A FAST LINE-BY-LINE RADIATIVE TRANSFER MODEL FOR TOVS
RADIANCE/TRANSMITTANCE STUDIES

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1. INTRODUCTION
Remote sounding relies on fast parameterized radiative transfer models in
order to process vast amounts of satellite measurements into useable data for
assimilation into numerical weather predictions models on an operational
basis. The alternative is to use a line-by-line radiative transfer model
(LBL). A LBL model is one that determines transmittances and/or radiances
from basic physics, that is — the position and shape of spectral lines are
explicitly accounted for. However, LBL's are inappropriate for operational
remote sensing applications since they are computationally expensive in
regards to execution time and memory. Nevertheless, LBL models are often used
as a standard against which various approximate methods are created and
tested, and are used in studies leading to model improvement.

The major bottleneck in calculating a transmittance or radiance using a
line-by-line code is the evaluation of the absorption coefficient, k. For
example, the top of the atmosphere, TOA, radiance is the sum of the attenuated
intensity from the surface at \( z_0 \), plus the attenuated emissions from the
atmosphere; ie,

\[
R = \int_{\Lambda_0} \left( B(\bar{\nu},T) \int_{z_0}^\infty e^{\int_{z_0}^z - \int_{z_0}^{z'} \mu k(\bar{\nu}) \rho dz'} B(\bar{\nu},T) k(\bar{\nu}) \rho dz' \right) d\bar{\nu} \tag{1}
\]

where \( B(\bar{\nu},T) \) is the surface intensity at wavenumber, \( \bar{\nu} \), and temperature \( T \),
\( \rho \) is the number density, \( B(\bar{\nu},T) \) is the Planck function, and \( \mu \) the secant of
the zenith angle. \( B, T, \rho \) and \( k \) are all implicit functions of \( z \).

The absorption coefficient appears to be simple, but in fact it is the sum
of the individual absorption coefficients from all spectral lines across the
spectrum plus continuum contributions; ie,

\[
k(\bar{\nu}) = \sum_{\text{spectrum}} S_{\text{line}}^i (\bar{\nu}_{oi}) \cdot f(\bar{\nu}-\bar{\nu}_{oi}) + \sum_{\text{continuum}} k_{\text{cont}}^j (\bar{\nu}) \tag{2}
\]

where \( S_i \) is the linestrength of the \( i \)th line and \( f \) is a spectral line shape
function.

The absorption coefficient is computationally intensive for two reasons.
Firstly, in principle the summation is over the entire spectrum, although in
practice only significantly contributing lines are summed. Still, a
relatively narrow region of spectral space may contain thousands of lines.

Secondly, the evaluation of the line shape function can be computationally
intensive. The commonly used the Voigt function, for example, is non-
analytical and must be evaluated numerically. Consequently, a significant amount of computational time is devoted to its evaluation which is reflected by the amount of literature devoted to evaluating this function quickly and efficiently.

These two factors in combination can easily consume upwards of 75% of the total computational time. Unquestionably, a significant amount of time can be saved by concentrating on reducing the time required to evaluate the total absorption coefficient.

2. AN ABSORPTION COEFFICIENT LOOKUP TABLE

The computation of Eq. 2 can be reduced greatly by replacing the k-generation subroutines by a suitable pre-computed set of lookup tables. Such tables depend on wavenumber, pressure, temperature and absorber amount. As a matter of convenience there is a single table per absorbing species.

Potentially a table can be quite large, however there is a way to reduce it by making an assumption. The shape function is usually dependent on absorber amount through the Lorentz half-width, ie,

\[ \alpha_L(\nu) = \alpha_{\text{ref}}^a(\nu) \frac{P}{P_0} \left( \frac{T_{\text{ref}}}{T} \right)^n (1 + \beta(\nu) \, c), \quad \beta(\nu) = \left( \frac{\alpha_{\text{ref}}^a(\nu)}{\alpha_{\text{ref}}^a(\nu)} + 1 \right) \]

where \( P_0 \) is 1013.25 mb, \( \alpha^a \) and \( \alpha^b \) are the air-broadened and self-broadened half-widths respectively at the reference temperature, \( T_{\text{ref}} \), \( n \) is a temperature dependent coefficient and \( c \) is the volume mixing ratio. However for practically all atmospheric cases \( \beta c \) is negligible. Therefore it can be reasonably assumed that \( k_{\text{line}} \) is independent of absorber amount, ie \( \beta c = 0 \), thus eliminating the need for the table to depend on absorber amount.

The construction of a table is straightforward. A spectral resolution is chosen, in this case 0.005 (cm\(^{-1}\)), and a conventional line-by-line model, such as GENASIS (Drummond et al, 1993), is utilized to calculate absorption coefficients at predetermined values of pressure and temperature. The combinations of pressure and temperature (Table I) are chosen such that virtually all possible atmospheric p-T profiles lie within the table boundaries. The resulting coefficients, stored as log(k), are then re-organized into a lookup table.

Once created, the implicit summations for evaluating \( k \) for arbitrary \( p \) and \( T \), are replaced by a simple access to a table, followed by a two dimensional cubic polynomial interpolation scheme. First, an arbitrary \( p \) and \( T \) pair is transformed to log\((p/p_0)\) and \( T/T_0 \), then the appropriate 4x4 section of the table containing the desired point \((p,T)\) is located. Four polynomial interpolations are performed in the log\((p/p_0)\)-direction to obtain values at the points log\([k(p,T_j)]\), \( j = 1, 4 \). The final log\([k(p,T)]\) is determined by an interpolation in the \( T/T_0 \)-direction. Finally, the estimated log\([k(p,T)]\) is transformed into \( k(p,T) \).

Although constructing each absorption coefficient table consumes a sizable
amount of computation time, the time consumed represents most of the LBL computational work and is not duplicated when using the tables for radiative transfer calculations.

Currently a set of 6 tables exist from 500(cm⁻¹) to 1700(cm⁻¹), (ie, the HIRS longwave channels) at 0.005(cm⁻¹) resolution. The tables were created with the aid of GENASIS and took about 7 CPU days to create.

The effectiveness of the method is illustrated by the following example. The TOA radiance due to atmospheric emissions (2nd term in Eq. 1) between 1180 and 1580 (cm⁻¹) was determined using two methods: the GENASIS suite, and using the pre-computed tables to estimate k. The model atmosphere, consisting of H₂O, CO₂, O₃, N₂O, CH₄ and O₂ (AFGL Model 6, Anderson et al, 1986), was divided into 80 layers. The boundaries of these layers correspond to the TOVS levels with an additional level located in between at \( \sqrt{\frac{P_i P_{i-1}}{2}} \). The GENASIS simulation took about 1300 CPU minutes and using the tables, 16 CPU minutes. The resulting TOA radiance is plotted in figure 1 along with the percentage difference between the two methods. As can be seen the difference between the simulations is generally below 1%. If the radiance is convoluted with the response function the difference is less than 0.5%.

Since implementation of tables to evaluate radiative transfer is notably faster than conventional LBL methods, such a method can be referred to as a fast line-by-line method (FLBL).

3. AN APPLICATION EXAMPLE

The TOVS transmittance model assumes that the total mean transmittance is the product of three independent mean transmittances; ie,

\[
\tau_{\text{UMG+H₂O+O₃}}(p) - \tau_{\text{UMG}}(p) \tau_{\text{H₂O}}(p) \tau_{\text{O₃}}(p) = 0
\]

This is equivalent to stating that there is no spectral overlap between three absorbing groups; the so-called uniformly mixed gases (CO₂, N₂O, CH₄ and O₂), designated as UMG, water vapour, and ozone. This assumption is not necessarily true.

Equation 2 is evaluated using FLBL methods for 1103 atmospheres (see Appendix). The results are plotted in figure 2 as a function of \( \tau(\text{UMG+H₂O+O₃}) \). Deviations from zero are indicative of the effect of ignoring spectral overlap between different absorption groups. It should be noted that O₃ contribution in these channels is trivial, hence the curve is more of a measure of the overlap between UMG and H₂O. The deviations are greatest near the peak of the weighting function where the channel is most sensitive. In HIRS 10 and 11, the assumption leads to an underestimate of transmittance of \( \approx 4\% \) and \( \approx 2\% \) respectively and an overestimate of transmittance of \( \approx 9\% \) in HIRS 12.

The effect of the transmittances on the TOA radiance from a black surface located at pressure p, or 'black cloud', is considered in figure 3. The radiances are calculated using FLBL generated mean transmittances as follows,
\[ R_{\text{TOA}}^{\text{OA}}(p_i) = B(T_i) \tau(p_i) + \sum_{j=1}^{i} \frac{1}{2} \left[ B(T_j) + B(T_{j-1}) \right] \left[ \tau(p_{j-1}) - \tau(p_j) \right] \]

where \( B(T) \) is evaluated using the appropriate band correction coefficients (Planet, 1988). Figure 3 shows, as percentages, the difference between Eq. 5 evaluated using \( \tau(\text{UMG+H}_2\text{O+O}_3) \) and using \( \tau(\text{UMG})\tau(\text{H}_2\text{O})\tau(\text{O}_3) \). Figure 4 is displays the differences as brightness temperatures. In terms of brightness temperature the effect of ignoring overlap can lead to errors of about .25K, .6K and .15K in HIRS 10, 11 and 12 respectively for 'clear skies' (a black surface at 1000mb). It is apparent that ignoring overlap leads to significant errors in HIRS channel 11.

4. SUMMARY

The FLBL method uses conventional LBL methods to precalculate a large number of absorption coefficients as a function of pressure, temperature and wavenumber. In subsequent radiative transfer calculations the time consuming explicit calculation of absorption coefficients is replaced by table lookups. This method, excluding the time required to construct the table, can reduce the time to simulate a TOVS radiance by almost two orders of magnitude compared to a conventional LBL. The FLBL results are within a couple of percent of the LBL. The use of FLBL methods will undoubtedly increase the ease of performing sensitivity studies and developing of improved parameterized models for TOVS and other instruments.

An application of the FLBL to study the effect of ignoring overlap between absorbing species (UMG and \( \text{H}_2\text{O} \)) demonstrated that work is required to improve the fast transmittance models for the HIRS water vapour channels with regards to spectral overlap.

5. APPENDIX  SAGEII/NMC DATA SET

In order to carry out the study in section 3, a dataset containing temperature, ozone and water profiles to the effective top of the atmosphere, TOA, was required. Other dominant absorbers, such as \( \text{CO}_2 \), are considered to be invariant. To fulfill this need, the GEDEX dataset (Olsen et al, 1992) was obtained. Within this dataset can be found temperature profiles, and water vapour and ozone profiles for the upper atmosphere as determined by the Stratospheric Aerosol and Gas Experiment II, SAGEII (Wang et al, 1992). In order to complete the water vapour profiles down to the surface, data from National Meterological Center’s global numerical weather analysis cycle was collocated and splined onto the upper water vapour profile. Unfortunately the same could not be done for ozone, hence the tropospheric portion was completed using one of six AFGL reference atmospheres (Anderson et al, 1986).

The resulting combined dataset contains about 3300 profile sets of temperature, ozone and water vapour from 1986 that are representative of the mid-latitudes. The polar regions are not included, nor are the tropical
regions represented. The latter is an unfortunate byproduct of the reduction of the dataset during the collocation process.

6. REFERENCES
Olsen, L.M. and A Wanock III, 1992: Greenhouse Effect Detection Experiment (GEDEX), Selected Data Sets, NASA Climate Data System, NASA — Goddard Space Flight Center, Greenbelt, Maryland, USA.

<table>
<thead>
<tr>
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<table>
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<th>temperature knots (K)</th>
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<td>180.000</td>
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TABLE: 1 Values of pressure and temperature used to define the k-table.
Figure 1: Comparison of the TOA atmospheric emission of Eq. 1 calculated using the LBL method and the FLBL method across the 6.7μm H2O spectral region. The percentage difference between the mean radiances is 0.40%, -0.06% and -0.04% for HIRS 10, 11 & 12. The NOAA 10 response functions for HIRS 10, 11 & 12 are shown.
Figure 2: Comparison of the convoluted FLBL TOA mean transmittances properly mixed and the triple band product for selected pressures. Each set of points represents a profile taken from the SAGE/NMC dataset.
Figure 3: Comparison of the TOA radiance from a black surface located at one of the selected pressures using the transmittances in figure 2.
Figure 4: Same as figure 3, except in terms of brightness temperature differences.
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