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The Effect of Dynamics on the Composition of Titan's Upper Atmosphere

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Abstract

Using a global time-dependent general circulation model, we calculate the distribution of constituents in Titan's thermosphere resulting from transport caused by winds and molecular and eddy diffusion. Our simulations reveal that thermospheric winds effectively mix constituents in Titan's upper atmosphere. Consequently, the large eddy coefficients inferred from Voyager UVS observations may be a result of vigorous thermospheric circulation on Titan. Thermospheric winds also cause large diurnal variations in composition, with equatorial CH₄ mole fractions near 1400 *km* ranging from ~ 15 % in the late afternoon to ~ 58 % in the early morning at equinox. The predicted variations should be observed with Cassini's INMS instrument.

1. Introduction

The distribution of gases in an atmosphere is controlled by chemistry and transport through winds, molecular and eddy diffusion. Given a vertical profile of constituent densities and atmospheric temperature, it is possible to calculate the eddy diffusion coefficient and thus quantify the degree of mixing of atmospheric gases. Analysis of the CH_4 densities measured in Titan's thermosphere by the Voyager Ultraviolet Spectrometer (UVS) solar occultation experiment [Smith, 1982; Strobel *et al.*, 1992; Vervack *et al.*, 2001] imply an eddy diffusion coefficient nearly two orders of magnitude larger than inferred for other planetary thermospheres. Strobel *et al.* [1992] determined an eddy coefficient of $(0.4 - 2.6) \times 10^9 \text{cm}^2 \text{s}^{-1}$ between ~ 985 and 1125 km altitude, near the ionospheric peak, where the pressure is $\sim 5 \times 10^{-5} \mu\text{bar}$. For comparison, the eddy diffusion coefficients at comparable levels inferred from 1-D models of the thermospheres of Earth, Venus, and Mars are 2×10^5 , 3×10^7 and $4 \times 10^7 \text{cm}^2 \text{s}^{-1}$ respectively [Allen *et al.*, 1981; Massie *et al.*, 1983; Krasnopolsky, 1993].

Müller-Wodarg *et al.* [2000], using a Thermospheric General Circulation Model (TGCM), have calculated horizontal and vertical winds speeds in Titan's upper atmosphere, driven by solar energy deposition, to be large, reaching values of $u \sim 60 \text{ ms}^{-1}$ and $w \sim 1 \text{ ms}^{-1}$, respectively. Scale analysis suggests that the eddy coefficient, K , is related to the scale height H and vertical velocity through $K \sim wH \sim 10^9 \text{cm}^2 \text{s}^{-1}$, assuming $H \sim 100 \text{ km}$. Thus, the large vertical wind may, at least in part, be responsible for the rapid vertical mixing in Titan's upper atmosphere. In the following, we test this hypothesis by replacing the non-interactive, globally averaged neutral composition assumed in the TGCM simulations of Müller-Wodarg *et al.* [2000] with self-consistent calculations of global gas transport by winds and diffusion.

2. Theory

The basic equations solved by our TGCM have been presented by Müller-Wodarg *et al.* [2000]. The model solves self-consistently the equations of momentum, energy and continuity by explicit time integration, considering altitudes between 600 and $\sim 1400 \text{ km}$ ($0.15 - 1 \times 10^{-6} \mu\text{bar}$). To include composition we consider molecular and eddy diffusion, but only in the vertical direction, since vertical gradients are much larger than horizontal gradients. The molec-

ular diffusion velocities are given by

$$\frac{\partial Y_i}{\partial z} - \left(1 - \frac{m_i}{m} - \frac{H}{m} \frac{\partial m}{\partial z}\right) \frac{Y_i}{H} = - \sum_{j \neq i} \frac{m Y_i Y_j}{m_j D_{ij}} (w_i^D - w_j^D) \quad (1)$$

where $Y_i = \rho_i/\rho$ and m_i are the mass fraction and molecular mass of the i th constituent, m is the mean molecular mass of the atmosphere, H is the pressure scale height, D_{ij} is the binary diffusion coefficient, and w_i^D is the vertical diffusion velocity of the i th constituent [Chapman and Cowling, 1970]. Molecular constituents are also subject to eddy diffusion, which we calculate with

$$w_i^K = -K \frac{\partial \ln(Y_i)}{\partial z} \quad (2)$$

where K is the eddy diffusion coefficient. Here, K represents mixing due to small-scale motions not resolved by the TGCM. The diffusion velocities are then used in the continuity equation to calculate the time development of mass fractions. The continuity equation for the i th constituent is given by

$$\frac{\partial Y_i}{\partial t} + u \frac{\partial Y_i}{\partial x} + v \frac{\partial Y_i}{\partial y} + \omega \frac{\partial Y_i}{\partial p} = g \frac{\partial}{\partial p} \left(\rho Y_i (w_i^D + w_i^K) \right) + J_i \quad (3)$$

where u and v are zonal and meridional velocities, $\omega = dp/dt$ is the vertical velocity of the atmosphere relative to a pressure level, ρ is the mass density, g gravity, and J_i is the net chemical source rate [Dickinson and Ridley, 1975]. The velocities u , v , and ω represent the mean velocity of the atmosphere, defined as the average of the velocities of individual constituents, weighted by their mass densities.

Our TGCM calculations include the three thermally active species in Titan's thermosphere, N_2 , CH_4 and HCN . Our intention is to study dynamical mixing, so we keep the chemistry as simple as possible. N_2 and CH_4 are treated as inert because the time constant for loss through photolysis is much longer than the diffusion time constant. The density profiles for these constituents are determined by advective and diffusive processes in the thermosphere, assuming zero vertical fluxes at the top boundary. The HCN density is modelled by specifying an empirical daytime production rate in the thermosphere and requiring $w_{\text{HCN}}^K = -K/H$ at the lower boundary. We assume a Gaussian distribution of the HCN production, which is centered around 850 km altitude, using a height-integrated production rate of $1 \times 10^9 \text{cm}^{-2} \text{s}^{-1}$, consistent with studies by Fox and Yelle [1997]. For CH_4 we assume a constant number mixing ratio of 1.7 % at the bottom boundary.

Molecular diffusion coefficients, in cgs units, are calculated with the formula $D = A(p_o/p)(T/T_o)^s$ where $p_o = 0.147 \mu\text{bar}$, $T_o = 135^\circ \text{K}$, and A (s) for pairs $\text{CH}_4 - \text{HCN}$, $\text{N}_2 - \text{HCN}$ and $\text{N}_2 - \text{CH}_4$ are given by 3.64×10^5 (1.749), 2.12×10^5 (2.012), and 3.64×10^5 (1.749), respectively. We adopt an eddy coefficient for small scale motions of $K = 5 \times 10^7 \text{cm}^2 \text{s}^{-1}$, assumed constant with altitude. Our calculations use spatial resolutions of 6° latitude by 10° longitude by 0.25 scale heights vertically and integrate with a 20 sec time step. Steady state is reached after 12 Titan days, with the continuity equation being satisfied to within 0.1 %. We present TGCM simulations for equinox at solar maximum, corresponding roughly to conditions during the Voyager 1 encounter with Titan in 1980.

3. Results and Discussion

3.1. Mixing by global circulation

The solid curves in Fig. 1 are altitude profiles of latitudinally averaged CH_4 and HCN mass fractions for dusk conditions calculated by the TGCM. The CH_4 values are roughly constant with height between 600 and 750 km altitude at around 1.7 %, increasing to 15 % near 1400 km . The profile of HCN increases from 7×10^{-6} at 600 km to 1.7×10^{-3} at 1060 km and falls to $\sim 1.6 \times 10^{-3}$ near 1400 km . The thermospheric peak in HCN mole fraction near 1060 km altitude is a result of the dayside HCN production through photolysis of N_2 and CH_4 .

Analyzing the TGCM output with a 1-D diffusion model in a manner equivalent to that used to analyze Voyager UVS data, we can derive an eddy diffusion coefficient from the TGCM output that represents total mixing caused by large scale dynamics resolved by the model. The result, shown in Fig. 1 (dashed curves) confirms the hypothesis that the large eddy diffusion coefficient on Titan is consistent with vigorous thermospheric mixing by large scale winds. The dashed curves are eddy coefficients derived from the TGCM CH_4 profile in the dusk sector (K_1) and its global average (K_2). To validate our calculation techniques, we carried out an additional TGCM simulation in which we artificially set to zero the advection terms of the continuity equation (3). The eddy coefficient from the global average CH_4 profile of this simulation is curve K_3 . Therefore, differences between K_3 and K_1 or K_2 are due entirely to transport of constituents by thermospheric winds.

K_1 (K_2) rises from around $5 \times 10^7 \text{cm}^2 \text{s}^{-1}$ below

850 km altitude to $1 \times 10^9 \text{cm}^2 \text{s}^{-1}$ ($8 \times 10^8 \text{cm}^2 \text{s}^{-1}$) near 1100 km altitude, while K_3 is constant up to 1200 km altitude at around $5 \times 10^7 \text{cm}^2 \text{s}^{-1}$, the value of the implemented eddy coefficient. The behavior of K_3 illustrates that our technique extracts the correct eddy coefficient up to around 1200 km altitude, but becomes increasingly unreliable above that, due to the technique's numerical inaccuracies at those heights. K_1 and K_2 are consistent with the range of values derived for dusk conditions from Voyager UVS observations by *Strobel et al.* [1992]. They suggested the high K values to be caused by vertical mixing due to saturating internal gravity waves. Our simulations show that global-scale solar-driven thermospheric circulation is sufficient to produce the large K values.

Differences between K_1 and K_2 are due to the differences in the globally averaged and the dusk sector vertical composition profiles (shown in Fig. 2 for the equator). This illustrates the potential variability of K profiles extracted at different local times. The general shape of K_1 and K_2 in Fig. 1 is closely related to the vertical behavior of thermospheric solar driven winds which become largest above $\sim 1100 \text{km}$ altitude and approach zero below 900 km . Below 900 km , therefore, mixing by winds is negligible in our simulations, resulting in K_1 and K_2 approaching the implemented eddy coefficient. However, as discussed by *Müller-Wodarg et al.* [2000], Titan's lower thermosphere may contain strong winds forced from lower altitudes. We have not included these winds in our simulations, but if they exist they probably cause rapid mixing also at those lower heights. We do not currently expect our calculations of dynamics below 900 km to represent real conditions on Titan. It is therefore not clear whether the K value at those heights is due to small scale turbulence or larger scale winds.

Titan's large scale mixing is caused by a diurnal solar heating generating horizontal day to night winds. Continuity requires the diverging (converging) horizontal dayside (nightside) winds to be accompanied by upwelling(downwelling). A global scale eddy is generated which continuously mixes the atmosphere by transporting gases up on the dayside, horizontally towards the nightside and then down, where a horizontal return flow ensures conservation of mass. With average horizontal and vertical wind speeds of $u \sim 30 \text{ms}^{-1}$ and $w \sim 0.5 \text{ms}^{-1}$, respectively, gas particles can be transported during a quarter Titan day by around 10,000 km horizontally and 170 km vertically. This corresponds to 145° latitude and 2 scale

heights near 1400 *km* altitude. So, winds on Titan are strong enough to transport gases over significant distances within a day. This is partly a consequence of Titan's small size and slow rotation rate. Recent calculations with a 2-dimensional model by *Lebonnois et al.* [2001] have shown stratospheric winds on Titan also to play an important role in mixing constituents below 300 *km*.

The homopause is defined as the altitude where values of the molecular and eddy coefficients are equal. Following this definition, the homopause altitude in our TGCM simulation range from around 900 to 1000 *km* (see Fig. 1).

Simulations by *Bougher et al.*[1999] have shown thermospheric circulation on Mars and Venus to cause significant mixing in their thermospheres. Similar results have also been found by *Rishbeth and Müller-Wodarg* [1999] and *Fuller-Rowell* [1998] for the Earth's thermosphere. The importance of large scale circulation upon mixing thus appears to be common in the solar system.

3.2. Horizontal composition structure

The combination of circulation and diffusion causes considerable diurnal variations in the CH₄ mole fractions, shown in Fig. 2. The plot displays height profiles of equatorial CH₄ mole fractions for 16 : 40 *h* local solar time (LST) (curve A) and 04 : 00 *h* LST (C) as well as the diurnal averages (B). These local times correspond to the locations of minimum and maximum values for the CH₄ mole fraction near 1400 *km*. In addition, the diurnal average is shown from the simulation in which we set to zero the advection terms (curve D). The figure illustrates that thermospheric winds drive considerable diurnal changes in CH₄ mole fraction, with values near 1400 *km* ranging from ~ 15 % in the afternoon sector to ~ 58 % in the early morning sector. The smaller daytime CH₄ mole fraction values are a result of the upwelling which transports gases from lower heights, where the CH₄ mole fractions are smaller, to higher altitudes. The larger nighttime values are caused by the reverse process through downwelling. Wind-driven diurnal changes are substantial above 1000 *km* and become smaller lower down, due to the absence of sufficiently large winds and the importance of turbulent diffusion.

Using our derived value of $K_1 \sim 1 \times 10^9 \text{cm}^2 \text{s}^{-1}$ near 1100 *km* altitude (Fig. 1) and the expression $\tau_K = H^2/K$, we calculate the diffusion time scale to be $\tau_K \sim 28 \text{h}$, corresponding to 1.8 *h* LST on Titan, which is roughly consistent with the time shifts of

CH₄ mole fraction extrema with respect to the sub-solar and anti-solar points. A similar value is found for vertical wind transport time scales, so the two are equivalent. Thus, on Titan the transport time scale is ~ 5 – 10 % of a local day (15.8 Earth days). This shift in local time distribution of minor species can be used to infer wind speeds from compositional measurements.

Comparison between curves B and D shows that the diurnally averaged CH₄ mixing ratios are larger by a fraction of up to ~ 15 % when ignoring dynamics. This shows that the winds generate *net* mixing of the thermosphere, which results in higher net relative abundances of the heavier constituents. This is due to diffusive time scales being sufficiently small compared to dynamical time scales.

Given that CH₄, HCN and N₂ are thermally active constituents, we expect their horizontal distribution to affect the day-night temperature behavior, which in turn affects the winds. This two-way interplay of dynamics and composition on Titan indeed appears in our simulations and will be subject of a future more comprehensive study.

The local time variations in CH₄ mole fraction in Fig. 2 are opposite to those found by *Vervack et al.* [2001] from their reanalysis of Voyager UVS data, which suggested CH₄ densities near 18 *h* LST to be larger than those at 06 *h* LST. They pointed out the difficulty in understanding this behavior on the basis of solar input, proposing alternative processes, such as magnetospheric precipitation. Our simulations show that global dynamics can cause large horizontal variations in composition and therefore, if the variations detected by *Vervack et al.* [2001] are real, they may indicate a circulation pattern that differs from the solar driven case described here.

4. Conclusions

Our calculations have revealed that thermospheric winds effectively mix constituents in Titan's upper atmosphere. This suggests that the large eddy coefficient inferred from Voyager UVS observations may be caused by vigorous mixing through large scale winds rather than small-scale turbulence. The winds also cause considerable local time changes in composition. We find that Titan has a diffusive transport time scale unusual in our solar system, which causes distinct features in the horizontal distribution of constituents. The Ion-Neutral Mass Spectrometer (INMS) instrument on board the Cassini spacecraft should be able

to observe these, and our model can be used to understand better these anticipated measurements.

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Figure 1. Vertical profiles of latitudinally averaged CH_4 and HCN mass fractions (solid curves), effective eddy diffusion coefficient (dashed) and, for comparison, molecular diffusion coefficients used in the TGCM (dotted). Solid and dashed lines are TGCM calculations for dusk conditions.

Figure 2. Vertical profiles of CH_4 mole fractions at latitude 0, as calculated by the Titan GCM. The curves are for 16 *h* (A) and 04 *h* (C) Local Solar Time (LST) and diurnal averages (B). Curve D shows diurnally averaged mole fractions for a simulation ignoring transport by winds.

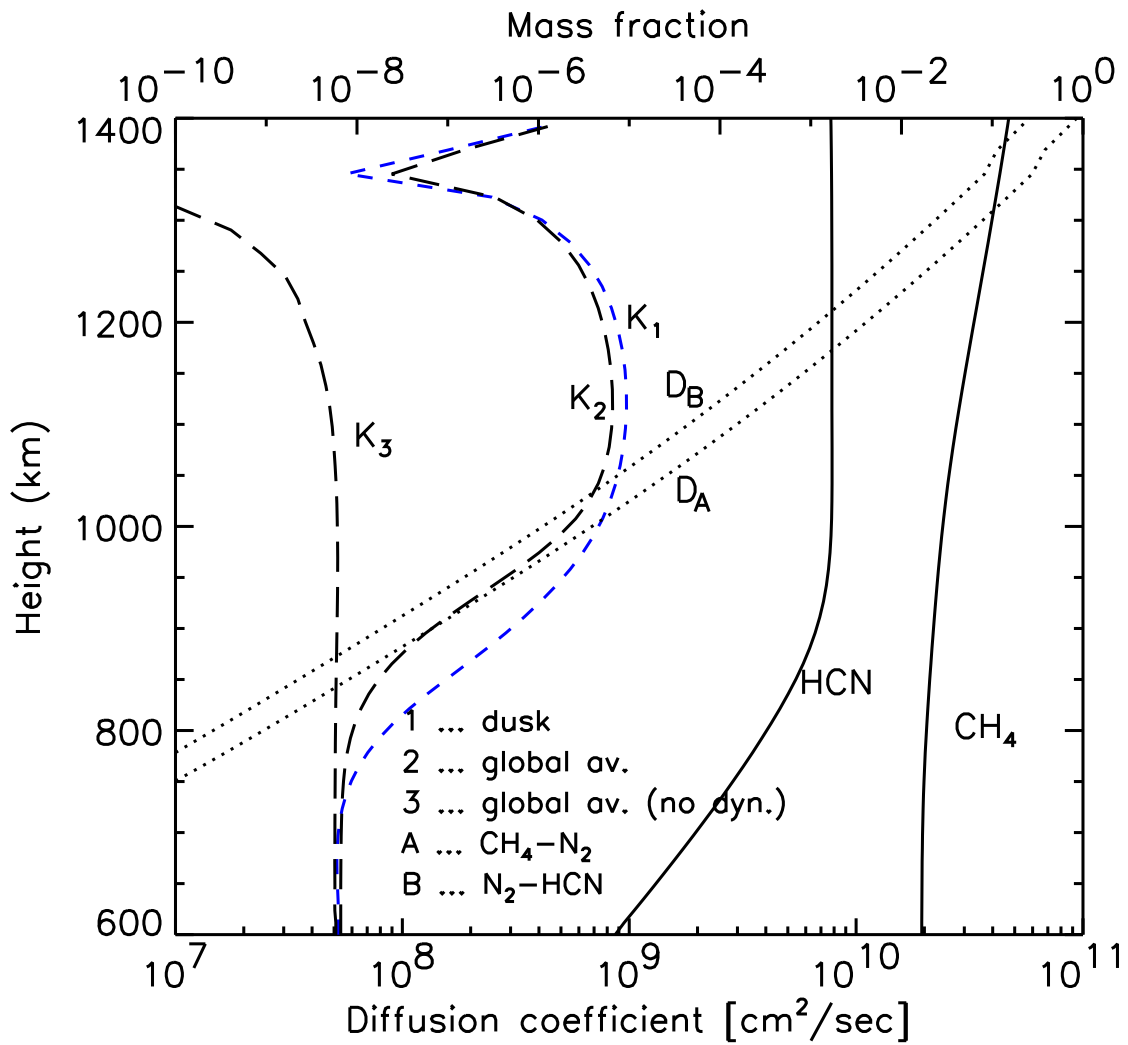


Fig. 1

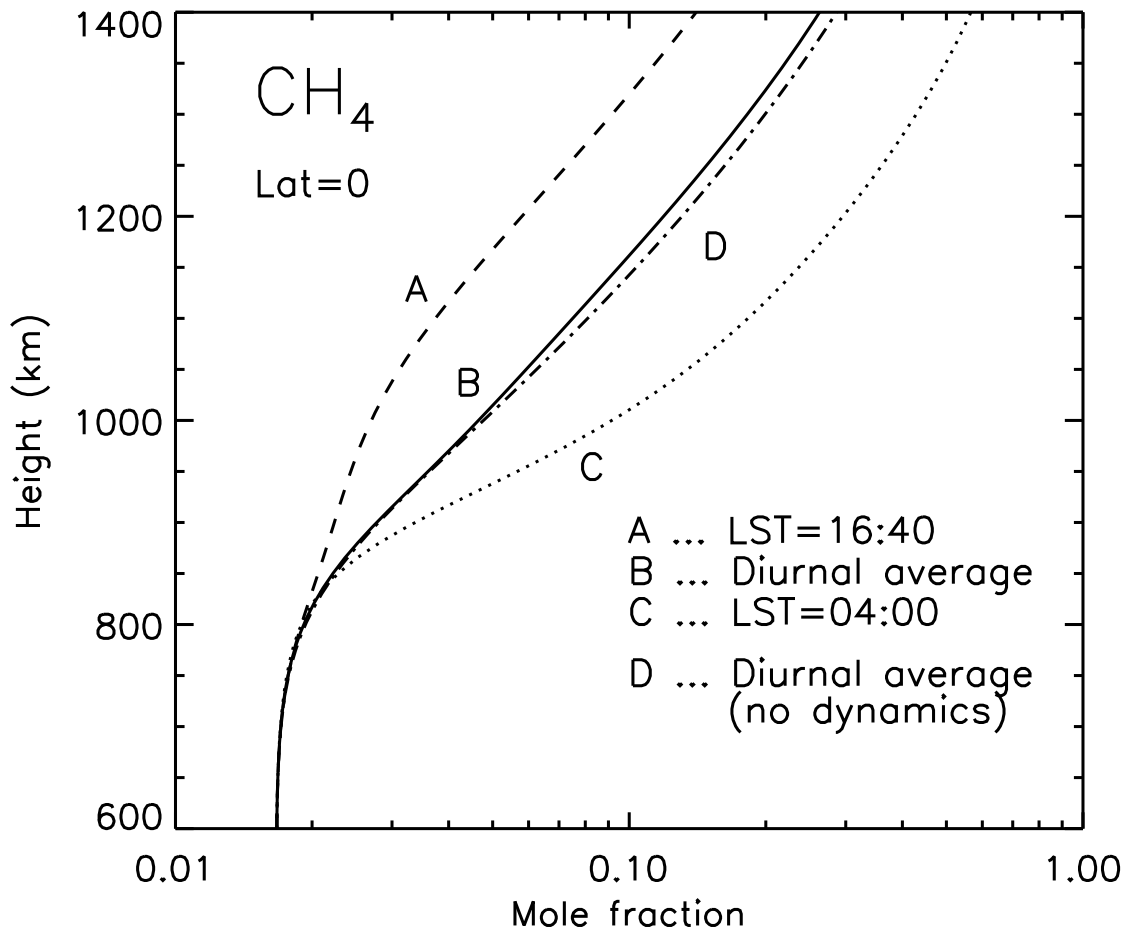


Fig. 2