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COMPARISON OF WEIGHTING FUNCTION CALCULATIONS BY LINEARIZED RADIATIVE TRANSFER MODELS

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Linearized radiative transfer models provide efficient algorithms to calculate the weighting functions and the layer efficient air mass factors (AMFs), which are used for solution of inverse problems for determination of gas distribution in the atmosphere. Limb scattered geometry, which is used in a few new space observation systems (OSIRIS, SOLSE/LORE, SCIAMACHY, GOMOS), is most sensitive to specialties of an algorithm for calculation of the weighting functions, because it has the sharp weighting functions. The first results of a comparison of the weighting function computations by the MCC++ spherical model and the CDI pseudospherical model are presented.

Compared characteristics

Traditional radiative transfer models allow estimating fluxes or intensities of radiation. Development of optical remote sounding stimulates designing of models able to an efficient calculation of derivatives of radiance with respect to optical parameters of an atmosphere, which are necessary for solution of inverse problems. We present the first results of comparison of such derivatives calculated for limb geometry and spherical atmosphere.

In another notation these derivatives are termed weighting functions. In case of spherical shell atmosphere, we may use also the efficient air mass factor (AMF), $m(h)$, of the layer located at the altitude *h*, which is proportional to the weighting function at *h*, $w(h)$:

$$w(h) = -L_{+} \cdot \sigma \cdot m(h) \cdot I \, .$$

Here L_{+} - is the geometric thickness of the atmospheric layer under investigation, σ - cross section of the gas, I - intensity of scattered light. The factor $m(h)$ has meaning similar to air mass factor for direct light. For a layer of a finite thickness, the effective AMF is equal to the weighted mean of the pathlength of photons, falling to a detector, normalized to the layer thickness. The magnification for the light path as compared to the geometric thickness of the layer, is caused by the facts that light may multiply and not-normally cross the layer.

Radiative transfer models

Two linearized radiative transfer models took part in the comparison:

(1) The MCC++ model (denoted in figures like OP) uses the Monte Carlo method for simulation of the multiple scattering light [*Marchuk et al. 1980*]. The model calculates radiance [Postylyakov et al. 2001] and weighting functions for a spherical shell atmosphere with polarization exactly. The current version of the model efficiently calculates weighting functions with respect to gaseous absorption [*Postylyakov 2003a, 2003b*]. A theoretical background for calculation of weighting functions with respect to aerosol scattering was developed [*Postylyakov 2003c*].

(2) The CDI/CDIPI model (denoted in figures like AR) is able to calculate the radiation field in a spherical shell atmosphere without polarization. The weighting functions with respect to absorption are calculated approximately for a pseudospherical atmosphere

using the CDI code. The suggested approach involves the Picard iterative approximation to solve the radiative transfer equation in its integral form [*Rozanov 2001*]. The radiation field calculated by solving the integro-differential radiative transfer equation in a pseudo-spherical atmosphere is used as an initial guess for the iterative scheme.

Modifications of the models, which took into account Lambertian reflection of surface, but ignore polarization and refraction took part in the comparison.

Optical model of atmosphere

A comparison was carried out for limb-viewing geometry coinciding with experiment SOLSE/LORE in the shuttle flight STS-87 [*Oikarinen et al. 2001*, *Loughman et al. 2003*]. Solar angles for line of sight tangent point: zenith 39.29°, azimuth 111.74°.

Tropical air density and ozone concentration profiles were taken from the MODTRAN model [*Berk et al., 1989*]. Total ozone column was scaled to 275 DU. Ozone cross section taken from Burrows et al. [*1999*] and Rayleigh scattering cross section from Bates [*1984*] were used. Aerosol extinction profile corresponds to MODTRAN one with surface visible range 50 km and background stratospheric condition (Fig.1). Henyey-Greenstein phase function with asymmetry factor g=0.7 at all altitudes and wavelengths was implemented. Albedo was equal to 0.95.

We determine optical parameters of atmosphere at grid with step 1 km up to 100 km, and performed calculations at wavelengths equal to 325 nm, 345 nm and 600 nm.

The efficient AMFs were calculated for layers with 1 km thickness.

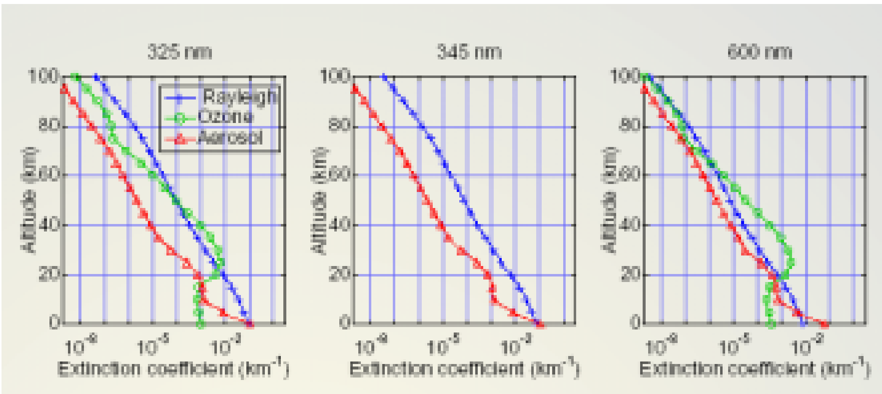

Fig.1. Extinction profiles used in comparison [*Oikarinen et al. 2001*].

Analysis of results

Percentage differences ((AR-OP)/OP) of intensities calculated by the models under comparison is shown in Fig.2. The single-scattering intensities differ by no more than 0.2%, what confirms a good agreement of ways of usage of the optical parameters of an atmosphere by two models. The differences of total intensity are less that 0.8% at 325 nm, and less than 2.8% at 345 and 600 nm. Some of possible causes of such differences are discussed in [*Loughman et al. 2003, Postylyakov et al. 2003*].

As a sample, the layer AMFs at 325 nm calculated by the MCC++ (OP) model for the total scattering light is shown in Fig 3a. The maximum of the layer AMF is located above the tangent height of the line of sight. If the tangent point is situated bellow the ozone maximum, than the layer AMFs have a fuzzy maximum. Else they are sharp and have the maximum just at the tangent height. The AMFs for tangent height bellow the ozone maximum have smaller maximal values. Such effect of the ozone on the layer AMFs is absent at 345 and 600 nm.

Percentage differences of the AMFs calculated by two models for single scattering at 325 nm is shown in Fig. 3b. The differences are less than tenths percent for most of altitudes. The maximal differences are less than 1%, and are located just above the tangent heights. Such location of the maximal difference is a manifestation of a high sensitivity of the limb AMFs to grid step and to features of algorithms, simulating radiative transfer.

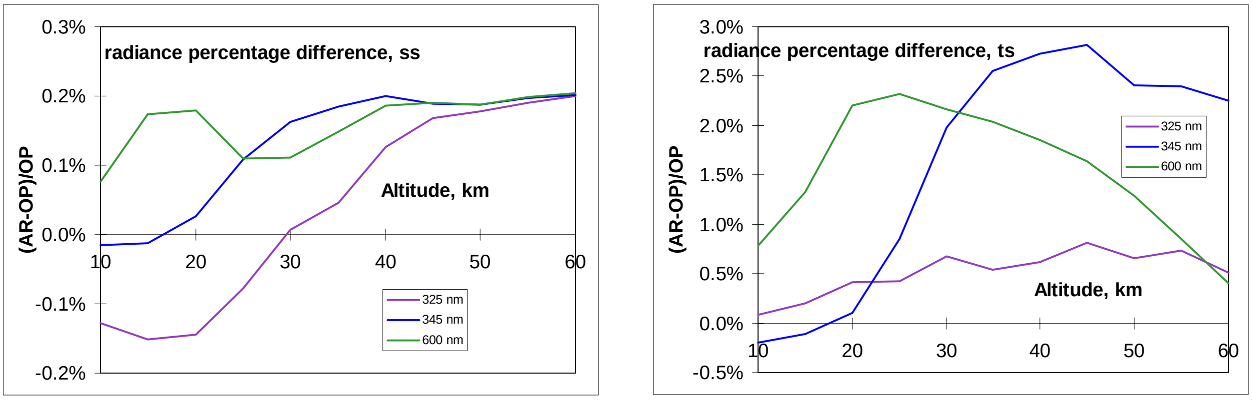

Fig. 2. Percentage differences of scattered limb intensities for single (a) and total (b) scattering.

The comparison of the AMFs calculated with account of total scattering (Figs.3c, 3d, 4d, 5d) identifies three main atmospheric zones with the specific manifestations of features of the computational methods and their accuracy.

(1) The first zone is located two layers over the tangent height. In this zone, the difference between two models did not exceed 1%. The AMFs are high here (as a rule, they range from 40 to 8 and decrease as the height increases). The AMFs are predominantly determined by single scattering (Lower stratospheric layers at 325 nm represent exceptions.)

(2) The second zone represents two layers located just over the tangent height h_0 . Because of weak absorbtion in layers above, the AMFs in the third zone sharply varies with height *h* approximately like $1/\text{sqrt}(h-h_0)$. This peculiarity causes a strong dependence of the computed AMFs on the algorithm and its actual height resolution. It is necessary to give attention to the agreement between the resolutions of the computational algorithm and measuring instrument. For this zone, the typical AMFs range between 60 and 80. When 1 km grid was used, the difference between the MCC++ and the CDI calculations of AMFs averaged over two layers of this zone was no more than 1.5%. To reach a good agreement for each 1-km layer inside second zone, the CDI model made calculation at grid with step of 1/45 km. In this case differences were no more than 1% for each 1-km layer.

(3) The third zone is located below the tangent height. In this zone, the layer AMF are determined completely by multiple scattering. The AMFs range typically between 1.8 and 2.2 and increase up to 3.8 for the troposphere and the visible spectral region. The absolute difference between two models is still small; however, the relative difference reaches 32% for heights of 50-60 km. Apparently, these differences are caused by discrepancies occurring in the multiple scattering computations performed with the spherical (MCC++) and pseudospherical (CDI) models, which is known issue for these heights. Notice that the retrieval errors should be scarcely affected by these discrepancies because the AMFs in the third zone are small.

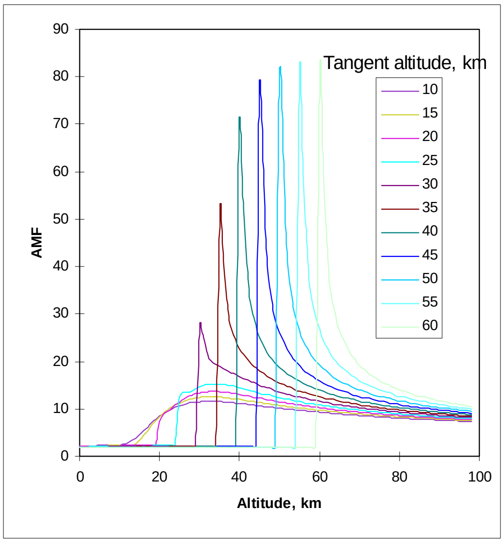

Fig. 3a. The layer air mass factors for 325 nm, calculated by the MCC++ (OP) model for all orders of scattering for different tangent altitudes) of the direction of observation.

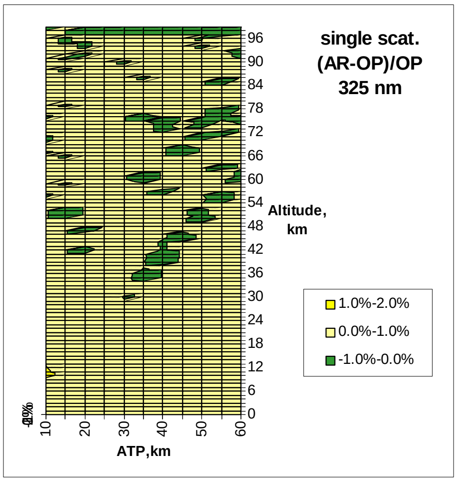

Fig. 3b. Percentage differences of the layer air mass factors calculated by the MCC++ (OP) and CDI (AR) models for single scattering vs altitude of the layer and altitude of the tangent point (ATP) of the line of sight. Wavelength=325 nm.

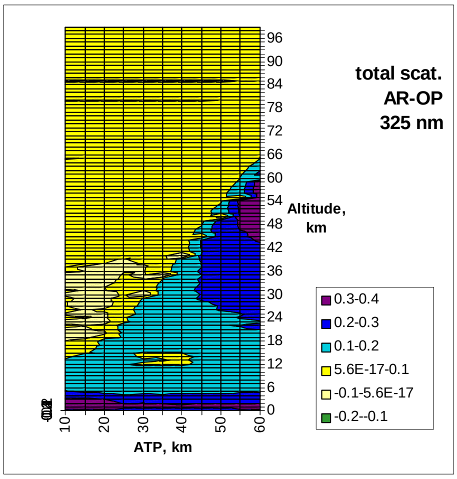

Fig. 3c. Absolute differences of the layer air mass factors calculated by the MCC++ (OP) and the CDI (AR) models for total scattering vs altitude of the layer and altitude of the tangent point (ATP) of the line of sight. Wavelength=325 nm.

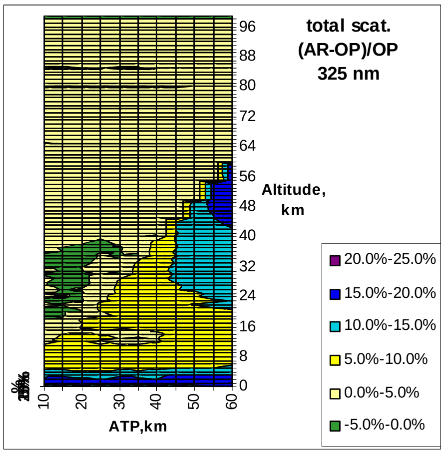

Fig. 3d. The same what in Fig.3b, but for total scattering.

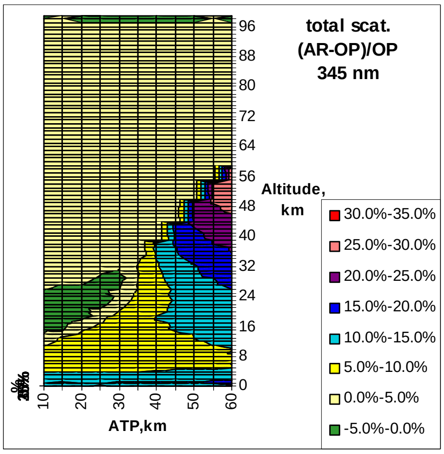

Fig. 4d. The same what in Fig.4, but for total scattering and for 345 nm.

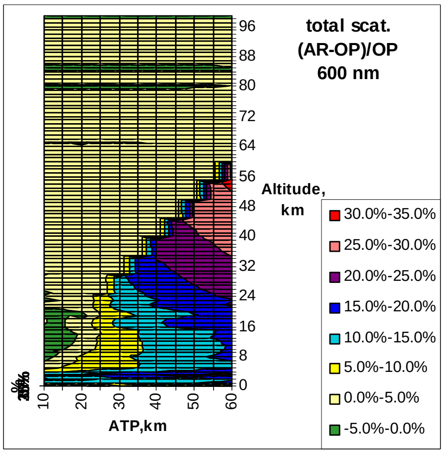

Fig. 5d. The same what in Fig.4, but for total scattering and for 600 nm.

Conclusions

The comparison shows overall reasonable agreement between the intensity and the efficient AMF (weighting function) calculations preformed by two linearized radiative transfer models, MCC++ and CDI/CDIPI, for all orders of scattering in a spherical atmosphere.

The differences of intensity calculation were less than 1% at 325 nm, and less that 3.8% at 345 and 600 nm.

The efficient AMFs calculated by two models have differences less than 1% above the line of sight (LOS).

The absolute differences of the efficient AMFs below the LOS are less than 0.4. This gives up to 30% of the AMFs at altitudes near 50-60 km and near the ground. The more probable cause of differences near 50-60 km is the different accuracy of calculation of multiple scattered radiance by the full spherical (MCC++) and approximate pseudospherical models (CPI). The single-scattering AMFs exactly calculated by both models hide differences of multiple-scattering AMFs above the LOS. These differences and the increased differences in the single-scattering AMFs near the LOS may help to understand differences in intensity calculation and are an area of the future research.

Comparing the absolute AMF differences below the LOS with the maximal AMFs at 345 and 600 nm, typically reaching 70-90, we assume that such difference may be not very important, when the AMFs are used for solution of inverse problem, using these wavelengths, and investigated gas has smooth vertical profile. If a gas has a maximum in near-ground layers, the AMF diverse near ground may provoke distortion of retrieval at all altitude. At 325 nm the AMF maximums decrease that may increase the effect of the AMF diverse.

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LINEARIZED SPHERICALRADIATIVE TRANSFER MODEL MCC++

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A linearized spherical radiative transfer model MCC++ was designed for usage in retrieval algorithms. It may efficiently calculates the weighting functions and the air mass factors simultaneously with the intensities taking into account multiple scattering. Scattered radiance is calculated for a spherical atmosphere taking into account the polarization of light, aerosol loading of atmosphere and the Lambertian surface albedo. The MCC++ model is shortly presented. The weighting functions and air mass factors calculated for NDSC twilight measurements for single scattering and for total scattering are compared. Time of calculations for different observation geometries was calculated.

1. Applications of linearized radiative transfer models

Linearized radiative transfer models allow to calculate efficiently both radiance and its derivatives with respect to the optical characteristics of an atmosphere (gas absorption, aerosol scattering, surface albedo, aerosol phase matrix, etc). These values may be applied for [*Postylyakov 2003a*]:

- Solution of inversion problem:

  Equation describing dependence of measured radiance $I(\mathbf{n})$ from vector of optical characteristics $\mathbf{n} = (n^1(h) \quad n^2(h) .... \quad n^i(h) \; ... \; n^{m-1}(h) \quad n^m(h)) = \mathbf{n}_0 + \Delta\mathbf{n}$ for retrieval:

  $$I(\mathbf{n}) = I(\mathbf{n}_0) + \sum_{i=1}^{m} \int \frac{\partial I(\mathbf{n}_0)}{\partial n^i} \Delta n^i(h) dh + o(\|\Delta\mathbf{n}\|) + \nu ,$$

  ν - noise of measurement.

  Radiance $I(\mathbf{n})$ and derivatives $\frac{\partial I(\mathbf{n}_0)}{\partial n^i}$ are calculated by a linearized models.

- Fast calculation of spectral radiance:

  Radiance at wavelength λ:

  $$I(\lambda) = I(\lambda_0) + \frac{\partial I(\lambda_0)}{\partial \lambda}(\lambda - \lambda_0) + o(\lambda - \lambda_0) =$$

  $$I(\lambda_0) + \sum_{i=1}^{m} \int \frac{\partial I(\mathbf{n}(\lambda_0))}{\partial n^i} \frac{\partial n^i(\lambda_0)}{\partial \lambda} dh(\lambda - \lambda_0) + o(\lambda - \lambda_0)$$

Radiance $I(\lambda)$ and derivatives $\frac{\partial I(\lambda_0)}{\partial n^i}$ are calculated by a linearized models. Here $\frac{\partial n^i(\lambda_0)}{\partial \lambda}$ - differential cross section.

2. Model MCC++

The model MCC++ [*Postylyakov 2003a 2003b*] simulates radiative transfer in the spherical atmosphere using Monte Carlo and direct integration methods. To simulate multiple scattering, the MCC++ model realizes two Monte Carlo methods: the method of conjugate walk and the method of modified double local estimation [*Marchuk et al. 1980*]. The method of double local estimation has a better computation time if the simulation is performed for twilight under conditions of large solar deep angles exceeding 3 - 5^o. To compute the single-scattering radiance, a procedure of direct integration of the source function is realized in line with the Monte Carlo one. A combination of the Monte Carlo method to simulate multiple scattering with the direct integration procedure to simulate single scattering has the best time of the computer simulation. The approximation of the spherically symmetrical atmosphere is applied also to shorten the time of the simulation. A new quick algorithm [*Postylyakov 2003b*] for simultaneous evaluation of the weighting functions (derivatives) with respect to gas concentration and air mass factors together with intensity was implemented in the model. This algorithm spends only 1.2-1.8 times as much time as calculation of intensity alone. The MCC++ code has vector (with polarization) and scalar versions, and takes into account surface albedo, aerosol scattering and absorption. The model is using C++, what makes possible to release like the C++ templates different versions of algorithm and widely to use code recycling.

3. Validation of the MCC++ model

The vector and scalar versions of the MCC++ code have been validated against other spherical and pseudospherical radiative transfer models for different geometries of observations, and against field measurements:

- Comparison of models for ground-based zenith-viewing twilight geometry [*Postylyakov et al. 2001*];
- Comparison with twilight field measurements of polarized radiance [*Postylyakov et al. 2003b*];
- Comparison of weighting function calculations for limb-viewing geometry [*Postylyakov and Rozanov 2003b*];
- Limb-viewing scattered light calculations [*Loughman et al. 2003*];
- Fine comparison of models for limb-viewing geometry [*Postylyakov et al. 2003c*].

4. Time of radiance calculation for different geometries

The MCC++ model took part in a comparison of computation times for limb-viewing geometry [*Loughman et al. 2003*]. Time of a computation of the MCC++ model for both the scalar and the vector cases for 1% precision was approximately equal to time of the pseudospherical codes (see Table 1). The other exact spherical models had times within 5-13 min. Table 1 shows also times of a later version 03/2002 of the MCC++ code capable to compute the intensities and all layer AMFs simultaneously. These times are still comparable with times spend by pseudospherical codes to calculate intensities only.

Table 1. Computation times of a simulation of limb scattered radiance by the MCC++ and pseudospherical models. Time for one wavelength and all tangent altitudes from 10 to 60 km at step of 5 km is given.

Model	Time of computation	Computer
Pseudospherical models, scalar code, pure Rayleigh atmosphere, times from Loughman et al. [2003]		
CDI	5 sec	Athlon 750 MHz
LIMBTRAN	5-10 sec (depending on grid)	SGI
Spherical model, pure Rayleigh atmosphere, times from Loughman et al. [2003]		
MCC++ (scalar), 01/2001	$3^{(*)}$ –$17^{(**)}$ sec	Pentium II 450 MHz
MCC++ (vector) , 01/2001	$3^{(*)}$ –$23^{(**)}$ sec	Pentium II 450 MHz
Spherical model, atmosphere with aerosol		
MCC++ (scalar), 03/2002	$5^{(*)}$ -$6^{(**)}$ sec	Athlon 1460 MHz
Simultaneous computation of radiance and weighting function, spherical model, atmosphere with aerosol		
MCC++ (vector), 03/2002	$6^{(*)}$ -$10^{(**)}$ sec	Athlon 1460 MHz

$^{(*)}$ - time for 600 nm, $^{(**)}$ - time for 325 nm or 345 nm.

The MCC++ model allows to calculate the weighting functions necessary for inversion of Umkehr ozone measurements for 18 min (see also Section 6). The Umkehr weighting functions are calculated simultaneously at 6 wavelengths from 306.3 to 329.5 nm and 8 solar zenith angles from 77^O to 90^O. for 20 atmospheric layers. Time was estimated for calculation with accuracy 0.1-1% at the single processor PC based on the AMD Athlon 1460 MHz.

Table 2 shows time of calculation of the weighting functions for retrieval the vertical profile of nitrogen dioxide. Measurements of solar radiation scattered in the zenith during twilight at 430-450 nm are used for retrieval (see also Section 5). Time of calculation varies as solar zenith angle changes. Time was estimated for atmosphere with 96 layers up to 120 km. The same computer as for Umkehr method was used.

Table 2. Time of calculation of the weighting functions at 450 nm with 1% precision for different solar zenith angles *Z* by the MCC++ model.

Z	Time, min
84	0.003
86	0.005
88	0.009
89	0.012
90	0.019
91	0.033
92	0.066
93	0.163
94	0.465
95	1.670
96	12.064

5. AMFs of twilight sounding of NO_2 by the DOAS method

Spectral measurements of intensity of light scattered in the zenith during twilight give information about vertical distribution of nitrogen dioxide below 45 km. The DOAS technique is used to derive slant column of NO_2 from the intensity. A comparison of layer air mass factors (AMFs) calculated using total scattering with approximate AMFs evaluated for single scattering is shown in Figure 1. Approximate AMFs underestimate AMFs below altitude of 20 km and overestimate above 30 km for all solar zenith angle from $z=84^0$ to $z=96^0$. Differences reach their maximum between 5 and 10 km for all solar zenith angles z. The difference is equal here to -30% of AMFs at $z=84^0$ and to -70% of AMFs at $z=96^0$. Between 20 and 30 km single-scattering AMFs give more than 95% of AMFs at $z<93^0$, but difference runs up to -25% at $z=96^0$. Approximate calculations have negligible difference from AMFs above 30 km for $z<93^0$. But difference increases from $z=94^0$ and amount to +20% at $z=96^0$.

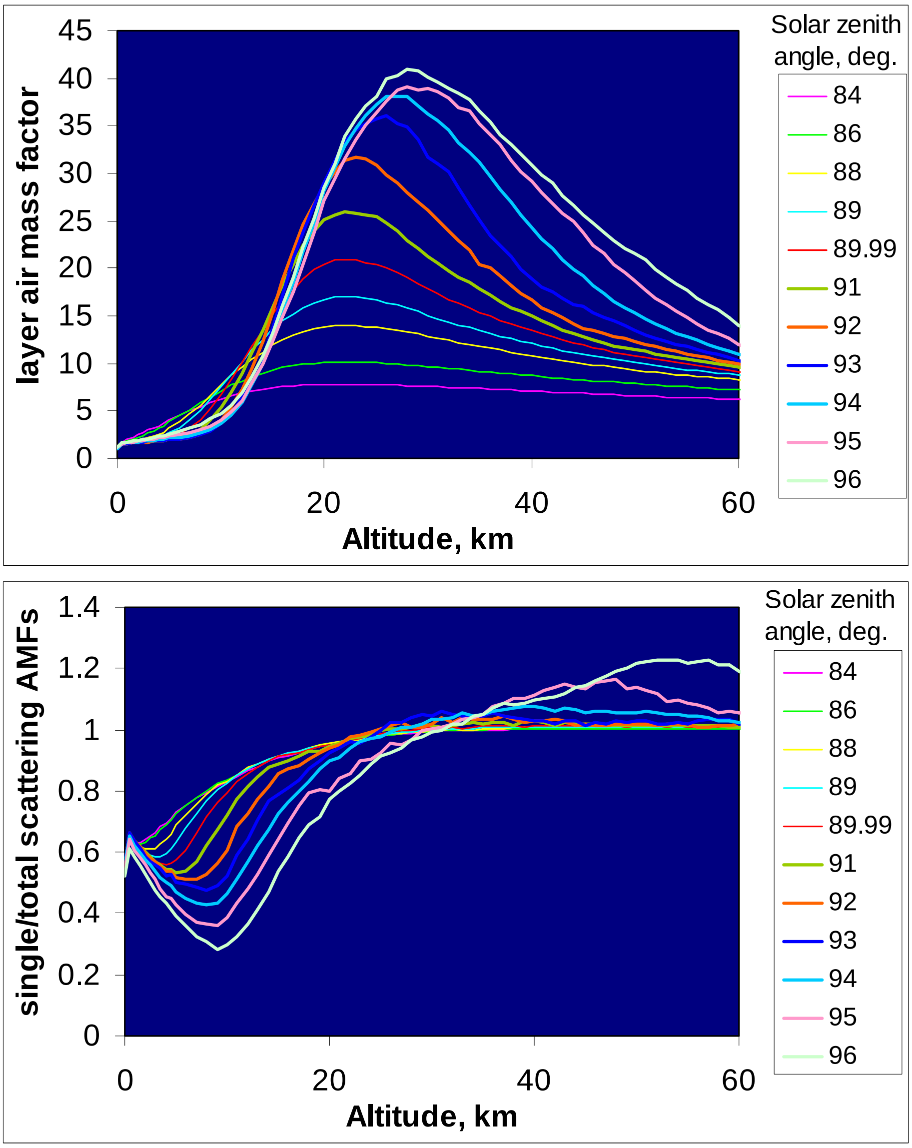

Fig. 1. The exact AMFs for NO_2 twilight observations (450 nm) and ratio approximate/exact AMFs. Albedo is equal to 0.5.

6. Effect of single-scattering weighting function on accuracy of Umkehr ozone

The Umkehr measurements at network of the Brewer spectrophotometers are source for determination of the ozone vertical distribution. A standard network retrieval algorithm uses approximative scheme to compute multiple scattering of light. A multiple scattering correction is subtracted from measured intensities, but the algorithm uses the weighting functions (WFs) calculated for the single scattering approximation. The simplified scheme for consideration of the WFs results in increased errors of the ozone retrieval, which was first noticed in paper [*Elansky and Postylyakov, 2000*]. The standard network and the extended [*Elansky et al., 1999*] Umkehr retrieval algorithms are considered. Figure 3 shows the errors of ozone retrieval by the algorithms, using the approximate WFs computed for single scattering, against ones, based on the exact WFs computed for total scattering. All algorithms used the intensity computed for total scattering. Inaccuracies of the WFs lead to an enhanced uncertainty in the ozone retrieval not only below 15-20 km, where the effect of multiple scattering is significant, but also for higher atmospheric layers.

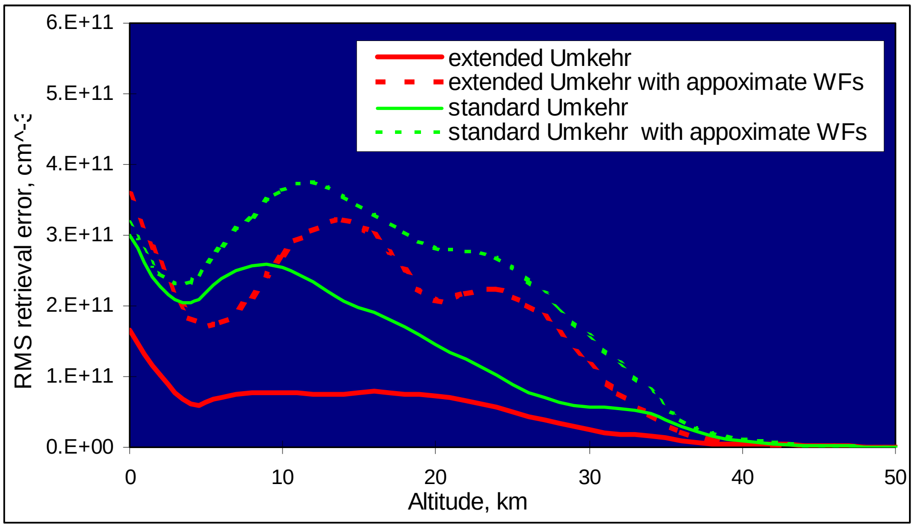

Fig. 3. Ozone retrieval rms errors of the extended and standard Umkehr algorithms for the exact and approximative WFs.

7. Conclusions

A new linearized radiative transfer model MCC++ was developed. The model calculates the weighting functions/derivatives with respect to absorption in atmospheric layers simultaneously with intensities. It simulates radiative transfer in spherically symmetrical atmosphere, taking into account polarization and surface albedo. The MCC++ code successfully passed comparisons against other RT models, which included the comparison of the weighting function calculations, the comparison for Sun up to 6^{O} bellow the horizon for simulation of ground-based observations, the comparison for scattering limb geometry. The developed model efficiently uses computational time. Theory of calculation of the weighting functions/derivatives with respect to aerosol scattering, taking into account polarization of light, was developed. Implementation of their calculation in a program code to be carried out.

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