

NASA AMES MARS GCM WITH PHOTOCHEMISTRY: MODELING O₂ IR NIGHTGLOW EMISSION

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Introduction:

The coupling of the NASA Ames Mars GCM (MGCM) and a photochemical scheme provides 3D chemical fields that interact spatially and temporally with the evolving temperature and wind fields. The addition of photochemistry is critical for modeling an extended atmosphere (surface to middle atmosphere). Further, photochemical interactions can provide constraints for investigations of dynamical processes. Simulations will be presented of the O₂ (a1Δg) emission in the 1.27 μm band on the nightside (IR nightglow emission). The O₂ IR nightglow emission that occurs aloft over the winter pole is an observable feature that is produced by the transport of trace species from low to high latitudes. This nightglow signature can therefore provide insight into the strength of meridional transport processes and the nature of the mean meridional circulation.

Motivation:

The first ever data has been reported concerning the O₂ IR nightglow emission by Bertaux et al., 2012 and Fedorova et al., 2012. The O₂ IR nightglow emission is the result of a three-body recombination ($O+O+CO_2 \rightarrow O_2^*+CO_2$) that occurs predominantly mainly in the polar night. The atomic oxygen, needed for recombination, is a product of photolysis of CO₂ and O₃ and is transported (with other trace species) within the mean meridional circulation from the equator towards higher latitudes. The descending branch near the poles transports the species to a region optimal for recombination and subsequent de-excitation (i.e. nightglow emission) to occur.

The O₂ nightglow emission has only been recently observed due to its low intensity compared to Venus and Earth. It appears mostly over high (70° – 90°) northern and southern latitudes between 40 and 60 km in altitude. The first observation of the nightside emission was conducted by MEx/OMEGA observing at the limb. Three vertical profiles were detected (Bertaux et al. 2012). The observance of the O₂ IR nightglow emission has been confirmed by two other instruments orbiting Mars. One, the SPICAM IR instrument onboard the MEx spacecraft collected seven profiles that are in good agreement with the OMEGA profiles (Fedorova et al., 2012). Two, the CRISM instrument onboard the MRO obtained over 100 profiles ranging over most of Mars seasons, high latitudes, local times, and longitudes between 2009 and 2011 (Clancy et al., 2012; Clancy et al., 2013). One of the trends observed was the O₂

IR nightglow emission in the northern winter solstice (L_s=270°) has a more intense peak emission than southern winter solstice (L_s=90°). Another trend was that the lowest peak altitude occurred during northern winter solstice (L_s=270°).

The observed trends of the nightglow seem to follow the standard concept of the meridional circulation. However, there have been minimal numerical studies (due to the previous lack of observations) and the work that has been published does not completely capture the location and intensity of the observed nightglow. Moreover, the few numerical studies that have been done do not do detailed work to isolate and quantify the relative contribution of any forcings upon the nightglow. The only dedicated numerical study with the recent observations was by Gagne et al. (2012) and they utilized atmospheric composition from Laboratoire de Meteorologie Dynamique (LMD) Mars GCM (Forget et al., 2009) as input for a detailed 1D airglow model. The modeled integrated intensity was usually smaller than the observed intensity, which was most likely due to the lack of a full connection to dynamics. The observation papers (Bertaux et al., 2012; Fedorova et al., 2012; Clancy et al., 2012, 2013) compare their observations to simulated O₂ IR nightglow emission from the same 3D GCM, the LMD Mars GCM (Forget et al., 2009). In the three works, it was found the LMD GCM simulations had a greater seasonal and vertical variation than observed and usually over predicted the peak altitude and peak intensity. These comparisons were conducted with a “standard” simulated Mars atmosphere and brief sensitivity studies were focused on temperature, reaction rates, and kinetic parameters.

Modeling:

The NASA Ames Mars Global Climate Model (GCM) will be utilized for this work. It solves the primitive equations and utilizes a finite difference dynamical core (based on an Arakawa “C”-grid). The horizontal resolution is 5° in latitude by 6° in longitude. The standard vertical sigma-coordinate is 24 layers and goes from the surface to ~80 km. The MGCM has been coupled with a photochemical scheme, which is described in detail by Lefèvre et al., 2004. Briefly, the chemical package accounts for and transports 11 species (O, O(¹D), O₂, O₃, H, OH, HO₂, H₂O₂, H₂, H₂O, and CO). To save computational resources, the photolysis rates are calculated off-line using the Madronich et al. (1998) model adapted to Martian conditions. The rates are stored

into a four-dimensional lookup table as a function of the overhead CO₂ column, the overhead O₃ column, the solar zenith angle, and the temperature. The model interpolates the table values to calculate the photolysis rate for the actual sunlight grid point. The Gas-phase reaction rate coefficients were mostly adopted from Sander et al., 2003. The rate coefficients of three-body reactions are increased by a factor of 2.5, to account for the higher efficiency of CO₂ as a third body in comparison with N₂ and O₂. Chemical families were adopted for O_x and HO_x species (O_x = O + O₃; HO_x = H + OH + HO₂) in order to reduce computational time. The chemical long-lived species (O₂, H₂, H₂O, CO, HO_x, O_x) are solved for by using the implicit method described by Shimazaki et al., 1985. The short-lived species are assumed to be in photochemical equilibrium (O₃, O(¹D), OH, HO₂).

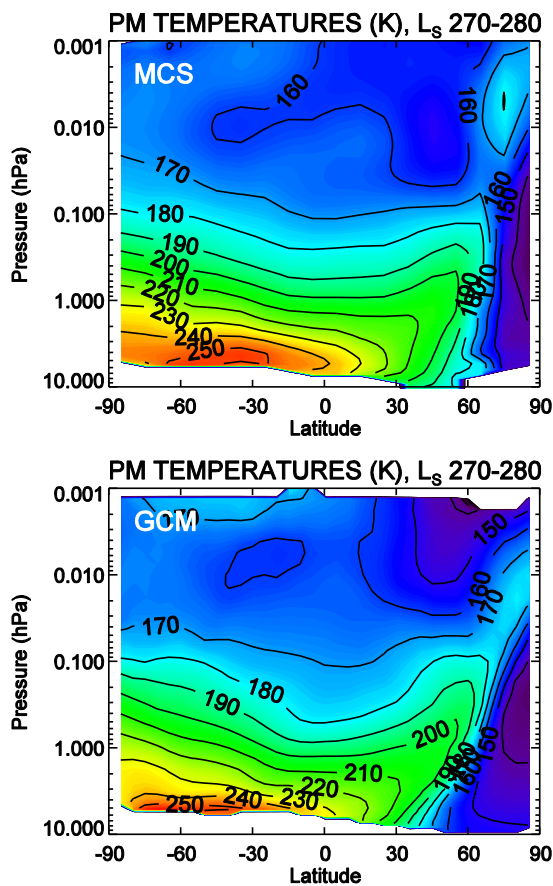


Figure 1: Zonally averaged temperatures for a local time range of 14 – 17 hours and seasonal averaged of Ls = 270–280. Top panel is MRO/MCS observations. Bottom panel is NASA Ames Mars GCM simulation.

The volume emission rate (VER) of the excited state O₂^{*} is simply described as the ratio of the production to the loss of the excited species, weighted by its lifetime. This ratio results in the number of photons emitted per unit time per unit volume from

radiative relaxation out of the O₂^{*} state into all lower states. For the VER of the excited O₂^{*} calculation implementation into the Mars GCM, we will initially use the photochemical equilibrium expression stated as follows: $\varepsilon(O_2^*) = \alpha k_1 [O][O][CO_2] / (1 + \tau(k_{CO_2}[CO_2]))$; where α is the total yield of O₂^{*}, k_1 is the rate coefficient for the three-body recombination reaction, [O] and [CO₂] are concentrations for the specific specie, τ is the lifetime by radiative relaxation of the specific excited state O₂^{*}, lastly k_{CO_2} is the quenching coefficient for CO₂. As initial values: $\alpha = 0.75$, $k_1 = 9.46 \times 10^{-34} \exp(485/T) \text{ cm}^6 \text{ molecule}^{-1} \text{ s}^{-1}$, $\tau = 4470 \text{ s}$, and $k_{CO_2} = 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The uncertainty in the effective yield and k_1 can produce differences in the oxygen profile, so sensitivity tests are needed.

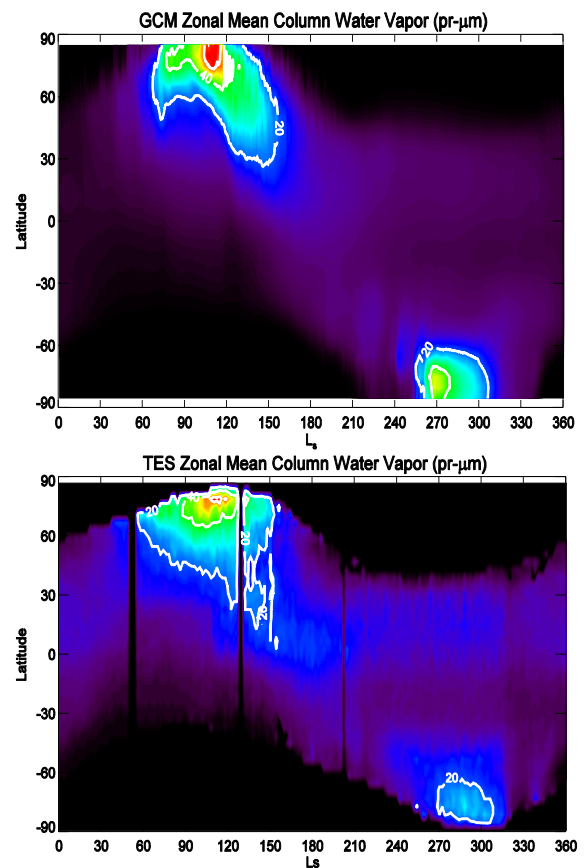


Fig. 2: Zonally averaged water vapor column abundance (pr-μm). Top panel is NASA Ames Mars GCM simulation. Bottom panel is TES observations.

Current Status:

The Lefèvre photochemistry scheme has been implemented into the Ames MGCM, but challenges remain. The current state of the MGCM captures the mean meridional circulation, temperatures (as compared to MCS observations, figure 1), and water cycle (as compared to TES observations, figure 2). Having a good water cycle is important due to the

anti-correlation between water and ozone; odd hydrogen catalytic cycles destroys ozone while water vapor is a source of HO_x. The resulting zonally averaged ozone column abundances are an order of magnitude less in the polar regions but are similar near the equator when compared to Lefèvre et al., 2004 results and observations. The simulated atomic oxygen has a similar trend as the ozone.

Expected Results:

We are actively addressing these issues and are optimistic that they will be resolved in the near future. At that point, we will focus on simulating the O₂ IR nightglow emission and comparing them to the observed trends. We plan to present the details needed to successfully implement the photochemistry scheme (or the important tests done in order to understand how to properly implement the scheme). Furthermore, the resulting ozone and more specifically the O₂ IR nightglow will be shown. We want to understand the sensitivity of the nightglow within the Ames MGCM. Lastly, including nightglow emission into the MGCM will also help in the future to deduce the relative importance of various forcing mechanisms of the meridional transport.

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