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Memorie della

MAGRATHEA cross section database

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Abstract. The search for exoplanets is a new-born field of astrophysics, whose importance can be hardly overstated. Currently, more than 5000 planets (or candidates) have been discovered and even more are expected in the near future with the launch of new generation space facilities. In this framework, where new data are about to come and need to be analyzed, a theoretical approach via numerical computation becomes mandatory, in order to plan and develop observational protocols, identify peculiar cases, and have hints about some of the phenomena only partly understood. Our project aims to study the role of the chemical composition, pressure, and planetary/stellar parameters on the atmospheric thermal profiles of terrestrial exoplanets.

1. Introduction

Thanks to the high computational capability offered by a previous CINECA B class project - INA17_C3B15 - we had the chance to explore a vast range of physical and chemical parameters of Early Earth atmospheres. We managed to model the atmospheres of thousands exoplanets considering a dry atmosphere composed of different combination of CO_2 and N_2 (Petralia et al. 2020). In this project we extend our opacity tables to water vapor, in order to be able to describe present Earth-like atmospheres (Alei et al. in preparation). Moreover, due to the fast access to computational resources via the MoU CINECA-INAF, the parallel (MPI) FORTRAN 90 code to produce our opacity tables have been tested and optimized in a relatively short time.

To build our line by line absorption spectrum, we exploit the HITRAN2016 Molecular Spectroscopic Database (Gordon et al. 2017) in the interval 0.24-1000 μm ($10 - 42000 cm^{-1}$). The line profiles are Voigt functions, opportunely modified for H_2O and CO_2. Carbon dioxide line profiles are observed to be sub-lorentzian away from the line center. We use the scaling factor suggested by Perrin & Hartmann (1989) beyond $3 cm^{-1}$ from the line center. Moreover, to adjust for the asymmetry of the line profile we applied the normalized correction factor given in van Vleck & Huber (1977). The CO_2 continuum is computed using a semi-empirical model, which provides the foreign continuum from 1 to 1000 μm or 0-10000 cm^{-1} (Mlawer et al. 2012). The CO_2 molecule also experiences collision induced absorption due to encounters with other CO_2 molecules. We account for these effects using the theoretical results of Gruzska & Borysow (1997) in the interval 33-1000 μm (10-300 cm^{-1}) and interpolating the experimental results of Baranov et al. (2004) in the interval 5-9 μm (1100-2000 cm^{-1}). To avoid an overestimate of the absorption, each CO_2 line is calculated out to 25 cm^{-1} from the line center, hence (as suggested by Mlawer et al. 2012) we consider continuum all the absorption produced further.

In the case of H_2O we follow the prescriptions of Halevy et al. (2009) and Mischna et al.

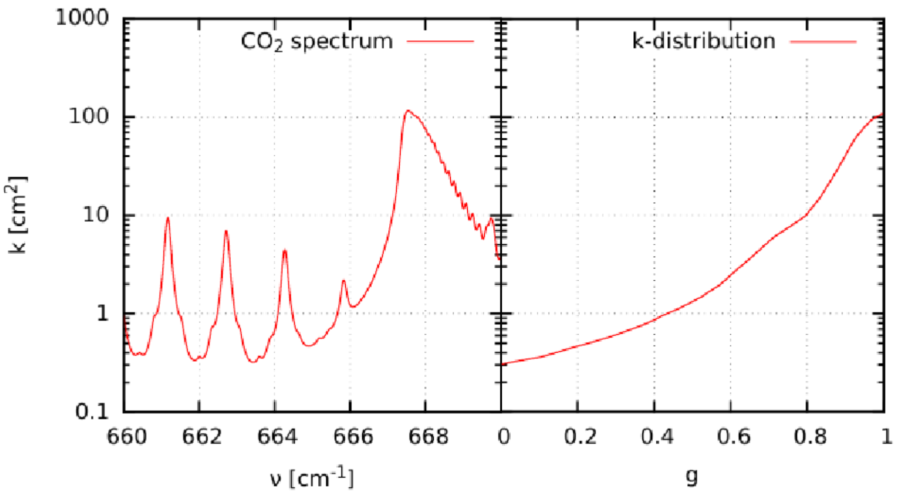

Fig. 1. Left panel: CO_2 spectrum in the 660 - 670 cm^{-1} interval for a gas at pressure p = 1 atm and temperature T = 296 K. Right panel: derived k-distribution.

Table 1. Opacity table at different values of pressure, temperature, CO_2 and H_2O mixing ratios.

Parameter	Values
Pressure (bar)	10^{-4} , 10^{-3} , 2.5×10^{-3} , 10^{-2} ,2.5×10^{-2} , 10^{-1} , 2.5×10^{-1}, 1 ,10 , 10^{2}
Temperature (K)	100, 150, 200, 250, 300, 350, 400, 450, 500
ω_{CO_2} and ω_{H_2O}	10^{-6} , 10^{-5} , 10^{-4} , 10^{-3} , 10^{-2} , 10^{-1} , 9.5×10^{-1}

(2012). We compute a Voigt profile within 40 times the Doppler width from the line center, and a Van Vleck and Weisskopf profile out to 25 cm^{-1} from the natural wavenumber of the transition ν_0. Also for water, we use the continuum model given in Mlawer et al. (2012), which provides both foreign and self continuum from 0.5 to 1000 μm (0 to 20000 cm^{-1}). Such a model derives H_2O line shapes by fitting the continuum in spectral regions where it is best constrained by measurements. The same line shape is extended to spectral regions where the continuum is not well constrained or simply never been measured.

Following Mischna, Lee & Richardson (2012) we divide the wavelength range 0.24-1000 μm in 14 bands. Each band is then further partitioned in 10 sub-bands, obtaining a total of 140 bands, and this is the spacing where we apply the k-distribution technique. The externally stored k-distributed values are defined in Table 1 and they are read and interpolated, according to the required values.

The k-distributed transmission is condensed in a few tens of points (i.e. 32) for each band (ex. Figure 1), making the storage of absorption coefficients fast and simple. A second fundamental benefit of this method is that absorption coefficients at largely different temperature and pressure are now degraded at the same resolution, still maintaining the precise information on the value of the transmission.

2. Future perspectives

As a future perspective, we plan to extend the opacity tables to O_2 , O_3, CH_4 and SO_2 via a larger ISCRA project.

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