Developing a self-consistent description of Titan’s upper atmosphere without hydrodynamic escape

Jared M. Bell1, J. Hunter Waite Jr.2,3, Joseph H. Westlake4, Stephen W. Bougher5, Aaron J. Ridley2, Rebecca Perryman2, and Kathleen Mandt2

1 Center for Planetary Atmospheres and Flight Sciences, National Institute of Aerospace, Hampton, Virginia, USA, 2 Division of Space Science and Engineering, Southwest Research Institute, San Antonio, Texas, USA, 3 Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, Texas, USA, 4 Johns Hopkins University Applied Physics Laboratory, Michigan, USA, 5 Department of Atmospheric, Oceanic, and Space Sciences, University of Michigan, Ann Arbor, Michigan, USA

Abstract In this study, we develop a best fit description of Titan’s upper atmosphere between 500 km and 1500 km, using a one-dimensional (1-D) version of the three-dimensional (3-D) Titan Global Ionosphere-Thermosphere Model. For this modeling, we use constraints from several lower atmospheric Cassini-Huygens investigations and validate our simulation results against in situ Cassini Ion-Neutral Mass Spectrometer (INMS) measurements of N2, CH4, H2, 40Ar, HCN, and the major stable isotopic ratios of 14N/15N in N2. We focus our investigation on aspects of Titan’s upper atmosphere that determine the amount of atmospheric escape required to match the INMS measurements: the amount of turbulence, the inclusion of chemistry, and the effects of including a self-consistent thermal balance. We systematically examine both hydrodynamic escape scenarios for methane and scenarios with significantly reduced atmospheric escape. Our results show that the optimum configuration of Titan’s upper atmosphere is one with a methane homopause near 1000 km and atmospheric escape rates of $1.41 \times 10^{-14}$ CH$_4$ m$^{-2}$ s$^{-1}$ and $1.08 \times 10^{-14}$ H$_2$ m$^{-2}$ s$^{-1}$ (scaled relative to the surface). We also demonstrate that simulations consistent with hydrodynamic escape of methane systematically produce inferior fits to the multiple validation points presented here.

1. Introduction

Atmospheric loss of constituents to space is a major process by which atmospheres evolve over time [Yung and Demore, 1999]. Titan is unique in the solar system because it is the only terrestrial body besides Earth that has a substantial N$_2$-dominated atmosphere, making it a possible analogue for an early, prebiotic Earth [cf. Clarke and Ferris, 1997; Sagan and Thompson, 1984; Yung et al., 1984]. Thus, understanding Titan’s atmospheric evolution is key to determining how Earth’s atmosphere may have transitioned into its current state [Yung and Demore, 1999]. Models that describe Titan’s atmospheric evolution are sensitive to the assumed atmospheric escape rates of methane (CH$_4$) and molecular hydrogen (H$_2$) over geologic time [e.g., Mandt et al., 2009; Mandt et al., 2012; Lorenz et al., 1999]. Therefore, quantifying current atmospheric escape rates is central to understanding the evolutionary trajectory of Titan’s atmosphere. And, more broadly, this quantification may provide clues about how Earth’s atmosphere evolved into its current life-sustaining environment.

Unfortunately, direct measurements of neutral atmospheric escape are not made by instruments on the Cassini orbiter and there are currently no published constraints on neutral methane escape from magnetospheric measurements. Thus, we must rely upon numerical models, usually one-dimensional (1-D), to infer atmospheric escape rates from Titan. These 1-D models are constrained to simultaneously match atmosphere composition below 500 km and Cassini Ion-Neutral Mass Spectrometer (INMS) data above 1000 km. Key parameters, such as eddy diffusion and topside escape rates, are then adjusted until the simulated densities and mixing ratios match INMS data.

Using this approach, Strobel [2009], Yelle et al. [2008], and Cui et al. [2012] estimated that large escape rates of methane (between ~2.0 and $3.0 \times 10^{13}$ CH$_4$ m$^{-2}$ s$^{-1}$ or ~40 and 60 kg s$^{-1}$ globally) are required to reproduce the INMS composition measurements. Strobel [2008, 2009] concluded that these inferred atmospheric escape rates of CH$_4$ were evidence of hydrodynamic escape. Conversely, several studies have suggested that hydrodynamic escape rates of CH$_4$ are not required to match INMS data. Tucker and Johnson [2009], and
Table 1. Global Parameter Settings for 1-D T-GITM

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_{10.7}$ radio flux</td>
<td>$8.0 \times 10^{-22}$ W/m$^2$/Hz</td>
</tr>
<tr>
<td>Solar zenith angle</td>
<td>60°</td>
</tr>
<tr>
<td>Saturn-Sun radial distance</td>
<td>9.25 AU</td>
</tr>
<tr>
<td>Model radial resolution</td>
<td>10 km</td>
</tr>
</tbody>
</table>

This methane escape controversy is mirrored by an apparent mismatch between the INMS $H_2$ density and mixing ratios using a methane homopause near 1000 km and escape rates of $\sim 1.0 \times 10^8$ CH$_4$ m$^{-2}$ s$^{-1}$. Similarly, Bell et al. [2010a, 2010b, 2011b] used a 1-D version of the Titan Global Ionosphere-Thermosphere Model (T-GITM) to reproduce the INMS densities and mixing ratios using a methane homopause near 1000 km and escape rates of $\sim 1.0 \times 10^8$ CH$_4$ m$^{-2}$ s$^{-1}$. Thus, our goal in this manuscript is to address simultaneously the controversy in CH$_4$ escape rates and the apparent mismatch between the upper and lower atmosphere $H_2$ composition measurements. We will do this by building upon our previous work in Bell et al. [2010a, 2010b, 2011b], where we identified three key aspects of our 1-D simulations that determined the amount of atmospheric escape of CH$_4$ and $H_2$ needed to match INMS measurements: (1) the amount of turbulence used in the model, (2) the net chemical destruction of methane (net production of $H_2$) included in the model (i.e., the sum over direct photolytic, ion-neutral, and neutral-neutral chemical losses), and (3) the inclusion of a self-consistent thermal balance calculation. We have designed a series of numerical experiments that explore each of these aspects sequentially, building from highly simplified simulations to fully coupled simulations that combine all three aspects into a global mean description of Titan's upper atmosphere.

Thus, our goal in this manuscript is to address simultaneously the controversy in CH$_4$ escape rates and the apparent mismatch between the upper and lower atmosphere $H_2$ composition measurements. We will do this by building upon our previous work in Bell et al. [2010a, 2010b, 2011b], where we identified three key aspects of our 1-D simulations that determined the amount of atmospheric escape of CH$_4$ and $H_2$ needed to match INMS measurements: (1) the amount of turbulence used in the model, (2) the net chemical destruction of methane (net production of $H_2$) included in the model (i.e., the sum over direct photolytic, ion-neutral, and neutral-neutral chemical losses), and (3) the inclusion of a self-consistent thermal balance calculation. We have designed a series of numerical experiments that explore each of these aspects sequentially, building from highly simplified simulations to fully coupled simulations that combine all three aspects into a global mean description of Titan's upper atmosphere.

2. The T-GITM Framework

The Titan Global Ionosphere-Thermosphere Model (T-GITM) is a three-dimensional (3-D) nonhydrostatic global circulation model (GCM) that solves the time-dependent Navier-Stokes equations between 500 km and 1500 km on a spherical altitude grid (see Appendix A for more details). The T-GITM numerical solvers in the vertical (i.e., radial) direction have been updated to use the Advection Upstream Splitting Method (AUSM$^{+}$-up) of [Liou, 2006] as well as the fourth-order Runge-Kutta time-stepping scheme outlined in Ullrich and Jablonowski [2012]. T-GITM currently carries 15 neutral species ($N_2$, CH$_4$, $H_2$, $^{14}N/^{15}N$, HCN, and $^{40}$Ar) and 5 ion species ($N_2^+$, $N^+$, HCN$^+$, CH$_3^+$, and $C_2H_5^+$), and electrons equal to the total ion content to provide charge neutrality.

All species are coupled through a reduced ion-neutral chemical scheme that focuses on the formation of HCN [Bell et al., 2010a]. However, this chemical scheme does not liberate the amount of $H_2$ inferred from Tucker et al. [2013], using a direct simulation Monte Carlo method, have reproduced the INMS measurements in the upper atmosphere while using only thermal escape rates of methane (less than $1.0 \times 10^9$ CH$_4$ m$^{-2}$ s$^{-1}$). Similarly, Bell et al. [2010a, 2010b, 2011b] used a 1-D version of the Titan Global Ionosphere-Thermosphere Model (T-GITM) to reproduce the INMS densities and mixing ratios using a methane homopause near 1000 km and escape rates of $\sim 1.0 \times 10^8$ CH$_4$ m$^{-2}$ s$^{-1}$. Thus, our goal in this manuscript is to address simultaneously the controversy in CH$_4$ escape rates and the apparent mismatch between the upper and lower atmosphere $H_2$ composition measurements. We will do this by building upon our previous work in Bell et al. [2010a, 2010b, 2011b], where we identified three key aspects of our 1-D simulations that determined the amount of atmospheric escape of CH$_4$ and $H_2$ needed to match INMS measurements: (1) the amount of turbulence used in the model, (2) the net chemical destruction of methane (net production of $H_2$) included in the model (i.e., the sum over direct photolytic, ion-neutral, and neutral-neutral chemical losses), and (3) the inclusion of a self-consistent thermal balance calculation. We have designed a series of numerical experiments that explore each of these aspects sequentially, building from highly simplified simulations to fully coupled simulations that combine all three aspects into a global mean description of Titan's upper atmosphere.

2. The T-GITM Framework

The Titan Global Ionosphere-Thermosphere Model (T-GITM) is a three-dimensional (3-D) nonhydrostatic global circulation model (GCM) that solves the time-dependent Navier-Stokes equations between 500 km and 1500 km on a spherical altitude grid (see Appendix A for more details). The T-GITM numerical solvers in the vertical (i.e., radial) direction have been updated to use the Advection Upstream Splitting Method (AUSM$^{+}$-up) of [Liou, 2006] as well as the fourth-order Runge-Kutta time-stepping scheme outlined in Ullrich and Jablonowski [2012]. T-GITM currently carries 15 neutral species ($N_2$, CH$_4$, $H_2$, $^{14}N/^{15}N$, HCN, and $^{40}$Ar) and 5 ion species ($N_2^+$, $N^+$, HCN$^+$, CH$_3^+$, and $C_2H_5^+$), and electrons equal to the total ion content to provide charge neutrality.

All species are coupled through a reduced ion-neutral chemical scheme that focuses on the formation of HCN [Bell et al., 2010a]. However, this chemical scheme does not liberate the amount of $H_2$ inferred from Tucker et al. [2013], using a direct simulation Monte Carlo method, have reproduced the INMS measurements in the upper atmosphere while using only thermal escape rates of methane (less than $1.0 \times 10^9$ CH$_4$ m$^{-2}$ s$^{-1}$). Similarly, Bell et al. [2010a, 2010b, 2011b] used a 1-D version of the Titan Global Ionosphere-Thermosphere Model (T-GITM) to reproduce the INMS densities and mixing ratios using a methane homopause near 1000 km and escape rates of $\sim 1.0 \times 10^8$ CH$_4$ m$^{-2}$ s$^{-1}$. Thus, our goal in this manuscript is to address simultaneously the controversy in CH$_4$ escape rates and the apparent mismatch between the upper and lower atmosphere $H_2$ composition measurements. We will do this by building upon our previous work in Bell et al. [2010a, 2010b, 2011b], where we identified three key aspects of our 1-D simulations that determined the amount of atmospheric escape of CH$_4$ and $H_2$ needed to match INMS measurements: (1) the amount of turbulence used in the model, (2) the net chemical destruction of methane (net production of $H_2$) included in the model (i.e., the sum over direct photolytic, ion-neutral, and neutral-neutral chemical losses), and (3) the inclusion of a self-consistent thermal balance calculation. We have designed a series of numerical experiments that explore each of these aspects sequentially, building from highly simplified simulations to fully coupled simulations that combine all three aspects into a global mean description of Titan's upper atmosphere.

2. The T-GITM Framework

The Titan Global Ionosphere-Thermosphere Model (T-GITM) is a three-dimensional (3-D) nonhydrostatic global circulation model (GCM) that solves the time-dependent Navier-Stokes equations between 500 km and 1500 km on a spherical altitude grid (see Appendix A for more details). The T-GITM numerical solvers in the vertical (i.e., radial) direction have been updated to use the Advection Upstream Splitting Method (AUSM$^{+}$-up) of [Liou, 2006] as well as the fourth-order Runge-Kutta time-stepping scheme outlined in Ullrich and Jablonowski [2012]. T-GITM currently carries 15 neutral species ($N_2$, CH$_4$, $H_2$, $^{14}N/^{15}N$, HCN, and $^{40}$Ar) and 5 ion species ($N_2^+$, $N^+$, HCN$^+$, CH$_3^+$, and $C_2H_5^+$), and electrons equal to the total ion content to provide charge neutrality.

All species are coupled through a reduced ion-neutral chemical scheme that focuses on the formation of HCN [Bell et al., 2010a]. However, this chemical scheme does not liberate the amount of $H_2$ inferred from Tucker et al. [2013], using a direct simulation Monte Carlo method, have reproduced the INMS measurements in the upper atmosphere while using only thermal escape rates of methane (less than $1.0 \times 10^9$ CH$_4$ m$^{-2}$ s$^{-1}$). Similarly, Bell et al. [2010a, 2010b, 2011b] used a 1-D version of the Titan Global Ionosphere-Thermosphere Model (T-GITM) to reproduce the INMS densities and mixing ratios using a methane homopause near 1000 km and escape rates of $\sim 1.0 \times 10^8$ CH$_4$ m$^{-2}$ s$^{-1}$. Thus, our goal in this manuscript is to address simultaneously the controversy in CH$_4$ escape rates and the apparent mismatch between the upper and lower atmosphere $H_2$ composition measurements. We will do this by building upon our previous work in Bell et al. [2010a, 2010b, 2011b], where we identified three key aspects of our 1-D simulations that determined the amount of atmospheric escape of CH$_4$ and $H_2$ needed to match INMS measurements: (1) the amount of turbulence used in the model, (2) the net chemical destruction of methane (net production of $H_2$) included in the model (i.e., the sum over direct photolytic, ion-neutral, and neutral-neutral chemical losses), and (3) the inclusion of a self-consistent thermal balance calculation. We have designed a series of numerical experiments that explore each of these aspects sequentially, building from highly simplified simulations to fully coupled simulations that combine all three aspects into a global mean description of Titan's upper atmosphere.
Table 2. T-GITM Lower Boundary Settings at 500 km Altitude and Cassini-Huygens Constraints

<table>
<thead>
<tr>
<th>T-GITM Lower Boundary Field</th>
<th>Cassini-Huygens Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_{CH_4} = 1.48%$</td>
<td>$1.48 \pm 0.9%$ (GCMSa) and $1.6 \pm 0.5%$ (CIRSb)</td>
</tr>
<tr>
<td>$\chi_{H_2} = 2.00 \times 10^{-3}$</td>
<td>$1.0 \pm 0.5 \times 10^{-3}$ (CIRS) and $1.01 \pm 0.16 \times 10^{-3}$ (GCMSa)</td>
</tr>
<tr>
<td>$\chi_{Ar^{40}} = 3.30 \times 10^{-5}$</td>
<td>$3.39 \pm 0.12 \times 10^{-5}$ (GCMSa)</td>
</tr>
<tr>
<td>$14N/15N = 167.7$</td>
<td>$167.7 \pm 0.6$ (GCMSa)</td>
</tr>
<tr>
<td>$n = 9.0 \times 10^{19}$ (m$^{-3}$)</td>
<td>$\sim 8.2 \times 10^{19}$ (m$^{-3}$) (HASf)</td>
</tr>
</tbody>
</table>

aNiemann et al. [2010].
bFlasar et al. [2005].
cJennings et al. [2009].
dYeany et al. [2007].
eAchterberg et al. [2008].
fFulchignoni et al. [2005].

an analysis of the Cassini INMS heavy hydrocarbon data by Waite et al. [2007] and Westlake et al. [2012], which indicate that the heavy hydrocarbons have a carbon to hydrogen ratio of roughly 1:1.7. This 1:1.7 C to H ratio suggests that 1.15 H$_2$ molecules are liberated for every CH$_4$ molecule consumed by chemistry. We approximate this amount of H$_2$ production by employing a semiempirical H$_2$ production rate in the T-GITM continuity equation given by $P_{H_2} = 1.15 \times L_{CH_4}$. While this approach is ad hoc, we examine the sensitivity of the simulated H$_2$ to chemistry in section 5.

For the purposes of simplicity, we perform 1-D T-GITM simulations that have identical orbital, seasonal, and solar cycle settings, which are outlined in Table 1 and are consistent with a global average. The 1-D simulations have a uniform 10 km vertical resolution and have a specified 60° solar zenith angle. We approximate a diurnal average by dividing the solar fluxes by a factor of 2.0. This approach differs from the settings in Bell et al. [2010a, 2010b, 2011b], but it matches other 1-D investigations of Titan’s upper atmosphere [e.g., Krasnopolsky, 2009, 2010; Strobel, 2010; Yelle et al., 2008].

T-GITM uses two layers of ghost cells (or boundary cells) for calculating gradients and specifying boundary conditions at the edges of the physical domain. At the lower boundary, we specify fixed densities and temperatures consistent with the Cassini-Huygens measurements listed in Table 2. However, for photochemically produced species, such as HCN, C$_2$H$_4$, and N(4S), we do not specify a fixed mixing ratio at 500 km, since (1) there are few reliable constraints and (2) doing so could bias their simulated densities. Instead, for these three photochemical species we extend the mixing ratios downward from the physical regime into the boundary cells. This approach allows the combined vertical dynamics and integrated chemistry to determine the mixing ratios in the T-GITM simulations. At the upper boundary (1500 km), we extend the temperatures and densities from the physical calculation domain into the boundary cells.

For the vertical velocities of most species, we do not specify boundary conditions at either boundary and we simply extend the velocities downward and upward from the calculation domain. For light species, such as H and H$_2$, we calculate their classical Jeans escape velocities at 1500 km in order to capture their thermal escape. Moreover, we specify hydrodynamic escape velocities of CH$_4$ in some simulations and we impose this escape by forcing a flux condition on either the lower or upper boundary of the model.

3. The Data Sets Used

In this section, we outline the key aspects of the INMS data used to infer atmospheric escape rates. There are currently two peer-reviewed methods for analyzing the INMS raw data: (1) the methods developed by Magee et al. [2009] and (2) the methods developed by Cui et al. [2008] and Cui et al. [2012]. Both methods produce similar results for the major species densities but differ in their minor species composition. For the purposes of this investigation, we rely on results obtained using the methods of Magee et al. [2009], but we emphasize that either method could be used with equal validity. In order to correct for a systematic underestimate of the neutral densities relative to other investigations, the INMS neutral densities have been multiplied by a uniform factor of 2.7 [Bell et al., 2010b]. Moreover, we average the flyby densities
between TA and T40 to create a prime mission average, properly propagating both the counting statistical and geophysical variabilities into our averages [Bell et al., 2010a, 2010b].

Our fixed simulation settings outlined in Table 1 are roughly consistent with the mean conditions of the Cassini Prime Phase between TA and T40, which according to Westlake et al. [2011] has a mean solar zenith angle of ∼103°, F10.7−cm value of 75 × 10−22 W m−2 s−1 Hz−1, a mean latitude of ∼36.6°N, and Sun-Saturn distance of roughly 9.20 AU. Ideally, we should run 3-D T-GITM simulations that account for the different flyby trajectories, at different orbital positions, and with more precise solar flux values. However, our main objective is to generate 1-D simulations that are (1) more directly comparable with other 1-D efforts and (2) representative of a global mean state of Titan’s atmosphere during the TA–T40 timeframe.

In order to validate T-GITM, we calculate arithmetic mean deviations between simulated densities and mixing ratios and the INMS measurements:

\[
\text{Percent deviation} = 100 \times \sum \frac{\psi_{\text{GITM}} - \psi_{\text{INMS}}}{\psi_{\text{INMS}}}.
\]

where \( \psi \) represents a specific mixing ratio or density, the subscript GITM denotes a model field, INMS the data field, and the index “i” ranges over the altitudes between 1050 km and 1500 km. We interpolate the INMS data and uncertainties onto the T-GITM uniform 10 km grid between 1050 km and 1500 km.

4. T-GITM Simulation Results

In the following four subsections, we outline a series of T-GITM simulations that systematically isolate and investigate the different processes that impact atmospheric escape. In sections 4.1–4.3, we begin with simulations that have a specified thermal structure that is unchanging over the course of the simulation (i.e., we omit the energy balance calculations). In section 4.1, we examine how the method for including turbulence impacts simulated mixing ratios of 40Ar—a key tracer of eddy diffusion. In section 4.2, we isolate the impacts of varying the amount of turbulence in T-GITM simulations. Section 4.3 outlines the impacts of either including or omitting chemical losses of CH4 on our estimates of atmospheric escape. Finally, in section 4.4, we introduce Navier-Stokes simulations that include fully coupled composition, momentum, and energy balance calculations.

4.1. Examining Different Eddy Diffusion Formulations

Eddy diffusion is a heuristic parameter that approximates the effects of subgrid scale turbulence on atmospheric models [see Atreya, 1986]. In T-GITM, this parameter obeys the following formula:

\[
K_{E}(r) = K_0 \sqrt{\frac{N_0}{N(r)}}, \quad K_E(r) \leq K_{\text{Max}},
\]

where \( K_E \) is the eddy diffusion coefficient (in m² s⁻¹), \( K_0 \) is the reference coefficient at the model lower boundary, \( N(r) \) is the total neutral density (in m⁻³), \( K_{\text{Max}} \) is the upper limit on eddy diffusion that we can adjust to enforce a desired homopause altitude, and \( N_0 \) is the total density at 500 km. As noted in Krasnopolsky [2009], this functional form approximates the effects of upward propagating gravity waves. By adjusting the upper limit, \( K_{\text{Max}} \), the eddy diffusion coefficient will dictate the amount of mixing in the atmosphere and the altitude at which the atmosphere goes from a well-mixed state to a molecular diffusive state—the homopause.

As found in Bell et al. [2010a, 2010b, 2011b], Yelle et al. [2008], and Strobel [2012], changing the magnitude of the eddy diffusion coefficient will significantly impact the amount of atmospheric escape of CH4 required by models to reproduce the INMS densities and mixing ratios. Thus, a method for reliably capturing the effects of this turbulence is central to inferring atmospheric escape. Since Cassini’s arrival to the Saturnian system, INMS densities and mixing ratios have been used to constrain the amount of turbulence in the upper atmosphere. In particular, Yelle et al. [2008] suggested that INMS measurements of 40Ar could act as a tracer in numerical models.

Because of this, we use 40Ar mixing ratios to benchmark the eddy diffusion coefficient used in T-GITM simulations. However, various modeling studies incorporate eddy diffusion using different methods. Thus, for a given eddy diffusion coefficient, we must test whether or not we obtain the same simulated vertical profile of 40Ar mixing ratios when using different numerical methods. In order to investigate this, we consider
Figure 1. Three methods for including turbulence (eddy diffusion) into T-GITM: the momentum equation (solid), the continuity equation (dashed), and the hydrostatic diffusion model (dash-dotted). (a) The neutral temperatures, (b) the molecular diffusion coefficients (black) and eddy diffusion coefficients (blue), (c) the effects of eddy diffusion on $^{40}$Ar mixing ratios, and (d) neutral densities (black) with INMS data of Magee et al. [2009] in red.

three methods (see Appendix A) for including turbulence in 1-D simulations: (1) the hydrostatic diffusion approach of Yelle et al. [2006, 2008] and Cui et al. [2012], (2) the inclusion of turbulence in the continuity equation like Strobel [2008, 2009, 2010, 2012], and (3) the inclusion of turbulence in the momentum equation like Bell et al. [2010a].

Figure 1 shows a comparison among the three methods for turbulence. These three simulations share the same composition and eddy diffusion constraints. Moreover, the temperatures are specified at all times in the simulations. Thus, only the method for including turbulence varies among these three simulations. Figure 1a depicts the specified thermal structure used in all three simulations, and Figure 1d depicts the simulated N$_2$ neutral densities (black lines) along with the INMS N$_2$ densities (red circles and horizontal uncertainties). Figure 1b contains the molecular diffusion coefficient of CH$_4$ (in black) and the assumed eddy diffusion coefficients (in blue). As seen in Figure 1c, the effects of eddy diffusion on $^{40}$Ar mixing ratios are very consistent among all methods and any differences between the simulated mixing ratios are less than 5%. This demonstrates that the simulated effects of eddy diffusion are method independent. Based upon this result, we will continue to include the effects of eddy diffusion in the momentum equation.

4.2. Eddy Diffusion: Homopause

Next, we isolate the impacts of varying the eddy diffusion coefficient on the inferred methane escape rates in T-GITM simulations. In order to do this, we consider two broad cases of eddy diffusion: (1) a low-methane homopause case near 880 km (consistent with Strobel [2009], Yelle et al. [2008], and Cui et al. [2012]) and (2) a high-methane homopause case near 1000 km (consistent with Bell et al. [2010b] and Mandt et al. [2012]). To test these methane homopause cases, we introduce three T-GITM simulations: model A, a high-homopause simulation; model B, a low-homopause simulation; and model B (HE), a low-homopause simulation with hydrodynamic escape imposed as a boundary condition because T-GITM cannot self-consistently calculate it. As in section 4.1, these three T-GITM simulations share the same fixed thermal structure of Figure 1a, which means that no energy balance calculations are performed. Models A, B, and B (HE) also share the same lower boundary constraints and the same chemical scheme. Thus, only the eddy diffusion coefficient and topside escape rates vary among these simulations.

The key characteristics of models A, B, and B (HE) are summarized in Table 3, and the resulting fields are presented in Figures 2 and 3. In this table, we highlight the topside escape rates for CH$_4$ and H$_2$ (scaled relative to the surface of Titan), the integrated chemical destruction of CH$_4$ (scaled relative to the surface of Titan),

BELL ET AL. ©2014. American Geophysical Union. All Rights Reserved. 4961
K_{\text{Max}} values, and the homopause altitudes for each T-GITM simulation. Operationally, we obtain different methane homopause altitudes by adjusting the K_{\text{Max}} values, where the low-homopause altitudes of 880 km correspond to K_{\text{Max}} = 1750 \text{ m}^2 \text{ s}^{-1} and the high-methane homopause altitude of 990 km corresponds to K_{\text{Max}} = 1.0 \times 10^6 \text{ m}^2 \text{ s}^{-1}. Additionally, all simulations share the same K_0 values and the same functional form given by equation (2). Finally, Table 4 summarizes how these models compare with the INMS data, based upon the percent deviation outlined above in equation (1).

Figure 2 summarizes the major composition results from these three simulations. Figures 2a and 2b show the simulated major neutral densities and mixing ratios, respectively. The black lines represent T-GITM simulations, and the red circles represent the average INMS measurements during the prime mission as determined by Magee et al. [2009] (please note that horizontal uncertainties are a convolution of both counting statistical uncertainties and geophysical variabilities). The CIRS and GCMS ranges for these species are shown in Figures 2c and 2d, respectively. The cyan and yellow data represent GCMS and CIRS constraints, respectively. (a) Neutral temperatures, (b) neutral densities, (c) volume mixing ratios of methane and hydrogen, and (d) volume mixing ratios of HCN and Argon.

Table 3. T-GITM Simulation Parameters (Fluxes/Integrated Values Scaled Relative to Surface)

<table>
<thead>
<tr>
<th></th>
<th>$\Phi_{\text{CH}_4}$ (CH$_4$/m$^2$/s)</th>
<th>$\Phi_{\text{H}_2}$ (H$_2$/m$^2$/s)</th>
<th>Integrated Chemical Loss (CH$_4$/m$^2$/s)</th>
<th>$K_{\text{Max}}$ (m$^2$/s)</th>
<th>CH$_4$ Homopause Altitude (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Section 4.1:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eddy diffusion</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>tests with frozen</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>temperatures</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model A (1)</td>
<td>$1.41 \times 10^{11}$</td>
<td>$1.08 \times 10^{14}$</td>
<td>$5.13 \times 10^{13}$</td>
<td>$10^6$</td>
<td>$\sim$ 990 km</td>
</tr>
<tr>
<td>Model B (2)</td>
<td>$3.15 \times 10^{11}$</td>
<td>$1.10 \times 10^{14}$</td>
<td>$5.14 \times 10^{13}$</td>
<td>$1750.0$</td>
<td>$\sim$ 880 km</td>
</tr>
<tr>
<td>Model B (HE) (3)</td>
<td>$2.60 \times 10^{13}$</td>
<td>$1.08 \times 10^{14}$</td>
<td>$5.14 \times 10^{13}$</td>
<td>$1750.0$</td>
<td>$\sim$ 880 km</td>
</tr>
<tr>
<td><strong>Section 4.2:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methane chemistry</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>tests with frozen</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>temperatures</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model A (NC) (4)</td>
<td>$1.10 \times 10^{11}$</td>
<td>$1.08 \times 10^{14}$</td>
<td>$5.11 \times 10^{13}$</td>
<td>$10^6$</td>
<td>$\sim$ 990 km</td>
</tr>
<tr>
<td>Model A (NC HE)</td>
<td>$1.71 \times 10^{11}$</td>
<td></td>
<td>(No chemistry)</td>
<td>$10^6$</td>
<td>$\sim$ 990 km</td>
</tr>
<tr>
<td><strong>Section 4.3:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Energy balance</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>calculations</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>with $Q_{\text{Plasma}} = 3.04 \times 10^9$ (eV/cm$^2$/s)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model C (5)</td>
<td>$1.47 \times 10^{11}$</td>
<td>$1.07 \times 10^{14}$</td>
<td>$5.14 \times 10^{13}$</td>
<td>$10^6$</td>
<td>$\sim$ 990 km</td>
</tr>
<tr>
<td>Model D (6)</td>
<td>$2.55 \times 10^{11}$</td>
<td>$1.10 \times 10^{14}$</td>
<td>$5.11 \times 10^{13}$</td>
<td>$1750.0$</td>
<td>$\sim$ 880 km</td>
</tr>
<tr>
<td>Model D (HE) (7)</td>
<td>$2.49 \times 10^{13}$</td>
<td>$1.09 \times 10^{14}$</td>
<td>$5.04 \times 10^{13}$</td>
<td>$1750.0$</td>
<td>$\sim$ 880 km</td>
</tr>
</tbody>
</table>

a(HE) means hydrodynamic escape rates are specified as a boundary condition.
b(NC) means that simulation neglects methane chemical losses.

Figure 2. T-GITM simulations with different methane homopause altitudes: models A, solid; B, dashed; and B (HE), dash-dotted. Red data are from Magee et al. [2009], and dark blue points are from Yelle et al. [2008]. The cyan and yellow data represent GCMS and CIRS constraints, respectively. (a) Neutral temperatures, (b) neutral densities, (c) volume mixing ratios of methane and hydrogen, and (d) volume mixing ratios of HCN and Argon.
Figure 3. Dynamical fields from models A, solid; B, dashed; and B (HE), dash-dotted. Species are color coded: CH$_4$, red; and H$_2$, blue. Total chemical loss rates represent the summation over all chemical loss mechanisms (for CH$_4$) or production mechanisms (for H$_2$). (a) The radial (vertical) velocities of methane and hydrogen, (b) their radial fluxes, (c) their total chemical losses, and (d) their molecular diffusion coefficients—note that the eddy diffusion coefficient is included as the gray curve.

are shown as horizontal yellow and cyan bars, respectively. Figure 2c shows the T-GITM simulated $^{40}$Ar mixing ratios (black) lines and the INMS measurements reported by Magee et al. [2009] (red circles with horizontal uncertainties) and those of Yelle et al. [2008] (blue circles and horizontal uncertainties). Similarly, Figure 2d shows the simulated and measured major stable isotopic ratios of $^{14}$N/$^{15}$N in N$_2$.

From Figures 2a and 2b and Table 4, we note that the methane densities and mixing ratios simulated by models A and B (HE) reproduce the INMS measurements equivalently well, whereas model B produces a significantly inferior fit to the data. This suggests that, when using a CH$_4$ homopause altitude of $\sim$880 km, we must impose hydrodynamic methane escape rates in T-GITM to reproduce the INMS methane data. This is seen in Table 3 by comparing model B (HE), in which we impose a hydrodynamic-like escape rate of $\sim$2.60 $\times$ 10$^{13}$ CH$_4$ m$^{-2}$ s$^{-1}$, with model B, where T-GITM simulates a methane escape rate of $\sim$3.15 $\times$ 10$^{11}$ CH$_4$ m$^{-2}$ s$^{-1}$.

<table>
<thead>
<tr>
<th>Section</th>
<th>N$_2$ Density</th>
<th>CH$_4$ Density</th>
<th>H$_2$ Density</th>
<th>CH$_4$ Mixing</th>
<th>H$_2$ Mixing</th>
<th>$^{40}$Ar Mixing</th>
<th>$^{14}$N/$^{15}$N Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.1: Eddy diffusion tests with frozen temperatures</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model A</td>
<td>5.8</td>
<td>6.6</td>
<td>4.5</td>
<td>4.1</td>
<td>5.6</td>
<td>12.7</td>
<td>0.8</td>
</tr>
<tr>
<td>Model B</td>
<td>5.3</td>
<td>100.5</td>
<td>5.5</td>
<td>84.0</td>
<td>6.0</td>
<td>36.6</td>
<td>8.2</td>
</tr>
<tr>
<td>Model B (HE)$^a$</td>
<td>5.6</td>
<td>2.8</td>
<td>8.8</td>
<td>4.2</td>
<td>6.4</td>
<td>35.6</td>
<td>8.4</td>
</tr>
<tr>
<td>4.2: Methane chemistry tests with frozen temperatures</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model A</td>
<td>5.8</td>
<td>6.6</td>
<td>4.5</td>
<td>4.1</td>
<td>5.6</td>
<td>12.7</td>
<td>0.8</td>
</tr>
<tr>
<td>Model A (NC)$^b$</td>
<td>5.9</td>
<td>40.1</td>
<td>4.9</td>
<td>30.9</td>
<td>5.8</td>
<td>12.1</td>
<td>0.9</td>
</tr>
<tr>
<td>Model A (NC HE)$^{a,b}$</td>
<td>6.0</td>
<td>9.2</td>
<td>4.5</td>
<td>6.4</td>
<td>5.5</td>
<td>12.6</td>
<td>0.8</td>
</tr>
<tr>
<td>4.3: Energy balance calculations with $Q_{\text{Plasma}} = 3.04 \times 10^8$ (eV/cm$^2$/s)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model C</td>
<td>9.5</td>
<td>3.4</td>
<td>8.3</td>
<td>6.0</td>
<td>5.1</td>
<td>9.6</td>
<td>0.8</td>
</tr>
<tr>
<td>Model D</td>
<td>30.0</td>
<td>64.0</td>
<td>13.8</td>
<td>109.0</td>
<td>6.5</td>
<td>13.5</td>
<td>9.7</td>
</tr>
<tr>
<td>Model D (HE)$^a$</td>
<td>53.0</td>
<td>30.9</td>
<td>24.1</td>
<td>40.9</td>
<td>99.0</td>
<td>48.0</td>
<td>11.6</td>
</tr>
</tbody>
</table>

$^a$(HE) means hydrodynamic escape rates are specified as a boundary condition.

$^b$(NC) means that simulation neglects methane chemical losses.
As seen in Figure 2c, the different T-GITM simulations match different $^{40}$Ar data sets. Model A matches the mixing ratios derived by Magee et al. [2009], while models B and B (HE) both match those determined by Yelle et al. [2008]. Figure 2d contains a comparison between the isotopic ratios simulated by T-GITM and measured by INMS. As seen in this figure and as quantified in Table 4, model A represents a superior fit to these isotopic ratios. Moreover, as noted in Mandt et al. [2012], these isotope ratios possess lower counting statistical uncertainties and may function as a more reliable diagnostic for eddy diffusion than $^{40}$Ar.

Figure 3 provides details about the dynamics and chemistry in models A, B, and B (HE). Figure 3a depicts the three species’ velocities: $N_2$ is shown in black, $CH_4$ in red, and $H_2$ in blue. The different simulations are designated by the same line styles as they are in Figure 2. In Figure 3a, models A and B simulate consistent velocities for all of the species, suggesting that the main driver for the vertical dynamics (pressure-gravity balance) is largely the same. By contrast, the $CH_4$ velocities simulated by model B (HE) deviate significantly from the other two, due to the hydrodynamically escape rates specified at the upper boundary. This suggests that the $CH_4$ vertical dynamics in model B (HE) are driven by the hydrodynamic escape boundary condition rather than the physics within T-GITM.

Figure 3b depicts the vertical fluxes of $H_2$ (blue) and $CH_4$ (red) for each simulation as well as the limiting fluxes for both $H_2$ in light green and $CH_4$ in magenta. The $H_2$ fluxes (blue) in all three simulations are nearly identical and cannot be distinguished from one another. Due to the chemical production seen in Figure 3c (blue curves), the $H_2$ fluxes increase with altitude. The $H_2$ fluxes increase until they reach values very close to the $H_2$ limiting flux profile (green). After rising to meet the limiting flux curve between 900 and 1000 km altitude, the $H_2$ fluxes then become asymptotic, suggesting that the limiting flux is setting the eventual escape flux of $H_2$ out of the atmosphere—consistent with Strobel [2010, 2012] and Cui et al. [2008].

By contrast, the methane vertical fluxes show systematic differences between the three T-GITM simulations. First, we note that the $CH_4$ fluxes systematically decrease with altitude, due to the chemical destruction (red) shown in Figure 3c. For models A and B, the chemistry reduces the upward fluxes by over 2 orders of magnitude. By contrast, in the hydrodynamic escape case of model B (HE), T-GITM must adjust the lower boundary fluxes to accommodate both the chemistry and the imposed topside escape rates. As seen in Figure 3c, this combined effect causes the model B (HE) vertical methane fluxes (red dash-dotted line) to exceed the limiting fluxes (magenta dash-dotted line) between 500 and 900 km, which then produces a decrease in the dash-dotted $CH_4$ volume mixing ratio seen in the previous Figure 2b.

Lastly, in Figure 3d we compare the eddy diffusion coefficients (gray) with both the methane (red) and molecular hydrogen (blue) molecular diffusion coefficients. The eddy diffusion coefficients for models B and B (HE) asymptote at a value of $K_{Max} = 1750.0 \text{ m}^2 \text{s}^{-1}$, whereas model A does not reach its $K_{Max}$ value listed in Table 3. The intersection altitude of $K_{E}$ and $D_{CH4}$ defines the methane homopause altitudes listed in Table 3. Similarly, we note that the $H_2$ homopause occurs well below the region where the limiting fluxes are set, explaining why the simulated $H_2$ densities remain insensitive to the homopause altitude.

4.3. Impact of Methane Chemistry

Some studies suggest that methane chemistry does not significantly impact estimates for methane escape [cf. Cui et al., 2012; Strobel, 2012; Yelle et al., 2008]. However, Bell et al. [2011b] indicated that chemistry may play a pivotal role, and we now seek to isolate the impacts of including or excluding methane chemical destruction. For this purpose, we examine three more simulations: model A from Figures 2 and 3, a new model A (NC) that is identical to model A but ignores the chemical losses of methane (i.e., no chemistry, NC), and finally model A (NC HE) which is identical to model A (NC) but now includes specified hydrodynamic escape rates at the upper boundary (i.e., no chemistry, hydrodynamic escape, NC HE).

These three models use the same homopause altitude of 990 km, the same frozen thermal structure seen in Figure 1a, and the same composition constraints at 500 km used in section 4.2 and Table 2. Thus, only the column-integrated total methane chemistry and topside escape rates are being varied (listed in Table 3 and scaled relative to the surface). Note that, when we exclude the chemical losses of $CH_4$, we must still calculate the products of methane chemistry in order to capture $H_2$ production.

The results of this study are shown in Figure 4. In Figure 4a, we compare simulated $CH_4$ and $H_2$ mixing ratios (black) against the INMS data (red). While all of the models match the data to within the error bars shown,
Figure 4. (a) Volume mixing ratios of methane and hydrogen, (b) their radial fluxes. Figure 4a shows methane chemistry study: model A, solid; model A (NC), dashed; and model A (NC HE), dash-dotted line. Red circles are data from Magee et al. [2009]. In Figure 4b, the red lines represent CH$_4$, and the blue lines represent H$_2$.

Table 4 shows that model A (NC) exhibits the highest deviation from the INMS measurements. By contrast, when hydrodynamic escape rates are imposed at the upper boundary in model A (NC HE), the simulated methane mixing ratios better reproduce the INMS data. Comparing models A (NC) and model A (NC HE) suggests that, when omitting methane chemical destruction, the only way to match INMS measurements is to impose hydrodynamic-like escape rates on the model. By contrast, model A is able to match the INMS methane mixing ratios with much lower methane escape rates, because it incorporates self-consistent chemical destruction of methane from direct photolytic, ion-neutral, and neutral-neutral chemistry [Bell et al., 2010a, 2011b].

Figure 4b shows the vertical fluxes (scaled relative to the surface) for each species in the same format as Figure 3b. The vertical methane fluxes for model A (NC) and model A (NC HE) are constant with altitude (to within 1%), while model A shows the characteristic decrease with altitude due to the column-integrated chemical destruction of CH$_4$. Thus, these simulations also highlight that the methane chemistry has both compositional and dynamical impacts in the T-GITM simulations, emphasizing the highly coupled nature of Titan’s upper atmosphere.

4.4. Coupled Energy Calculations

The T-GITM simulations in sections 4.1–4.3 were highly simplified by imposing a frozen temperature structure. However, this ignores the very important coupling between dynamics, composition, and energy balance. Thus, we next examine how estimates of CH$_4$ and H$_2$ atmospheric escape are altered by including the full Navier-Stokes equations in Appendix A by introducing three new T-GITM simulations: model C, a high-homopause simulation (990 km); model D, a low-homopause simulation (880 km); and model D (HE), a low-homopause simulation with hydrodynamic escape imposed. These new simulations are the analogues to models A, B, and B (HE) from section 4.1, as seen in Table 3.

For the self-consistent simulations, we include Solar EUV/UV heating, HCN rotational cooling, and finally a magnetospheric plasma heating term that was used in Bell et al. [2011a]. We use a fixed column-integrated magnetospheric plasma heating rate of 1.45 × 10$^{10}$ eV cm$^{-2}$ s$^{-1}$ (scaled relative to the surface) for all three simulations, which amounts to roughly 10% of the integrated solar EUV/UV heating (1.36 × 10$^{10}$ eV cm$^{-2}$ s$^{-1}$). Thus, models C, D, and D (HE) all share identical orbital, seasonal, and solar cycle parameters given in Table 1 and only the eddy diffusion coefficient and topside escape rates of methane are varying among these simulations (as seen in Table 3).

As seen in Figure 5, there is a systematic decrease in thermosphere temperatures going from model C to model D to model D (HE). Model C possesses the highest methane homopause of 990 km and the lowest escape rates of methane (see Table 3). The effects of this higher homopause altitude are evident in Figures 5b–5d. As was found in sections 4.2 and 4.3, the inclusion of the higher homopause altitude allows model C to match the CH$_4$ and 40Ar mixing ratios without the need for hydrodynamic escape.

Model C also possesses the lowest simulated HCN mixing ratios in Figure 5d and most closely approximates the HCN mixing ratios measured by INMS as reported in Magee et al. [2009] (red vertical bar). This is because the higher turbulence transports HCN more efficiently downward through the model’s lower boundary (i.e., into the lower atmosphere). HCN is considered to be the “thermostat” for Titan’s upper atmosphere and efficiently cools the thermosphere through rotational line emission [Yelle, 1991]. Thus, less HCN abundances...
Figure 5. (a) Neutral temperatures, (b) neutral densities, (c) volume mixing ratios of methane and hydrogen, and (d) Argon mixing ratios. Shown are fully coupled Navier-Stokes simulations: model C, solid line; model D, dashed line, and model D (HE), dash-dotted line. Red data are from Magee et al. [2009], and blue data are from Yelle et al. [2008]. GCMS and CIRS constraints are cyan and yellow lines. The vertical red bar in Figure 5d is the INMS measurements of HCN reported in Magee et al. [2009].

in model C produce less radiative cooling and a warmer thermosphere. As indicated in Magee et al. [2009] the reported HCN mixing ratios are likely lower limits, due to antechamber sticking. Therefore, model C’s overestimate of HCN values relative to those reported in Magee et al. [2009] is acceptable.

By contrast, the lower homopause altitudes in models D and D (HE) produce greater HCN mixing ratios above 1000 km, which increases the radiative cooling in the thermosphere and reduces the thermosphere temperatures in Figure 5a. These colder temperatures produce N₂, CH₄, and H₂ densities that do not match the INMS measurements as well as model C in Figures 5b and 5c. Even when including hydrodynamic escape in model D (HE), this model remains inferior to that of model C based upon its match to INMS data. Similarly, the H₂ mixing ratios in Figure 5c simulated by models D and D (HE) show increased deviations from INMS measurements due to the cold thermosphere temperatures that reduce thermal escape.

Finally, the major heating and cooling rates for the 1-D T-GITM are presented in Figure 6a in units of K s⁻¹, which capture the actual response of the simulated thermosphere to these different processes. As seen in Figure 6a and noted in Bell et al. [2010a], the dominant drivers for the thermosphere are the HCN cooling (blue) and the solar EUV/UV heating (red). Thermal conduction also plays a major role (black), as does a specified ion precipitation heating (magenta) that is adopted based upon the work by Bell et al. [2011a] and
5. The Impacts of H₂ Chemistry

As with CH₄, quantifying H₂ escape by reproducing the observations of H₂ is central to understanding the evolutionary history of Titan’s atmosphere. As noted in Strobel [2010, 2012], there is an apparent mismatch between the lower atmosphere and the upper atmosphere measurements of H₂. Essentially, 1-D models cannot reproduce the INMS H₂ measurements when using GCMS and/or CIRS constraints, and this difficulty can be seen in the H₂ mixing ratios of Figures 2 and 5. In these figures, we must use lower boundary H₂ mixing ratios in T-GITM that are higher than any measurements suggested by either CIRS (yellow horizontal lines) or GCMS (cyan lines). The horizontal CIRS range (yellow) also includes a factor of 2.0 enhancement in the near-surface H₂ mixing ratios in the midlatitudes to high latitudes reported by Courtin et al. [2008].

Next, we examine how variations in the H₂ chemical production can impact our ability to reconcile measurements of H₂ in the lower and upper atmosphere. As outlined in section 2, we have employed an empirical chemical production of H₂ given by $P_{H_2} = 1.15 \times L_{CH_4}$, which is loosely based upon the measurements of heavy hydrocarbon C/H ratios made by INMS [Waite et al., 2007; Westlake et al., 2012]. This scheme liberates significantly more H₂ than the original scheme of Bell et al. [2010a], and we now examine the implications of this added H₂ production on T-GITM simulated H₂ densities and mixing ratios.

In Figure 7, we compare three new T-GITM simulations that are identical to model A (high-methane homopause and fixed temperature), except that the H₂ chemistry and lower boundary conditions are altered in each case. The column-integrated H₂ production (scaled relative to the surface) is shown in Table 5. The baseline simulation is model A (shown in solid black). The second simulation is model A with the

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Integrated Production</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model A</td>
<td>$5.91 \times 10^{13}$</td>
</tr>
<tr>
<td>Model A with Bell et al. [2010a] chemistry</td>
<td>$2.13 \times 10^{13}$</td>
</tr>
<tr>
<td>Model A with Bell et al. [2010a] + adjusted mixing ratio</td>
<td>$2.08 \times 10^{13}$</td>
</tr>
</tbody>
</table>
semiempirical H₂ chemistry replaced with the scheme outlined in Bell et al. [2010a] (dashed black line), which liberates significantly less H₂ than the empirical method. The third simulation is model A with the Bell et al. [2010a] chemical scheme and an altered H₂ mixing ratio of 2.75 × 10⁻³ at 500 km, which is a mixing ratio consistent with previous work in Bell et al. [2010a] and Strobel [2010].

Figure 7 also shows the available constraints from the Huygens GCMS (light blue), the Cassini CIRS (yellow), and a range of mixing ratios from recent photochemical modeling studies in Krasnopolsky [2009] and Krasnopolsky [2010] (magenta). The data from GCMS and CIRS are obtained from much lower altitudes (near ~100–200 km), while the mixing ratio from the photochemical modeling are appropriate for 500 km. There are two primary observations to be made from this comparison. First, the semiempirical H₂ chemistry derived from the high-mass hydrocarbons allows T-GITM to match INMS using lower boundary mixing ratios that are closer to those measured by GCMS and CIRS deeper in the atmosphere. Second, when using the lower H₂ production of Bell et al. [2010a], we must adopt a higher lower boundary mixing ratio of H₂ that is consistent with recent photochemical models in the middle atmosphere but much higher than mixing ratios measured by either CIRS or GCMS.

6. Summary and Conclusions

Since the arrival of Cassini-Huygens to the Saturnian system, there has been an ongoing debate about the amount of CH₄ escaping that is required by models to match the INMS data. These inferred CH₄ atmospheric escape rates have ranged from ∼1.0 × 10⁸ CH₄ m⁻² s⁻¹ in Bell et al. [2010a, 2010b, 2011b] up to ∼2.0 × 10¹³ CH₄ m⁻² s⁻¹ in Yelle et al. [2008], Strobel [2009, 2010, 2012], and Cui et al. [2012]. Moreover, Strobel [2012] and others maintain that the highest CH₄ escape rates are evidence of a hydrodynamic escape mechanism, although hydrodynamic escape is typically defined as the bulk outflow of the whole atmosphere in response to intense heating [cf. Tian et al., 2008].

Our previous simulations in Bell et al. [2010a, 2010b, 2011b] demonstrated that hydrodynamic escape is only one possible model configuration consistent with INMS data. However, direct model-to-model comparisons between Bell et al. [2011b] and those such as Strobel [2010] were complicated by the fact that we included several factors including Sun-Saturn orbital distance variations over time as well as diurnal variations into our calculations which were ignored in the studies by Yelle et al. [2008], Strobel [2009, 2010, 2012], and Cui et al. [2012]. In the present work, we have reconfigured our T-GITM simulations to more closely approximate the approaches taken in other investigations into methane and molecular hydrogen escape.

When trying to reproduce the INMS data with models, it is well established that the amount of turbulence greatly impacts the amount of atmospheric methane escape required to match the INMS CH₄ data. Operationally, models parameterize turbulence using an adjustable eddy diffusion coefficient, and, thus, most studies use the inert gas ⁴⁰Ar to constrain it. When comparing different studies of atmospheric escape, one notices two major differences among them: (1) the method for including turbulence (i.e., how they parameterize it) and (2) the source for their ⁴⁰Ar data (either that of Magee et al. [2009] or Cui et al. [2008, 2012]). Fortunately, as seen in section 4.1 and Figure 1, the dynamical effects on ⁴⁰Ar are almost completely method invariant, whether you choose to use a hydrostatic diffusion approach (as in Cui et al. [2012] or Yelle et al. [2008]), include eddy diffusion in the continuity equation (as in Strobel [2009, 2010, 2012]), or include turbulence directly in the momentum equation (as in Bell et al. [2010a, 2010b, 2011b]). Thus, the primary differences among the various atmospheric escape studies must lie in the INMS ⁴⁰Ar mixing ratios used to constrain these eddy diffusion coefficients.

The large uncertainties in INMS retrieved ⁴⁰Ar mixing ratios are apparent in Figure 2c, which are so large that all of the simulated ⁴⁰Ar mixing ratios fall within this error range. These uncertainties in the ⁴⁰Ar data are due to (1) poor counting statistics, (2) the difficulty and nonuniqueness in subtracting other species, and (3) the relatively large geophysical variations from pass to pass. The end result is that a very minor species with very large uncertainties is being used almost exclusively to constrain turbulence effects in Titan’s atmosphere. As an added complication, recent laboratory and Huygens probe data analysis has revealed that noble gases are efficiently “trapped” in Titan’s atmospheric hazes [cf., Bar-Nun et al., 2007, 2008, Jacovi and Bar-Nun, 2008]. Thus, in addition to very large observational uncertainties, ⁴⁰Ar is most likely not truly inert.

Mandt et al. [2012] suggested that the major stable isotopes of ¹⁴N/¹⁵N in N₂, when combined with ⁴⁰Ar, could provide improved constraints on turbulence. The authors point out that ¹⁴N/¹⁵N ratios possess
significantly improved counting statistics, which is evident in Figure 2d. As can be seen in Figure 2d and in Table 4, the models using a lower methane homopause, models B and B (HE), calculate isotope ratios outside the INMS uncertainties. Thus, when using the combination of $^{40}$Ar and $^{14}$N/$^{15}$N to constrain the eddy diffusion coefficient, we find that model A (high-methane homopause simulation) is superior to both models B and model B (HE).

Section 4.2 also reproduces and explains the results obtained by Yelle et al. [2008], Cui et al. [2009], and Strobel [2012]. These earlier studies maintain that the methane homopause is near 880 km, which is obtained by matching the blue data points in Figure 2c. As seen by comparing models B and B (HE), in order to match the INMS CH$_4$ data using this lower homopause altitude, we must then impose hydrodynamic escape rates of CH$_4$. This is what has been concluded by Yelle et al. [2008], Cui et al. [2009], and Strobel [2012].

In addition to turbulence, chemical destruction of methane also plays a major role in determining the amount of topside escape that is required by models to match INMS data. As seen in Figures 4a and 4b, when ignoring the methane chemistry T-GITM cannot match the INMS data without imposing hydrodynamic CH$_4$ escape rates on the model, since model A (HCHE) fits the data much better than model A (NC). This is essentially the same result obtained by Yelle et al. [2008] and Cui et al. [2012], who also ignore chemistry. Thus, when ignoring chemistry, one must compensate by imposing hydrodynamic outflow to match INMS data. By contrast, by including direct photolytic, neutral-neutral, and ion-neutral methane chemical losses, model A is able to match INMS data while simulating escape rates that are consistent with pre-Cassini estimates [see Johnson et al., 2009].

Finally, including a self-consistent thermal balance calculation that responds to changing composition and dynamics further modifies estimates of atmospheric escape, as seen in section 4.4 and Figure 5. This section demonstrated that, as the homopause altitude decreases, the HCN mixing ratios increase, resulting in higher overall cooling of the thermosphere and highlighting the intimate connection between composition, dynamics, and energy balance. Because of this coupling, the lower methane homopause simulations—models D and D (HE)—did not match the available INMS measurements as well as the high-methane homopause simulation of model C (see Table 4). This thermal balance interplay has not been discussed before, since neither Yelle et al. [2008] nor Cui et al. [2012] include thermal balance calculations and Strobel [2012] does not include the self-consistent HCN chemistry.

In contrast to CH$_4$, H$_2$ escape is comparatively simple. When freezing the thermal structure, the H$_2$ escape rates required to match INMS data are given by classical Jeans escape, which is consistent with recent kinetic modeling by Tucker et al. [2012]. Moreover, when freezing the thermal structure, H$_2$ is invariant to our choice of methane homopause, which conflicts with the findings of Strobel [2012] who suggested that a high-methane homopause impacted simulated hydrogen densities. In fact, when examining the fully self-consistent T-GITM simulations of section 4.4, we find that model C, which has the highest methane homopause, best reproduces the measured H$_2$ densities and mixing ratios. Finally, the results in section 5 reveal that, for a given thermal structure, simulated H$_2$ densities are most sensitive to the chemical scheme used. If we liberate more H$_2$ from chemistry, then we are better able to reconcile lower and upper atmosphere H$_2$ measurements, suggesting that the key to reconciling the GCMS and CIRS H$_2$ measurements with INMS data lies in the chemical scheme used.

Ultimately, we have demonstrated that it is possible to reconcile simultaneously both the lower and upper atmosphere measurements of CH$_4$ and H$_2$ and that there is no need for hydrodynamic escape of methane. Our best fit configurations of T-GITM (models A and C) have methane homopauses near 990 km, and they match both lower and upper atmospheric measurements of CH$_4$, $^{40}$Ar, HCN, and the $^{14}$N/$^{15}$N isotopic ratio in N$_2$. Our estimates of upwelling methane fluxes are at most $\sim 1.5 \times 10^{11}$ CH$_4$ m$^{-2}$ s$^{-1}$ (or $\sim 10^{25}$ CH$_4$ s$^{-1}$ globally), which is consistent with recent nonthermal escape rates estimated by De La Haye et al. [2008] and Johnson et al. [2009]. Moreover, these are global mean upper limits on neutral methane escape, since (1) T-GITM likely underestimates methane chemical losses and (2) kinetic treatments are needed to estimate actual escape fluxes (such as Tucker and Johnson [2009] or Tucker et al. [2012]). Finally, our studies suggest that the key to reconciling the apparent mismatch between lower and upper atmospheric measurements of H$_2$ lies in the complex chemistry of Titan’s atmosphere between 200 km and 1000 km.
Appendix A: Methods for Including Eddy Diffusion

The Titan-Global Ionosphere-Thermosphere Model (T-GITM) solves the time-dependent, coupled Navier-Stokes continuity, momentum, and energy equations outlined in Bell et al. [2010a]. We assume that each neutral species possesses its own continuity equation and its own vertical velocity (radial velocity). However, T-GITM assumes that all neutral species share the same background temperature [Ridley et al., 2006]. The continuity equation is given by

$$ \frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s) = P_s - L_s, $$

(A1)

where \( \rho_s \) represents the mass density (kg m\(^{-3}\)), \( \mathbf{u}_s \) the velocity (m s\(^{-1}\)), \( P_s \) the chemical sources (kg m\(^{-3}\) s\(^{-1}\)), and finally \( L_s \) the chemical losses (kg m\(^{-3}\) s\(^{-1}\)) for a species, "s." Next, the species-specific momentum equation is given by

$$ \rho_s \frac{\partial \mathbf{u}_s}{\partial t} + \rho_s \mathbf{u}_s \cdot \nabla \mathbf{u}_s + \nabla P_s + \nabla \cdot \tau_s - \rho_s \mathbf{g} + \rho_s \left[ 2 \mathbf{\Omega} \times \mathbf{u}_s + \mathbf{\Omega} \times (\mathbf{\Omega} \times \mathbf{r}) \right] = \sum_{i=1}^{s} \rho_{s_i} \mathbf{v}_{st} (\mathbf{u}_s - \mathbf{u}_{s_i}) + \sum_{i=1}^{s} \rho_{s_i} \mathbf{v}_{st} (\mathbf{a}_{s_i} - \mathbf{a}_s). $$

(A2)

In equation (A2), \( \tau_s \) is the velocity stress tensor (in Pa), \( \mathbf{g} \) the gravitational acceleration (in m s\(^{-2}\)), \( \mathbf{\Omega} \) Titan's rotational angular velocity (rads\(^{-1}\)), \( v_{st} \) the momentum collision frequency (s\(^{-1}\)), and \( \omega_s \) the eddy diffusion velocity (in m s\(^{-1}\)). The eddy diffusion velocity is given by Colegrove et al. [1966] as

$$ \omega_s = -K_E(r) \frac{1}{\chi_i} \frac{\partial \chi_i}{\partial r}, $$

(A3)

where \( K_E(r) \) is the eddy diffusion coefficient and \( \chi_i \) is the species' volume mixing ratio. Finally, the energy equation solved by T-GITM is given by

$$ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T + (\gamma - 1) T \nabla \cdot \mathbf{u} + \frac{\tau_s \cdot \nabla \mathbf{u}}{\rho_c} = \frac{1}{\rho_{c_v}} (Q_{\text{total}} - \nabla \cdot \mathbf{q}). $$

(A4)

Here \( T \) represents the bulk background temperature (K), \( \mathbf{u} \) the mass-weighted mean velocity, \( \tau \) the mean velocity stress tensor, \( \rho \) the mean mass density, \( c_v \) the specific heat at a constant volume (J kg\(^{-1}\) K\(^{-1}\)), \( Q_{\text{total}} \) is the total energy sources in units of (W m\(^{-3}\)), and \( \mathbf{q} \) thermal conduction. \( Q_{\text{total}} \) has several contributions, including solar EUV/UV heating, HCN rotational cooling, and magnetospheric ion precipitation heating, such that \( Q_{\text{total}} = Q_{\text{EUV}} + Q_{\text{magn}} - Q_{\text{HCN}} \). We close the Navier-Stokes equations with the collision-dominated versions of the viscosity stress tensor and heat flux vector as follows:

$$ \tau_s = \eta_s \left[ \nabla \mathbf{u}_s + \left( \nabla \mathbf{u}_s \right)^T - \frac{2}{3} (\nabla \cdot \mathbf{u}_s) I \right], $$

(A5)

$$ \mathbf{q} = -\lambda \nabla T, $$

(A6)

where \( \lambda \) is the thermal conduction coefficient (W m\(^{-1}\) K\(^{-1}\)), \( \eta_s \) is the viscosity coefficient (kg m\(^{-1}\) s\(^{-1}\)), and \( I \) is the second-order unit tensor.

Next, we outline three methods for including turbulence in 1-D simulations of Titan's upper atmosphere. The first method is shown above in equations (A1)–(A3), where we include the effects of turbulence directly in the momentum equation, as done by both Bell et al. [2010a] and Boqueho and Blelly [2005]. This is our preferred method and is denoted “GITM Momentum Eqn” in Figure 1. A second method for dealing with turbulence is to use a purely hydrostatic diffusion approach consistent with Cui et al. [2012], Yelle et al. [2006], and Yelle et al. [2008]:

1. Continuity

$$ \nabla \cdot (\Phi_s) = 0. $$

(A7)

2. Momentum

$$ \frac{1}{\chi_i} \frac{\partial \chi_i}{\partial r} = \frac{D_i}{D_i + K_E} \left[ \frac{1}{H_{\text{atm}}} - \frac{1}{H_i} \right] \left( 1 - \frac{\Phi_s}{\Phi_{i,s}} \right). $$

(A8)
3. Diffusion limited flux

\[ \Phi_{ls} = D_s N \left( \frac{1}{H_{\text{atm}}} - \frac{1}{H_s} \right) \chi_s. \]  

(A9)

4. Hydrostatic equilibrium of the atmosphere

\[ \frac{1}{N} \frac{dN}{dr} + \frac{1}{T} \frac{dT}{dr} = - \left( \frac{1}{H_{\text{atm}}} \right). \]  

(A10)

In these expressions, \( \Phi_s \) is the species-specific flux (in molecules \( m^{-2} \ s^{-1} \)), where \( \Phi_s = n_s V_s \) and \( \Phi_{ls} \) represents the diffusion limited flux of Hunten (1973). \( H_{\text{atm}} \) is the atmospheric scale height (in m), and \( H_s \) is the species-specific scale height. \( D_s \) represents the total diffusion coefficient for species "s" (in \( m^2 \ s^{-1} \)). All other variables are the same as in equations (A1)–(A4). This approach is denoted “Diffusion Eqn” in Figure 1.

The third and final method approximates that of Strobel (2009, 2010, 2012), who includes turbulence effects in the continuity equation:

1. Continuity

\[ \frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s) + \nabla \cdot \mathbf{P}_s + \tau_s - \rho_s \mathbf{G}^t = \sum_{s\neq} \rho_s \mathbf{v}_{st} (\mathbf{u}_s - \mathbf{u}_t). \]  

(A12)

where all of the variables are the same as in the standard T-GITM formulation in equations (A1)–(A4). This method is denoted as “GITM Continuity Eqn” in Figure 1.

Acknowledgments

J. Bell would like to thank A. Nagy and all of the INMS team members for their input and guidance. Also, the authors would like to thank the Center for Space Environment Modeling (CSEM) at the University of Michigan for continued use of their computational facilities and expertise. This work was supported by the NASA grant NAS503001NM0710023, subcontracted through JPL. The NASA High End Computing (HEC) and the University of Texas Advanced Computing Center (TACC) supported the simulations presented here.

Michael Balikhin thanks Thomas Cravens and Philippe Garnier for their assistance in evaluating this paper.

References


