The broadband continuum implementation

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Abstract: Two possibilities for the simulation of a broadband continuum are described: the direct input of cross-sections and number density profiles or the calculation of cross-sections by a KORA-internal Mie model with aerosol size distribution parameters and refraction indices as input. Analytical derivatives with respect to various parameters are supported.

1 Forward calculation

Two different possibilities are implemented in KOPRA to consider the effects of a broadband continuum:

- Direct use of profiles of wavenumber dependent absorption and extinction cross sections and a profile of particle number density.
- Use of profiles of wavenumber dependent refraction indices (real and imaginary parts), of a profile of particle number density and profiles for parameters describing the particle distribution in a KOPRA-internal Mie-model to calculate the absorption and extinction cross sections.

1.1 Cross-section input

Input necessary for this mode of operation:

- Altitude profiles of the aerosol number density [particles/cm^3]
- Altitude profiles of absorption and extincition cross sections [cm^2/particle]. These are wavenumber depedent and can be given on an arbitrary wavenumber grid. Directly after reading, the cross sections are interpolated for each microwindow to a 5 cm^{-1} grid. (It is asumed here that 5 cm^{-1} are sufficient to describe wavenumber dependence of aerosols.)

In the next step, during ray-tracing, particle columns [particles/cm^2] for each atmospheric path are determined from the number density profiles (assuming linear interpolation between two altitude levels.) Further, Curtis-Godson values for each path are calculated for the wavenumber dependent absorption and extinction cross sections (using the number density for weighting).
During radiative transfer the cross sections for each path are multiplied with the particle columns to get the absorption and extinction optical depths. During this procedure it is necessary to interpolate the cross sections to the non-equidistant fine grid on which the radiative transfer is performed. This interpolation is performed linearly.

1.2 Mie-model input

Input necessary for this mode of operation:

- Altitude profiles of the aerosol number density N_{tot}[particles/cm^3].
- Number of modes for the particle distribution *nmode* (1- or 2- modal size distributions are supported).
- Altitude profiles of refraction indices (real and imaginary part). These are wavenumber depedent and can be given on an arbitrary wavenumber grid. Directly after reading, the refraction indices are interpolated for each microwindow to a 5 cm^{-1} grid. (It is asumed here that 5 cm^{-1} are sufficient to describe the detailed wavenumber dependence of aerosols.)
- Altitude profiles for mode radius r_i [μm], mode width s_i, and ratio of particles in mode 1 to the total number of particles v_N. (Number density and particle distribution parameters are given on the same altitude grid.)

It is assumed that the aerosols are spherical and homogeneous. The formula for the 1 or 2-modal log-normal size distribution density which is supported by KOPRA reads:

$$n(r) = \sum_{i=1}^{nmode} \frac{N_i}{\sqrt{2\pi} r s_i} \exp - \frac{(\ln \frac{r}{r_i})^2}{2 s_i^2}, \tag{1}$$

where r is the aerosol radius, $N_1 = N_{tot}$ for $nmode = 1$, and $N_1 = v_N N_{tot}, N_2 = (1 - v_N) N_{tot}$ for $nmode = 2$.
The integral over the size distribution density for all radii is the total aerosol number density

$$N_{tot} = \int_0^\infty n(r) dr. \tag{2}$$

During ray-tracing, particle columns [particles/cm^2] for each path are determined from the number density profiles (assuming linear interpolation between two altitude levels.) Further, Curtis-Godson values for each path are calculated for the particle distribution parameters and the wavenumber dependent refraction indices (using the number density for weighting) .
An essential difference to the previous section is that there the cross-sections are an input while in this section they have to be calculated from the Curtis-Godson path values of the particle distribution parameters and the refraction indices. This is performed by a Mie model which is called in the module where the absorption cross sections for the other species are also determined (Mie_call@abco_m).
Input for the Mie-model are the particle size distribution parameters and refraction indices. The model is described in detail in [1] and [2] . However, it was not possible to use this program unchanged since the integration over the particle distribution was rather slow. Therefore, the integration was optimized for the log-normal size distributions which are supported by KOPRA. During the Mie-calulations integrals of the form $\int_0^\infty f(r)n(r)dr$ are determined. By substituting $z^2 = (\ln r/r_i)^2/2s_i^2$ they are transformed into $\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} f(r(z)) \exp -z^2 dz$. This integrals can very efficiently be solved by using the Gauss-Hermite quadrature formula [3].
Output of the Mie-model are the absorption and extinction cross sections on the same wavenumber grid as the refraction indices.
As in the previous section during radiative transfer these cross sections for each path are multiplied with the particle columns and linearly interpolated to the wavenumber fine-grid to get the absorption and extinction optical depths.

2 Derivative calculation

KOPRA calculates analytical derivatives with respect to various parameters determinining the continuum contribution in the spectra.

2.1 Cross-section input

In this case the derivatives of the spectrum with respect to the aerosol number density is determined.
During the determination of path column values of aerosol particles in the raytracing module the derivatives of these column amounts with respect to the altitude retrieval-parameters of the number density are calculated. Afterwards, during radiative transfer first the derivatives of the spectrum with respect to the aerosol path column values are determined. Then, the post-derivation is performed by multiplication with the previously calculated derivatives of the column with respect to the altitude parameters of the number density.

2.2 Mie-model input

In addition to the derivatives with respect to number density which was already described in the previous section, derivative spectra with respect to the aerosol size distribution parameters (r_i, s_i, v_N) are produced.
As for number density, during the Curtis-Godson calculation the derivatives of the path values for r, s and v_N with respect to their altitude retrieval-parameterization are calculated. When the Mie-model is called with the Curtis-Godson layer values as input, parallel to the determination of the absorption and extinciton cross sections their derivatives with respect to the size distribution parameters are computed. (By analytic derivative of the log-normal size distribution functions with respect to r_i, s_i and v_N.)

During radiative transfer the following 3 steps are performed to get the final derivative spectra with respect to the size distribution altitude parametrization:

- Derivative of the radiance with respect to the absorption and extinction cross sections
- Multiplication by the derivative of these cross sections with respect to the Curtis-Godson layer values.
- Multiplication by the derivative of the Curtis-Godson layer values with respect to the altitude retrieval-parameter values

Bibliography

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[3] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran, 2nd edition, Cambridge University Press, p. 147 1992.