Comparison of single and multiple scattering approaches for
the simulation of limb-emission observations in the mid-IR

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Abstract

The validity of single scattering radiative transfer calculations for simulation of limb-emission measurements of clouds in the mid-infrared spectral region was investigated by comparison with a multiple scattering model. For in limb direction optically thin clouds, like polar stratospheric clouds, errors of the single scattering scheme range below 3%. For optically thick clouds deviations are below 3% in case of low single scattering albedo ($\omega_0 = 0.24$) increasing up to 10–30% for $\omega_0 = 0.84$. Clouds which are optically thick in limb, but thin in nadir direction, can cause limb radiances which are by a factor of 1.7 higher than the blackbody radiance at cloud altitude.

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1. Introduction

Due to their long pathlength through the atmosphere mid-infrared limb-emission sounders are especially suited for the detection of thin clouds, like polar stratospheric or sub-visible cirrus clouds. Recently it was proven by balloon borne measurements with the Michelson Interferometer for Passive Atmospheric Sounding-Balloon (MIPAS-B) instrument that scattering of radiation

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from the earth’s surface and the troposphere into the line-of-sight of the instrument must not be neglected in radiative transfer simulations of such observations [1]. By using the single scattering radiative transfer model KOPRA (Karlsruhe Optimized and Precise Radiative transfer Algorithm) the impact of various types of polar stratospheric clouds on satellite limb-emission measurements was investigated in a subsequent study [2]. In these papers it was argued, however not proven, that the single scattering approach is sufficient for the modelling of limb radiative transfer in such optically thin clouds. In the present work we investigate the accuracy of the single scattering as implemented in KOPRA by intercomparison with results of the most recently developed multiple scattering scheme in the Atmospheric Radiative Transfer Simulator (ARTS). This investigation assesses the applicability of relatively fast single scattering calculations which is important for data analysis of measurements of polar stratospheric and of cirrus clouds by current and future satellite borne spectrally high-resolution limb-emission sounders like MIPAS on Envisat [3], launched in March 2002, or (TES) Tropospheric Emission Spectrometer on EOS-Aura [4], scheduled to be launched in 2004.

2. The ARTS multiple scattering model

The first version of the model ARTS-1 is a one-dimensional (1D) unpolarized radiative transfer model, which is sufficiently fast for operational use and can also be applied for sensor characterization studies [5]. A new version, ARTS-2, is currently being developed in order to simulate the influence of multiple scattering on measured radiances, polarization effects emerging from ice particle scattering and Zeeman splitting, and in addition three-dimensional (3D) effects resulting from horizontal inhomogeneities in the atmosphere. For the intercomparison with KOPRA being presented in this paper, the 1D unpolarized mode of the new ARTS version was applied.

The unpolarized radiative transfer equation for spherical particles or an ensemble of randomly oriented non-spherical particles can be written as

$$\frac{dI_v(n, s)}{ds} = -k_{e,v}(s)I_v(n, s) + k_{a,v}(s)B_v(s) + S_v(n, s).$$

(1)

Here \(I\) is the intensity, \(k_e\) and \(k_a\) the extinction and absorption coefficients of the gases and particle distributions, \(B\) the Planck function and \(S\) the scattering integral. Furthermore \(v\) is the frequency of the radiation and \(n\) the propagation direction. The scattering integral can be written as

$$S_v(n, s) = \int_{4\pi} d\Omega' Z_v(n, n', s)I_v(n', s),$$

(2)

where \(Z\) is the phase function averaged over the ensemble of all particles.

ARTS uses the Discrete Ordinate Iterative (DOIT) method to solve the radiative transfer equation. The method is described in detail in the ARTS user guide [6] and in [7] where the same approach has been applied and investigated in a plane parallel 1D radiative transfer model. The scattering problem is solved in a restricted part of the atmosphere, denoted as “cloudbox”. The cloudbox is discretized in the spatial domain and also in the angular domain of the propagation.
directions. The intensity field is calculated for each discrete point. Boundary condition is the incoming radiation field on the boundary of the cloudbox calculated by clear-sky radiative transfer calculations.

In order to obtain a first guess for the scattering integral field, the clear-sky field is interpolated on all cloudbox points. The interpolated field is taken as a first guess to evaluate the scattering integral term. Putting the result of the integration into Eq. (1) leads to

$$\frac{dI_v^i(n, s)}{ds} = -k_{c,v}(s)I_v^i(n, s) + k_{a,v}(s)B_v(s) + S_v^{(i-1)}(n, s), \quad (3)$$

$$S_v^{(i-1)}(n, s) = \int_{4\pi} dn'Z_v(n, n', s)I_v^{(i-1)}(n', s). \quad (4)$$

Assuming that the coefficients are constant between the discrete grid points, Eq. (3) can be solved analytically using an exponential approach. In practice averaged values for the coefficients are taken. This approximation is valid if the discretization of the cloudbox is sufficiently fine.

The first iteration field, i.e. the field obtained by solving Eq. (3) ($i = 1$), is compared to the first guess field ($i = 0$). Assume that the first iteration field is closer to the solution field than the first guess field. In this case it makes sense to repeat the procedure which is to calculate the scattering integral now using the first iteration field and then solving again Eq. (3). In this way the second iteration field ($i = 2$) is obtained. On the assumption that the method converges two successive iteration fields must be equal within a numerical accuracy limit. If this is fulfilled after the $n$th iteration, then the $n$th iteration field is taken as solution of Eq. (1).

3. The KOPRA single scattering model

KOPRA was especially developed for the analysis of spectrally high resolved remote sensing measurements of the earth’s atmosphere in the mid-infrared [8,9]. The part of the model describing radiative transfer in the gaseous atmosphere has been validated extensively [10–13]. Based on a layer-by-layer approach KOPRA models the radiative transfer as a succession of extinction, emission and scattering in homogeneous layers.

The analytic solution of Eq. (1) for a homogeneous layer of thickness $s$ is

$$I_v(n, s) = I_v(n, 0) \exp(-k_{c,v}s) + \frac{k_{a,v}B_v + S_v(n)}{k_{c,v}} [1 - \exp(-k_{c,v}s)], \quad (5)$$

where $I_v(n, 0)$ denotes the background radiance. If the instrumental line-of-sight traverses $L$ layers the discretized radiative transfer equation reads:

$$I_v(n, s^{obs}) = I_v(n, 0) \prod_{l=1}^{L} \tau_{v,l} + \sum_{l=1}^{L} \left[ \frac{k_{a,v,l}B_{v,l} + S_{v,l}(n)}{k_{c,v,l}} (1 - \tau_{v,l}) \prod_{j=l+1}^{L} \tau_{v,j} \right] \quad (6)$$

with the index on the layers $l$. $\tau_{v,l} = \exp(-k_{c,v,l}s_l)$ is the transmission of layer $l$ with thickness $s_l$. For determination of the scattering integral $S_{v,l}(n) = \int_{4\pi} dn'Z_{v,l}(n, n')I_{v,l}(n')$ the incoming
radiances are calculated neglecting the scattering source term

\[
I_{v,l}(n') = I_v(n',0) \prod_{l'=1}^{L'} \tau_{v,l'} + \sum_{l'=1}^{L'} \left[ \frac{k_{a,v,l'} B_{v,l'}}{k_{c,v,l'}} (1 - \tau_{v,l'}) \prod_{j=l'+1}^{L'} \tau_{v,j} \right].
\]  

(7)

The prime symbol denotes that the variables belong to the first-order scattering rays. Below, four different options of scattering in KOPRA will be compared with ARTS:

- \textit{KOPRA(0):} Zero scattering scheme neglecting the scattering source term \( S_{v,l}(n) \) in Eq. (6).
- \textit{KOPRA(1):} Zero scattering scheme neglecting the scattering source term \( S_{v,l}(n) \) and replacing \( k_{a,v,l} \) by \( k_{c,v,l} \) in Eq. (6).
- \textit{KOPRA(2):} Single scattering scheme using Eqs. (6) and (7).
- \textit{KOPRA(3):} Single scattering scheme using Eqs. (6) and (7) in which \( k_{a,v,l} \) is replaced by \( k_{c,v,l} \).

4. Definition of scenarios

In order to avoid any problems with differences in line-by-line calculations during the model intercomparison, for the selected spectral interval (946.149–950.837 cm\(^{-1}\)) absorption cross-sections for the gases CO\(_2 \) and H\(_2\)O were calculated with KOPRA for the atmospheric pressure–temperature profile on a 0.5 km grid. These precalculated cross-sections were used to calculate the gaseous radiance contributions with the ARTS model.

The altitude profile of the cloud was defined between 9.5 and 12.5 km altitude with linearly increasing (from 0 cm\(^{-3}\)) values of number density from 9.5 to 10 km and decreasing (to 0 cm\(^{-3}\)) from 12 to 12.5 km. Between 10 and 12 km the number density was constant. A log-normal size distribution of spherical ice-cloud particles was assumed with a median-radius of 4 \( \mu \)m and a width of 0.3. Table 1 summarizes the five scenarios of increasing density. Here, the smallest volume density is in the order of that of typical polar stratospheric clouds of type I containing a large fraction of HNO\(_3 \) and scenario 2 is representative of polar stratospheric clouds of type II consisting of ice particles.

<table>
<thead>
<tr>
<th>Cloud scenario</th>
<th>Number density [cm(^{-3})]</th>
<th>Volume density [( \mu )m(^3) cm(^{-3})]</th>
<th>Optical depth</th>
<th>Optical depth</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>nadir</td>
<td>limb(^a)</td>
</tr>
<tr>
<td>1</td>
<td>0.01</td>
<td>4.0194</td>
<td>1.68(1.75) \times 10(^{-3})</td>
<td>0.17(0.176)</td>
</tr>
<tr>
<td>2</td>
<td>0.1</td>
<td>40.194</td>
<td>1.68(1.75) \times 10(^{-2})</td>
<td>1.7(1.76)</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>401.94</td>
<td>1.68(1.75) \times 10(^{-1})</td>
<td>17.0(17.6)</td>
</tr>
<tr>
<td>4</td>
<td>10</td>
<td>4019.4</td>
<td>1.68(1.75)</td>
<td>170(176)</td>
</tr>
<tr>
<td>5</td>
<td>100</td>
<td>40194</td>
<td>16.8(17.5)</td>
<td>1700(1760)</td>
</tr>
</tbody>
</table>

Optical depths are given for the two cases \( \omega_0 = 0.24 \) and 0.84 (in brackets).

\(^a\)11 km tangent altitude.
For determination of single scattering properties, Mie calculations were used on basis of refractive indices of ice by Toon et al. [14]. In the middle of the defined spectral interval the refractive index is \( (1.07 + 0.17i) \) leading to an absorption cross-section of \( 5.1 \times 10^{-7} \text{ cm}^2 \) and a scattering cross-section of \( 1.6 \times 10^{-7} \text{ cm}^2 \), resulting in a single scattering albedo \( \omega_0 = 0.24 \). Thus, this is a case of relatively strong absorption, since the chosen wavenumber region is situated at the edge of an ice absorption peak in the mid-IR with a maximum around 830 cm\(^{-1}\). To cover also a case of strong scattering and weak absorption we used an index of refraction of \( (1.25 + 0.018i) \) for the same wavenumber region. This resulted in absorption and scattering cross-sections of \( 1.1 \times 10^{-7} \) and \( 5.9 \times 10^{-7} \text{ cm}^2 \), respectively \( (\omega_0 = 0.84) \). Optical depths for the different cloud scenarios are given in Table 1 for nadir direction and limb view with a tangent altitude at 11 km in the middle of the cloud. In case of nadir geometry only scenario 5 is optically thick, while in limb direction scenarios 3–5 are opaque.

5. Results for case \( \omega_0 = 0.24 \)

Fig. 1 shows the intercomparison between results from ARTS, and KOPRA(0) to KOPRA(3) for the case of strong absorption and for a line-of-sight crossing the middle of the cloud layer at 11 km tangent altitude. Spectra for lower altitudes are not shown here because results were very similar. As reference, the top row compares the cloud-free model runs. In the region between the strong emission lines where the gaseous atmosphere is optically thin and to which, thus, the comparison between the cloud calculations will refer, differences are below 0.5%.

The very thin cloud of scenarios 1 mainly introduces a broadband offset above the clear-sky spectrum due to the emission by the cloud particles and the scattering of radiation from the troposphere and the earth’s surface. The scattered contribution is the difference between KOPRA(0) and ARTS and accounts for about 35% of the total radiance. Since the second zero scattering scheme KOPRA(1) models a larger emission from the cloud particles the difference to ARTS is with 15% somewhat reduced compared to KOPRA(0). The results of both single scattering models, KOPRA(2) and KOPRA(3) are nearly identical to the multiple scattering approach with less than 0.5% difference.

In scenario 2, the radiance continuum is strongly increased and reaches with 2000 nW/(cm\(^2\) sr cm\(^{-1}\)) the value of the Planck function for the temperature at cloud altitude. The spectra of the single and multiple scattering models clearly show signs of radiance of tropospheric origin, like the downward pointing absorption features of the water vapor lines. These structures are missing in the calculations by both zero scattering schemes KOPRA(0) and KOPRA(1). The difference between those and ARTS are of the same magnitude as in scenario 1. The accuracies of KOPRA(2) and KOPRA(3) with less than 1% are still much better in case of neglecting scattering. However, with less than 0.5% KOPRA(3) fits closer to ARTS than KOPRA(2) with 1%.

In scenario 3 there is a further increase of the continuum radiance compared to scenario 2. The background value for the scattering models is now larger than radiation of a blackbody at the cloud position which is given by the result of KOPRA(1). The cloud is optically thick in limb, but not in nadir direction. Thus radiance from the warm troposphere and the earth’s surface increases the total signal. This is obvious from the fact that those calculated spectra which include
scattering, still exhibit the downward pointing features of the tropospheric water absorption lines. Differences show that the zero scattering models still underestimate the radiance by more than 10%. However, also the single scattering models differ from the ARTS reference by about 4.5% for KOPRA(2) and 2% for KOPRA(3).

The continuum radiance in scenario 4 is lower than in case of scenario 3 due to the fact that, though the cloud is still not opaque in nadir direction, less radiation from the troposphere reaches the particles along the line-of-sight which could scatter into the direction of the observer.
Furthermore, the typical tropospheric absorption features are not visible anymore. KOPRA(1) is with 3% closer to ARTS than KOPRA(2) with about 9% difference. This is due to neglecting second-order scattering in the scattering source function of first-order scattering radiances. KOPRA(3) with 2.5% deviation from ARTS still delivers the best result.

In case of scenario 5, which is optically thick in nadir and limb direction, the cloud closely resembles a black body. Thus, KOPRA(1) deviates from the multiple scattering model by only 0.1%. KOPRA(3) shows differences of 2% and KOPRA(2) of 11%.

6. Results for case \( \omega_0 = 0.84 \)

Results of the model intercomparison for the case of large scattering \( (\omega_0 = 0.84) \) are shown in Fig. 2. Though the optical depth of both cases is not very different (see Table 1) the continuum signal in the optically thin scenario 1 is increased by a factor of 1.4 compared to the case of strong absorption. This is due to the increased scattering of radiation originating in the warmer troposphere and on ground. Further, the flanks of the water vapor lines show downward pointing broader features also caused by scattered tropospheric radiation. With differences of 40% and more, the zero scattering models KOPRA(0) and KOPRA(1) are far off the reference while the single scattering schemes KOPRA(2) and KOPRA(3) deviate by only 1.5% and 1% from ARTS.

With about 3000 nW/(cm\(^2\) sr cm\(^{-1}\)) the background radiance of the reference spectrum for scenario 2 is 50% higher than the blackbody radiance at cloud altitude. Very strong absorption features appear at the position of the water vapor and in the flanks of the CO\(_2\) lines. Thus, as in scenario 1 zero scattering models are not capable to model these effects. However, compared to scenario 2 of the strong absorption case, also single scattering models have larger differences from the ARTS reference: KOPRA(2) underestimates the radiance by about 7% while KOPRA(3) calculates 3% lower values than ARTS.

For the first in limb direction optically thick scenario 3, the radiance calculated by ARTS reaches its maximum with about 3400 nW/(cm\(^2\) sr cm\(^{-1}\)), by a factor of 1.7 larger than the blackbody at cloud position. The single scattering model, however, does not follow this further increase, but results in lower radiances than in scenario 2. Thus, the differences with respect to the multiple scattering calculation increase up to 20% for KOPRA(3) and 35% for KOPRA(2).

In case of scenario 4 the ARTS radiances decreased and are only 1.2 times higher than the blackbody. Therefore, the zero scattering model KOPRA(1) compares best, with differences of 13%. The single scattering approach of KOPRA(3) is far off with up to 32% lower radiances.

In the optically thick scenario 5 ARTS and blackbody calculations (KOPRA(1)) are nearly identical with less than 1% difference. Thus, quasi no radiation from the lower troposphere reaches the instrument any more. The comparison with KOPRA(3) is with 8% differences much better than for scenarios 3 and 4.

7. Conclusion

The range of validity of zero and single scattering calculations for simulation of mid-IR limb-emission measurements of clouds was investigated by comparison with a multiple scattering code.
Scenarios from optically thin to thick clouds for the two cases of low ($\omega_0 = 0.24$) and high ($\omega_0 = 0.84$) single scattering albedo were used as baseline for the calculations. Fig. 3 shows the single scattering albedo for spherical ice particles in the mid-infrared as a function of wavenumber and particle radius. Obviously, the chosen values for $\omega_0$ cover a large fraction of the overall variability.

For the two in limb direction optically thin cloud scenarios 1 and 2, which resemble the cases of polar stratospheric clouds and subvisible cirrus clouds the single scattering approaches achieve...
results with maximum errors of a few percent. Thus, single scattering models are sufficient for evaluation of such measurements. Zero scattering schemes, however, show errors of more than 15% and 40%, depending on the single scattering albedo. From Fig. 3 it is clear that the zero scattering approaches can only be used for particle radii less than about 1 μm at the lower and less than 0.2 μm at the higher end of the shown spectral interval.

For in limb direction optically thick clouds the quality of single scattering calculations strongly depends on the single scattering albedo. The differences for the model KOPRA(3) range from only 2–3% for \( \omega_0 = 0.24 \) up to 10–30% for \( \omega_0 = 0.84 \). For the latter case larger errors appear for clouds which are optically thick in limb, but not in nadir direction and which, thus, still scatter a large amount of lower tropospheric radiation into the instrumental line of sight. Combining these results with Fig. 3 it is clear that for the regions with \( \omega_0 > 0.8 \) which are situated mainly above 1000 cm\(^{-1} \) for radii between 1 and 10–20 μm the single scattering approaches deliver results with uncertainties in the range of the investigated high scattering case. However, in the atmospheric window below 1000 cm\(^{-1} \), where the ice absorption peak is located, single scattering simulations in case of optically thick clouds should be reliable for particles less than 10–20 μm. For larger particles the single scattering albedo is around 0.5 over the whole wavelength region. There, we estimate that the accuracy of single scattering calculations lies between our extreme cases and is in the range of about 5–15%.

Comparing the results of different KOPRA options, in case of zero scattering KOPRA(l) and in case of single scattering KOPRA(3) achieve for all scenarios and cases better results than KOPRA(0) and KOPRA(2), respectively. The latter implementations underestimate radiances because they neglect the scattering source term while KOPRA(1) and KOPRA(3) compensate for this by increasing the locally emitted radiation through replacing the absorption coefficient by the extinction coefficient in the direct and the scattered rays, respectively.

A further outcome of this study is that in case of large single scattering albedo and clouds which are optically thick in limb, but thin in nadir direction the continuum radiance can be by a factor of up to 1.7 enhanced with respect to the blackbody radiation at cloud top altitude. This is a consequence of the scattering of radiation from the warm troposphere and the earth’s surface into the line-of-sight of a limb viewing instrument. Such strong effects are expected to be detectable in recently measured spectra by MIPAS on Envisat or in data of previous missions of mid-IR limb-
emission sounders like CRISTA (Cryogenic Spectrometers and Telescopes for the Atmosphere) [15] or CLAES (Cryogenic Limb Array Etalon Spectrometer) [16].

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References

