowed sufficiently with respect to neutrals in
the Enceladus torus, then charge exchange produces a sufficient number of particles with
velocities capable of spreading the dense $\text{H}_2\text{O}$ Enceladus torus into the cloud observed by
Shemansky et al. [1993].

Farmer [2009] pointed out the importance of dipole–dipole interactions in collisions
involving $\text{H}_2\text{O}$ molecules. She showed that collisions inside the dense Enceladus torus
(parameterized by macroscopic viscosity) are alone sufficient for the creation of the ex-
tended component of Saturn’s neutral cloud. Cassidy and Johnson [2010] later argued
that Farmer’s fluid treatment is inappropriate for neutral–neutral collisions in the Ence-
ladus torus, where the mean free path is on the order of the torus size itself. Instead,
Cassidy and Johnson [2010] approached the problem with a direct simulation Monte Carlo
(DSMC) model. Their model self-consistently included losses due to charge exchange, dis-
sociation, and ionization, whereas Farmer [2009] accounted for losses to charge exchange
and ionization by evolving the neutral cloud for the time scales (months to a few years)
found in Sittler et al. [2008]. Both studies agree that neutral–neutral collisions are neces-
sary for the inflation of Saturn’s neutral cloud.

Collisions between neutrals occur at a rate proportional to the square of the neutral
density. Thus, where neutral densities peak near the orbit of Enceladus, neutral–neutral
collisions occur more often than either charge exchange or dissociation, whereas near 6
$R_\text{S}$, neutral densities drop and all three processes become comparable (see Fig. 3, Cassidy
and Johnson [2010]). Models involving neutral collisions have recently been validated
with Herschel observations by Hartogh et al. [2011], who attribute a warm and broadened
Enceladus torus to heating via neutral–neutral collisions; the effect of these interactions
should therefore be included in any attempt to fully model Saturn’s neutral clouds. Nev-
ertheless, several first-order conclusions can be drawn by revisiting charge exchange and
dissociation.

Previous neutral cloud models approach charge exchange from the neutrals’ point of
view, whereas we follow the ion along its trajectory, thus allowing us to identify the
gyrophase at which an ion undergoes charge exchange. We find that including the phase
dependence doubles OH densities at the orbit of Enceladus, decreases oxygen density by
\( \lesssim 10\% \), and has no effect on H\(_2\)O (section 3.1). Also, the velocity-dependence of charge
exchange varies by species. Previous studies (e.g., Johnson et al. [2006]; Cassidy and
Johnson [2010]) have considered velocity-dependence, but have used a single cross section
to represent all charge exchanges. We show in section 3.1 that symmetric reactions such as
H\(_2\)O + H\(_2\)O\(^+\) \rightarrow H\(_2\)O\(^+\) + H\(_2\)O\(^*\) (the asterisk identifies a neutral released with the speed of
the reacting ion) tend to distribute neutrals closer to Saturn, while asymmetric exchanges
such as H\(_2\)O + O\(^+\) \rightarrow H\(_2\)O\(^+\) + O\(^*\) populate a more extended cloud, with less absorption
on Saturn.

With regard to dissociation, OH produced by impact/photodissociation of H\(_2\)O has pre-
viously been modeled with an initial speed of 1 km s\(^{-1}\) [Jurac and Richardson, 2005; Cas-
sidy and Johnson, 2010], whereas recent laboratory measurements span 1 to 1.6 km s\(^{-1}\),
depending on the molecule’s internal energy [Wu and Chen, 1993; Makarov et al., 2004].
We model this parameter space and find that, relative to charge exchange, most OH found
inside 9 R\(_S\) is produced by dissociation when OH is dissociated from H\(_2\)O at 1 km s\(^{-1}\),
with that location extended to 15 R\(_S\) when OH is dissociated from H\(_2\)O at 1.6 km s\(^{-1}\)
instead.
This paper is organized as follows. The model for the production of neutrals via dissociation and three illustrative charge exchanges is explained in section 2. Our results are found in section 3, followed by a discussion in section 4. The important points are summarized in section 5.

2. Model

We begin with a few words on nomenclature. The neutral torus in this paper pertains to the primary neutral torus (not plasma torus) supplied directly by Enceladus's plumes. The neutral clouds refer to the secondary neutrals produced from charge exchange and dissociation in the neutral torus.

The production of Saturn’s neutral cloud is modeled in two steps. We first construct a dense $\text{H}_2\text{O}$ torus from a plume positioned at Enceladus’s south pole with specifications based on several Cassini Enceladus flybys (Smith et al. [2010]; see also Smith et al. [2004], Smith [2006], and Smith et al. [2007]). Secondary neutrals are then produced from the primary neutral torus by charge exchange and dissociation, some of which remain gravitationally bound to Saturn and form the neutral clouds. On the basis that they spend most of the time outside the neutral torus and plasma sheet, we assume their lifetimes to be determined solely by photo-processes, though in section 3.3, we consider the effects of charge exchange and electron impact.

2.1. Neutral torus model

The neutral torus and Enceladus plume models are described in the following subsections.

2.1.1. Enceladus $\text{H}_2\text{O}$ torus
Our aim is to study the effects of several important reactions occurring in Enceladus’s orbit. The primary neutral torus, fed directly by Enceladus, is produced in the model by evolving water molecules released from Enceladus into a dense neutral torus centered on Enceladus’s orbit (3.95 R₆). The assumption is that all H₂O is initially produced by a single plume at Enceladus’s south pole. In reality, more than one plume has been observed [Porco et al., 2006], and researchers such as Saur et al. [2008] and Smith et al. [2010] have studied their signature on flyby observations. For our purposes, the detailed influence of multiple plumes can be neglected. The plume particles’ radial speed distribution is prescribed as a one-dimensional Maxwellian with temperature $T = 180$ K [Spencer et al., 2006; Hansen et al., 2006]:

$$f(v) = \left(\frac{m_{\text{H}_2\text{O}}}{2\pi k T}\right)^{1/2} \exp\left(-\frac{m_{\text{H}_2\text{O}}}{2kT}(v - v_{\text{bulk}})^2\right),$$  \hspace{1cm} (1)

where $v_{\text{bulk}}$ is the bulk speed, equal to $720$ m s⁻¹, 1.8× the thermal speed estimated by Smith et al. [2010] ($v_{\text{therm}} = \sqrt{2kT/m_{\text{H}_2\text{O}}} = 400$ m s⁻¹). Additionally, a raised cosine distribution is used to determine where the molecules are released:

$$g(\theta) = \begin{cases} \frac{1}{\theta_0} \left[1 + \cos\left(\frac{\theta}{\theta_0}\pi\right)\right] & \text{if } \theta < \theta_0 = 30^\circ \\ 0 & \text{otherwise.} \end{cases}$$  \hspace{1cm} (2)

Co-latitude theta is measured from Enceladus’s south pole, and $\theta_0 = 30^\circ$ is the plume half-width, based on INMS in situ observations [Smith et al., 2010]. We assume no azimuthal dependence.

Enceladus’s gravity is ignored since the escape velocity, $v_{\text{esc}} = 240$ m s⁻¹, is greatly exceeded for most molecules (99%), where $v_{\text{bulk}} > v_{\text{therm}} > v_{\text{esc}}$; our results differ by less than one percent whether Enceladus’s gravity is considered or not. Particles released from Enceladus are thus assumed to move on Keplerian orbits with respect to Saturn. Each
water molecule is allowed to orbit inside the torus for a period determined by the collective lifetimes against photodissociation, electron-impact dissociation, and charge exchange. To be clear, the molecules forming the neutral torus are subject to all of the losses stated, while the neutral cloud is subject to photo-processes only (section 2.2). Further reaction details are important for modeling plasma characteristics but only the timescales given below are required to model the neutral torus.

Photodissociation: The photodissociation lifetime for H$_2$O, $\tau_{\text{phot}} = 9.1 \times 10^6$ s, comes directly from Huebner and Carpenter [1979], scaled to Saturn’s distance from the Sun. At peak solar activity, neutral abundances attributed to dissociation double [Jackman and Arridge, 2011].

Impact dissociation: In the case of impact dissociation, suprathermal (hot) electrons dominate [Fleshman et al., 2010b]. Assuming the conditions near Enceladus’s orbit apply throughout the neutral torus, we estimate the hot electron density and temperature to be 160 eV and 0.3 cm$^{-3}$ from Fleshman et al. [2010b], which fit within a range of recent observations (cf., Young et al. [2005], Sittler et al. [2008]). The rate coefficient for impact dissociation of water is found by convolving $\sigma(v)v$ with a 160 eV Maxwellian distribution to find $\kappa_{\text{imp}} = 1.5 \times 10^{-6}$ cm$^3$ s$^{-1}$ (Fleshman et al. [2010b], table S9). Above 100 eV, $\kappa_{\text{imp}}$ is insensitive to temperature, making this estimate valid for a range of observations. Assuming the hot electron density, $n_{\text{eh}}$, is constant over the neutral torus, the lifetime against impact dissociation is $\tau_{\text{imp}} \approx [\kappa_{\text{imp}} n_{\text{eh}}]^{-1} = 2.2 \times 10^6$ s. Dissociation via thermal electrons—whose temperature and density are 2 eV and 60 cm$^{-3}$—is also expected, but such collisions occur 5× less often (Fleshman et al. [2010b], table S9) and are thus ignored here.
Charge exchange: The following three reactions are included in this study:

\[
\begin{align*}
\text{H}_2\text{O} + \text{H}_2\text{O}^+ & \rightarrow \text{H}_2\text{O}^+ + \text{H}_2\text{O}^* \\
\text{H}_2\text{O} + \text{H}_2\text{O}^+ & \rightarrow \text{H}_3\text{O}^+ + \text{OH}^* \\
\text{H}_2\text{O} + \text{O}^+ & \rightarrow \text{H}_2\text{O}^+ + \text{O}^*. 
\end{align*}
\]

(3a) (3b) (3c)

Other charge exchanges are important in the neutral torus, some of which involve ions reacting with secondary neutrals such as H, O, and OH. To model their effect properly, one would calculate these neutral densities as in a conventional time-dependent neutral cloud model. We estimate that including all such reactions would increase our estimates on neutral cloud densities by approximately a factor of two. The primary purpose of choosing this combination of reactions is to study three classes of charge exchanges, for which the collision frequency decreases with, increases with, or is independent of the relative speed of the reacting pair (reactions 3b, 3c, and 3a, respectively). We return to this point in section 2.2.2.

An estimate of the charge exchange lifetime can be made by adding the rate coefficients for reactions 3a–3c. Multiplying by the observed \(\text{H}_2\text{O}^+\) and \(\text{O}^+\) densities near the orbit of Enceladus (6 and 12 cm\(^{-3}\), Sittler et al. [2008]), we find \(\tau_{\text{chex}} = \left[\kappa_{\text{H}_2\text{O}^+}\text{n}_{\text{H}_2\text{O}^+} + \kappa_{\text{O}^+}\text{n}_{\text{O}^+}\right]^{-1} = [6.0 + 2.8]^{-1} \times 10^8 \text{ s} = 1.1 \times 10^7 \text{ s}\). The reaction rates are from Lishawa et al. [1990] and Albritton [1978] for \(\kappa_{\text{H}_2\text{O}^+}\) and \(\kappa_{\text{O}^+}\), respectively. The lifetime of \(\text{H}_2\text{O}\) against the sum of these processes is then

\[
\tau_{\text{torus}} = \left[\frac{1}{\tau_{\text{phot}}} + \frac{1}{\tau_{\text{imp}}} + \frac{1}{\tau_{\text{chex}}}\right]^{-1} = (1.1 + 4.5 + 0.91)^{-1} \times 10^7 \text{ s} = 1.6 \times 10^6 \text{ s} \approx 20 \text{ days.} \] (4)
These estimates can be compared to Fig. 3 of Cassidy and Johnson [2010]: for example, our lifetime against dissociation is $1.7 \times 10^6$ s, while they use $7 \times 10^6$ s near $4 R_S$. The discrepancy comes mostly from the impact dissociation timescale. Cassidy’s dissociation rate was calculated using Schippers et al. [2008], wherein CAPS ELS data were fitted and extrapolated down from $5.5 R_S$, while our own estimate hinges on a hot electron density derived from our chemistry model [Fleshman et al., 2010b]. For charge exchange, we have a lifetime of $1.1 \times 10^7$ s, and Cassidy and Johnson [2010] have a comparable $8 \times 10^6$ s.

Particles are created and tracked in each of our model runs, and the results are scaled to the number of water molecules in the real neutral torus. The total number is estimated from an assumed neutral source rate from Enceladus of $\dot{M} = 200$ kg s$^{-1}$ [Jurac and Richardson, 2005; Hansen et al., 2006, 2011] and lifetime, $\tau_{\text{torus}}$ (Eq. 4):

$$N_{\text{torus}} = \dot{M}\tau_{\text{torus}}/m_{\text{H}_2\text{O}} \approx 1.1 \times 10^{34} \text{ H}_2\text{O molecules.}(5)$$

We bin and azimuthally average the results to find a 2-D density function, $n_{\text{torus}}(r, \theta)$ (radius and latitude), through which to introduce ions for charge exchange. This function also determines from where dissociated neutrals are produced.

### 2.1.2. Plume model

Before describing dissociation and charge exchange within the torus, we address a calculation with the purpose of comparing the neutral production near Enceladus with that from the entire torus. In doing so, we prescribe a plume whose density is consistent with Eqs. 1 and 2. In this case, the ambient neutral density can be ignored compared to the neutrals leaving the surface of Enceladus directly.

The densities are determined everywhere by imposing integrated flux ($\int n(r, \theta)v(r, \theta)dA$) and energy ($mv^2/2 - mM_EG/r$) conservation at a given distance $r$. The picture can be
simplified, however, since most neutrals have at least twice Enceladus’s escape velocity. The speeds are thus independent of $r$ in the immediate vicinity of Enceladus. By equating the integrated flux at the surface of Enceladus to the same integral at another distance $r > R_E$, we find a familiar $1/r^2$ dependence:

$$n_{\text{plume}}(r, \theta) = n(\theta) \left( \frac{R_E}{r} \right)^2 \exp \left[ - \left( \frac{r - R_E}{H_r} \right) \right].$$ (6)

The trailing exponential factor is imposed ad hoc to keep the total plume content finite, and reflects Saturn’s influence as the molecules leave Enceladus. Consistent with Saur et al. [2008], $H_r$ is set at 4 times the Hill radius of 948 km. The angular dependence is consistent with our velocity distribution in the previous section (Eq. 1),

$$n(\theta) = \begin{cases} \frac{n_0}{2} \left[ 1 + \cos \left( \frac{\theta \pi}{\theta_0} \right) \right] & \text{if } \theta < \theta_0 = 30^\circ \\ 0 & \text{otherwise,} \end{cases}$$ (7)

which is normalized such that $n(0) = n_0$, where the plume strength $n_0$ is found to be $5.9 \times 10^8$ cm$^{-3}$ by integrating $n(\theta)v_{\text{bulk}}$ over the area spanning the south pole of Enceladus from $\theta = 0^\circ$ to $\theta = \theta_0 = 30^\circ$, and setting that result equal to the plume production rate of $\dot{M}/m_{\text{H}_2\text{O}} = (200 \text{ kg s}^{-1})/m_{\text{H}_2\text{O}} = 6.7 \times 10^{27}$ molecules per second.

In section 3, we compare the results of charge exchange with the plume ($n_{\text{plume}}$) to that with the entire torus ($n_{\text{torus}}$).

2.2. Neutral cloud model

Production of Saturn’s neutral clouds entails following the neutrals produced by dissociation and charge exchange occurring within the neutral torus. The treatment of each of these processes are described below.

2.2.1. Dissociation
The hydroxyl radical, OH, produced largely by dissociated H$_2$O, has previously been modeled with a single speed of 1 km s$^{-1}$ (i.e., Jurac and Richardson [2005], Cassidy and Johnson [2010]). Dissociated OH has been measured however with speeds between 1 and 1.6 km s$^{-1}$ [Wu and Chen, 1993; Makarov et al., 2004]. Here we bound this range by modeling the OH neutral clouds produced from an azimuthally-symmetric source (with respect to Saturn) with velocities drawn from Maxwellian distributions with temperatures $T = \frac{1}{2}m_{OH}v^2_{mp}$, where the most probable speed, $v_{mp}$, is set to 1 and 1.6 km s$^{-1}$, representing the low- and high-speed limits.

The initial locations of the ejected OH are determined by the spatial distribution of neutrals in the Enceladus torus ($n_{\text{torus}}(r, \theta)$, section 2.1.1), and the directions of their release are chosen randomly and isotropically. The molecules orbit Saturn until they are photodissociated and removed from the system.

By assuming a volume over which dissociations occur, the number of modeled OH molecules can be scaled to a realistic value. We take the volume to be a torus centered on Enceladus (3.95 Rs), with a minor radius of 1 Rs:

$$V \approx 2\pi(4\text{ Rs})(2\text{ Rs})^2 = 2 \times 10^{31} \text{ cm}^3.$$  \hspace{1cm} (8)

For impact dissociation, we then expect a contribution of

$$N^\text{imp}_{\text{cloud}} = k_{\text{imp}}\tau_{\text{phot}}^\text{OH}V = 2.8 \times 10^{34} \text{ OH molecules},$$  \hspace{1cm} (9)

where $k_{\text{imp}} = 7.9 \times 10^{-5} \text{ cm}^{-3} \text{ s}^{-1}$ is the rate (per volume) of impact dissociations occurring between suprathermal electrons and H$_2$O molecules in the torus [Fleshman et al., 2010b] and $\tau_{\text{phot}}^\text{OH} = 1.8 \times 10^7 \text{ s}$ is the photodissociation lifetime of OH at Saturn [Huebner and Carpenter, 1979]. The number of OH molecules produced by photodissociation in the
torus is similarly given by

\[ N_{\text{cloud}}^{\text{phot}} = k_{\text{phot}}^{\text{OH}} V = 7.6 \times 10^{33} \text{ OH molecules}, \]  

where \( k_{\text{phot}} = 2.1 \times 10^{-5} \text{ cm}^{-3} \text{ s}^{-1} \) is the rate (per volume) of \( \text{H}_2\text{O} \) photodissociations occurring in the Enceladus torus (Fleshman et al. [2010b], Table S9). The total abundance attributed to dissociation is then given by the sum of Eqs. 9 and 10. Cassidy and Johnson [2010] constrained their study with HST observations [Melin et al., 2009] and found a similar OH content (see comparison in Fig. 10c, this paper).

That neutral production by photo- and impact dissociation are comparable in magnitude is itself noteworthy. This condition is not shared by systems with hotter and denser plasma. For example, electron impact dissociation and ionization dominate over photon-driven processes in Jupiter’s Io torus, where the plasma is warmer where the pick-up energies are four times higher than at Enceladus [Delamere et al., 2007; Fleshman et al., 2010b]. We also note that unlike with Io, long neutral lifetimes in the Enceladus neutral torus inhibit the response of Saturn’s neutral clouds to short-term plume variability, though variability on the order of months has been studied by Smith et al. [2010].

2.2.2. Charge exchange

We now describe the model for producing and following neutrals from charge exchange. Cassidy and Johnson [2010] and Jurac and Richardson [2005] also considered velocity-dependent charge exchange, but unlike these previous studies, we capture the gyrophase at which the reactions occur by following ions along their trajectories (section 3.1). We also prescribe cross sections specific to each reaction, being particularly interested in the effects of low-velocity charge exchange.
At very high speeds, the cross sections go to zero for all charge exchanges \([Johnson, 1990]\). At low relative velocities, however (few \(\text{km s}^{-1}\)), the details of the collision are determined by the nature of the reacting species. If the reactants and products are identical, apart from an electron (\(i.e., \text{H}_2\text{O} + \text{H}_2\text{O}^+ \rightarrow \text{H}_2\text{O}^+ + \text{H}_2\text{O}^*\)), the reaction is termed resonant, or symmetric, and the cross sections grow as the inverse of the relative speed. If the reactants differ, as with \(\text{H}_2\text{O} + \text{O}^+ \rightarrow \text{H}_2\text{O}^+ + \text{O}^*\), the cross sections are likely to vanish at low speeds \([Rapp and Francis, 1962]\)—the difference being that the energy of the electron configurations is unchanged for symmetric-type charge exchanges \([Johnson, 1990]\). Neutrals produced from resonant charge exchange therefore tend to have lower velocities than do neutrals produced from non-resonant (asymmetric) charge exchange. This is a key point central to much of our discussion in section 3.

Individual ions are followed as they traverse the neutral torus (section 2.1). This approach allows their gyrophase to be determined the instant that charge exchanges occur (see Fig. 1). The implicit assumption is that the collision is elastic, and that the neutral product has an initial velocity given by the ion velocity just before the exchange takes place.

The ions are introduced into the model from two Maxwellian speed distributions,

\[
f_\perp(v_\perp) = \frac{m_{\text{ion}}}{kT_\perp} v_\perp \exp \left[ -\frac{m_{\text{ion}} v_\perp^2}{2kT_\perp} \right] \quad \text{(speeds perpendicular to } B) \tag{11}\]

\[
f_\parallel(v_\parallel) = \sqrt{\frac{m_{\text{ion}}}{2\pi kT_\parallel}} \exp \left[ -\frac{m_{\text{ion}} v_\parallel^2}{2kT_\parallel} \right] \quad \text{(speeds parallel to } B) \tag{12}\]

with a temperature anisotropy of

\[
\frac{kT_\perp}{kT_\parallel} = \frac{27 \text{ eV}}{5.4 \text{ eV}} = 5 \tag{13}\]
for both O\(^+\) and H\(_2\)O\(^+\) [Sittler et al., 2008]. The perpendicular temperature is derived from the pick-up ion velocity at the orbit of Enceladus, determined from CAPS data by Wilson et al. [2009] \(kT_\perp = \frac{1}{2}m_{W^+}(v_\phi - v_{Kep})^2\). The ions also rotate around a guiding center (field line) moving at \(v_\phi = 18\) km s\(^{-1}\) in a frame rotating with the neutrals.

For the component of our study aimed at estimating local neutral production (section 2.1.2), ions passing near Enceladus are diverted (treating Enceladus as a rigid cylinder) and are slowed to 10% of the ambient flow speed to account for the effects of mass-loading (see Fleshman et al. [2010a]).

Time steps are taken at less than 1% of an ion’s gyroperiod:

\[
\Delta t = R \times T_{gyro} = R \times \frac{2\pi m}{qB},
\]

where \(R\) is a random number between 0 and 0.01, \(T_{gyro}\) is the ion’s gyroperiod (3.6 s for H\(_2\)O\(^+\)), \(B = 325\) nT, and \(q\) and \(m\) are the charge and mass, respectively, of the reacting ion. Such resolution is necessary in order to capture the significance of the energy dependence at low relative speeds. After each time step, the collision frequency \(\nu\) is calculated from

\[
\nu(r, \theta, v_{rel}) = n(r, \theta)\sigma(v_{rel})v_{rel},
\]

where \(n(r, \theta)\) is the local H\(_2\)O density (section 2.1), \(v_{rel}\) is the relative velocity between the reacting ion and neutral, and \(\sigma(v_{rel})\) is the velocity-dependent cross section. Poisson statistics are used to test the likelihood of one or more reactions having occurred within \(\Delta t\). If \(\exp(-\nu\Delta t)\) is less than a second random number between 0 and 1, then a reaction occurs. The possibility of multiple reactions occurring over \(\Delta t\) is taken into account, but it is neglectable (appendix A).
As with OH produced by dissociation (section 2.2.1), neutrals produced by charge exchange are followed under the influence of Saturn’s gravity until they are photodissociated or photoionized. Their initial location and velocity are taken to be that of the reacting ion, pre-transfer.

The model runs are centered on the orbit of Enceladus spanning 10 $R_E$ in the direction of corotation ($R_E = 250$ km = radius of Enceladus) and $\pm 120 R_E$ (0.5 $R_S$) in both the radial and $z$ directions to adequately sample the $H_2O$ torus (section 2.1.1). Ions are introduced into the model on the upstream boundary, and their guiding centers flow downstream at a speed $v_{\text{plasma}} = 18$ km s$^{-1}$ relative to the neutrals. Their starting location in ($r,z$) is chosen randomly.

**Scaling:** The neutral clouds formed *via* charge exchange are done so in our model by following a relatively small number of ions, and must thus be scaled to facilitate comparison with observations and other models. The number of neutrals in our modeled clouds have been scaled by accounting for the following. First, the number of representative ions used to produce the neutral clouds *via* charge exchange falls short of, and must be scaled to, the number of ions present in the actual plasma torus, $n_{\text{iom}}V$. The volume of the plasma torus, $V$, is given in Eq. 8, and $n = 12$ and 6 cm$^{-3}$ for $O^+$ and $H_2O^+$, respectively [Sittler et al., 2008]. Second, we have argued that photo-processes are more likely to occur than either charge exchange or electron-impact processes throughout the neutral clouds with the exception of very near the neutral torus. In keeping with this assumption, the plasma torus thus feeds the extended neutral clouds *via* charge exchange for a photodissociation (photoionization in the case of oxygen) time scale before equilibrium of the neutral cloud is achieved: $\tau_{\text{phot}} = 14, 0.6, 0.3$ years for O, OH, and $H_2O$, respectively [Fleshman...
et al., 2010b]. Our model runs followed $10^5$ ions for 100 seconds, and the resulting neutral clouds were scaled as described.

3. Results

In the following sections, we present and discuss the neutral clouds resulting from dissociation and charge exchange in our model.

3.1. Charge exchange

In the neutrals’ reference frame, ions oscillate between $\approx 0$ km s$^{-1}$ and twice the local pick-up speed ($v_\phi \approx 18$ km s$^{-1}$) due to gyro-motion. A cartoon of this can be seen in Fig. 1, where $v_{\text{rel}} \approx 0$ at the cusp of the ion trajectory and reaches a maximum of $v_{\text{rel}} \approx 2v_\phi$ along the flow direction. Shown are several trajectories for which $v_\perp$ is either less than, greater than, or approximately equal to the bulk flow velocity. The neutrals formed via charge exchange follow the trajectories indicated in red.

The velocity dependence of reactions 3a–3c are determined by the details of the reacting species [Johnson, 1990]. Essentially, symmetric charge exchanges have cross sections that increase monotonically with decreasing velocity, whereas cross sections for asymmetric exchange peak and then vanish at low relative speeds. The implication is that symmetric exchanges produce lower velocity neutrals and a more compact neutral cloud than do asymmetric reactions.

With symmetric charge exchange, the cross sections go as $v_{\text{rel}}^{-1}$, so that the collision frequency ($n\sigma v$) is independent of $v$, as with reaction 3a, whereas asymmetric exchanges are defined by cross sections (and collision frequencies) which tend rapidly toward zero at low relative velocities ($\sim v_{\text{rel}}^4$, Rapp and Francis [1962]).
The cross sections \((10^{-16} \text{ cm}^2)\) used in this paper to study reactions 3a–3c plotted in Fig. 2a are given by

Reaction 3a: \(\text{H}_2\text{O} + \text{H}_2\text{O}^+ \rightarrow \text{H}_2\text{O}^+ + \text{H}_2\text{O}^*\)

\[\sigma_{\text{H}_2\text{O}} = 38E_{\text{rel}}^{-0.5}\]

(16a)

Reaction 3b: \(\text{H}_2\text{O} + \text{H}_2\text{O}^+ \rightarrow \text{H}_3\text{O}^+ + \text{OH}^*\)

\[\sigma_{\text{OH}} = 38E_{\text{rel}}^{-0.88} - 0.39 \exp \left( -\frac{1}{2} \left( \frac{E_{\text{rel}} - 57}{12} \right)^2 \right)\]

(16b)

Reaction 3c: \(\text{H}_2\text{O} + \text{O}^+ \rightarrow \text{H}_2\text{O}^+ + \text{O}^*\)

\[\sigma_{\text{O}} = 69E_{\text{rel}}^{-0.29} + 30 \exp \left( -\frac{1}{2} \left( \frac{E_{\text{rel}} - 65}{18} \right)^2 \right)\]

(16c)

The Gaussian terms in Eqs. 16b and 16c account for downward and upward trends in the associated data sets near 30 km s\(^{-1}\), but have little consequence on the neutral cloud, given that most bound particles are produced at lower velocities.

Symmetric exchanges occur between like species by definition, although unlike species also exhibit symmetric behavior on occasion. Therefore, we explore several hypothetical behaviors for the OH*-producing reaction 3b at low energies. This test is separate from, but related to, the comparison between reactions 3a–3c themselves, and it motivates the point that both high and low energy behaviors have an important effect on the neutral cloud. With \(\sigma_{\text{OH}}^{\text{extrapolated}}\), we have extrapolated the best-fit curve (Eq. 16b) to the lowest energies. Symmetric and asymmetric behaviors are explored with \(\sigma_{\text{OH}}^{\text{symmetric}}\) and \(\sigma_{\text{OH}}^{\text{asymmetric}}\) [Rapp and Francis, 1962; Johnson, 1990]. \(\sigma_{\text{OH}}^{\text{symmetric}}\) is the same as \(\sigma_{\text{OH}}^{\text{extrapolated}}\) except that below 1.5 eV, \(\sigma_{\text{OH}}^{\text{symmetric}} = 30E_{\text{rel}}^{-0.5} \times 10^{-16} \text{ cm}^2\). Notice that a similar energy dependence also applies to Eq. 16a, consistent with symmetric charge exchange. \(\sigma_{\text{OH}}^{\text{asymmetric}}\) is the same as \(\sigma_{\text{OH}}^{\text{extrapolated}}\) except that below 1.5 eV, \(\sigma_{\text{OH}}^{\text{asymmetric}} = 11E_{\text{rel}}^2 \times 10^{-16} \text{ cm}^2\). Although it could
be argued that $\sigma_{\text{OH}}^{\text{symmetric}}$ better fits the data if the two measurements at 2 eV are ignored, our results for reaction 3b were obtained with $\sigma_{\text{OH}}^{\text{extrapolated}}$ unless noted otherwise. We will discuss the implications of choosing $\sigma_{\text{OH}}^{\text{extrapolated}}$ over $\sigma_{\text{OH}}^{\text{symmetric}}$ and $\sigma_{\text{OH}}^{\text{asymmetric}}$ shortly.

The collision frequencies ($n\sigma v$) are plotted in Fig. 2b for a given neutral density—in this case for $n_{\text{H}_2\text{O}} = 10^3$ cm$^{-3}$. The collision frequency for oxygen increases with relative speed, while it is constant for water, and peaks at low velocities for OH. The significance is that the oxygen cloud tends to be more extended than either the OH or H$_2$O clouds. The average collision frequency is also much higher for oxygen ($\times10$) than for either OH or H$_2$O, resulting in greater oxygen abundance.

The equatorial neutral cloud densities resulting from reactions 3a–3c are plotted in Fig. 3. Only neutrals produced from charge exchange are shown; neither the Enceladus neutral torus, nor the neutrals produced via dissociation have been included. Oxygen is two orders of magnitude more abundant than either OH or H$_2$O because of the higher rate of production, but also because oxygen has a longer lifetime against photoionization than either OH or H$_2$O have against photodissociation. Unlike Cassidy and Johnson [2010], dissociated neutrals from the latter processes are not tracked in our model. Beyond the scope of the present study, this additional heating source would serve to further inflate the oxygen and OH clouds. Fig. 3b is the same as 3a, except that the profiles are normalized to the peak density at the orbit of Enceladus. The oxygen cloud is seen to be the most extended, followed by water, and finally by OH, with an order of magnitude separating the three species at 20 $R_S$.

The effects of low-velocity charge exchange are shown in Fig. 4. In Fig. 4a, we see that the peak density (as well as the total neutral cloud content) is the highest with $\sigma_{\text{OH}}^{\text{extrapolated}}$
because more low-velocity neutrals are produced than with either \( \sigma_{\text{OH}}^{\text{symmetric}} \) or \( \sigma_{\text{OH}}^{\text{asymmetric}} \).

Conversely, fewer low-velocity neutrals are available to populate the region near Enceladus’s orbit with \( \sigma_{\text{OH}}^{\text{asymmetric}} \) when compared to either \( \sigma_{\text{OH}}^{\text{extrapolated}} \) or \( \sigma_{\text{OH}}^{\text{symmetric}} \). Stated another way, \( \sigma_{\text{OH}}^{\text{extrapolated}} \) yields a neutral cloud with the steepest slope, and \( \sigma_{\text{OH}}^{\text{asymmetric}} \), the shallowest. Fig. 4b is identical to Fig. 4a, apart from normalization. In this case, the slope of the density profile should not be confused with the effect of inflating (spreading) the OH cloud. It should be viewed, rather, as the enhancement or depletion of low velocity neutrals to fill the region inside of \( \approx 10 \, R_S \). In other words, neutrals beyond 10 \( R_S \) are mostly formed in charge exchanges at high velocities, for which all \( \sigma_{\text{OH}} \) converge to the same curve (Fig. 2).

We have assumed to this point that the plasma is sub-corotating in Enceladus’s orbit (18 \( \text{km s}^{-1} \), Wilson et al. [2009]). One might expect, however, that the neutral cloud would be affected in a measurable way if instead, the plasma corotates at 26 \( \text{km s}^{-1} \).

The H\(_2\)O cloud would be least affected, given that the collision frequency of reaction 3a is independent of speed (Fig. 2b), but what about reactions such as 3b and 3c, whose collision frequencies are velocity-dependent? Increasing the plasma speed amounts to shifting the spread of ion velocities in Fig. 2 to the right, which would on average increase the speed of the neutral products. This is indeed the case, and in such a test where we increased the plasma speed from 18 to 26 \( \text{km s}^{-1} \), the oxygen cloud increased in abundance and became even more extended. The OH cloud also expanded somewhat, but decreased in total abundance. Unfortunately, the differences were less than 10% in both the slope of the distribution and in total oxygen abundance, suggesting that neutral cloud observations are in this way unlikely to predict plasma speeds in the torus.
3.1.1. Neutral cloud sources: plume vs. neutral torus

We described in section 2.1 the production in our model of the neutral H$_2$O torus from the Enceladus plumes. The plumes themselves have also been prescribed as a separate background density ($n_{\text{plume}}$, section 2.1.2) so that we can compare charge exchange occurring throughout the neutral torus to that occurring only within the Enceladus plumes.

The results are shown in Fig. 5, where we have plotted the oxygen clouds produced from charge exchange within both the Enceladus plumes (local) and the entire neutral torus (global). The results are for reaction 3c, but the same test with reactions 3a and 3b produces similar results. Immediately noticeable is that the local production is $\approx 0.1\%$ of the overall neutral production. The torus’s dominance of neutral production can be explained as follows. First, the volume of the torus where reactions are occurring can be estimated as $2\pi(4R_S)(0.2R_S)^2$, where $0.1R_S$ is roughly the torus’s scale height. The volume of the plume can be estimated from Eq. 6, where the dimensions are on the order of a cylinder with width $2R_E$ and height $H_r \approx 16R_E$. Dividing these volumes gives roughly $250(R_E/R_S)^3 \approx 10^{-5}$. Further, the collision frequencies are proportional to the neutral density, which in the plume are on the order of $10^7$ cm$^{-3}$, whereas typical torus densities are $10^5$ cm$^{-3}$, making collisions in the plume $100\times$ more frequent per volume than in the torus. All told, the ratio of the volumes ($10^{-5}$) combined with the ratio of densities ($10^2$) explain the local-to-global neutral production ratio of $10^{-3}$ shown in Fig. 5a. A similar pattern has been shown to exist at Jupiter by Bagenal [1997] and Dols et al. [2008], where the majority of plasma is produced throughout the neutral torus, rather than near the interaction at Io itself.
The slopes of the neutral clouds from the plume and torus are most easily compared in Fig. 5b, in which the density profiles have been normalized. The local source produces a more confined neutral cloud because the ions from which they originate have been slowed near the plume to account for the effect of mass-loading (Fleshman et al. [2010a]). Nevertheless, such a signature would be difficult to untangle in the data since global exceeds local production so overwhelmingly.

3.2. Dissociation

A major component of the OH cloud is produced by dissociation within the neutral torus, whereby the initial velocities of the OH products range from 1 to 1.6 km s$^{-1}$ [Wu and Chen, 1993; Makarov et al., 2004]. In Fig. 6, the clouds resulting from the high- and low-speed cases are plotted along with the result from velocity-dependent charge exchange in section 3.1. First note that dissociation contributes $100\times$ more OH than does charge exchange at the orbit of Enceladus (4 RS); the total cloud mass is almost $100\times$ greater as well. Second, dissociation dominates over charge exchange from the Enceladus torus out to 9 and 15 RS in the low- and high-speed cases, respectively. The OH cloud content will only be marginally affected by variable solar activity [Jackman and Arridge, 2011], given that impact dissociation contributes $4\times$ more neutrals than does photodissociation, by virtue of the respective reaction rates (section 2.2.1). In both cases, few neutrals are absorbed by the rings, and even less by Saturn itself. The same is not true of charge exchange, where $\approx 50\%$ of the neutrals are absorbed by Saturn (section 3.3).

Fig. 7c is a two-dimensional version of Fig. 6, where the dissociation results have been averaged and added to the results from charge exchange. Saturn is at the left, and the Enceladus’s orbit is located on the equator at 4 RS. In addition to being confined radially,
the dissociated neutrals are also bound tightly to the equator, while neutrals from charge
exchange tenuously fill the magnetosphere.

Fig. 7a shows the hydrogen cloud that accompanies the dissociated OH clouds
\((\text{H}_2\text{O} + \text{e}, \gamma \rightarrow \text{OH}^* + \text{H}^*)\). To conserve momentum, the hydrogen atoms have \(17\times\) the
speed of the dissociated OH molecules, and thus range between 17 and 27 km s\(^{-1}\), with
a relatively large, diffuse neutral cloud. Shown is the result for the low-speed case, which
produces more bound particles and thus a more substantial neutral cloud. Charge ex-
change from reactions such as \(\text{H}_2\text{O} + \text{H}^+ \rightarrow \text{H}_2\text{O}^+ + \text{H}^*\) are also responsible for H-cloud
production, and deserve attention in future studies.

### 3.3. Fates of neutral atoms and molecules

In our model, neutrals created by dissociation and charge exchange are eventually either
absorbed by Saturn, escape the system, or orbit until they are destroyed (ionized) by
photons. In Fig. 8a the fates for each species are given by percentage. In the case of
hydrogen, the results are from the dissociation model, described in section 3.2. The
enormous amount of escape (84\%) is due to the high velocities (\(\approx 17\) km s\(^{-1}\)) with which
hydrogen is created following \(\text{H}_2\text{O}\) dissociation, and the 8\% absorption is largely comprised
of hydrogen which would escape the system otherwise.

Oxygen is produced purely from charge exchange in our model (reaction 3c). About one-
half escapes, one-third is absorbed, and the remaining 13\% contributes to the neutral cloud
before being photoionized. Water is also produced purely by charge exchange (reaction
3a) with 18\% contributing to the neutral cloud. Percentage-wise, more water is absorbed
than oxygen because oxygen is produced with higher speeds and generally larger orbits
(section 3.1).
The fate of OH is dominated by dissociation: 96% feed the neutral cloud (ultimately ionized), 4% are absorbed, and virtually none escape. The reason for the large percentage of bound and unabsorbed neutrals is that dissociated OH has a velocity spread of 1 to 1.6 km s\(^{-1}\) in the neutral frame, compared to the escape speed of \(\approx 5\) km s\(^{-1}\) in the same frame. Looking only at OH produced by charge exchange (minor compared to dissociation), 58% are absorbed, 23% supply the neutral cloud, and 20% escape. Compared to H\(_2\)O, an even greater percentage of charge-exchanged OH is absorbed because the cross sections favor production of low-velocity OH molecules (Fig. 2b).

The production of oxygen via dissociation of H\(_2\)O has been ignored in this paper on the grounds that, unlike OH, oxygen is largely produced by charge exchange. The cross section for oxygen-producing charge exchange is an order of magnitude higher than that for the OH-producing reaction near the plasma flow speed of \(v_{\text{plasma}} = 18\) km s\(^{-1}\) (Fig. 2a), while the photodissociation rates are an order of magnitude smaller [Huebner and Carpenter, 1979]. We estimate that including oxygen produced from dissociation would increase the total oxygen cloud content by less than 20%.

Charge exchange and dissociation play a large role in creating Saturn’s neutral clouds from the plume-fed neutral torus. The reactions we have included have been chosen to demonstrate the effects of low velocity charge exchange and dissociation, but they are also among the most important. The neutral cloud densities presented in this paper are expected to undershoot the results from models which include the additional reactions found in Fig. 3, of Fleshman et al. [2010b] by no more than a factor of two. With this caveat in mind, we now compare the present results with several other recent models.

3.3.1. Comparison with other models
Fig. 8b: J06 is the work of Johnson et al. [2006], where they also investigated the neutral clouds created from low-velocity charge exchange in the stagnated flows in Enceladus’s orbit. Fig. 8b: J07 is from Jurac and Richardson [2007], where the authors were primarily interested in the interaction between the neutral cloud and Saturn’s rings. The most recent model comes from Cassidy and Johnson [2010] (C10), where they investigated the spreading of the neutral cloud from neutral–neutral collisions.

To compare with these studies, we first had to weight our H, O, OH, and H$_2$O clouds. We did this for two limiting cases. In the first case ($\tau_{\text{phot}}$, Fig. 8b), we assume, as we have thus far, that the neutral clouds evolve until destroyed by either photoionization or photodissociation: H, O, OH, H$_2$O = 40, 14, 0.6, 0.3 years, respectively. These lifetimes yield an upper limit since charge exchange and electron impact are not included as losses.

In the second case ($\tau_{\text{all}}$), we derived a lower limit to the lifetimes from Table 2 of Fleshman et al. [2010b] by summing the additional losses due to charge exchange and electron impact, finding: H, O, OH, H$_2$O = 0.4, 0.4, 0.2, 0.03 years, respectively. Notice in particular the drastically different times scales for H and O, where including the additional sinks reduce the size of the H cloud by a factor of 40/0.4 = 100, and the oxygen cloud by 14/0.4 = 35. This case represents an extreme limit, given that the neutrals spend almost all of their time orbiting outside of the Enceladus torus, where compared to photo-processes, the chances of charge exchange and electron impact are relatively unlikely. We mention, however, that Rymer et al. [2007, 2008] has shown that circulation patterns inside of 12 R$_S$ at Saturn gives rise to ‘butterfly’ hot electron pitch angle distributions, related to low temperature anisotropy ($T_\perp/T_\parallel$), on which proton field-aligned distributions depend [Sittler et al., 2008].
The individual clouds (excluding hydrogen) were weighted by the stated time scales and totaled in Fig. 8b. When only losses to photodissociation/ionization are considered ($\tau_{\text{phot}}$), the neutral cloud is dominated by oxygen, whose fate thus determines that of the neutral cloud. When charge exchange and electron impact are also included ($\tau_{\text{all}}$), dissociated OH contributes significantly, driving the neutral cloud (ionized) percentage up, and the escape percentage down. We note that the neutral fates presented in Bagenal and Delamere [2011] (escape = 44%, ionized = 17%, absorbed = 39%) were based on an earlier version of our model which only included H$_2$O.

The particles that are neither absorbed nor lost by escape make up the neutral clouds. In the case where the cloud evolves for $\tau_{\text{phot}}$, oxygen and hydrogen dominate since they are far less likely to be photoionized than are OH and H$_2$O to be photodissociated. With charge exchange and electron impact included ($\tau_{\text{all}}$), however, more oxygen and hydrogen are removed from the system, which then tends to favor a molecular OH–H$_2$O cloud. In terms of total mass the same applies, although hydrogen accounts for only a few percent at most. We find that the total cloud mass is bounded between $\approx 1$ and 10 Mtons, for $\tau_{\text{all}}$ and $\tau_{\text{phot}}$, respectively.

It is worth pausing to re-emphasize that the system is in reality better represented by the $\tau_{\text{phot}}$ case, from which all neutral clouds in this paper have been derived. The $\tau_{\text{all}}$ case is strictly valid only for neutrals within the Enceladus torus, though reactions with electrons and protons may also prove important, as discussed above. What is illustrated, however, is that Saturn’s magnetosphere is less oxygen-dominated than suggested by looking at losses from photo-processes alone. These results suggest that our oxygen abundances are somewhat overestimated, likely by less than a factor of two.
3.3.2. Neutral absorption

The particles absorbed by Saturn and its rings are plotted by species and latitude in Fig. 9. In Fig. 9b, we see that most absorption comes from oxygen (74%), followed by H$_2$O (11%), OH (9%), and finally by hydrogen (6%). Absorption is equally divided between Saturn and its rings except in the case of OH, where twice as much falls on Saturn’s rings. This is because OH is largely produced by impact dissociation, which creates slower neutrals than does charge exchange, whereby in our model, H$_2$O and oxygen arise exclusively.

In Fig. 9b, absorption is plotted against Saturn’s latitude. Because the model is symmetric about the equator, the results apply to either hemisphere. Oxygen, water, and OH follow the same trends because they all originate from charge exchange (dissociated OH is slow and does not reach Saturn), and have been created from ions with similar velocity distributions. Any second-order differences due to the velocity-dependence of the respective cross sections are not immediately apparent. Hydrogen, on the other hand, is produced entirely by dissociation in the model and exhibits a more uniform flux across Saturn. The explanation is that the velocity distribution from which hydrogen is produced is isotropic, whereas that which produces charge-exchanged neutrals is bi-Maxwellian (section 2.2.2). The fluxes shown in Fig. 9b are consistent with Hartogh et al. [2011], who modeled recent Herschel observations of Saturn’s water torus and found an average flux of $6 \times 10^5$ cm$^{-2}$ s$^{-1}$ for H$_2$O + OH impinging on Saturn.

4. Discussion

Some useful conclusions can be drawn by further contrasting our results with Cassidy and Johnson [2010] (C10). It is important that we first mention a profound difference
between our models. The model of C10 effectively carries out resonant charge exchange only, which does not chemically alter the neutral population; neutrals in their model are produced either directly from Enceladus or from subsequent dissociations. Neutrals in our model, on the other hand, originate from Enceladus (H$_2$O). OH is then created via dissociation (as with C10), but secondary O, OH, and H$_2$O populations are created from H$_2$O via charge exchange with the dense plume-fed Enceladus torus. The C10 model redistributes neutrals around Saturn, while we redistribute and chemically re-assign neutral abundances by allowing for asymmetric charge exchanges. Thus, it may well be a coincidence that our models are similar in total abundance. While it may be difficult to compare our total abundances, the slope of our radial density profiles can be contrasted directly because our redistribution mechanisms (charge exchange and dissociation) are similar. Differences are due largely to C10’s inclusion of neutral collisions and our prescribing unique velocity-dependent charge exchange for each of the O-, OH-, and H$_2$O-producing reactions (reactions 3a–3c).

Our neutral clouds are compared with C10 in Fig. 10. All of our clouds include contributions from charge exchange, but the H$_2$O cloud is mostly comprised of water sourced directly from Enceladus (3.95 R$_S$), and OH includes the additional source from dissociation. In the C10 model, the water molecules were spread due to neutral–neutral collisions, which explains our higher H$_2$O densities near Enceladus’s orbit (Fig. 10a). The slope of the oxygen profile agrees best with C10 because their charge exchange cross section most resembles our own (Eq. 16c). Our H$_2$O profiles agree less, and our OH slopes, the least, due mainly to the strong effect that neutral collisions have on those more polar molecules. In particular, C10 used a much larger cross section for neutral collisions involving H$_2$O
and OH [Teske et al., 2005] than for atomic oxygen [Bondi, 1964]. This helps to further explain our agreement with their oxygen profile since we exclude neutral–neutral collisions from our model altogether. We conclude that neutral–neutral collisions appear to play a less significant role with atomic species, such as oxygen and hydrogen.

The column densities (Fig. 10b) are similar to C10, who constrained their O and OH clouds with the most recent Cassini UVIS results of Melin et al. [2009]. Our oxygen density—as well as our total oxygen content (Fig. 10c)—is higher for two reasons. First, we use a larger cross section than does C10 for reaction 3c, and second, the clouds presented here have been limited only by photoionization. Charge exchange and electron impact are second order losses beyond 6 Rs, but including them would favorably reduce the oxygen content more than OH and H2O (section 3.3), bringing our models into better agreement.

Our total H2O content is 4× less than C10 found (Fig. 10c). This is partly because we have subjected H2O molecules in the primary (plume-fed) neutral torus to the shortest lifetimes possible (section 2.1.1), whereas C10 tracks molecules that get kicked out of the densest plasma via neutral collisions, and thus survive longer, being less susceptible to both charge exchange and electron impact. That their total H2O content is higher than ours (Fig. 10c), does not contradict the fact that their H2O column density is lower; neutral–neutral collisions would spread out the torus, lowering the column density, while allowing neutrals to survive longer, increasing the total abundance.

Our model would benefit by including the redistribution attributed to neutral collisions by allowing particles to interact in a direct simulation Monte Carlo (DSMC) model such as in C10. Likewise, DSMC models would benefit by including charge exchange cross
sections specific to each reaction. Such models should also take into account asymmetric charge exchanges, which affects neutral cloud composition.

The reactions modeled in this study were chosen in order to measure the effect of symmetric and asymmetric charge exchange at low velocities. Building upon our findings, future studies should include additional neutral-producing charge exchanges, such as \( \text{OH}^+ + \text{H}_2\text{O} \rightarrow \text{OH}^* + \text{H}_2\text{O}^+ \), \( \text{H}^+ + \text{H}_2\text{O} \rightarrow \text{H}^* + \text{H}_2\text{O}^+ \), and \( \text{OH}^+ + \text{H}_2\text{O} \rightarrow \text{O}^* + \text{H}_3\text{O}^+ \), as well as dissociative recombination of \( \text{H}_2\text{O}^+ \).

5. Conclusions

We have modeled low-velocity charge exchange from the point of view of the ions, allowing us to study the effects of velocity as well as gyrophase. With reactions 3a–3c, we have been able to offer an estimate on the size and shape of the neutral clouds at Saturn, while simultaneously exploring the sensitivity of the neutral clouds to a variety of velocity-dependent reactions.

We have also re-visited the production of OH following \( \text{H}_2\text{O} \) dissociation in the primary neutral torus. Previous models have used 1 km s\(^{-1}\) as the initial velocity for OH, while measurements suggest a range of speeds from 1 to 1.6 km s\(^{-1}\). In our model, the higher speed increases the range within which dissociation dominates neutral production from 9 to 15 \( \text{R}_S \).

Additional findings are:

(1.) Charge exchange cross sections that increase steeply at low speeds tend to produce neutral clouds more confined to the orbit of Enceladus, implying the most spreading for oxygen, moderate spreading for \( \text{H}_2\text{O} \), and the least for OH (Fig. 3). Accounting for
gyrophase doubles the local OH density within Enceladus’s orbit, has $\approx$ no effect on H$_2$O, and decreases oxygen density by less than 10%.

(2.) Enceladus is solely responsible for the creation of the neutral H$_2$O torus via thermal ejection from its plumes. However, Saturn’s neutral clouds are overwhelmingly produced by charge exchange and dissociation occurring throughout the torus (99%), and not near Enceladus itself (Fig. 5).

(3.) We estimate that roughly half of all neutrals escape the system, with the remaining equally divided between absorption by the rings/planet and the neutral clouds (Fig. 8). Less than 50 kg s$^{-1}$ is thus ionized and transported out of the system as plasma. This number is expected to represent an upper limit, given we have assumed that all particles forming the neutral clouds are ultimately ionized; a more accurate result would require modeling the detailed effects of charge exchange and neutral–neutral collisions within the neutral clouds. This estimate can be compared to Sittler et al. [2008], whose Figs. 14 and 17 give roughly $(NL^2/W^2/L^2) \times m_{W^+}/\tau_{\text{transport}} \approx 3 \times 10^{31} \times m_{W^+}/10^5$ s $\approx 10$ kg s$^{-1}$ at $L = 10$.

(4.) Saturn’s neutral cloud has a total mass of at least 1 Mton, but likely much closer to 10 Mtons. The primary plume-fed neutral torus (0.3 Mtons) is comprised entirely of water in our model, while the secondary neutral clouds are broken down into H ($\lesssim 5\%$), O ($\lesssim 82\%$), OH ($\gtrsim 13\%$), and H$_2$O ($\approx 1\%$). Atomic oxygen dominates the composition both because of a high production rate from charge exchange as well as a long lifetime against photoionization. Charge exchange and reactions with electrons favorably remove hydrogen and oxygen, but are secondary loss mechanisms throughout the majority of the magnetosphere.
Our model predicts fluxes on Saturn from charge exchange of $\approx 6 \times 10^5$ cm$^{-2}$ s$^{-1}$ for both OH and H$_2$O (consistent with Herschel observations by Hartogh et al. [2011]), and oxygen is about 5× higher. Absorption is divided equally between Saturn and its rings (Fig. 9a).

Our total neutral abundances are similar to Cassidy and Johnson [2010] (C10) for both OH and H$_2$O, and 4× higher for oxygen (Fig. 10). Differences in the slopes of our equatorial density profiles are in part due to our not including neutral–neutral collisions, while this fact appears to have no effect on the oxygen profile. On the other hand, C10 did not include the effects on neutral chemistry following asymmetric charge exchanges, nor did they use velocity-dependent cross sections particular to each reaction. Herschel observations by Hartogh et al. [2011] confirm the importance of neutral–neutral collisions for H$_2$O, but if oxygen is the dominant neutral species in Saturn's magnetosphere, as our model predicts, neutral–neutral collisions may play a smaller role in Saturn's neutral cloud than previously expected.

Given the effect on both the size and shape of the neutral clouds, we suggest that future neutral cloud models include charge exchange cross sections unique to each reaction. Asymmetric charge exchange also has an important effect on neutral chemistry that should be implemented. Regarding the ions' gyrophase, Monte Carlo models can account for its effect by using phase-dependent probability distributions. Finally, the range of OH velocities studied here should be considered when modeling dissociation.

Moving forward, we plan to implement these suggestions into the neutral cloud model of C10 and to couple that model with the chemistry model of Fleshman et al. [2010b]. Constrained by Cassini plasma observations, the chemistry model uses C10's neutrals as
input, and provides ion temperatures and densities throughout the magnetosphere (< 20 R\(_S\)), which C10 in turn uses to update neutral densities. An improved understanding of two issues is planned: (1) Where does plasma transport become important? (2) What is the role of hot electrons with regard to ion–neutral chemistry inside 20 R\(_S\)?

**Appendix A: Collision probability**

The average number of collisions occurring during a time interval \(\Delta t\) is given by \(\lambda \equiv \nu \Delta t\), where \(\nu = n_{\text{neutrals}} \sigma(\nu_{\text{rel}}) v_{\text{rel}}\) is the local collision frequency, assumed to be constant during \(\Delta t\). Statistics are applied to determine if and how many reactions occur during \(\Delta t\).

The Poisson distribution [Zwillinger and Company, 1996; Reif, 1965] gives the probability of suffering exactly \(n\) collisions for a given \(\lambda\):

\[
f(n; \lambda) = \frac{e^{-\lambda} \lambda^n}{n!}. \tag{A1}
\]

Notice that Eq. A1 peaks at \(n = \lambda\) if one treats \(n\) as a continuous variable. Summing Eq. A1 discretely from \(n = k\) to \(n = \infty\) gives the probability of suffering at least \(k\) collisions during \(\Delta t\),

\[
P_k(\lambda) = e^{-\lambda} \sum_{n=k}^{\infty} \frac{\lambda^n}{n!}. \tag{A2}
\]

Because Eq. A1 is normalized \((e^{-\lambda} \sum_{n=0}^{\infty} \lambda^n/n! = e^{-\lambda} e^{\lambda} = 1)\), Eq. A2 can be conveniently rewritten as

\[
P_k(\lambda) = 1 - e^{-\lambda} \sum_{n=0}^{k-1} \frac{\lambda^n}{n!}. \tag{A3}
\]

A random number \((0 < N < 1)\) is compared to each \(P_k\) at each timestep. The largest \(k\) for which \(P_k > N\) determines how many fast neutrals (collisions), \(k\), are produced during \(\Delta t\).
In practice, it is only necessary to compare to the first few $P_k$ when $\lambda \ll 1$, made evident by the leading terms in Eq. A2 for $k + 1$ and $k$:

$$\frac{P_{k+1}}{P_k} \approx \frac{f(k + 1; \lambda)}{f(k; \lambda)} = \frac{\lambda^{k+1}/(k + 1)!}{\lambda^k/k!} = \frac{\lambda}{k + 1 \to 0}. \quad (A4)$$

Multiple collisions are thus increasingly unlikely when $\lambda \ll 1$. In such cases, comparison with $P_1 = 1 - e^{-\lambda} \approx \lambda = \nu \Delta t$ is sufficient.

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Figure 1. Sketch of gyrating ions in the neutral frame with guiding centers moving along a prescribed flow field, shown here near Enceladus for scale. Warm ions ($v_{\perp} > v_{\text{flow}}$) move on trajectories that coil around themselves and do not reach zero relative velocity with respect to the neutrals at any point. Cool ions ($v_{\perp} < v_{\text{flow}}$) essentially trace their guiding centers with ‘snake-like’ trajectories, and also do not obtain zero relative velocity. Fresh pick-up ions ($v_{\perp} \approx v_{\text{flow}}$) do, however, obtain zero relative velocity at the cusps of their cycloidal trajectories. Neutrals produced by charge exchange (whose trajectories are indicated by the red lines) tend to be created with velocities at which the respective reaction rates peak (Fig. 2).
Figure 2. (a.) Cross sections for the reactions listed in the legend. Data for reactions 3a and 3b are from Lishawa et al. [1990], and data for reaction 3c is from Li et al. [1995]. $\sigma_{\text{extrapolated}}^{\text{OH}}$, $\sigma_{\text{symmetric}}^{\text{OH}}$, and $\sigma_{\text{asymmetric}}^{\text{OH}}$ are hypothetical fits applying to the OH*-producing reaction, and are explored in Fig. 4. Ions oscillate between $\approx 0$ and $36$ km s$^{-1}$ in the Enceladus torus. (b.) Collision frequency, $n\sigma(v)v$, for a given density of $n_{\text{H}_2\text{O}} = 10^3$ cm$^{-3}$ plotted over the same energy range. The collision frequency increases with energy in the oxygen-forming reaction, while the water-forming reaction is independent of energy and the OH-forming reaction declines with energy.
Figure 3. Neutral clouds produced by the reactions shown in Fig. 2. (a.) Oxygen is the most abundant because the cross section section is $10 \times$ higher than with O and OH. The lifetime of oxygen against photoionization is also much longer than the lifetime for either OH or H$_2$O against photodissociation. (b.) Same as above, but normalized to peak. Oxygen shows the most spreading because reactants are produced with higher velocities (Fig. 2b), which expands the cloud. The same trend holds with H$_2$O and OH, where OH tends to be created with the lowest velocities (Fig. 2, $\sigma_{\text{OH}}^{\text{extrapolated}}$).
Figure 4. Neutral OH clouds produced from three hypothetical charge exchange cross sections: $\sigma_{\text{OH}}^{\text{extrapolated}}$, $\sigma_{\text{OH}}^{\text{symmetric}}$, and $\sigma_{\text{OH}}^{\text{asymmetric}}$ (Fig. 2). (a.) $\sigma_{\text{OH}}^{\text{extrapolated}}$ produces the highest density ($\sigma_{\text{OH}}^{\text{asymmetric}}$, the lowest) at Enceladus because of the creation of additional low-velocity particles. (b.) Same as above, but normalized to peak. The differences in density in the tail is not an indication of spreading, but rather further illustrates the deficiency in the peak density, going from $\sigma_{\text{OH}}^{\text{extrapolated}}$ to $\sigma_{\text{OH}}^{\text{asymmetric}}$. 
Figure 5. (a) Comparison between charge exchanged neutrals produced near the Enceladus plume and those produced from the neutral torus as a whole—in this case for oxygen. (b.) Though shown here for oxygen, all charge exchange reactions near the plume result in a cloud with less spreading than their global counterpart due to the imposed slowing of the plasma (and hence, the release of slower neutral products) near the plume in response to mass-loading [Fleshman et al., 2010a].
Figure 6. OH clouds produced from charge exchange and high- and low-speed dissociation. Dissociation dominates neutral cloud production inside 9–15 $R_S$, at which point charge exchange becomes the dominant contributor.
Figure 7. Neutral cloud densities in the $r$–$z$ plane. (a.) Hydrogen produced purely from $\text{H}_2\text{O}$ dissociation. (b.) Oxygen produced purely from charge exchange (reaction 3c). (c.) Hydroxyl produced from the combination of charge exchange and dissociation. Dissociation dominates inward of $9$–$15$ R$_S$ along the equator, while charge exchange (reaction 3b) tenuously fills the magnetosphere elsewhere. (d.) Water produced entirely by charge exchange (reaction 3a). (e.) Dense torus fed directly by the Enceladus plumes (section 2.1.2).
Figure 8. The fates of neutrals in our model along with the results from other models. (a.) Dissociation produces low-velocity neutrals and OH is thus not likely to escape or to be absorbed. Conversely, dissociation also produces hydrogen which largely leaves the system. (b.) The results of J06 \cite{Johnson2006}, J07 \cite{Jurac2007}, and C10 \cite{Cassidy2010}, along with our own weighted totals (excluding hydrogen; see section 3.3.1). In the case of $\tau_{\text{phot}}$, the lifetime of the cloud is determined by photoionization/dissociation only, whereas with $\tau_{\text{all}}$, we limit the lifetimes by also including electron impact and charge exchange. These limiting cases bound the previous studies, except that C10 has more absorption attributed to neutral–neutral collisions.
Figure 9. (a.) Neutrals absorbed by Saturn, plotted by species. Partitions with horizontal lines indicate percentages absorbed by Saturn’s rings. (b.) Neutral flux on Saturn as a function of latitude. Neutrals produced by charge exchange (H₂O, OH, and O) peak in flux at low latitudes due to the nature of the ion distributions from which they originate, which have initial velocity vectors predominantly in the ring plane. Conversely, hydrogen flux is constant across Saturn because it originates from dissociation, whose velocity distribution is prescribed as isotropic. Note that OH produced by dissociation is not energetic enough to reach Saturn.
Figure 10. (a.) Total neutral clouds from our model, compared with Cassidy and Johnson [2010] (C10). All clouds include contributions from charge exchange (reactions 3a–3c), while H$_2$O is largely comprised of water sourced directly from Enceladus, and OH includes contributions from dissociation. The cloud densities are limited by photodissociation for OH and H$_2$O and by photoionization for O. Including charge exchange as a loss for cloud neutrals would reduce the lifetime for O more than for either the OH or H$_2$O, and would lower the relative oxygen abundance accordingly. (b.) Equatorial column densities found by integrating the plotted equatorial densities. The H$_2$O column density is similar to C10, despite their having a very different radial distributions. (c.) Total neutral cloud content. Our total H$_2$O content is less than C10 found, while our H$_2$O column density is higher because our H$_2$O cloud is not subjected to neutral collisions and is thus more confined.