MODTRAN3: Suitability as a Flux-Divergence Code

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Introduction

The Moderate Resolution Atmospheric Radiance and Transmittance Model (MODTRAN3) is the developmental version of MODTRAN (Abreu et al. 1991) and MODTRAN2 (Anderson et al. 1993). The Geophysics Directorate, Phillips Laboratory, released a beta version of this model in October 1994. It encompasses all the capabilities of LOWTRAN 7 (Kneizys 1988), the historic 20 cm^{-1} resolution (full width at half maximum, FWHM) radiance code, but incorporates a much more sensitive molecular band model with 2 cm^{-1} resolution. The band model is based directly upon the HITRAN (Rothman et al. 1992) spectral parameters, including both temperature and pressure (line shape) dependencies. Validation against full Voigt line-by-line calculations (e.g., FASCODE [Clough et al. 1988; Clough et al. 1981]) has shown excellent agreement (Anderson et al. 1993). In addition, simple timing runs demonstrate potential improvement of more than a factor of 100 for a typical 500 cm^{-1} spectral interval and comparable vertical layering.

Not only is MODTRAN an excellent band model for "full path" calculations (that is, radiance and/or transmittance from point A to point B), but it replicates layer-specific quantities to a very high degree of accuracy (Theriault et al. 1993). Such layer quantities, derived from ratios and differences of longer path MODTRAN calculations from point A to adjacent layer boundaries, can be used to provide inversion algorithm weighting functions or similarly formulated quantities. One of the most exciting new applications is the rapid calculation of reliable IR cooling rates (Kimball 1993), including species, altitude, and spectral distinctions, as well as the standard spectrally integrated quantities. Comparisons with prior line-by-line cooling rate calculations are excellent, (Clough et al. 1992; Ellingson and Fouquart 1991) and the techniques can be extended to incorporate global climatologies of both standard and trace atmospheric species (Summers 1993).

MODTRAN Description

Background

Because MODTRAN and MODTRAN2, along with LOWTRAN 7, have been previously described in the literature, only a brief discussion of additional enhancements is included here. The MODTRAN series of codes encompasses the same set of common elements (e.g., spherical refractive geometry, solar and lunar source functions, scattering [Rayleigh, Mie, single and multiple], default atmospheric profile descriptions [gases, aerosols, clouds, fogs, and rain], plus molecular continua [H_2O, CO_2, O_3, O_2, N_2] and simplified user interfaces for more specific atmospheric and instrumental characterization [Isaacs et al. 1986; Anderson et al. 1986; Shettle 1990; Clough et al. 1989]).

The 2 cm^{-1} spectral resolution of the MODTRAN band model is based on the original development of Berk, Bernstein, and Robertson (1989), with recent modifications for 0_3 and CO_2 (Acharya et al. 1993). With the release of the HITRAN94 data base, the two-parameter equivalent width band model (sensitive to both temperature and pressure) will be immediately updated to accommodate the new spectroscopy. In addition, the water vapor continua (both self and foreign) will be modified to remain consistent with those in FASCODE and the combined DOD/DOE (line-by-line radiative transfer model) recommendations. If necessary, multiple options for the continua will be maintained. The band model parameters have been calculated for 12 species at five temperatures from 200-300K, basically spanning the range of primary interest for atmospheric applications under conditions of local thermodynamic equilibrium. The band model temperature ranges will ultimately be extended slightly in MODTRAN3 to accommodate the colder tropopause temperatures encountered in the winter polar regions.

Other New and Proposed Modifications

Some specific new enhancements have been implemented for MODTRAN3. These include three solar corrections: a correction/replacement of the vis/near IR solar irradiance;[(a)] a more exact single scattered low sun geometry where refractive bending is sufficiently accurate to determine path tangent altitude;[(b)] and an accommodation for direct very low sun irradiances (solar zenith angles greater than 90°).[(c)]

Two of the more important enhancements to appear in MODTRAN3 relate directly to climate change studies. First, the chloro-fluorocarbon (CFC) and other heavy molecules (whose spectroscopic properties appear on the HITRAN92 data base as temperature-dependent cross sections) have been incorporated into pseudo-band models (see Figure 1, as implemented by Zachov et al. 1994). Second, the ability to alter the maximum number of layers in MODTRAN through the use of a parameter statement replaces the original artificially imposed 33-layer limitation, but requires that the code be recompiled (Conant 1993). A third important modification will be the eventual adoption of the DISORT (discrete ordinate) multiple scattering algorithm (Stamnes et al. 1988).

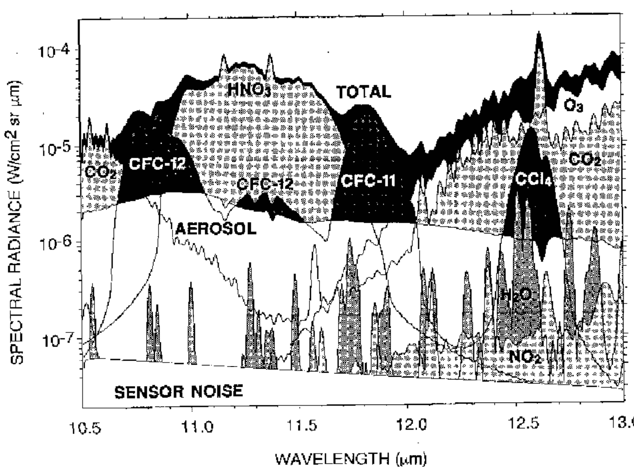

Figure 1. MODTRAN3 radiance contributions by species, including CFCs; 15-km tangent height.

(a) As suggested by B.-C. Gao and R. Green, private communication.
(b) A. Berk, private communication.
(c) G. Anderson, private communication.

The extension of the code into the ultraviolet will include O_2 (Conant 1993; Anderson et al. 1992), SO_2 and $N0_2$, along with upgraded ozone Chappuis and Wulf bands in the visible and near-IR.[(a)]

Calculation of Atmospheric Cooling Rates Using MODTRAN2/3

Technique

A preliminary technique for calculating atmospheric cooling rates has been developed based on infrared radiance calculations, initially using MODTRAN2, and more recently using the developing MODTRAN3 with a much more sophisticated radiance algorithm (Bernstein 1994). Comparisons of both versions against benchmark line-by-line calculations shows very good agreement. However, the "linear in tau" approximation, suggested by Wiscomb (1976) and Ridgway et al. (1991) as currently implemented in the released version of MODTRAN3, is used here to correct for the layer temperature-gradient problem in optically thick layers. The more exact Bernstein approach provides a correction for arbitrary opacities across the temperature gradient.

All the inferred cooling rate calculations presented here are currently for clear sky using several model atmospheres. The initial cooling rate results are compared with similar calculations performed with FASCODE for water vapor only (Clough et al. 1992). The current method follows that of Clough as closely as possible so that differences in the results can be attributed primarily to the differences between the line-by-line and band models. Additional MODTRAN3 cooling rate comparisons for CO_2 and O_3 have also been made to published LBL results (Ellingson and Fouquart 1991) yielding excellent agreement.[(b)] Note that the comparisons use the original FASCODE continua (Clough et al. 1989), rather than the newer proposed values.

(a) E. Shettle and P. Acharya, private communication.
(b) Bernstein, L. S., P. K. Acharya, D. C. Robertson, G. P. Anderson, J. H. Chetwynd, L. M. Kimball; Very Narrow Band Model Calculations of Atmospheric Fluxes and Cooling Rates Using the MODTRAN Code; in preparation.

Radiance Calculation

The radiance calculations, as noted, follow the development of Clough et al. (1992) and will not be repeated here. However, for a band model, it is necessary to replace the exact Beer's Law quantities with $\tau_{eff'}$ and $T_{eff'}$ (both still functions of v), the effective layer optical depths and transmittances, respectively. These are derived from the ratios and the log ratios of the full path transmittances (T_ℓ, the transmittance from the observer to layer ℓ) between adjacent layers, e.g., $\tau_{eff'} = \ln (T_\ell/T_{\ell+1})$ and $T_{eff'} = (T_\ell/T_{\ell+1})$.

Comparison of Transmittance and Radiance Calculations: FASCODE vs. MODTRAN3

Anderson et al. (1993) show a comparison of MODTRAN2 vs. FASCODE transmittances for a horizontal path (15-m altitude and 500-km range) for the spectral range 500 to 3000 cm^{-1}. The accompanying statistical comparisons suggest that the improved MODTRAN3 will usually be within one percent RMS difference for the full spectral range, with specific errors as large as 10% over narrow spectral ranges associated with the edges of the strong CO_2 bands. A very preliminary comparison of MODTRAN3 radiances with the new ICRCCM (InterComparison of Radiative Codes in Climate Models) comparison data appears in Figure 2.[(a)]

Flux Calculation

The up-welling and down-welling thermal fluxes of radiant energy at a given atmospheric level are calculated by integrating the radiance, I_v (μ), at wavenumber *u* over the appropriate hemisphere, again as described in Clough et al. (1992). The required integration for determining the up-welling and down-welling fluxes for this study employed standard two-point, first-moment Gaussian quadrature, as opposed to the three-point quadrature employed by Clough. The agreement was not noticeably affected. Figure 3 provides a composite of the spectrally integrated (0-3000 cm^{-1}) mid-latitude summer (MLS) and sub-arctic winter (SAW) up-down flux differences between MODTRAN3 and the Clough FASCODE calculations, well within a few percent at all altitudes except the surface.

(a) R. G. Ellingson, private communication.

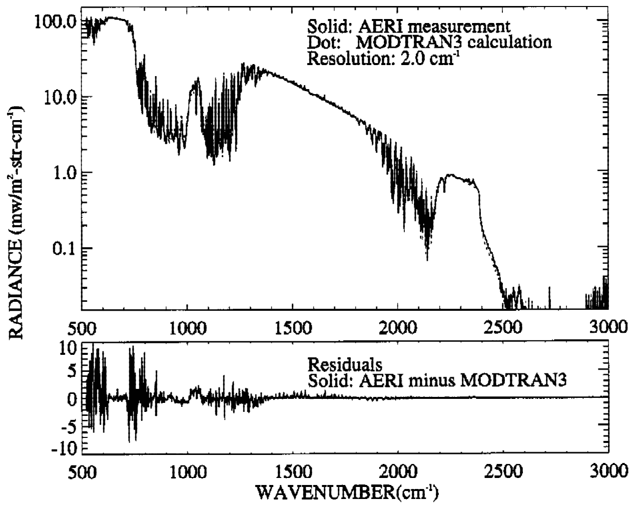

Figure 2. Preliminary comparison between MODTRAN3 and the 1993 ICRCCM Comparison Data Set (Case 3, Ellingson 1993); 2 cm^{-1} resolution, decade offset.

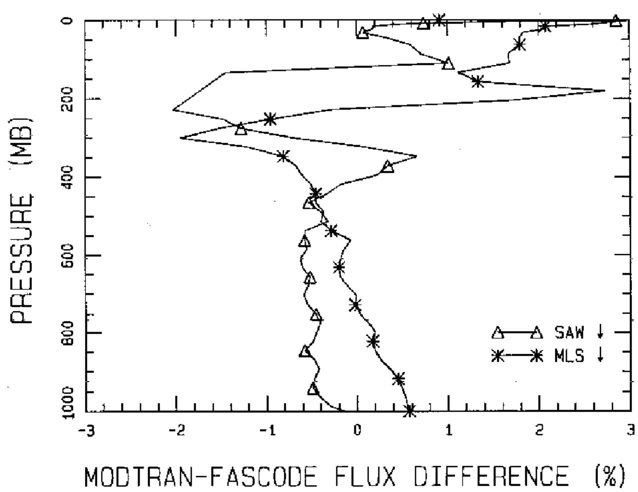

Figure 3. Flux differences (%), as a function of pressure, between MODTRAN3 and FASCODE for mid-latitude summer and sub-arctic winter (see text).

Cooling Rate Calculation

The divergence of the net flux at atmospheric level ℓ represents the rate of energy loss per unit volume of atmosphere, or the cooling rate $Q_v = \Delta F_v$. The monochromatic cooling rate for the atmospheric layer bounded by levels ℓ and ℓ-1 is computed in terms of change in temperature, θ, with respect to time, t, by the usual finite difference formula (Wiscombe 1976)

$$\frac{\partial\theta}{\partial t}\Big|_{\nu;\ \ell,\ \ell-1} = \frac{g(F_{\nu;\ \ell} - F_{\nu;\ \ell-1})}{C_p(P_\ell - P_{\ell-1})}$$

where g is gravitational acceleration, C_p is the specific heat of air at constant pressure, and P is pressure. A value of 8.422 (mbar K d^{-1}) per (W m^{-2}) is used for the ratio g/C_p, independent of altitude.

Comparison of Cooling Rate Results

Both the MODTRAN2 and 3 calculations were originally based on 60 atmospheric layers as defined by Clough et al. (1992). Layers were spaced at increments of approximately 20 mb pressure from 0 mb to 1013 mb. Cooling rates were found to be sensitive to the choice of layering at both the top and bottom of the atmospheric profile and have been redefined for improved sampling. Data for layer temperatures and water vapor densities were interpolated from the published ICRCCM data (Ellingson and Fouquart 1991).

Some recent MODTRAN3 results are presented in Figure 4, again for MLS and SAW cases. The integrated cooling rates are remarkably close for these “water vapor only” cases. A companion contour plot (Figure 5 [Kimball 1993]) with spectral separation at 10 cm^{-1} resolution also shows the same detailed structure found in FASCODE results, as discussed by Clough et al. (1992). Two additional preliminary comparisons (one for $C0_2$ cooling [MLS] with alternate LBL codes (Ellingson and Fouquart 1991); the other a very primitive assessment of cooling rates due to the addition of CFC11 and CFC12) suggest that MODTRAN3’s capabilities are well in agreement with more exact approaches.

Conclusions

This entire study, however initially successful, is still in the “proof of concept” stage; both coding optimization and spectral resolution enhancements (as much as a factor of

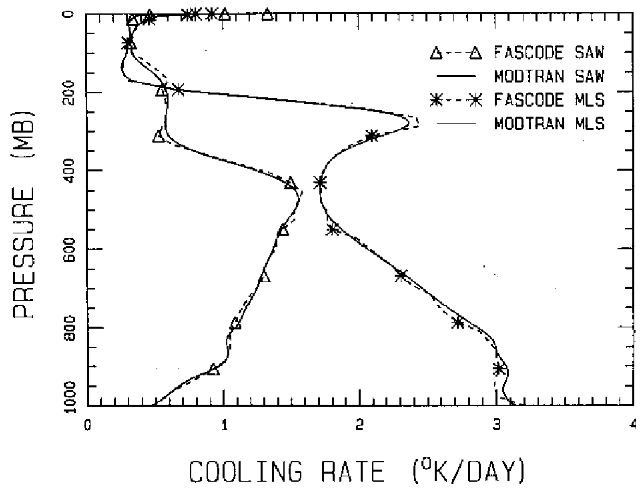

Figure 4. Spectrally integrated water vapor cooling rate (K/day) comparisons between FASCODE and MODTRAN3 for mid-latitude summer and sub-arctic winter (see text).

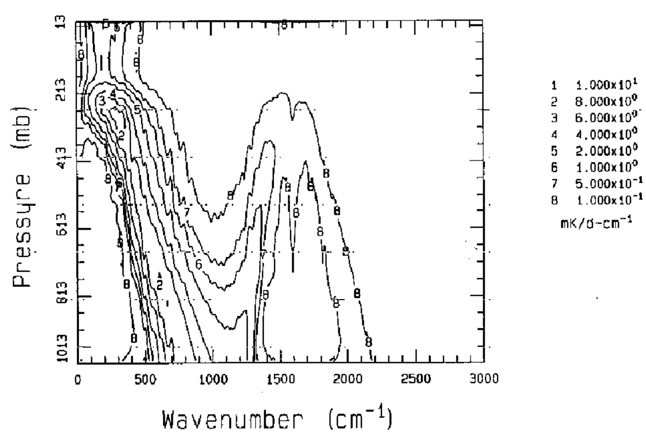

Figure 5. Contour plot of preliminary cooling rate calculations for water vapor, mid-latitude summer, from Kimball (1993).

10, from 2 to 0. 2 cm^{-1}) may permit the accommodation of $C0_2$ line coupling parameterizations and, ultimately, the important energy exchange mechanisms between the troposphere and the middle and upper atmosphere (stratosphere and lower mesosphere) through the inclusion of non-local thermodynamic equilibrium effects. Other necessary enhancements will center on more complete accounting of the non-clear atmosphere, using new cloud formulations. The beginnings of these efforts can be simulated now through the use of semi-opaque cirrus cloud models, but much more work will be necessary to successfully incorporate the more realistic descriptions being developed by the climate change community.

Finally, to make the MODTRAN band model logistically more appropriate for flux-divergence calculations, the multiple runs (one each for 2 or 3 angles, 2 directions, and 60+ layer boundaries) can be recast with multitask processing and storage, such that the spectral calculations can be done in parallel. This change will result in remarkable timing improvement and no loss in accuracy.

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