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Coupling Photochemistry to the NASA Mars Climate Modeling Center 3D Mars Global Circulation Model (gcm2.1v24)

A. Brecht (1, 2), M. Kahre (2), R. Haberle (2), J. Hollingsworth(2), and F. Lefèvre(3)

(1) Bay Area Environmental Research Institute, Petaluma, CA, USA, (2) NASA Ames Research Center, Moffett Field, CA, USA, (3) LATMOS, Guyancourt, France (Amanda.s.brecht@nasa.gov / Fax: 650-604-6779)

Abstract

In the work to be presented, a photochemical model has been coupled to the NASA Mars Climate Modeling Center (MCMC) 3D Mars global circulation model (Mars GCM) (gcm2.1v24). This photochemistry coupling provides 3D chemical fields which interact spatially and temporally with the evolving temperature and winds fields. The addition of photochemistry is recognized to be critical in the effort in extending the Mars GCM to middle atmospheric levels and further to provide more constraints in understanding the Martian global atmospheric circulation.

1. Introduction

The NASA MCMC 3D Mars GCM (gcm2.1v24) has been extended to incorporate the middle atmosphere (~80 km to ~120 km). The model extension is important because it provides an integrated framework with a deeper domain to examine seasonal mean fields and large-scale wave activity with insight into circulation patterns in the middle atmosphere.

Temperatures from the Mars GCM with the extension (i.e. incorporation of Non-Local Thermodynamic Equilibrium (NLTE) heating and cooling) have been compared to observations, specifically observations from the ESA MEx SPICAM instrument. The comparison between SPICAM and Mars GCM are not in great agreement [2]. Results from the comparison show the simulation is very warm at lower pressures (<1E-3) compared to SPICAM profiles (see Fig. 1). The main reason for the extra warming is the underestimated fixed atomic oxygen profile used for the CO_2 15-µm cooling parameterization. [4] performed a study and found the fixed reference atomic oxygen profile used within the cooling parameterization (which is currently utilized within the Mars GCM) are below the actual abundance levels. Furthermore, it has been suggested that the CO_2 15-µm cooling is sensitive to the abundance of atomic oxygen ([1],[6]). The sensitivity to the atomic oxygen profile has been reproduced with test cases utilizing the Mars GCM (not shown). Therefore, this leads into incorporating calculated/updated chemistry (photochemical scheme) in the Mars GCM.

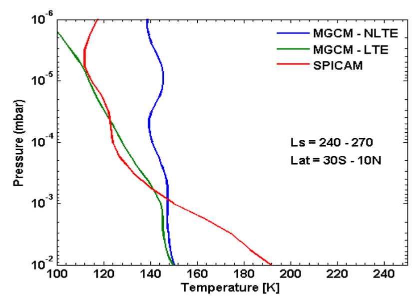

Figure 1: Comparison of zonally averaged temperature profiles from Mars GCM simulations (NLTE – blue solid line and LTE – green solid line) and SPICAM observations (red solid line).

2. Photochemistry within the Mars GCM

To properly simulate the middle atmosphere, specifically the temperatures, the Mars GCM needs updating chemistry for the CO_2 15-µm cooling scheme.

2.1 Photochemistry Scheme

The implemented photochemistry scheme within the Mars GCM is described in detail by [5]. The chemical package calculates oxygen, hydrogen, and CO. More specifically, the scheme accounts and transports 12 species (O, $O(^1D)$, O_2, O_3, H, OH, HO_2, H_2O_2, H_2, H_2O, CO, and CO_2). To save computational resources, the photolysis rates are calculated off-line using the [7] model adapted to Martian conditions. The rates are stored into a four-dimensional lookup table as a function of the overhead CO_2 column, the overhead O_3 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 [8]. The rate coefficients of three-body reactions are increased by a factor of 2.5, to account for the higher efficiency of CO_2 as a third body in comparison with N_2 and O_2. Chemical families were adopted for O_x and HO_x species ($O_x = O + O_3$; $HO_x = H + OH + HO_2$) in order to reduce computational time. The chemical long-lived species (O_2, H_2, H_2O, CO, HO_x, O_x) are solved for by using the implicit method described by [9]. The short-lived species are assumed to be in photochemical equilibrium (O_3, $O(^1D)$, OH, HO_2).

2.2 Discussion

The important species for the NLTE CO_2 15-µm cooling scheme, besides CO_2, is atomic O. However, at this time measurements of atomic O are not possible. Therefore, ozone will be used as an initial study and constraint for atomic O.

Ozone is produced in two steps. The first step is photolysis of CO_2 and O_2; secondly, the recombination of the product of O and O_2. It is destroyed by two mechanisms: (1) photolysis and (2) the reaction with HO_x radicals (OH, HO_2). Because ozone is destroyed by HO_2, ozone is expected and predicted to be strongly anti-correlated with water vapor (e.g. [5]). Ozone has also been observed to vary seasonally and diurnally (e.g. [3]). The seasonal peak concentration has been observed in the Northern and Southern polar winters. The simulated results from the Mars GCM will be compared to observations and other published GCM results (i.e. LMD GCM). The anti-correlation, seasonal variation, and diurnal variation will be presented.

6. Summary and Conclusions

A photochemical package has been coupled to the NASA MCMC Mars GCM. One of the reasons for this coupling is to provide a more realistic atmosphere for the CO_2 15-µm parameterization, which is key to modeling the middle atmosphere temperatures. The initial testing of the photochemical package is to compare the simulated ozone to observations and other published GCM results, which will be presented. Furthermore, the current status of the NASA MCMC Mars MGCM vertical grid extension will be presented.

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