PROGRESS IN MODELLING NON-LTE PROCESSES IN THE MARTIAN ATMOSPHERE.

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Introduction

Non-local thermodynamic equilibrium (non-LTE) situations in the upper atmospheres of the planets need to be understood in order to perform meaningful simulations of the radiative balance of these atmospheres. Also they are needed in order to validate and analyse the increasing number of measurements of those high altitudes, either from ground observatories or from instruments on board orbiting satellites, which can be a useful technique for sounding these highly unexplored layers.

In the case of Mars, the first objective, that related to the radiative balance of the non-LTE atmosphere, is specially important above about 60 km, where the emissions by CO_2 at 15-microns dominate the cooling rate of the atmosphere (Bougher and Dickinson, 1988). Also the direct absorption of solar radiation in the near-IR spectrum, between 1 and 5 micron, represents an important term in the radiation budget beetwen 50 and 120 km approximately (Bougher et al, 1994). And regarding the second aim of non-LTE studies in Mars, an avalanche of new measurements of the infrared emissions of a number of gases in the upper Martian atmosphere is being taken from instruments on board Mars Express, which are currently being analyzed. In the case of the atmosphere of Mars, these emissions offer the fascinating chance to research on a real model-data symbiosis, as the theoretical models available can be employed in data validation tasks on one hand, and on the other, the data may allow us to test and improve the model simulations also.

In this presentation, we will describe the progress made recently in the modeling and understanding of non-LTE processes in the CO_2 atmosphere of Mars, based on the analysis of the new data from Mars Express. We will mention how such analysis is improving the models and how the new knowledge can be used to extend the present paramaterizations of the radiation field in the upper atmosphere currently in use in most Martian GCMs.

Analysis of Mars Express data

We focus here in the brief description of the two IR instruments on board Mars Express which are supplying useful data to test and improve our current non-LTE models, and on how these theoretical tools, on another hand, are helping to validate the Mars Express data sets.

PFS and OMEGA observations

Two are the Mars Express instruments of largest and direct interest for us, the Planetary Fourier Spectrometer (PFS), and the Visible and Infrared Mineralogical Mapping Spectrometer (OMEGA). With different spectral resolutions and coverages and with different fields of view, these instruments are supplying fully new infrared observations in nadir and limb geometries of atmospheric emissions which come from the whole range of altitudes in the atmosphere of Mars, although we focus here on those above about 60 km. Regardig the spectral characteristics, the resolution of PFS, around 1.5 cm-1, is better than that of OMEGA, around 10 cm-1, and both cover the strong CO_2 and CO atmospheric emissions between 2.5 and 5.0 μm. Regarding the field of view, OMEGA is better than PFS, as the nominal values at typical tangent heights is of the order of 1 km for OMEGA and around 25 km for PFS. Two contributions to the present volume are directly connected with the present work, as they present some of the limb measurements of these instruments. One of them, by Pierre Drossart and co-workers, describes the fluorescence of CO_2 in the 4.3 μm region observed by OMEGA, and the other, by Vittorio Formisano and coworkers, presents also infrared emissions by CO_2 and CO obtained in the limb, a work which is expanded in more detail by Formisano et al (2006). And a third work, by Lopez-Valverde et al (2005), was devoted to some of the nadir PFS data which show clear signs of non-LTE. All these measurements form the basis of this work; we will briefly mention here the main characteristics of these data sets and we will focus on the modeling of the emissions. Needless to recall the large advantage of having two instruments on board Mars Express measuring similar emissions with different characteristics. The state of the analysis at present is still more individual, with focus on internal validation, being the mutual correlation of data sets an exciting task for the near future.

Improvements in non-LTE modelling

At the Instituto de Astrofisica de Andalucia (IAA-CSIC), in Granada, and for more than a decade, we have been working on the development of a theoretical model of the non-LTE emissions of CO_2 and CO in the Martian atmosphere (Lopez-Valverde and Lopez-Puertas, 1994a,b; Lopez-Puertas and Lopez-Valverde, 1995). Due to the scarcity of the data available from the upper atmosphere, there is a need to validate such theoretical tool. The Mars Express datasets mentioned above are particularly valuable as they offer a unique opportunity for such validation exercise, with repeated measurements of the upper atmosphere in very different illumination conditions and for a full Martian year. Also the two instruments, OMEGA and PFS, represent a unique and fruitful scenario, as the model can be tested with confidence by two independent and correlated measurements.

The analysis of the data follow two steps.
First, the theoretical non-LTE model is used to compute the populations of the vibrational states. Appropriate geophysical conditions should be employed in the calculation, like the actual temperature and pressure profiles and the surface temperature and pressure, in addition to solar illumination conditions and abundances of the different species. So far, all these parameters are not know for all the observations, and averaged reference atmospheres are used instead. This is not a big problem at the present state of the analysis, because in a first approximation, the major non-LTE populations are not very affected during daytime by the actual temperature structure.
And second, a forward model calculation is performed. Here, we also need to take into account the model atmosphere, together with the vibrational populations obtained in the first case. This is done for this study using the Reference Forward Model (RFM) code , a version of the GENLN2 package (Edwards, 1992), developed at Oxford University for the analysis of MIPAS/Envisat data (Dudhia, 2000). This model was modified in order to handle non-LTE emissions (Edwards et al, 1993) and is particularly suitable for our work.

PFS NADIR MEASUREMENTS

A first validation test for the non-LTE model was the study of the 4.3 μm nadir observations of PFS (Lopez-Valverde et al 2005). A comparison of data and simulation is shown in their Figure 1. This spectral region is dominated by a deep atmospheric absorption of the surface IR emission in the strongest IR band of CO_2 at this wavelength. The PFS data showed two distinct emission features in the centre of the absorption region, typical of much higher emission temperatures than any reasonable Martian tropospheric value. As they seem to be located in the optically thick core of the CO_2 rotational lines, whose optical thickness is very large in Mars, we interpreted this emission as originated at much higher up in the atmosphere. Contributions from different CO_2 bands were computed and showed that the emission contains a strong component from the second hot (SH) bands of the main isotope (626), those with upper states 10001 and 02011). These states are excited by solar absorption in the 2.7μm fundamental bands and their populations reach much higher values than in thermal equilibrium above about 40 km (Lopez-Valverde and Lopez-Puertas, 2004b). Or using the concept of vibrational temperature, an equivalent magnitude to quantify the population enhancement, the SH vibrational temperatures were much higher than the kinetic temperature. This result was well known from the existing theoretical non-LTE models in Mars (Stepanova and Shved, 1985; Deming and Mumma, 1983; Lopez-Valverde and Lopez-Puertas, 1994b). But these are not the sole solar pumped states with emitting bands in the spectral region at 4.3 μm, and Lopez-Valverde et al (2005) showed how a number of features in the PFS nadir spectrum seemed to be correlated to a diversity of other bands, mostly fundamental and hot bands of the four major isotopes. All these emissions seem to come from the Martian mesosphere and lower thermosphere.

It is worth mentioning that similar emission features in the center of the 4.3 μm absorption band in Mars had been observed previously by ISO (Lellouch et al, 2000). The data were noisy and these authors could only assign the emission to solar non-LTE in the SH bands of CO_2. A first tentative simulation with our non-LTE model produced a too large emission. In the work by Lopez-Valverde et al (2005), the PFS and ISO data sets were compared in some detail, and a revision of the non-LTE model was performed, regarding the handling of the lower states of the 4.3 SH bands, the Fermi states (020). It was then possible to lower the large emission obtained earlier by a factor 4, and a good agreement with PFS was obtained and to some extent also with ISO. This agreement gave us confidence on the way the major emissions are included in the model.

PFS AND OMEGA LIMB OBSERVATIONS

For the study of the limb measurements by OMEGA we also performed a number of model runs in order to understand the main features observed. We refer the reader to the presentations by Drossart et al. and by Formisano et al. in this volume for details of the observations.

The data in the region at 4.3 μm showed in the limb distinct features in addition to a major two-peaks structure similar to that observed already in nadir, and produced by the SH bands of the 626 isotope. However, two major intriguing results called our attention. First, and very clear in both, PFS and OMEGA datasets, the apparently large contribution at shorter wavenumbers than the P branch of the SH bands, which should be produced by weaker CO_2 bands to be identified. And second, the different peak emissions of the SH bands which were supposed to be responsible for the main structure of the whole region. This was particularly evident in the OMEGA data, and it was intriguing that the asymetry was observed only at tangent heights below about 120 km only.

A number of numerical exercises were performed to understand both results. In a recent work, Formisano et al (2006) studied the variability observed in the weak

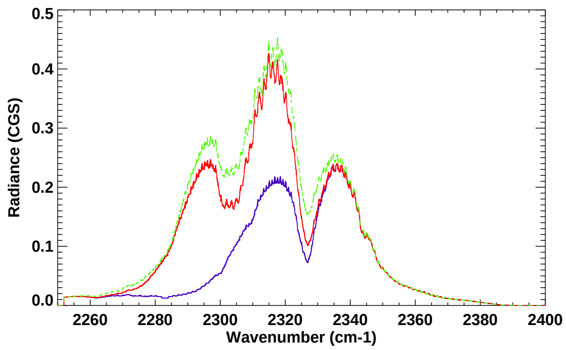

Figure 1: Non-LTE limb spectra at 4.3 μm at 80 km tangent altitude. See text for details.

CO_2 bands which should be responsible for the contribution outside the major SH bands. Regarding the assymetric behaviour of the SH emissions, several hypothesis have been proposed, like being produced by CO_2 ice particles (Drossart et al, 2005). This last possibility was based on a recent laboratory determination of the absorption by CO_2 ice, and it motivated extensive calculations to find out a tentative cloud of CO_2 ice clouds with the appropriate size and vertical distribution. However, the ubiquitous nature of the assymetry found by OMEGA (Drossart et al, this volumen) moved us to look for alternatives.

A possible solution has recently emerged for both problems. It comes from an improvement in the forward model calculations performed so far. We extended it to a larger number of CO_2 infrared bands of the 626 isotope. The theoretical model is able to compute the populations of a larger number of vibrational states than in routine mode. Lopez-Valverde and Lopez-Puertas (1994b) studied for example more than a dozen CO_2-626 vibrational levels with large non-thermal populations after solar absorptions around 1.2, 1.4, 1.6 and 2.0 μm. Part of this solar excitation is eventually lost by radiative decay in hot and combination bands also in the 4.3 um region. These were not included in the forward model computation of the emerging radiances so far. Most of these ro-vibrational transitions are too weak but their populations are strongly out of LTE during daytime in the stronger absorption CO_2 bands mentioned above. We have recently included them in the forward calculations and the result is that all these minor bands do give a significant contribution to the emerging radiance. And not only in the spectral region adjacent to the P-branch of the SH bands, but also to the peak of the P branch, precisely as observed by PFS and OMEGA. For all these weak new bands, their maximum contribution occurs in the optically thick conditions of a limb geometry. In nadir observations their inclusion is less relevant.

Figure 1 shows the result of such calculation, including these bands on a limb calculation at 80 km tangent height, for a spectral resolution similar to PFS. The states included are those excited by solar absorption in the fundamental transitions of the 626 isotope of CO_2 at 1.2, 1.4, 1.6 and 2.0 μm, and in the first hot (FH) bands at 2.7 μm. We also performed calculations of individual band contributions, which show that the largest contribution comes from the solar absorption by three 2.0 μm states (20013, 20012, and 20011). Three lines are shown in Figure 1: one in violet including the 4.3 fundamental, FH and SH bands of the four main isotopes, which was the system considered so far; a second line (red) adding the 2.0 μm bands to the system, and a third one, in green, which is the total emission by all the bands included. Calculations for tangent heights of 120 or higher do show that these three lines coincide. These bands are specially strong in the mesosphere, where their absorptions peak. At the extremely low densities at higher altitudes, in the thermosphere, all of these weak bands are so optically thin that do not give any significant contribution. Such a behavior of the weak bands is well known, as it has been observed in many cases in the Earths upper atmosphere (Lopez-Puertas et al, 1998; Lopez-Puertas and Taylor, 2001).

Parameterizations of heating/cooling rates

In the framework of the European Mars Climate Database project, funded by ESA and CNES, and in collaboration with LMD-CNRS and with the Oxford University, the first non-LTE parameterizations of the thermal cooling rate at 15 microns in the Martian atmosphere were developed (Lopez-Valverde and Lopez-Puertas, 2001; Lopez-Valverde et al, 2003). Also a parameterization for the near-IR solar heating rates was proposed, based on the tabulation of solar heating by Lopez-Valverde et al (1998). These are in used in most Martian GCMs nowadays, but need to be improved in several directions, being this one of the objectives of the new phase of this European project.

The revision of the model mentioned above, triggered by the analysis of Mars Express, is improving the way the high energy states are handled by the model, and will supply a new component to the solar heating rate. This is due to the new set of weak ro-vibrational bands from high combinational states, including also those of the minor isotopes. The impact of these bands is surely small but needs to be evaluated and implemented in a future version of the solar heating rates.

Conclusions and future work

The improvements in the analysis of the Mars Express data, from revisions of the theoretical tool and the forward model calculations, are starting to give good agreements with the data, not only in the nadir but also in the interesting limb datasets of PFS and OMEGA. This gives us confidence on the theoretical modeling, and estimulates further improvements and extensions.

First, we want to extend the number of states handled by the model to all the states of the Hitran database, including the weak high combination states of all the CO_2 minor isotopes. Their contributions may be smaller than the 626 isotope, but they need to be incorporated to be confident in the correctness of the limb data analysis.

Second, and as mentioned above, we want to evaluate the impact of all these minor bands on the energy balance of the upper atmosphere of Mars. All the new bands to implement are weak but numerous, and may have an impact on the near-IR solar heating. Such study should be extended to a revision of the current parameterization of the solar heating rates.

Finally, after the present phase of validation and interpretation of the measurements, and the improvements of the non-LTE model, we plan to use it into a non-LTE retrieval suite in order to derive abundances and non-LTE parameters, in a similar fashion as such retrievals are working operationally in the analysis of Earth's upper atmospheric data from Envisat.

Not only these activities are improving our understanding of the radiation field and the structure of the upper atmosphere of Mars, but will also pave a roadmap to similar studes in the Venus atmosphere, extracting the maximum out of the analysis of the instruments PFS and VIRTIS on board the Venus Express mission.

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