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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A modified band approach for the accurate calculation of on-line photolysis rates in stratospheric-tropospheric Chemical Transport Models" *by* J. E. Williams et al.

J. E. Williams et al.

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We would like to thank referee #1 for their concise and instructive review of our paper.

We feel that by adopting many of the suggestions of the referee we have made substantial improvements to the manuscript. We address the concerns and queries raised below:

General Remarks:

We acknowledge the point made by the referee regarding the clarity of the discussion performed throughout the paper. As a result we have dispensed with both of the appendices and brought all details related to the development of the pseudo-spherical

radiative transfer solver forward to section 3. Moreover, we have re-arranged to text in sections 2,3 and 4 so as to improve on the issue of forward referencing.

The referee mentions that further comparison of the various reference codes with either DISORT or the full spherical reference model would have been useful in determining the overall error of the scheme. As the DISORT model does not currently include a full sphericity component it does not serve as a good benchmark for simulations performed for high incident zenith angles. The full spherical reference model used in the manuscript is computationally expensive and therefore cannot be used to derive actinic fluxes for each spectral bin of the working grid throughout the entire column.

The product of both the absorption co-efficient and the quantum yield within a particular band interval for any chemical species determines the contribution each band interval makes towards the photolysis rate of that species. This is exemplified by the differences observed in the resulting errors for JO3 -> O1D as a result of updating the quantum yield (discussed in section 4.3, pg 3529). By considering this product with respect to wavelength one may make an estimate as to how sensitive a particular photolysis rate is to the occurrence of enhanced scaling ratios. In general, if a particular species has broad absorption characteristics the effect of enhanced scaling ratios will most likely be moderate due to the cancellation of errors which occurs across band intervals. However, if a species absorbs preferentially in the UV spectral region (lambda$<$320nm) the effects of enhanced ratios will be more important. We suggest that it is wise to assess the errors associated with each new chemical species by comparing the resulting profiles against a suitable reference.

In order to provide more details concerning the computational efficiency of the method we have included details regarding the computational expense of using the PIFM-PS solver and the modified band method for the one-dimensional model atmosphere used throughout the paper.

Specific Comments:

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Page 3514: The definition of the acronym has now been included.

Page 3527: The determination of the new scaling wavelengths was performed manually rather than by the use of any type of optimization procedure. The fact that the band limits for bands 2-4 have a large impact on the resulting errors introduced by the band approach meant that the number of permutations needed to obtain the optimal values was significantly reduced. The details concerning the selection criteria for the optimal band settings has been expanded in the text thus: “A criterion used for the selection of the optimal band settings was that the errors introduced by the band approach should not be greater than ś10% for the majority of the chemical species. Additionally, the errors should decrease compared to those obtained using the original band settings for almost all of the chemical species. “

Page 3529: The referee is referred to the remarks made in the General Comments section above concerning this point.

Page 3533: We agree with the referee’s comments regarding the emphasis of the discussion provided in Section 5.1. In response we have changed the emphasis of this section to focus on the error budgets calculated for select J values in the presence of aerosols.We also change the associted figure to show a contour plot of the associated error budgets in the sza range 72-85 deg.

Page 3535: The text has been amended accordingly.

Page 3540: In line with the suggestions of the referee we have moved the details contained in the Appendices forward to Section 3.

Page 3537: We have amended the text thus: “The errors on the resulting J values are generally of the order of approx. 2% for the middle and upper atmosphere. These increase up to approx. 40% below 20km for certain species (notably O3 and HNO4) although the magnitude of such rates at these high zenith angles is so small that the effect of such errors on the chemical tracer fields is minimal. “

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Figures: Figures 3 and 4 have been combined and the lighter colours changed to improve visibility. The figure legend for Fig. 3 has been modified accordingly taking into account the suggestions of the referee. Figures 5 through to 7 have been re-formulated so that direct comparisons can be made between the performance of the original and modified band methods. The differences between the error budgets shown in Figs. 10 and 11 for sza above and below 90 deg. arise from an erroneous comparison being made for the sza range of 85-90 deg. We have subsequently corrected the comparison and combined Figs. 10 and 11 so as to provide a continuous comparison over the sza range of 85-93 deg.

The colour scheme chosen for figures 5 to 9 has been re-defined in order to make the distinction between positive and negative errors more vivid. Due to the errors for the stratospheric species being relatively small near the top of the atmosphere we wish to retain our original contouring for figures 10 and 11 rather than using contours of 5% (as chosen for the tropospheric comparisons).

The purpose of performing comparisons versus a “final working version” of the code is to provide the potential user with a realistic error estimate which pertains to a version of the modified band method which will be implemented online. The authors feel that, even though removing the effects of the look-up tables would give smoother contours, such errors would not pertain to the version applied in a higher scale model.

Technical Corrections:

The suggestions and errors made by the referee have all been incorporated.

Interactive comment on Atmos. Chem. Phys. Discuss., 6, 3513, 2006.

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