NON-LTE RETRIEVALS OF CO_2 IN THE MARTIAN ATMOSPHERE FROM OMEGA LIMB DATA.

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Introduction

Several instruments on board Mars Express (MEx) have observed daytime atmospheric emissions in the IR, although the data at high altitudes and in a limb geometry have not been sufficiently exploited so far ([1], [9], [12]). Sounding in a limb geometry is a real challenge because this geometry favours optically thick conditions, difficult to handle. In addition, the emissions of the atmospheric species at the low pressures at these altitudes are no longer in LTE (local thermodynamic equilibrium), i.e. they cannot be described by the local kinetic temperature. This is normally a limitation compared to a classical (LTE) inversion scheme where the temperature is already known, and therefore the state populations. In the UPWARDS project (http://www.upwards-mars.eu) we aim at the retrieval of atmospheric densities of the carbon species (CO_2 and CO) and of temperature in the middle and upper atmosphere of Mars (50-160 km), from the daytime limb observations between 2.7 and 4.7 μm, carried out by two instruments on board MEx, OMEGA and PFS.

Both CO_2 and CO have strong ro-vibrational bands that produce intense atmospheric IR emissions during daytime due to well-known non-LTE pumping by solar excitation (also called solar fluorescence). Although these emissions have been studied before ([3], [9], [12]), they have not been used to retrieve density or temperature in the Martian atmosphere so far.

Non-LTE retrievals of CO and CO_2 from IR emissions at high altitude are common nowadays in the Earth upper atmosphere [7], and have recently been performed also in Venus ([4], [11]). However, these Venus retrievals were performed under the approximation of optically thin conditions (CO retrievals from VIRTIS/Venus Express [4]) or from a nadir down-looking geometry, with a fixed and well-known emission layer (in the case of CO_2, at 4.3 μm from VIRTIS [11]). The application of a non-LTE retrieval in a limb geometry which addresses optically thin and thick conditions and from the dominant species of the atmosphere is an entirely new challenge in planetary atmospheres, including the Earth.

For this investigation we need, first of all, to combine state-of-the-art non-LTE models and line-by-line retrieval techniques in order to simulate these emissions correctly (forward model), and then retrieve the abundances of the emitting species from the measurements.

This work in progress describes the design and test of a retrieval scheme suitable for the Mars non-LTE observations, and the preliminary results obtained from synthetic limb radiances and from actual OMEGA measurements.

The non-LTE Forward Model

The direct or *Forward Model* is an essential piece of every inversion or retrieval process and can be considered as the first part of such an inversion. Its primary goal is to simulate realistically the atmospheric emissions to be measured by a given instrument (on board a satellite around Mars, in our case) once the atmospheric state is known. Under LTE conditions, current state-of-the-art forward models basically consist of a precise line-by-line radiative transfer calculation and a careful handling of geometrical conditions, ray-tracing, angle integration, instrumental line shape and convolution functions. Under non-LTE conditions, the forward model additionally requires the simulation of the populations of the energy states of the molecular species responsible for the emissions of interest. In the IR part of the spectrum, in Mars, we are dealing with CO_2 and CO that have a large number of ro-vibrational bands. The non-LTE description shall include all the relevant energy exchange processes between states and isotopes, and a precise treatment of radiative exchanges between layers. A comprehensive and sophisticated non-LTE model is therefore needed, and has to be coupled with the line-by-line radiative transfer calculation mentioned above.

At the Instituto de Astrofísica de Andalucía (CSIC) we have ample experience in non-LTE modelling and retrieval techniques in planetary atmospheres [7]. In the case of the Mars and Venus atmospheres, a non-LTE model called MARVEN was developed and applied to a diversity of investigations. These studies included an energy balance, validation by simulating the emerging radiation field as measured from ground and from several instruments in Mars orbit, and also the creation of parametrizations and fast schemes to be included in global circulation models (GCMs) [8]. This model, however, has not been coupled to a line-by-line radiative transfer model in an efficient manner in order to tackle complex inversion problems. On the other hand, our team has been developing and applying non-LTE inversion methods to Earth's atmosphere observations, in collaboration with the Karlsruhe University ([2], [14]). The Earth's forward model used in such studies combines a generic non-LTE radiative transfer algorithm called GRANADA [2] with a well tested line-by-line radiative transfer model called KOPRA [13]. This is the forward model adopted in the present study.

Some characteristics and merits of the GRANADA model are:

- Calculation of rotational and vibrational populations and their derivatives with respect to the non-LTE retrieval parameters.
- Generalized scheme for all molecules: used for populations of CO_2, O_3, CO, NO, NO_2, H_2O, CH_4, HCN, etc.
- User-defined states and transitions, altitude range, iteration strategies, process definition, etc.
- Line-by-line and line independent radiative transfer (KOPRA).
- Inversion of multilevel steady state equation with the Lambda iteration or Curtis matrix formalism.

The Retrieval Processor

For the solution of the inverse problem, and following [6], we are using the so called *Retrieval Control Program* (RCP), conceived and developed at the Institute of Meteorology and Climate Research (IMK) of the Karlsruhe University with the non-LTE section implemented by the IAA/CSIC team.

RCP solves iteratively the retrieval problem, starting from an initial guess. The calculation of the spectra and Jacobians is performed with KOPRA, with inputs from the GRANADA non-LTE population model for the given atmospheric state at the current step. The measurement covariance matrix is calculated from the noise-equivalent spectral radiance of the measurements. The regularization matrix is a first order Tikhonov-type matrix. For stability, the RCP uses a Levenberg-Marquardt damping, which is forced to be zero in the last iteration. Convergence is reached when the change of the retrieval parameters with respect to the previous iteration is smaller than a given fraction of the noise retrieval error.

Therefore, the inputs to RCP are:

- a measured spectra (normally Level 1B), or alternatively, synthetic spectra generated by a given forward model (like KOPRA);
- an initial guess;
- an *a priori* information of the quantities to be retrieved.

And the principal outputs are the retrieved parameters, in addition to diagnostics such as the averaging kernels, the noise error covariance matrix or the vertical resolution.

The Mars non-LTE inversion scheme

Figure 1 schematically shows the interaction among the different modules of the retrieval processor. This retrieval scheme works following 5 stages:

- the *a priori* information is introduced in KOPRA and GRANADA;
- GRANADA calculates the non-LTE populations;
- KOPRA uses the non-LTE populations to compute the outgoing radiances and the Jacobians;
- the simulated spectra and the measured (or synthetic) spectra are introduced in the RCP for iteration;
- if the result does not satisfy the convergence criterion, it is sent back to KOPRA and GRANADA for recalculation, otherwise the retrieved data are obtained.

Besides the CO_2 density, a height-independent radiance offset is also fitted jointly in the retrieval, at each wavelength, to account for potential calibration offsets, i.e. instrumental non-zero (space) signal affecting the measurements at all tangent altitudes.

Two types of retrieval runs have been performed in order to test the scheme under Martian conditions and Mars Express instrumental characteristics. The first set of runs consisted of a number of synthetic retrievals, i.e. using simulated spectra. Once the retrieval behaviour was understood, we applied the scheme to OMEGA data.

For both sets, the *a priori* profiles were taken from specific runs of the LMD Mars GCM [5], using monthly averages and their temporal standard deviation (STD) as a measure of the *a priori* uncertainty. Spatial components to this STD have not been added but are under consideration. Also the extraction has been done at the finer GCM grid of 3.75 x 5.625 degree. Similarly, the model time step is 2 h. A multilineal interpolation, similar to that included in the Mars Climate Database version 5.2 [10] has been used.

The CO_2 profile is regularized by means of a Tikhonov-type smoothing with a strong diagonal constraint below 60 km in order to force the retrieved CO_2 to be close to the *climatological* density (*a priori*) in the lower mesosphere. Above 60 km, the constraint is optimised to obtain stable calculations with a precision high enough to allow for meaningful physical interpretation of the retrieved CO_2 abundance.

Preliminary Results

The retrieval scheme shown above, after being adapted to Martian conditions, has been applied to both synthetic

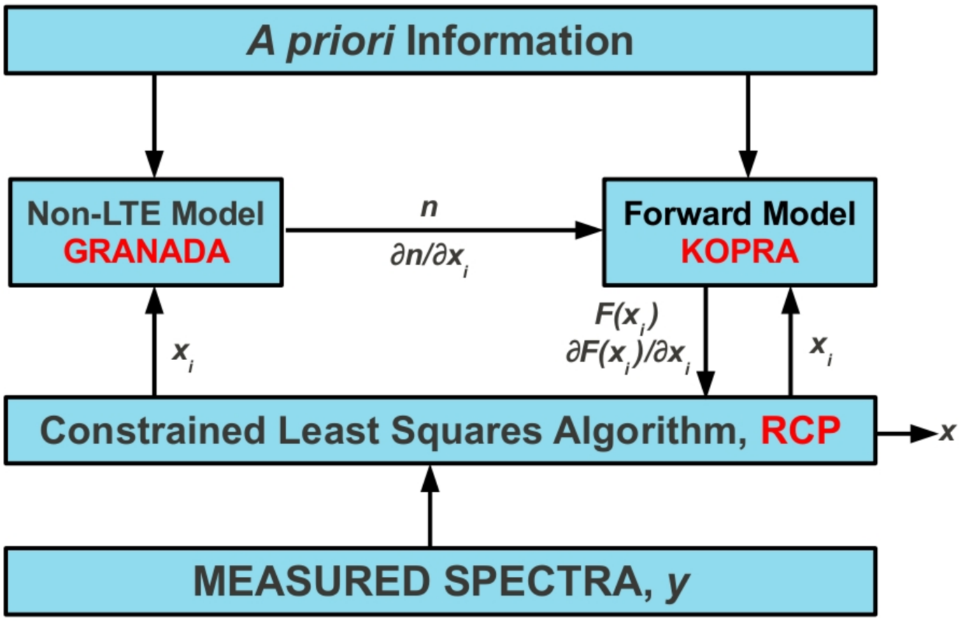

Figure 1: The IMK-IAA non-LTE retrieval scheme, adapted from [6]. x_i is the vector of the retrieval parameters at each iteration step, x is the output vector of retrieval parameter, and n are the non-LTE populations from GRANADA. KOPRA calculates the simulated spectra, $F(x_i)$, and the Jacobians, $\delta F(x_i)/\delta x_i$, at each iteration.

spectra and Mars Express OMEGA IR limb data, in order to retrieve CO_2 density profiles only, not temperatures.

While synthetic retrievals converge when the *a priori* profile is not far from the solution, most OMEGA spectra analysed so far do not achieve convergence. A few numerical issues have been found with the OMEGA cubesets studied, leading to convergence problems and/or to extremely high volume mixing ratios in the uppermost layers of the retrieval range.

To tackle this problem, a large set of variations to the input parameters, in both the reference atmosphere and the retrieval processor, were introduced. The goal was to search for a better agreement between the *a priori* knowledge of the atmosphere and the retrieval's outcome. These variations included: a reduction in the number of wavelengths and tangent altitudes; the study of data from different orbits; changes in the noise or regularization retrieval parameters; and hydrostatic effects like modifications in pressure and temperature. Some of these changes improved the retrieval convergence, but the retrieved vmr values were still unrealistic.

After the application of clustering techniques to the OMEGA data cubes, some peculiar spectra were found, suggesting that temperature may play an important role. Therefore we performed tests to evaluate the temperature sensitivity.

We found that the measurements are sensitive to variations of 1 K for altitudes between 90 and 110 km, and to variations of a few Kelvin outside this altitude range (above and below), for some of the spectral points under study. This is an ideal case, where the vmr is constant or, at least, known, meaning the sensitivity values obtained are rather optimistic. The result could, on the other hand, improve if the information at different wavelengths is combined.

The next steps of this ongoing project will be focused on the convergence problem, by further fine tuning the non-LTE model, and performing joint vmr and temperature retrievals. The comparison with PFS data will also be studied, after an ongoing work on collocated data from both instruments.

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