A Martian K-distribution model for fast radiative calculations from the surface to the thermosphere

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Introduction

Most applications of radiative transfer in the IR in planetary atmospheres require precise and fast calculations of atmospheric transmittances, fluxes and heating rates. The dense forest of CO2 spectral lines of varying intensities and widths existing in the Martian case is a good example. While the goal of a high precision calculation can be achieved with line-by-line models, approximations are still needed for fast solutions like those needed in General Circulation Models (GCM) and in long-term and evolution studies. The so called “k-distribution” methods are an example of procedures which combine precision and acceleration. They consist in replacing the complex spectral structure of the absorption coefficient by a simplified function, its cumulative distribution function, much smoother and faster to integrate (Goody et al., 1989; Lacis and Oinas, 1991) . The k-distribution formalism is suitable to combine absorption and scattering, and therefore is handy to study the lower, dusty Martian atmosphere. It also permits the handling of a mixed atmosphere with diverse radiatively active species, and the treatment of spectral line overlapping, at least in an approximate manner (Mlawer et al., 1997). For all these reasons, these methods are gaining popularity among GCM, evolutionary models, and even remote sensing problems, to mention a few recent applications.

Motivation

One area of research where these methods have not been applied yet in a more systematic manner is the study of radiative problems in the upper atmosphere. One of the reasons is the validity of diverse approximations in radiative transfer at those altitudes. Among the most common solutions we can mention the cool-to-space approximation, the neglect of overlapping between lines, the use of simplified line shapes, the replacement of the very time-consuming angle integrations with quadratures like the diffusivity approximation, etc. However, none of these is suitable for a precise calculation of cooling rates in a wide range of altitudes. For example, in the lower mesosphere the lines are still Lorentzian but not in the upper mesosphere and above. Also the cool-to-space approximation is inadequate at mesospheric altitudes for some important bands of CO2, its altitude of validity being specific, varying greatly from band to band depending on the optical thickness of the particular emission considered.

Another difficulty in the upper atmosphere comes from the breakdown of local thermodynamic equilibrium (LTE), which occurs at atmospheric layers with sufficiently low densities. Non-LTE situations are normally handled by specific theoretical models, which incorporate their own suite of approximations to solve the radiative transfer at those altitudes. The apparent separation of lower and upper atmosphere radiative transfer problems has limited the application of methods of the lower atmosphere to higher altitudes.

This work is intended to develop a k-distribution model for the Martian atmosphere which is free from some of the above approximations, can be used from the surface up to the thermosphere, can handle non-LTE situations in the CO2 strongest bands in the IR, and which also opens the possibility of studying effects of relevance in the lower Martian atmosphere, like the coupled absorption of gas and dust and the strong overlapping of CO2 ro-vibrational lines.

Model description

This k-distribution model is an on-going effort at the Instituto de Astrofísica de Andalucía/CSIC, in Granada, Spain. It is based on the formalism of Lacis and Oinas (1991) , whose first step is the computation of the cumulative distribution function of the absorption coefficient of the Martian atmosphere in a given spectral range of interest. In the case of the broad and all-important 15-um band of CO2, responsible for the largest cooling of this atmosphere in the IR, we are using a total of 19 sub-intervals. The distribution function, or g-function, is obtained from absorption coefficients at 0.0001 cm-1 resolution, from the Hitran2004 database. All this is intended to obtain accurate transmittances and to allow for separate treatment of diverse CO2 bands in the upper atmosphere.

Following previous developments, and in order to accelerate the k-distribution model we produced a tabulation of the absorption coefficients in a sufficiently wide range of temperature and pressure, with 20 K steps and 0.5 in log(Pressure). Bi-linear interpolation between grid points is used in the tabulation.

The second step of the computation is the vertical integration, which is performed by a discretization of the radiative transfer equation and imposing common boundary conditions at the surface, following also Lacis and Oinas (1991). The vertical integration requires some care in order to guarantee the correlation of spectral features. Normally some correlation technique is used for such purpose. We tested that of Edwards and Francis (2000) which produced only a minor improvement in the fundamental bands of the main CO2 isotopes compared to a non-correlated solution.

Variations in a few model parameters, like the number of points in the g-function and their distribution were explored. Our nominal calculations use 50 points, with a larger density near the g=1 value, as suggested by previous work (Mlawer et al., 1997; Edwards, 2000)

For further acceleration, a tabulation of g-functions was created, as an alternative to the tabulation of absorption coefficients. This table is of much smaller size and the code is significantly faster, with a very small reduction in the precision of transmittances and cooling rates in the 15-um band.

Application to non-LTE in the upper atmosphere

One problem inherent to the upper atmosphere and its low gas densities is the rupture of the LTE approximation. Under such conditions each CO2 level is studied separately by incorporating its strongest energy exchanges in collisional processes and its relevant ro-vibrational bands. The collisional and radiative couplings between states is normally very large and important for many states, and this requires to solve a large number of coupled equations. This is achieved normally by matrix inversion, or iteration, or a mixture of both. The availability of a fast and accurate calculation is therefore an interesting possibility to improve the usual radiative transfer methods within non-LTE models.

The non-LTE model used in this study is that developed by Lopez-Valverde and Lopez-Puertas (1994); which uses the well known Curtis Matrix formalism (Lopez-Puertas and Taylor, 2001). This requires the computation of a matrix of double differences of atmospheric transmittances, which need to be computed previously. In contrast to the most common applications of the k-distribution method, our key objective is to compute a large number of atmospheric transmittances, which will be part of the Curtis Matrix.

The transmittances in selected bands of the 15-um spectral region were compared to the two methods of calculation of atmospheric transmittances included in the non-LTE model so far. These two models are: (i) a fast line-independent model (LIMOD), which follows an histogramming technique (Lopez-Valverde and Lopez-Puertas, 1994), and (ii) a slow but more precise line-by-line model. We obtained that the k-distribution method represents a significant reduction in computing time for large atmospheric paths compared to the line-independent model, and at the same time, we confirmed as expected that its behavior is similar in terms of precision to the LIMOD.

Comparison to other k-distribution models

To date, an increasing number of correlated k-distribution models are being used in diverse Martian models. In addition to the usual testing against line-by-line models, their behavior and cross-comparison is a very needed exercise. This is not only a further testing exercise but may indicate biases between the different models. Such a task has been tackled recently by Mischna et al (2012), who developed a new k-distribution model for the ancient Mars and compared it with a selected number of other k-distribution models used in several Martian GCMs, and also with a well known line-by-line model. Therefore, we have compared our k-distribution model against the code of Mischna and co-workers. The work is still on going, specially regarding the study of the modification of parameters and the models' response to them, but a few results were obtained for the 15-um spectral region up to about 80 km altitude. A few small discrepancies were obtained both in the k-distribution and in the line-by-line models, which are surely inherent to atmospheric griding, surface boundary conditions, and spectral source data. When these are eliminated from the comparison, the agreement between both codes is good.

Conclusion and future work.

The k-distribution model designed was applied to the calculation of atmospheric transmittances in a few bands of CO2 in the 15-um region, and represents a step forward in the acceleration of non-LTE models in the Martian atmosphere.

A few extensions of the model are under investigation at this moment. One of them is the treatment of overlapping between the CO2 lines in the lower atmosphere, and its incorporation into the Curtis Matrix formalism. This will allow the extension of the non-LTE models to lower altitudes.

The second extension is the application of the k-distribution to the near-IR spectral region between 1-5 um, where strong CO2 bands absorb direct solar radiation and give a significant heating of the upper mesosphere. The application will be based on the results obtained in the 15-um region, and will also help in the acceleration of the calculation of the solar heating by CO2 under non-LTE conditions.

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