Introduction: Motivation and Requirements

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Abstract: In this paper we present the motivation to develop another radiative transfer code, namely KOPRA, besides the existing ones and the requirements set up by the MIPAS/ENVISAT mission in terms of observation scenarios, instrument characteristics, and retrieval strategy which were the drivers for the design details of KOPRA.

Retrieval of atmospheric state parameters from remote measurements depends on the accurate modeling of atmospheric radiative transfer. This is in particular true for limb emission spectrometry experiments like the MIPAS experiments [1, 2, 3] where a lot of demanding physics is involved in radiative transfer. Although a number of good radiative transfer codes are available [4, 5, 6, 7, 8, 9, 10], after some general preliminary considerations [11] we decided to design and develop a new code specifically suited for the data analysis of the space-borne Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) experiment [12] which is going to be launched on ESA's Environmental Satellite 1 (ENVISAT-1), for the following reasons: Due to global and altitudinal coverage and observation geometry, the MIPAS experiment sets up a number of specific requirements with respect to modeling of geophysical conditions which are not all fulfilled by the codes available; the modeling of the very specific instrumental response of MIPAS is a mandatory requirement which is not at all or not rigorously provided by other codes; the radiative transfer code must be integrated in an automated retrieval system being able to handle very high data amounts which sets up specific needs on the performance of the code and on the controlling options; and a code written by our own can be better designed in terms of flexibility and structure and easier adopted to future needs than a foreign one.

Therefore the Karlsruhe Optimized and Precise Radiative transfer Algorithm (KOPRA) has been developed. KOPRA is planned to be applied during data analysis within a dedicated scientific level-2 data processor to be developed and installed at IMK and within the MIPAS/ENVISAT processor at DFD/Oberpfaffenhofen. It models the mid-IR radiative transfer through the entire atmosphere (from the boundary layer to about 200km altitude) and considers - to our knowledge - all effects relevant in this spectral and altitude range. It is therefore suited for the data analysis of MIPAS which is going to be launched on ESA's Environmental Satellite 1 (ENVISAT-1) into a polar orbit in about 800 km altitude. MIPAS is designed to be a limb-viewing emission FTIR spectrometer with 0.025 cm^{-1} spectral resolution, covering the mid infrared from 685 cm^{-1} to 2410 cm^{-1} (14.6 - 4.15 μm) by five spectral channels. Observation modes supported are a rearward looking mode with possible azimuth sweep angles from 75^o to 110^o and a sideward looking mode in anti-sun direction with possible azimuth sweep angles from 160^o to 190^o. The elevation pointing range of the instrument results in scans with achievable tangent heights from about 5 to 150 km [13]. The field-of-view of MIPAS is about 30 km in horizontal direction and 0.9 mrad in vertical direction, resulting in about 3 km width at the tangent point, depending on tangent altitude. The standard limb sampling step width will be 3 km, which results in an averaging of air masses along the line-of-sight over about 400 km. The sampling rate is about 500 km along-track and about 2800 km across-track (at the equator). Thus, the observations will cover the complete globe for day, night, and twilight conditions from the middle troposphere to the thermosphere.

The viewing direction will be close to meridional which requires to take into account the oblateness of the Earth for calculation of the line-of-sight, including refraction in a non-spherical atmosphere with horizontal density inhomogeneities. In this viewing direction, horizontal inhomogeneities in temperature, pressure, and constituent abundances may occur often, for example when crossing with the line-of-sight the vortex edge, the boundary of the innertropical convergence zone, or the terminator. Cirrus clouds in the upper troposphere, or, during polar night observations, polar stratospheric clouds may be in the line of sight. This requires modeling of particle-caused continuum-like extinction in the mid-IR spectrum. Observation of the lower atmosphere down to the middle troposphere sets up the requirement of very accurate modeling of the absorption coefficients which has to cover all effects caused by high pressure, like pressure-broadening in combination of Doppler broad-

ening (Voigt line shape) and pressure-shift of the molecular transitions, line-mixing (in particular for Q-branches of ro-vibrational bands of CO_2, but also for other branches and molecules), duration-of-collision effects in the far line wings (water vapor and CO_2 "continua"), and a careful selection of lines contributing to the signal from outside of the observed spectral interval. In the lower to middle atmosphere a rather big number of trace species with high molecular weight contribute to the overall emission signal of the atmosphere. The ro-vibrational transitions of these species are too dense to be modeled line-by-line as it is common for other molecules. Therefore methods to utilize absorption cross-section spectra provided by several molecular spectroscopy labs and provided for a (sometimes rather small) number of pressure/temperature conditions had to be developed. Scientific questions to be investigated on the basis of the retrieved data further make it desirable to handle isotopomeric species of molecules (for example H_2O, HDO, and $^{18}H_2O$; CH_4 and CH_3D; the symmetric and asymmetric isotopomers of ozone $^{16}O_3$, $^{16}O^{16}O^{18}O$, and $^{16}O^{18}O^{16}O$) independently of each other and thus not to constrain their atmospheric concentration by a common profile. In the middle to upper atmosphere non-LTE (non-local thermodynamic equilibrium) population of the molecular states will be a major concern for emission sounders. Therefore the radiative transfer code must be able to handle the non-LTE effects in the radiance signal of the atmosphere, provided information on the non-LTE population of the molecular states is available. In this region, strong horizontal gradients of geophysical state parameters may also have a considerable impact on the observed spectrum and thus need to be modeled within KOPRA. In order to model the atmospheric signal as it is observed by the MIPAS instrument, the instrument response in terms of spectral resolution and apodized instrumental line shape (AILS), field-of-view (FOV) integration of the atmospheric radiance profile, and finite-FOV effects on the ILS has to be considered. Within a retrieval procedure, the radiative transfer code has to provide much more than the simulation of spectra.
In general terms a multi-geometry radiative transfer problem can be written linearily as

$$Y = \mathbf{K}X \tag{1}$$

where Y is a vector of form

$$(y_{1,1} \dots y_{1,mmax(1)}, y_{2,1} \dots y_{2,mmax(2)} \dots y_{nmax,1} \dots y_{nmax,mmax})^\tau,$$

containing spectra of $mmax(n)$ gridpoints, related to measurement geometry $n \leq nmax$; $\mathbf{K}$ is the $\sum_{n=1}^{nmax} mmax(n) \times imax$ Jacobian, containing the partial derivatives $\partial y_{n,m}/\partial x_i$; X is the imax-dimensional vector containing atmospheric and instrumental parameters. The retrieval problem then can be written as

$$X = (\mathbf{K}^\tau \mathbf{K} + \mathbf{R})^{-1} \mathbf{K}^\tau (Y_{measured} - Y_{calculated}) \tag{2}$$

where $Y_{measured}$ is a set of measurements, while $Y_{calculated}$ is the related set of spectra calculated on the basis of the best available estimate of X. $\mathbf{R}$ is a regularization parameter. Eq. 2 can easily be rewritten in a recursive manner, reflecting iterative processing in order to take account for nonlinearities in radiative transfer.
Random error estimation follows the formalism

$$\mathbf{S_x} = (\mathbf{K}^\tau \mathbf{S_y^{-1}} \mathbf{K})^{-1} \tag{3}$$

where $\mathbf{S}_x$ and $\mathbf{S}_y$ are the covariance matrices of the retrieval parameters and the measurement, respectively, while the mapping ΔX of uncertainty Δw of a priori information w on the retrieval of state parameter X can be approximated as

$$\Delta X = (\mathbf{K}^\tau \mathbf{K})^{-1} \mathbf{K}^\tau \left(\frac{\partial y_{1,1}}{\partial w} \ldots \frac{\partial y_{nmax,mmax}}{\partial w}\right) \Delta w \tag{4}$$

The requirement to the forward model is to provide at each iteration the set of spectra $Y_{calculated}$, the Jacobian $\mathbf{K}$, and, at the last iteration, the partials $\partial y_{n,m}/\partial w_j$ for all $jmax$ parameters to be considered in the systematic error assessment, while a standard forward code not run in environment of a retrieval code has to provide only once a single spectrum and no derivatives. $\mathbf{R}$ and $Y_{measured}$ are of relevance only in the inversion code. From the viewpoint of optimizing interfaces care has to be taken that:

1. Partial derivatives shall be calculated internally rather than by successive calls of the forward code for incremented x-values, whenever possible.

2. For calculation of derivatives, the vector spaces involved shall be matched. In the following some examples are given:

   (a) if the vertical profiles of state parameters are sampled finer inside the forward code than in the retrieval, inter-layer constraints have to be supported by the forward module.

   (b) an option has to be provided whether abundances of different isotopes of a molecule shall be treated as one parameter or as several independent parameters.

   (c) constraints between populations of energy levels have to be activatable and deactivatable

   (d) spectroscopic data have to be includable and excludable in/from the vector X of variable parameters.

3. Obvious behavior of partial derivatives shall be implemented in a hard-wired way; e.g. partial derivatives of spectral radiances of a spectrum of tangent altitude z (i.e. lower edge of the field of view) with respect to atmospheric parameters at altitudes below z always are zero.

4. Systematic error estimation needs partial derivatives of spectral radiances with respect to much more parameters $\partial y_{n,m}/\partial w$ than inversion. These partial derivatives obviously are needed only at the last iteration rather than at each iteration.

5. Redundant calculation of quantities shall be avoided whenever possible. This applies to

   (a) ray-tracing and airmass calculations which can be reused during several iterations;

   (b) absorption coefficients can be reused for other geometries and iterations;

Within KOPRA, the link to such a retrieval concept with high flexibility is given by the analytical calculation of spectral derivatives with respect to an in principle unlimited number of parameters, with a used-defined and completely flexible set-up of geophysical parameter vectors and by providing the options to run KOPRA in appropriate modi. The applicability in automated data processing is reflected in KOPRA's highly efficient and optimized calculation of atmospheric absorption cross

sections, its user-defined accuracy adjustment and the ability to avoid recalculation of redundant quantities when imbedded in a data processing loop. The user-defined accuracy-parameters control the calculation of absorption cross sections, the layering of the atmosphere, the mass integration along the ray path, and the accuracy of field of view and instrumental line shape modeling. However, the optimal choice of the accuracy-control parameters is not always obvious, and may depend on the actual case under investigation. This problem is accounted for in a dedicated study in order to allow optimized performance within the automated quasi-operational processing of MIPAS data.

With all these features, KOPRA reflects the requirements set up by this mission in terms of the instrument design details, the observation scenarii, the link to a retrieval concept with high flexibility, and the applicability within automated data processing. In this report, we will describe the algorithm of radiative transfer behind the coding of KOPRA, and the realization of this algorithm down to the data structure with respect to a variety of aspects in the various modules of KOPRA. We further add a study on the optimal choice of accuracy-control parameters. Although we attempted to include all physics known to be relevant for application to MIPAS in our data analysis, we were aware that some simplifications may be allowed which, however, should be made on basis of *a posteriori* decisions on the relevance of these effects by means of the full assessment of the forward modeling error and its mapping on the retrieval error. For this reason, the forward model error and its mapping on over-all retrieval error due to discarding these individual physical processes and properties of the atmosphere and the instrument has been assessed for a number of example cases. This study will serve as a guideline for designing the real MIPAS/ENVISAT data analysis. Finally we provide an installation guide with description of the line data format and an example of the complete set of input files necessary to run KOPRA.

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