1. Introduction

Both the Cassini and the New Horizons mission in the outer solar system are allowing scientists to critique previous ideas concerning atmospheric evolution and escape. While orbiting the Saturn system the Cassini satellite has been collecting data from Titan’s atmosphere for over 6 years, and the New Horizons spacecraft will collect data on Pluto’s atmosphere in 2015 as it travels to the Kupier Belt. Understanding the mechanisms that control escape in planetary atmospheres allows us to infer its original inventory. Titan, Saturn’s largest moon, has an N₂ rich atmosphere with a few percent CH₄, 10ths of a percent of H₂ and a sparse population of organic molecules. Pluto also has a N₂ rich atmosphere with a few percent CH₄ but there is also a sparse population of CO and its surface pressure is nearly (20-200) millionth of the surface pressure at Titan (Olkin et. al. 2003). Both of the outer solar system bodies are bombarded by the solar radiation at their respective distances from the sun Titan ~10AU and Pluto ~30AU (at perihelion), and, since they do not have intrinsic magnetic fields, they are also exposed to plasma bombardment: for Pluto it is the solar wind plasma and for Titan it is primarily the plasma trapped in Saturn’s magnetosphere. All of the previous mentioned effects can lead to escape in planetary atmospheres for particles with favorable velocities.

Several decades worth of atmospheric models have concluded that Pluto’s atmosphere is escaping through a process commonly referred to as ‘slow hydrodynamic escape’ which requires a significant escape flux in comparison to the theoretical Jeans flux (e.g.: Hunten and Watson 1982; McNutt 1989; Krasnolpolsky 1999; Strobel 2008a). Recently, this process has also been suggested to occur at Titan (Strobel 2008b) even though its mass is over an order of magnitude larger than that for Pluto. The slow hydrodynamic escape models use Cassini density data to constrain the mass loss rate from Titan. Density profiles of H₂ in the upper atmosphere confirm its escape, and the escape rate ~ 1x10²⁸ s⁻¹ is typically agreed upon (Johnson 2009). However, recent results from Monte Carlo simulations have determined the N₂ and CH₄ loss rates for Titan are not correct, and suggest that N₂ escape from Pluto is more like Jeans escape rather than hydrodynamic escape (Tucker and Johnson 2009). A Monte Carlo approach is necessary to model thermal escape from a rarefied atmosphere as opposed to a fluid approach. In the following sections the Direct Simulation Monte Carlo model is explained, including summaries of current results.

2. Exobase, Jeans Escape & Hydrodynamic Escape

Escape occurs most efficiently in the exosphere, a tenuous region in the upper atmosphere, where molecules can travel planetary scale distances and not collide with other molecules (Johnson et. al. 2008). The exobase is the lower boundary to this region, and it is defined as the altitude where the mean free path for collisions, \( \lambda_{\text{mfp}} = (2^{1/2} \pi n \sigma)^{-1} \), is comparable to the atmospheric scale height \( H = kT/mg \) (n – density, \( \sigma \) – collision cross-section, \( k \) – Boltzmann constant, \( T \) – temperature, \( m \) – molecule mass, \( g \) – gravity). In rarefied gas dynamics the ratio \( \lambda_{\text{mfp}}/H \) is referred to as the Knudsen number \( K_n \), and it provides the criterion for when a gas flows similarly to a fluid and can be modeled using solutions to the equilibrium fluid equations \( (K_n << 1) \), or when it becomes increasingly collisionless and must be modeled stochastically \( (K_n > 0.1) \). At the exobase \( K_n \sim 1 \), and it is the altitude in the atmosphere where the column density is \( N = \sigma^{-1} \).

Thermally driven atmospheric escape is characterized by the Jeans parameter it is the ratio of the gravitational potential energy to the thermal energy at the exobase \( \lambda_{\text{exo}} = GM_p m/(T_{\text{exo}} k) \), where \( M_p \) is the mass of the planet. For large jeans parameter values, the gravitational energy of the planet dominates the thermal energy of the atmosphere. Therefore, only a small fraction of particles at the tail end of the speed distribution can escape if they have proper velocity. In this case the escape flux is \( F_s = n_{\text{exo}} v_{\text{exo}} \exp[- \)
\[ \lambda_{exo} (1 + \lambda_{exo}), \text{ where } \langle v_{exo} \rangle \text{ is the mean thermal speed (Chamberlain and Hunten 1987). At the exobase for Titan and Pluto respectively the Jeans parameter is } \lambda_{exo} \approx 55, \text{ and } \approx 10. \]

If the gravitational energy of the planet is comparable to the thermal energy of the gas, \( \lambda_{exo} = 2 \), then the atmosphere can flow off the planet in bulk, like a fluid, and the escape is essentially hydrodynamic. Hydrodynamic escape is defined as an organized gas flow produced by thermal conduction from below the exobase which produces an expansion in the upper atmosphere in which the bulk flow speed exceeds the escape speed (Johnson et al. 2008). When the fluid equations are applied to a 1D radial atmosphere, the continuity equation leads to a constant atmospheric flux vs. radial distance from a lower boundary: \[ n(r) v(r) = F_H, \]
with \( n(r) \) the number density and \( v(r) \) the flow speed vs. \( r \) the radial distance from the center of the plane. \( F_H \) is re-written as a rate in the equations below.

The radial momentum (pressure) equation for molecules of mass \( m \) in which the viscous term is typically dropped, can be written

\[
\frac{dp}{dr} = n \left( \frac{d\Phi}{dr} \right) - n \left( \frac{d(mv^2/2)}{dr} \right) \tag{1a}
\]

where \( p \) is the pressure \((nkT)\) and \( \Phi \) the gravitational potential energy \((GM_p m/r)\). The corresponding energy equation can be written:

\[
\frac{d\varphi}{dr} = \left( \frac{C_p}{F_p} - \Phi \right) - 4\pi r^2 \kappa (dT/dr) = 4\pi r^2 Q(r) \tag{1b}
\]

where \( C_p \) is the heat capacity per molecule and \( \kappa = \kappa(T) \) the thermal conductivity (e.g., Johnson et al. 2008).

Throughout the remainder of the paper we will refer to the slow hydrodynamic escape model as SHE. The standard procedure in the SHE model is to use \( \varphi \neq 0 \), but set \( v = 0 \) in Eqs. (1a) and (1b) below an upper boundary that is above the exobase. The equations are then solved as a function of \( \varphi \) and \( dT/dr, \varphi \) from a lower boundary, \( r_o \), where \( n_o = n(r_o) \) and \( T_o = T(r_o) \) are specified, with the condition that \( n, T \rightarrow 0 \) as \( r \rightarrow \infty \).

The equations below the exobase with \( v = 0 \) are:

\[
\frac{d(nkT)}{dr} = n \left( \frac{d\Phi}{dr} \right) \tag{2a}
\]

and

\[
\frac{d[\varphi (C_p T - \Phi) - 4\pi r^2 \kappa (dT/dr)]}{dr} = 4\pi r^2 Q(r) \tag{2b}
\]

These integrate to give the pressure vs. \( r \) and an equation for the heat flux:

\[
p = p_o \exp[-\int_{r_o}^{r_o} (GM_p m/r^2)/kT \ dr] \tag{3a}
\]

with \( p = nkT \) and

\[
[\varphi (C_p T - \Phi) - 4\pi r^2 \kappa (dT/dr)] = \langle E\varphi \rangle_{r_o} + 4\pi r_o^2 \beta(r). \tag{3b}
\]

Here \( \langle E\varphi \rangle_{r_o} \) is the heat flux across \( r_o \), and, as in Strobel (2008a), \( \beta(r) = r_o^{-2} \left[ \int_{r_o}^{r_o} r^2 Q(r) \ dr \right] \) with \( \beta \rightarrow \beta_o \) as \( r \rightarrow \infty \).

The temperature is, therefore, assumed to be defined even in the exosphere, and the expression for thermal conductivity is not changed, hence remains independent of density. This procedure gives solutions of \( n(r) \) and \( T(r) \) for a range of escape rates. In addition the SHE model is usually solved in dimensionless variables scaled by \( \varphi \) which favors solutions with large escape fluxes (Watson et al. 1981). The ‘best’ solution is typically picked using available density data as a constraint. However, Tucker and Johnson (2009) have used Monte Carlo techniques to show that very different escape fluxes can produce similar density profiles for the atmosphere, shown below.

### 3. Direct Simulation Monte Carlo

The SHE model is suitable for the region of the atmosphere where \( Kn < 0.1 \) applying it beyond the exobase must be done with care. To describe the transition region in the atmosphere from below the exobase to beyond \( Kn > 0.1 \), solutions to the Boltzmann equation or Monte Carlo simulations are required. We use the Direct Simulation Monte Carlo model, DSMC, (Bird, 1994). The atmosphere is described using a set of representative molecules and its evolution is calculated by following the motion of these particles subject to gravity and collisions. Thermal conduction is explicitly included and depends on the cross sectional area for collisions as well as the local density. A 1D simulation is carried out, consistent with the 1D continuum models being tested. In the main flow direction, radially outward from Titan, the space is divided into cells with heights less than the local mean free path for collisions.
To accurately describe an atmosphere using such simulations three conditions are must be satisfied (Shematovich 2004): there should be a sufficient number of representative particles to describe the nature of the flow; the molecular motion between collisions is independent of the nature of the collisions; and the time between collisions must be much larger than the time step.

In Tucker and Johnson (2009), we describe the atmospheric corona over radial distances $r/r_o$ up to 2.2 with the upper boundary dependent on the Jeans parameter involved. Fixed densities and temperatures taken from the continuum models in Strobel (2008a; 2008b) and Yelle et. al. (2008) were applied at the lower boundary which is below the exobase. The upper boundary was placed many scale heights above the exobase to include any effects of collisions which may have occurred beyond the nominal exobase. Upward moving molecules with speeds greater than the escape speed were assumed to escape while the others were specularly reflected back to the simulation region. The reflected, non-escaping molecules represent ballistic particles that are returning allowing a shorter time to achieve steady state. If chosen high enough the upper boundary should not affect the results as shown in figure (2). Typically, on the order of a few hundred thousand particles were used to represent the atmosphere in order to have at least a few hundred particles in the very top cells. The weights for the representative molecules were determined in order to meet that condition. Using this number of representative molecules, we were able to obtain results with a relatively small statistical scattering. Even with this number of particles we cannot accurately simulate the escape that might occur well above the exobase if our lower boundary is the same as in the continuum models. Therefore, we use the continuum results at an altitude closer to the exobase and simulate the transition region $Kn \sim 0.01$.

### 4. SHE Model Results

Before presenting the results from the DSMC simulations we will briefly discuss some of the current SHE model results for a N$_2$ atmosphere, shown in table (1). It is interesting that for the ‘baseline case’ in which all the heat input into the atmosphere is deposited below the lower boundary, $Q(r) = 0$ above $r_o$ in (Strobel 2008a, Strobel 2008b), solutions with a significant escape flux ($q_{\text{H}} = 1 \times 10^{-27} \text{ s}^{-1}$ and $5 \times 10^{-30} \text{ s}^{-1}$) were obtained for both the atmospheres of Titan and Pluto respectively. These results represent lower limits to the escape rates in the absence of solar heating. Even though Titan has a Jeans parameter 5 times larger than that for Pluto, the SHE model concluded that Titan’s atmosphere should escape at a higher rate. For comparison purposes the corresponding Jeans flux values for Titan and Pluto would be $\phi_J = 3.0 \times 10^9 \text{ s}^{-1}$ and $5 \times 10^{25} \text{ s}^{-1}$.

<table>
<thead>
<tr>
<th>System</th>
<th>$r_{\text{exo}}/r_o$</th>
<th>$l_{\text{exo}}$</th>
<th>$Kn_o$</th>
<th>$\phi_H/\phi_J$ s$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Titan</td>
<td>1.5</td>
<td>55</td>
<td>$2 \times 10^8$</td>
<td>$3 \times 10^7$</td>
</tr>
<tr>
<td>Pluto</td>
<td>2.2</td>
<td>10</td>
<td>$1 \times 10^8$</td>
<td>10</td>
</tr>
</tbody>
</table>

*Based on data in Strobel (2008a, 2008b)

$\sigma = 4 \times 10^{-16} \text{ cm}^2$ (Strobel 2009)

$Kn_o$ - Knudsen number at lower boundary.

### 5. DSMC Results

DSMC is ideally suited to test the results from SHE model no assumptions are made about the temperature or density at the upper boundary, and thermal conduction is inherently a function of the local density. Therefore a series of simulations were done in Tucker and Johnson (2009) to test the SHE model results for $Q(r) = 0$ for Titan. We fixed the temperature and density at the lower boundary (3875 km) to the solution from the SHE model in (Strobel 2008b). The DSMC results are shown in figure (1). The density profiles between the methods are similar, but the temperature for the DSMC result is isothermal throughout the simulation region. And accordingly, the local speed distributions all matched the theoretical Maxell Boltzmann Speed distribution for a temperature of 141K. No test particles that escaped during the DSMC simulation. The simulations were performed for a suitable amount of time if 1 test particle would have escaped during the simulation the escape rate would have been 6 orders of magnitude less than the SHE model result. The gravitational binding energy at the DSMC exobase (4000km) is $\sim 0.6eV$, and the mean energy of the N$_2$ molecules at 141K is $\sim 0.01eV$. Only a very small fraction of particles at the tail of the distribution will have energy to escape, and for this case escape should occur very similar to the Jeans rate. In
our simulations we could not achieve the Jeans rate because it would have required several millions of particles, or extremely long simulations.

Figure (1): DSMC result (open triangles - dotted lines) using lower boundary conditions at 3875 km from case with no heating in Strobel (2008): temperature (inverted triangles - bottom axis) and density (upward triangles - top axis) (Tucker and Johnson 2009). Exobase is at 4000 km represented by horizontal line. Result is compared to SHE model solution from Strobel (2008b) (filled triangles – solid lines).

Figure (2): Temperature (inverted triangles - bottom axis) and density profiles upward triangles - top axis) vs. radial distance from Titan with T=600K at the lower boundary 4000km (Tucker and Johnson 2009). Solid line represents upper boundary at 7000km and triangles represent upper boundary at 6400km. \( \lambda_{exo} \) = 11 at exobase 4600 km. Difference in escape results between simulations less than 3%.

However, by artificial increasing the temperature to 600K at the lower boundary for Titan we were able to force escape to occur (Tucker and Johnson 2009). As shown in figure (2), the adiabatic cooling is indicative of the escape which occurred at a rate of 7x10^{-5} s^{-1}. We found that even at \( \lambda_{exo} \) ~ 11 escape still occurred similar to the Jeans theoretical values (1.5*Jeans) rather than hydro-dynamical. This result emphasized that for the baseline case thermal escape rates for \( \lambda_{exo} \) given by the SHE model are incorrect. Also, as shown in figure (2), the upper boundary did not affect the results for this artificial case. The average escape rate obtained using the different upper boundaries differed by less than 3%.

6. Combined DSMC/Fluid Approach

The DSMC results for the artificial 600K simulations where \( \lambda_{exo} \) =11 for Titan are consistent with results for Pluto where the Jeans parameter at the exobase is ~ 10. In these results as well, escape occurred similar to Jeans theoretical rate. At the DPS 2009 meeting in Puerto Rico we presented results from a combined Fluid/DSMC approach to determine improved escape rates which produced consistent solutions for density and temperature in the transition region, \( \mathrm{Kn} \sim 0.01 \), between the DSMC results, and the results from numerically solving the equilibrium fluid equations. In the region of Pluto’s atmosphere where the \( \mathrm{Kn} \ll 0.01 \), we numerically solve Eq. (3b) and use that in Eq. (3a) to obtain the density and temperature from \( r_e \) to \( r_{top} < r_{exo} \). The temperature and density at the lower boundary were fixed and the heat flux through the boundary was determined iteratively as discussed below. We do not assume, as in SHE, that \( T \to 0 \) as \( r \to \infty \). The results (density and temperature) at \( r_{top} \) are then used as the lower boundary conditions for DSMC. DSMC is applied to a region from \( r_{top} \) to \( r_{esc} \) an altitude many scale heights above the exobase. This boundary must be increased until the effect of the simulation is negligible. At \( r_{esc} \) we calculate both the particle escape rate \( \varphi \) and the average energy carried off from Pluto’s atmosphere. This energy flux is then used to resolve the equilibrium fluid equations which in turn provide new conditions at \( r_{top} \). This procedure is iterated until we obtain a convergent density, temperature and energy flux in the region where the fluid equation solution and the DSMC results are coupled. Our approach differs from the SHE model in that escape is determined on a particle by particle basis from the top of the atmosphere. The upper boundary is constrained by the energy flux across the lower boundary, which is in turn...
determined by the amount of energy that can be carried away to space by escaping molecules.

![Graph](image)

**Figure (3):** Comparison of the Fluid/DSMC iterative result solid lines/filled circles to the SHE model result for the case with no heating in Strobel (2008a) dashed lines. Temperature bottom axis and density top axis: the curves nearest the downward oriented axis represent temperature, and the curves nearest the upward pointed arrow represent density. Exobase is at radial distance ~3200 km.

In figure (3), it is seen the T(r) in the Fluid/DSMC model decreases much slower with altitude than in the SHE model result. Correspondingly, the Fluid/DSMC result is denser at higher altitudes. Thermally induced escape is occurring but differs from the SHE model result by an order of magnitude, 4x10^{25} s^{-1}. This rate is 1.3 times the Jeans rate (3.1x10^{25} s^{-1}) for the appropriate exobase altitude 3200km in the Fluid/DSMC solution. These results have shown that the density and temperature structure given by the SHE model is not consistent with the escape flux.

### 7. Summary/Future Work

Recent measurements by Cassini of density data in Titan’s upper atmosphere (Waite et. al. 2005) have led to several continuum models (eg. see Johnson 2009). In particular the SHE model in (Strobel 2008b) for a baseline case in which all the heat was assumed to occur below the lower boundary found the mass loss rate of N₂ from Titan to be several orders of magnitude larger than the Jeans rate even though Titan has a Jeans parameter of 55. The preferred results for the SHE model include solar heating is larger. These simulations were obtained using a pure N2 atmosphere, but the mass loss rate was attributed to CH₄ and H₂ (Strobel 2008b).

We have used DSMC simulations which includes thermal conduction explicitly to test the ‘baseline results from the SHE model. The DSMC results have shown that in the absence of any external energy input into the atmosphere that the escape of N₂ from Titan’s atmosphere would occur similar to Jeans escape. In addition, the temperature in Titan’s atmosphere was artificial increased 600K (Tucker and Johnson 2009) which lowered the Jeans parameter to 11, and forced escape. Although, thermal escape did occur it was essentially at the Jeans rate. These results suggest that the SHE model escape rates for Pluto’s atmosphere which has a Jeans parameter of ~11 could also be incorrect. Therefore, we have used a combined fluid/DSMC iterative procedure to obtain consistent escape rates, density profiles and temperature profiles between the DSMC model and the solutions to the equilibrium fluid equations without the assumption that n, T→0 as r→∞. In principle the DSMC can be used to simulate the entire simulation region but as Kn becomes << 0.1 the calculation becomes computationally expensive. We numerically solved the equilibrium equations in the region of the atmosphere where Kn<<0.1, and used the DSMC model in the tenuous region Kn>0.1 (section 6).

Significant thermally-driven escape from Pluto’s atmosphere does not occur for Q = 0 because the upward thermal heat flux produced using the parameters in Strobel (2008a) cannot support a flux that is significantly enhanced over the Jeans type flux. Our DSMC simulations obtain a baseline escape rate from Pluto’s atmosphere ~ 4.14e25 s⁻¹ which is ~1.3 times the Jeans rate. This result should be considered the true baseline result to which adding solar heating above 1450km will increase.
the stringent enough criterion. Therefore, using the available density data to constrain the estimated escape fluxes in the SHE model is not a stringent enough criterion. Currently we are configuring the DSMC model and the fluid/DSMC approach to include heating so we can obtain accurate estimates.

Understanding the $Q(r) = 0$ case for thermally induced escape is an important starting point, but to accurately estimate the escape rate it is necessary to include solar heating. Figure (3) shows a result from a DSMC simulation normalized the solutions from the SHE model in (Strobel 2008a) for solar medium conditions. In this case the SHE model escape rate is $2.5 \times 10^{27} \text{s}^{-1}$. However, the DSMC model results in a smaller temperature gradient and an escape rate, $8.0 \times 10^{26} \text{s}^{-1}$, 1.1 times the Jeans rate. These preliminary results again indicate that the $T(r)$ result from the SHE model may not be able to maintain the high escape rates. A common conclusion from our results is that for very different temperatures profiles it is possible to obtain similar density profiles, see figures (1) and (3). Therefore, using the available density data to constrain the estimated escape fluxes in the SHE model is not a stringent enough criterion. Currently we are configuring the DSMC model and the fluid/DSMC approach to include heating so we can obtain accurate estimates.

Furthermore, the bulk of this study thus far has focused on a single species atmosphere. It is important to note that for Titan one of the preferred results for the SHE model attributes an escaping mass flux to CH$_4$ $2.5 \times 10^{27} \text{s}^{-1}$ and H$_2$ $9 \times 10^{27} \text{s}^{-1}$ and none to N$_2$ (Strobel 2009). As shown in Figure 5, trial DSMC simulations using a two component atmosphere N$_2$ and CH$_4$ does not result in any significant CH$_4$ flux that was enhanced in comparison to the Jeans flux (Tucker and Johnson 2009). Throughout the simulation region both atmospheric species were in thermal equilibrium and the resulting density profiles compare well with the Cassini density data. Other DSMC simulations have been done that include H$_2$ which produce similar escape rates compared to the SHE model, but it appears H$_2$ may not be in thermal equilibrium with the other atmospheric components as assumed in the continuum models (Cui et. al. 2009; Strobel 2009). More tests are currently underway for larger simulation regions in Titan’s atmosphere. These results will be compared to Cassini data as well.

In all the simulations discussed above we used an energy independent cross-section, and assumed isotropic scattering. The accuracy of the DSMC results
is dependent on the proper choice of cross-section. For most results $n(r)$ and $T(r)$ do not change much when small changes are made to the cross-section, or when scattering is chosen to favor forward directed angles after a collision (Tucker and Johnson 2009). However, the average escape rate is very sensitive the previously mentioned properties as well as the upper boundary location. Additionally, DSMC molecules are inherently translational, so approximations are required to properly account for the internal energy of diatomic molecules. The next steps include addressing these topics to learn the most appropriate set of parameters and approximations to use with DSMC to determine the most accurate escape rates.

**Acknowledgements**

This work is supported by the NSF and the VSGC. Special thanks to Darrell F. Strobel for discussions and providing solar heating data. Thanks to Justin Erwin and Alexey Volkov for contributions to the paper.
References

Molecular Gas Dynamics and the Direct Simulation of


Cui, J., Yelle, R.V., Volk, K., 2008. Distribution and
escape of molecular hydrogen in Titan’s thermosphere


Johnson, R. E., 1990. Energetic Charged-Particle
Interactions with Atmospheres and Surfaces. Springer-
Verlag, Berlin.


Johnson, R.E., M.R. Combi, J.L. Fox, W-H. Ip, F.
Leblanc, M.A. McGrath, V.I. Shematovich, D.F.
Strobel, J.H. Waite Jr, "Exospheres and Atmospheric
Escape", Chapter in Comparative Aeronomy, Ed. A.

Johnson, R.E., Combi, M. R., Fox, J. L., Ip, W-H.,
Leblanc, F., McGrath, M. A., Kasting, J.F., Pollack,

atmospheric escape: Monte Carlo simulations for
Titan’s atmosphere. PSS 57, 1889-1894.

Trafton, L., 1980. Does Pluto Have a Substantial

Waite Jr., J.H., et. al., 2005. Ion neutral mass
spectrometer results from the first flyby of Titan.
Science 308, 982-986.

The dynamics of a rapidly escaping atmosphere:
Applications to the evolution of Earth and Venus.
Icarus 48, 150–166.

Yelle, R.V., Borggren, Cui, J., Muller-Wodarg, I.C.F.,