The effect of dynamics on the composition of Titan's upper atmosphere

I. C. F. Müller-Wodarg[1,2] and R. V. Yelle [3]

[1] 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 CH_4 mole fractions near 1400 km ranging from $\sim$15% in the late afternoon to $\sim$58% in the early morning at equinox.   *INDEX TERMS:* 3367 Meteorology and Atmospheric Dynamics: Theoretical modeling; 5405 Planetology: Solid Surface Planets: Atmospheres—composition and chemistry; 6280 Planetology: Solar System Objects: Saturnian satellites. **Citation:** Müller-Wodarg, I. C. F., and R. V. Yelle, The effect of dynamics on the composition of Titan's upper atmosphere, *Geophys. Res. Lett.*, *29*(23), 2139, doi:10.1029/2002GL016100, 2002.

1. Introduction

[2] 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 $(0.4-2.6) \times 10^9 \, cm^2 \, s^{-1}$ between $\sim$985 and 1125 km altitude, near the ionospheric peak, where the pressure is $\sim$5 $\times$ 10^{-5} µbar. 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 $4 \times 10^7 \, cm^2 \, s^{-1}$ respectively [*Allen et al.*, 1981; *Massie et al.*, 1983; *Krasnopolsky*, 1993].

[3] *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 $u \sim 60 \, ms^{-1}$ and $w \sim 1 \, ms^{-1}$, respectively. Scale analysis suggests that the eddy coefficient, K, is related to the scale height H and vertical velocity through $K \sim wH \sim 10^9 \, cm^2 \, s^{-1}$, assuming $H \sim 100 \, km$. 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

[4] 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 km ($0.15-1 \times 10^{-6}$ µbar). 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 molecular diffusion velocities are given by

$$\frac{\partial Y_i}{\partial z} - \left(1 - \frac{m_i}{m} - \frac{H}{m}\frac{\partial m}{\partial z}\right)\frac{Y_i}{H} = -\sum_{j/i} \frac{mY_iY_j}{m_jD_{ij}}\left(w_i^D - w_j^D\right) \quad (1)$$

where $Y_i = \rho_i/\rho$ and m_i are the mass fraction and molecular mass of the ith 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 ith 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 represets 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 ith constituent is given by

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

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.

[1]Atmospheric Physics Laboratory, University College London, London, UK.
[2]Also at Center for Space Physics, Boston University, Boston, Massachusetts.
[3]Lunar and Planetary Laboratory, University of Arizona, Tucson, USA.

[5] 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 $w_{HCN}^K = -K/H$ 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 $1 \times 10^9 cm^{-2} s^{-1}$, 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.

[6] Molecular diffusion coefficients, in cgs units, are calculated with the formula $D = A(p_6/p)(T/T_6)^s$ where $p_6 = 0.147$ μbar, $T_6 = 135°$ K, and A (s) for pairs CH_4-HCN, N_2-HCN and N_2-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 $K = 5 \times 10^7$ $cm^2 s^{-1}$, assumed constant with altitude. Numerical experiments showed that using a constant, as opposed to height-dependent value of K had a negligible effect on constituent abundances. 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. 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

[7] The solid curves in Figure 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.

[8] 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 Figure 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
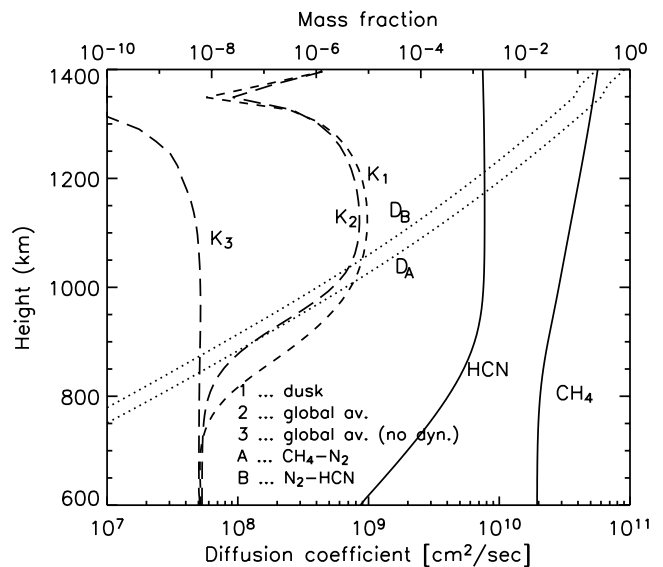

Figure 1. Vertical profiles of latitudinally averaged CH_4 and HCN mass fractions (solid curves), effective eddy diffusion coefficient (dashed) and, for comparison, molecular diffusion coefficients used in the TGCM (dotted). Solid and dashed lines are TGCM calculations for dusk conditions. The altitude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

are due entirely to transport of constituents by thermospheric winds.

[9] K_1 (K_2) rises from around 5×10^7 $cm^2 s^{-1}$ below 850 km altitude to $1 \times 10^9 cm^2 s^{-1}$ (8×10^8 $cm^2 s^{-1}$) near 1100 km altitude, while K_3 is constant up to 1200 km altitude at around 5×10^7 $cm^2 s^{-1}$, the value of the implemented "small scale" 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. For the same reason, the K_1 and K_2 curves above 1200 km are unreliable. K_1 and K_2 below 1200 km 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 in-situ thermospheric circulation is sufficient to produce the large K values.

[10] 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 Figure 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 Figure 1 is closely related to the vertical behavior of thermospheric solar driven winds which become largest above ~ 1100 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
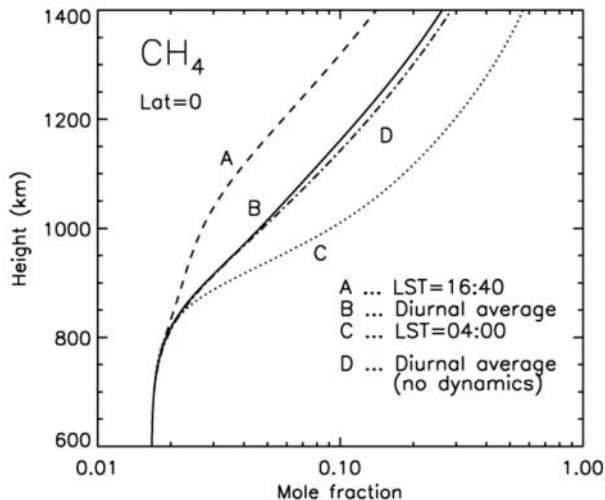
Figure 2. Vertical profiles of CH_4 mole fractions at latitude 0, as calculated by the Titan GCM. The curves are for 16 h (A) and 04 h (C) Local Solar Time (LST) and diurnal averages (B). Curve D shows diurnally averaged mole fractions for a simulation ignoring transport by winds. The altitude mapping of each parameter is done rigorously.

also at those lower heights. We do not currently expect our calculations of dynamics below 900 km to represent real conditions on Titan.

[11] A global scale diurnal eddy is generated by the solar heating and 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 $u \sim 30\ ms^{-1}$ and $\omega \sim 0.5\ ms^{-1}$, 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 2-dimensional calculations by *Lebonnois et al.* [2001] have shown stratospheric winds on Titan also to play an important role in mixing constituents below 300 km. Simulations by *Bougher et al.* [1999] showed thermospheric circulation on Mars and Venus to cause significant mixing in their thermospheres. The importance of large scale winds upon mixing thus appears to be common in the solar system.

[12] 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 Figure 1).

3.2. Horizontal Composition Structure

[13] The combination of circulation and diffusion causes considerable diurnal variations in the CH_4 mole fractions, shown in Figure 2. The plot displays height profiles of equatorial CH_4 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 CH_4 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 CH_4 mole fraction, with values near 1400 km ranging from $\sim$15% in the afternoon sector to $\sim$58% in the early morning sector. The smaller daytime CH_4 mole fraction values are a result of the upwelling which transports gases from lower heights, where the CH_4 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.

[14] Using our derived value of $K_1 \sim 1 \times 10^9\ cm^2\,s^{-1}$ near 1100 km altitude (Figure 1) and the expression $\tau_K = H^2/K$, we calculate the diffusion time scale to be $\tau_K \sim 28\ h$, corresponding to 1.8 h LST on Titan, which is roughly consistent with the time shifts of CH_4 mole fraction extrema with respect to the sub-solar and anti-solar points. Thus, on Titan the transport time scale is $\sim$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.

[15] Comparison between curves B and D shows that the diurnally averaged CH_4 mixing ratios are larger by a fraction of up to $\sim$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 comparable to dynamical time scales between $\sim$1000 and $\sim$1200 km height.

[16] The local time variations in CH_4 mole fraction in Figure 2 are opposite to those found by *Vervack et al.* [2001] from their reanalysis of Voyager UVS data, which suggested CH_4 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

[17] 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. 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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I. C. F. Müller-Wodarg, Atmospheric Physics Laboratory, Department of Physics and Astronomy, University College London, 67-73 Riding House Street, London W1P 7PP, UK. (i.mueller-wodarg@ucl.ac.uk)

R. V. Yelle, Lunar and Planetary Lab, University of Arizona, Tucson, AZ 85721, USA. (yelle@lpl.arizona.edu)