A NEW FAST RADIATIVE TRANSFER MODEL FOR TOVS

J.R. Eyre

European Centre for Medium-range Weather Forecasts,
Reading, U.K.

1. INTRODUCTION: BACKGROUND TO DEVELOPMENT OF THE MODEL

1.1 Intended applications

An essential component of a system for exploiting data from satellite sounding instruments is an accurate and fast radiative transfer (RT) scheme which computes the radiance emitted at the top of the atmosphere, along the viewing direction of the instrument and averaged over the spectral response of each instrument channel, for a given profile of atmospheric and surface conditions. The new RT model described here has been developed initially for use with data from the High-resolution Infra-red Radiation Sounder (HIRS) and Microwave Sounding Unit (MSU) – part of the TIROS Operational Vertical Sounder (TOVS) on the TIROS-N/NOAA series of polar-orbiting satellites (see Schwab, 1978 or Smith et al. 1979). However, its design has taken into account its future extension for other satellite sounding systems.

The development of the new model has been stimulated by recent research activities on data assimilation for numerical weather prediction (NWP), and specifically by the requirement at ECMWF to assimilate TOVS radiances directly within experimental schemes for 3- and 4-dimensional variational analysis (3DVAR and 4DVAR – see Pailleux, 1989, 1990). This application requires not only a RT model capable of performing calculations on global radiance data in a reasonable time, but also its associated tangent linear and adjoint models.

The model can also be used in more conventional approaches to the extraction of information from satellite radiances. Most "physical" retrieval schemes require rapid calculation of radiances as part of the inversion process. The new model has been developed for use in a retrieval scheme under development at ECMWF (see Eyre, 1990). This is a physical-statistical nonlinear scheme using a forecast profile and its expected error covariance as constraints with the method described by Eyre (1989). In the context of NWP data assimilation, this method is better described as one-dimensional variational analysis (1DVAR), and this work is closely related to the work on 3DVAR and 4DVAR. The 1DVAR requires both the RT model itself and its associated model for calculating the full gradient matrix, i.e. the partial derivatives of each radiance with respect to each atmospheric/surface variable. The new gradient model replaces the approximate model described by Eyre (1989).

In common with similar RT schemes, the new model will require careful tuning through comparison of measured TOVS radiances with those computed from collocated radiosonde and NWP model profiles. This aspect will be very important for successful use of the new model and is discussed further in section 2.5.

The new model is also intended to have a number of other applications. It could be used for off-line RT calculations needed
to generate various coefficients required by other retrieval schemes. With minor modifications (see section 2.4), it could also be used to calculate radiances for other sounding instruments, present and planned, and to simulate the performance of proposed future satellite systems.

1.2 Design requirements

The range of intended applications places a number of requirements on the scheme which have influenced its design:

- It must be fast enough to be of practical use with global data in near real-time. This entails both simple algorithms and an architecture leading to efficient vectorization.

- It must however be accurate. In practice the error introduced by approximations in the RT calculation should not add significantly to those from other sources (such as those inherent in the underlying spectroscopic data).

- It must be flexible in several respects, including:
  - allowing calculations with or without the presence of cloud,
  - allowing further development for TOVS, through inclusion of refinements to the RT physics,
  - allowing modifications to serve other instruments.

- In addition to the RT model itself, the program suite must include corresponding tangent linear, adjoint and gradient-matrix models. These should also be fast and preferably exact.

1.3 Features of the new model and relationships to earlier models

The approach to the RT calculation follows the general method used at NESDIS (and many other centres) and described by Weinreb et al. (1981). Corresponding code is used for TOVS RT calculations in the International TOVS Processing Package (ITPP) developed by CIMSS/NESDIS at the University of Wisconsin–Madison. A modified version of the ITPP RT code was implemented at the UK Meteorological Office as the "TOVSRAD" model (Eyre, 1984).

The new RT model described here took TOVSRAD as the starting point for most of the algorithms. However, the software has been completely re-coded with a different architecture; calculations for many profiles and/or channels (channels x profiles ~ 1000) can now be computed in parallel, in order to take advantage of vector hardware.

The main scientific change in the new model concerns the transmittance calculation, and particularly the treatment of water vapour. The method used by Weinreb et al. (1981) was found difficult to vectorize and hence slow. A new fast transmittance model has been developed to overcome this problem and to provide a common model for microwave and infra-red channels (which allows all
channels to be treated alike throughout the RT calculation and thus assists vectorization). Like the ITPP algorithm for transmittance of uniformly-mixed gases, the new model is of the McMinnin/Fleming type (see McMinnin and Fleming, 1976). It is an adaptation of the model of Eyre and Woolf (1988) which was developed for microwave channels. When this model was tested on HIRS channels, it was found to give poor accuracy for channels with strong water vapour absorption. The features which are different in the new model have been introduced mainly to overcome this problem. Whereas uniformly-mixed gases and water vapour were treated together in the Eyre/Woolf model, they have again been separated here. However, the angular dependence is now treated by one algorithm, rather than two. Ozone transmittance is still treated separately using a modified version of the algorithm given by Weinreb et al. (1981).

Other scientific features of the scheme include the treatment of cloud in the infra-red (a single layer in the present implementation). The architecture allows a general treatment of surface emissivity; the present implementation includes a fixed emissivity for each HIRS channel and a single variable emissivity for MSU. Provision has been made (although not yet implemented) for the treatment of cloud liquid water in the microwave and a more complex treatment of microwave surface emissivity.

Although the model described here has been developed initially for HIRS and MSU, it is anticipated that it will be used, with minor modifications, for several other instruments. Some planned and possible extensions to the RT model are discussed in section 2.4.

2 ALGORITHMS

2.1 The radiative transfer scheme

The radiance in channel \( i \) is given by:

\[
R_i = (1 - N_i) R_i^d + N_i R_i^o
\]  
(2.1.1)

where \( R_i^d \) is the clear-column radiance,
\( R_i^o \) is the overcast radiance, and
\( N_i \) is the effective fractional cloud cover (assumed to be in a single layer).

For infra-red channels, \( N_i = N_c \), the same for all channels, and \( N_c \) is an input variable. For all microwave channels, \( N_i = 0 \), since it is planned to include the effects of cloud liquid water through a contribution to the transmittance profile.

The clear-column radiance is given by:

\[
R_i^d = R_i^s + R_i^a
\]  
(2.1.2)

where \( R_i^s \) is the contribution from the surface, and
$R_i^a$ is the contribution from the atmosphere.

[An additional contribution for solar radiation reflected by the surface could also be added here.]

The surface contribution is given by:

$$R_i^s = \varepsilon_i^s B_i(T') \tau_i^s$$  \hspace{1cm} (2.1.3)

where $\varepsilon_i^s$ is the surface emissivity,
$B_i(T')$ is the modified Planck function for channel $i$ for the surface skin temperature $T'$, and
$\tau_i^s$ is the transmittance from the surface to space.

For infra-red channels, the surface emissivity is currently set to one for all channels. For microwave channels, the surface emissivity is an input variable. See section 2.4 for a discussion of possible future extensions for surface emissivity.

The modified Planck function takes account of the averaging of the true Planck function over the spectral response of channel $i$ for scene temperature $T$ and is given by:

$$B_i(T) = c_{1i} / \left[ \exp \left( c_{2i} / (a_i + b_i T) \right) - 1 \right]$$  \hspace{1cm} (2.1.4)

where $c_{1i}$, $c_{2i}$, $a_i$ and $b_i$ are pre-computed coefficients for each channel (see Weinreb et al 1981, Lauritson et al 1979). $c_{1i} = c_1 v_i^3$ and $c_{2i} = c_2 v_i$, where $c_1$ and $c_2$ are the normal Planck function coefficients and $v_i$ is the central frequency of the channel. $a_i$ and $b_i$ are the so-called "band correction coefficients".

The calculation of the surface transmittance, $\tau_i^s$, is described in section 2.2.

Returning to eq. 2.1.2, the atmospheric contribution includes both direct upward emission, $R_i^e$, and downward emission reflected back from the surface, $R_i^d$:

$$R_i^a = R_i^e + R_i^d.$$  \hspace{1cm} (2.1.5)

$R_i^e$ is obtained as a sum of the contributions from all emitting layers:

$$R_i^e = \sum_{j=1}^{N} R_{ij}^e$$  \hspace{1cm} (2.1.6)

where $R_{ij}^e = \frac{1}{2} \left( B_i(T_j) + B_i(T_{j-1}) \right) \{ \tau_{ij}^s - \tau_{ij}^l \}$  \hspace{1cm} (2.1.7)
and $T_j$ is the temperature at atmospheric level $j$, and $\tau_{ij}$ is the transmittance in channel $i$ from level $j$ to space along the viewing direction of the instrument (see section 2.2).

The atmospheric levels are numbered from the top down as follows:
- for $j = 0$, pressure $p_j = 0$, $T_j = T_1$ and $\tau_{ij} = 1$,
- for $j = 1$ to $N-1$, pressures $p_j$ are for standard levels described in section 2.3, and
- for $j = N$, $p_j$ = surface pressure, $T_j$ = surface air temperature and $\tau_{ij} = \tau_i^s$.

Note that eq. 2.1.7 is an approximation. It assumes that the form of the radiative transfer equation (RTE) for monochromatic radiation can be applied to the spectrally-averaged radiance and the spectrally-averaged transmittance. It also represents an integral by a finite summation and assumes that the mean emission from a layer is given by the average of its boundary values.

$R_d^i$ is obtained with a similar summation:

$$R_d^i = \sum_{j=1}^{N} R_{ij}^d$$  \hspace{1cm} (2.1.8)

where $R_{ij}^d = R_{ij}^s[1-e_i^s]/(\tau_i^s \tau_{i,j-1}^s)$  \hspace{1cm} (2.1.9)

This is equivalent to assuming that:
- the reflection at the surface is specular, and
- the total transmittance of an atmospheric path is the product of the transmittances of its constituent sub-paths (which is strictly true only for monochromatic radiation, but is usually a good approximation when the absorption is weak).

[The assumption of specular reflection could be changed to that of reflection from a mean incoming angle with a simple modification to eq. 2.1.9].

Returning to eq. 2.1.1, the overcast radiance $R_o^i$ is obtained as follows. The overcast radiance which would result from an opaque cloud top at pressure level $j$ is given by:

$$R_{ij}^o = B_i(T_j)\tau_{ij} + \sum_{j=1}^{j'} R_{ij}^n.$$  \hspace{1cm} (2.1.10)

This assumes that the opaque cloud is black and non-reflective. [It would be quite simple to modify eq. 2.1.10 to accommodate a non-black, reflective cloud. Reflection of both down-welling atmospheric emission and solar radiation could be included.]
If the cloud-top pressure, $p_c$, lies between pressure levels $J$ and $J-1$, then the overcast radiance at $p_c$ is obtained by linear interpolation:

$$R_i^o = (1-f_c)R_{iJ}^o + f_c R_{iJ-1}^o$$  \hfill (2.1.11)

where $f_c = (p_J - p_c) / (p_J - p_{J-1})$. \hfill (2.1.12)

Note that $p_c$ is an effective cloud-top pressure, i.e. the pressure at the effective radiating temperature of the cloud. It should represent a good approximation for clouds which are either optically thick in the upper layers or geometrically thin.

The radiance is converted to an equivalent black-body temperature (brightness temperature) using the inverse of eq. 2.1.4:

$$TB_i = \{c_{21}/(\ln(1 + c_{11}/R_i)) - a_i\}/b_i.$$ \hfill (2.1.13)

Note that the same form of the equations is used for microwave and infra-red channels; the Planck function is computed exactly for MSU channels even though a linearized approximation would be adequate at these frequencies.

2.2 The transmittance model

The absorption by uniformly-mixed gases is treated separately from that by water vapour. However, each is obtained with an algorithm of the same form. The optical depth for the layer from pressure level $j$ to space along a path at an angle $\theta$ to the vertical is obtained as follows: the ratio of the optical depths for adjacent pressure levels involves a polynomial with terms which are functions of temperature and specific humidity at and above these levels. If $d_y$ is the optical depth from level $j$ to space in channel $i$, then:

$$d_{ij} = d_{i,j-1} + Y_j \sum_{k=1}^{K} a_{ijk} X_{kj}. \hfill (2.2.1)$$

In the present implementation, $K = 10$ and the values of $X_{ij}$ and $Y_j$ for uniformly-mixed gases and water vapour models are as follows:
uniformly-mixed gases

\[ X_U \]
\[ \delta T_j \sec \theta \]
\[ X_{2U} \]
\[ \delta T_j^2 \sec \theta \]
\[ X_{3U} \]
\[ \delta T_j \sec \theta \]
\[ X_{4U} \]
\[ \frac{p}{p} \delta T_j \sec \theta \]
\[ X_{5U} \]
\[ \left( \sec \theta - 1 \right) \]
\[ X_{6U} \]
\[ \left( \sec \theta - 1 \right)^2 \]
\[ X_{7U} \]
\[ \delta T_j \left( \sec \theta - 1 \right) \]
\[ X_{8U} \]
\[ \frac{p}{p} \delta T_j \left( \sec \theta - 1 \right) \]
\[ X_{9U} \]
\[ \delta T_j \left( \sec \theta - 1 \right) \]
\[ X_{10U} \]
\[ 1 \]
\[ Y_j \]
\[ 1 \]

where

\[ \overline{\delta T_j} = \frac{1}{p_j} \sum_{i=1}^{p_j} \delta T_i (p_i - p_{i-1}) \]  \hspace{1cm} (2.2.2)

\[ \overline{p \delta T_j} = \frac{2}{p_j} \sum_{i=1}^{p_j} (p_i \delta T_i - p_{i-1}) \]  \hspace{1cm} (2.2.3)

\[ u_j = \frac{1}{2} (q_j + q_{j-1}) (p_j - p_{j-1}) \]  \hspace{1cm} (2.2.4)

\[ \delta T_j = \frac{1}{2} (T_j - T_j^{ref} + T_{j-1} - T_{j-1}^{ref}) \]  \hspace{1cm} (2.2.5)

\[ \delta q_j = \frac{1}{2} (q_j - q_j^{ref} + q_{j-1} - q_{j-1}^{ref}). \]  \hspace{1cm} (2.2.6)

\( T_j \) and \( q_j \) are the temperature and specific humidity (water vapour mass mixing ratio) profiles. \( T_j^{ref} \) and \( q_j^{ref} \) are corresponding reference profiles (the mean of a set of 1200 global profiles obtained from NESDIS has been used). Further information on the reasons for choosing this formulation, its accuracy and the method used to compute the coefficients \( a_{yk} \) are given in the Appendix.

The absorption by ozone is treated separately using a modified version of that described by Weinreb et al. (1981) and used in ITPP and TOVS/RAD. The new model for ozone optical depth is:

\[ d_{ij}^O = \sum_{k=1}^{2} \lambda_k \left( 1 + \left( \sec \theta - 1 \right) a_{ijk} \right) \ln \beta_{ijk} \]  \hspace{1cm} (2.2.7)

where \( \lambda_2 = (\Omega - 257)/253, \)

\[ \lambda_1 = 1 - \lambda_2, \] and

\( \Omega \) = total column ozone in Dobson units.
The correspondence between the original model and the new model is discussed in the Appendix.

If the optical depths for uniformly-mixed gases, water vapour and ozone are respectively \( d_{ij}^M \), \( d_{ij}^W \) and \( d_{ij}^O \), then their combined optical depth is:

\[
d_{ij} = d_{ij}^M + d_{ij}^W + d_{ij}^O.
\]  
(2.2.8)

[This is only exact for monochromatic calculations. An improved approximation is discussed in the Appendix.]

The common practice of allowing for the inclusion of an empirical correction to the transmittance model has been followed. This is usually done by raising the computed transmittance to the power \( \gamma_a \), where \( \gamma_a \) is determined empirically. This is equivalent to multiplying the computed optical depth by a factor \( \gamma_a \). Then the corrected optical depth \( d_{ij}^c \) is given by:

\[
d_{ij}^c = \gamma_a d_{ij}.
\]  
(2.2.9)

It is anticipated (see section 2.4) that versions of the scheme may be required in which the pressure levels used for the transmittance calculation are not the same as those used in the integration of the radiative transfer equation (RTE), and that some interpolation of the transmittance profile will be needed. The architecture of the code allows this to be added later. At present the RTE is integrated on the same standard levels on which the transmittances are calculated, and the only interpolation/extrapolation required is to obtain the surface transmittance. If the surface pressure \( p_s \) lies between standard levels \( L \) and \( L-1 \), then the optical depth at the surface, \( d_{IN}^c \), is obtained by linear interpolation:

\[
d_{IN}^c = d_{IL}^c + f_s \left( d_{IL-1}^c - d_{IL}^c \right)
\]  
(2.2.10)

where \( f_s = (p_s - p_L) / (p_L - p_{L-1}) \)  
(2.2.11)

If \( p_s \) exceeds the pressure of all the standard levels, then \( L \) is set to the last standard level (highest in pressure) and \( d_{IN}^c \) is extrapolated using the same equations.

Finally, optical depths are converted to transmittances:

\[
\tau_{ij} = \exp \left( - d_{ij}^c \right).
\]  
(2.2.12)

Note that, in this way, only one exponent calculation is required for each transmittance.
2.3 Treatment of the atmospheric profile

The transmittance and RT calculations are performed using atmospheric layers bounded by a number of standard pressure levels (plus surface pressure and cloud-top pressure). The 40 standard levels currently used are defined in Table 1. [Other sets of levels could easily be used. However transmittance coefficients corresponding to them would then be required.] The atmospheric profile of temperature and water vapour and all the related parameters required in the transmittance calculations must therefore be set up for these levels and the corresponding layers.

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Fixed pressure levels (in mb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 0.2</td>
<td>0.5 1 1.5 2 3 4 5 7</td>
</tr>
<tr>
<td>10 15</td>
<td>20 25 30 50 60 70 85 100</td>
</tr>
<tr>
<td>115 135</td>
<td>150 200 250 300 350 400 430 475</td>
</tr>
<tr>
<td>500 570</td>
<td>620 670 700 780 850 920 950 1000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2</th>
<th>Profile vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Element No</td>
<td>Description</td>
</tr>
<tr>
<td>1 - 40</td>
<td>temperature in K at 40 standard pressure levels</td>
</tr>
<tr>
<td>41 - 55</td>
<td>ln (specific humidity in g/Kg) at 15 lowest standard levels</td>
</tr>
<tr>
<td>56 57</td>
<td>surface air temperature in K</td>
</tr>
<tr>
<td>58</td>
<td>surface air ln (specific humidity in g/Kg)</td>
</tr>
<tr>
<td>59</td>
<td>surface skin temperature in K</td>
</tr>
<tr>
<td>60</td>
<td>surface pressure in mb</td>
</tr>
<tr>
<td>61</td>
<td>total column ozone in Dobson units</td>
</tr>
<tr>
<td>62</td>
<td>cloud-top pressure in mb</td>
</tr>
<tr>
<td>63</td>
<td>effective fractional cloud coverage</td>
</tr>
<tr>
<td>64 - 66</td>
<td>microwave surface emissivity (50.3 GHz)</td>
</tr>
<tr>
<td>67</td>
<td>microwave surface emissivity parameters - not used at present</td>
</tr>
<tr>
<td>68</td>
<td>total column cloud liquid water in mm - not used at present</td>
</tr>
</tbody>
</table>
The RT model takes as input a "profile vector" of 67 elements as defined in Table 2. Humidity is currently specified as
ln (specific humidity in g/Kg) for ease of use with the present
formulation of the lDVAR retrieval scheme. [It would be simple to
modify the code to accept other variables such as specific humidity
itself or relative humidity.] To simulate clear-column radiances,
\(N_e\) is set to zero, but \(p_s\) should be set to a realistic value. Only
the first parameter for microwave surface emissivity is currently
used and represents the emissivity at MSU frequencies. Planned
extensions to use the other parameters are discussed in section 2.4.
Similarly, total column cloud liquid water is not currently used.
The integration of the RTE only uses levels at and above the
surface. However, the interpolation of the surface transmittance
also makes use of a pressure level below the surface. It is
therefore important that the temperature and humidity at this level
are extrapolated in a realistic way or else set equal to the surface
air values.

The humidity profile is specified by the input only for the
lowest 15 levels (i.e. up to 300 mb). It is extrapolated internally
to give a reasonable stratospheric profile as follows: if \(p_j\) is
pressure in mb, then

\[
\begin{align*}
\text{for } & \quad 300 > p_j \geq 70, & q_j = \max \{q_{300} \left(\frac{p_j}{300}\right)^3, q_{\min}\} \\
\text{and for } & \quad p_j < 70, & q_j = q_{\min},
\end{align*}
\]

where \(q_{\min} = 0.003\, g/Kg\).

Using the temperature and humidity at standard levels, the total
column ozone, the surface pressure and the angle of the viewing
path, all the other profile variables required in the calculation of
optical depth are calculated as described in section 2.2

2.4 Potential developments

Some potential developments to the scheme have already been
mentioned in sections 2.1 - 2.3 and, regarding the transmittance
model, in the Appendix. This section elaborates on some of these
plans and possibilities.

Cloud liquid water

Provision has been made for inclusion of the effects of cloud
liquid water on microwave channels through an additional optical
depth profile. This would also require methods for distributing the
input of total column cloud liquid water between different layers in
a reasonable way, and then for converting the amount in each layer
to an optical depth. Alternatively, a more substantial change could
be made in order that the profile of cloud liquid water (rather than
the total) could be given as input.

Surface emissivity - microwave

At present the microwave surface emissivity is provided as a
single input variable for each profile. This is adequate for MSU
because the channels which "see" the surface are close in frequency. However, for other instruments (e.g. SSM/I, AMSU) this is not the case, and a different method must be used. Provision has been made for up to four variables. This should allow the implementation of parametric models such as that proposed by Grody (1988) in which a number of parameters define the emissivity as some function of frequency, where the function is appropriate for many natural surface types. Alternatively, if the surface type is known, then the surface type indicator — already an input to the model — could be used to drive a physical model of surface emissivity.

Surface emissivity - infra-red

The code allows for a number of surface types of which three are currently active (surface = black, sea or land), but infra-red surface emissivities are set to one for all channels for all surfaces. However this could easily be changed to more surface types and to a different value for each channel and surface type.

Ozone transmittance

The model used here for ozone transmittance is rather crude. It is probably adequate for the weak effects of ozone of HIRS channels 1 - 7. However, it is not adequate for HIRS channel 9 — the ozone channel at 9.7 µm. A better model, suitable for all channels, would be desirable. Given appropriate line-by-line calculations, a fast model of the same form as the water vapour transmittance model could be implemented.

Surface humidity

Although this is an input variable, it is not currently used because it does not affect the transmittance profile; the optical depth at the surface is obtained by interpolation/extrapolation from adjacent standard levels. A modification to this procedure would be desirable so that the input surface humidity did have some effect on the radiance through the surface transmittance.

Integration of the radiative transfer equation

This is currently performed on the same standard pressure levels as used in the transmittance calculation. Although this is usually quite accurate, there is evidence that it can lead to undesirably large errors in certain cases. The small numbers of levels around the tropopause and in the boundary layer are particular concerns. This could be remedied in the following ways:

- changing the standard pressure levels to more suitable values and perhaps increasing their number,

- using the standard levels only for the optical depth calculation and performing the RTE integration on another set of levels. If a NWP model profile is used as input, then the NWP model's levels/layers could be used for this purpose. In this case the profile would have to be interpolated to the standard levels for the optical depth calculation, and then the results interpolated back for the RTE integration.
Solar reflection

This is currently omitted, but provision has been made for its inclusion. It should be introduced consistently with the inclusion of non-black (reflective) surfaces and/or clouds. The solar zenith angle is already present as input for this purpose.

2.5 Tuning

Like similar RT models, the new model is not expected to give results sufficiently accurate for use with real data unless it has undergone empirical tuning through comparison of measured radiances with those calculated from collocated radiosonde and/or NWP model profiles. The method used in the ITFP and TOVSRAD models has been retained.

- A correction to the calculated transmittance by raising it to the power $\gamma$ (implemented here by multiplying the optical depth by $\gamma$ - see section 2.2). $\gamma$ is a different constant for each channel and is expected to be adjusted infrequently (e.g. once per satellite).

- A bias correction, $\delta$, to the calculated brightness temperatures. For flexibility, this has not been implemented within the RT scheme but should be applied to its output. It is expected that these values will have to be functions of latitude or air mass type and to require frequent tuning (e.g. once per month) as the biases in some channels may exhibit a seasonal cycle.

3. TANGENT LINEAR, ADJOINT AND GRADIENT MATRIX MODELS

If we represent the RT scheme as an operator for transforming an atmospheric profile vector, $\textbf{x}$, into a radiance (or brightness temperature) vector, $\textbf{y}$:

$$\textbf{y} = \textbf{F}(\textbf{x}), \quad (3.1)$$

then the tangent linear operation can be written in terms of the gradient of this equation:

$$\delta \textbf{y} = \textbf{K}(\textbf{x}).\delta \textbf{x}, \quad (3.2)$$

where $\textbf{K}(\textbf{x})$ is the matrix of partial derivatives of $\textbf{F}(\textbf{x})$ with respect to $\textbf{x}$. The adjoint of this operation can be written in terms of the transpose of $\textbf{K}(\textbf{x})$:

$$\text{grad}_x = \text{grad}_y.\text{grad}_y = \textbf{K}(\textbf{x})^T.\text{grad}_y. \quad (3.3)$$

Therefore, in principle, both the tangent linear and adjoint operations can be performed by computing the gradient matrix, $\textbf{K}(\textbf{x})$, and then performing the appropriate dot product. However, for very large systems it may not be feasible to calculate the full matrix, and we need to perform the tangent linear and adjoint operations without explicitly calculating the matrix $\textbf{K}(\textbf{x})$. In this case, we may represent the operations in a general way:
tangent linear: \[ \delta y = T_\mathbf{L}(\mathbf{x}, \delta \mathbf{x}) \]
adjoint: \[ \text{grad}_\mathbf{x} = A \mathbf{D}(\mathbf{x}, \text{grad}_\mathbf{y}). \]

For the direct RT model described above the three associated models - K, TL and AD - have all been coded (see section 4.2). All three models are exact (cf. the K-matrix model developed by Eyre (1989), which is only approximate). The method for TL and AD is the same as that followed by Thépaut and Moll (1990). It is possible to develop the K-matrix code either from that of the TL or AD models. In practice it was found much easier in this case to modify the AD model.

4. TECHNICAL ASPECTS AND SPEEDS

Technical details on the implementation of the new scheme as FORTRAN 77 routines are given in ECMWF Technical Memorandum 176 (Eyre, 1991).

The current implementation on the CRAY-YMP at ECMWF has achieved the following CPU speeds: for 19 TOVS channels processed in blocks of 50 profiles, the direct model requires 1.15 ms per profile on a single processor of the computer, and the tangent linear and adjoint routines require an additional 1.17 and 2.21 ms per profile respectively. When processing only one profile at a time, the direct model is 1.7 times slower.

From these values we can estimate the typical computer load in processing global TOVS data. When processed at a spacing of about 100 km, there are \( \approx 20000 \) TOVS soundings per satellite every 6 hours. For these data, and assuming one direct model computation per sounding (as might be required in a linearized, one-step retrieval scheme), the RT calculations would take only \( \approx 23s \) per satellite on one processor. For three-dimensional variational assimilation of TOVS radiances, one might expect \( \approx 10 \) iterations of the direct model plus its adjoint. At the same data spacing, this leads to a requirement of about 900s per satellite on one processor every 6 hours. These values suggest that, even with the most computationally demanding retrieval/assimilation techniques, the RT computations involved in processing global TOVS data should not represent a major load for the computers now available at major operational centres.

5. REFERENCES


APPENDIX. TRANSMITTANCE MODEL - FURTHER DETAILS

A.1 Calculation of coefficients

For a small number of diverse atmospheric profiles (32 were used here), transmittances were calculated. Ideally this should be done using a line-by-line model but so far the ITTP/TOVSRAD fast RT model has been used for this purpose. Results were calculated and stored separately for uniformly-mixed gases and for water vapour and, for this purpose, ozone was excluded. Transmittances were calculated for all 40 pressure levels (see table 1) and for five scan angles (at secθ = 1, 1.25, 1.5, 1.75 and 2). Coefficients aₘₙ
in equation 2.2.1 were then calculated by linear regression of \( \{d_{j_k}/d_{j-1}\}/Y_j \) against \( X_j \).

A.2 Rationale for the new model

The uniformly-mixed gases are treated in the same way as in the Eyre/Woolf model, except that the water vapour terms have been removed (since this component of the transmittance does not depend on them) and they have been replaced by terms representing the off-nadir effects.

The water vapour model is similar to the Eyre/Woolf model but has the following differences. Firstly, the angular dependence has been addressed in a single algorithm. Secondly, the relatively poor performance of the Eyre/Woolf model for water vapour channels was traced to the difficulty in calculating coefficients using a linear regression method when the absolute water vapour amounts vary by orders of magnitude between cold, dry profiles and warm, moist profiles. The performance is improved by replacing \( (d_j/d_{j-1}) \) by \( (d_j/d_{j-1})(\sec^6 \theta_j)^{-1/6} \) as the predictand in the regression; the latter can be considered as an "effective absorption coefficient" in the strong absorption limit and so varies only moderately from profile to profile. This is the origin of terms 1 to 4 in the expansion.

Terms 5 to 9, which correspond to fitting \( (d_j/d_{j-1})(\sec^6 \theta_j)^{-1} \), are included to allow for the behaviour when the water vapour absorption is dominated by either weak lines or continuum effects. It should be stressed however that the precise form of the terms included was arrived at empirically.

A.3 Accuracy

The accuracy of the model was checked by comparing the transmittances computed directly by the ITPP model with those from the new model. For the 32 profiles used as the dependent set (i.e. for the calculation of regression coefficients), the standard deviations of the error were calculated for uniformly-mixed gases only, for water vapour only and for their combination. The transmittance errors for uniformly-mixed gases were negligible, reaching a maximum of 0.2% in HIRS channel 5. Errors were larger by up to an order of magnitude for water vapour, the maximum standard deviation of error being about 1.6% in HIRS channel 12 at 620 mb. Comparable errors were also present at lower altitudes in most other channels, but they are only significant in the combined transmittance for HIRS channel 7-8, 10-11 and 19 and for MSU channel 1.

The accuracy was also checked for three independent samples of 32 profiles each: a mid-latitude, a high latitude and a low latitude set. Results were comparable with those for the dependent sample.

A.4 Water vapour transmittance in stratosphere

Water vapour transmittances are calculated for levels \( p_j \geq 100 \text{ mb} \) using an accurate integration of the water vapour amount
from $p_1$ to 0.1 mb. At present in the new model, no calculation is performed for $p_1 < 100$ mb, i.e. $\tau_1 = 1$. This is because no coefficients have been generated for $p_1 < 100$ mb due to an instability in the ITPP water vapour routine in this region. This does not lead to serious problems and could be corrected if regression coefficients were calculated using line-by-line transmittances.

$u_1$ is as defined in section 2.2 (i.e. the layer water vapour content), except (for consistency) at $p_1 = 100$ mb, where $u_1$ is the sum of the water vapour in all layers above 100 mb.

A.5 A possible extension

At present the new model follows the ITPP model in assuming that the three contributions to the transmittance are separable — see equation 2.2.8. This is equivalent to a monochromatic transmittance approximation and for real, non-monochromatic channels may not always be accurate. It could be improved if line-by-line optical depth calculations were available for:

- uniformly-mixed gases only, and
- uniformly-mixed gases plus water vapour.

The total optical depth could be calculated as:

$$d_j = d_j^N + d_j^{M-W-M} + d_j^O$$

where $d_j^{M-W-M}$ is the optical depth for (mixed gases plus water vapour) minus the optical depth for mixed gases alone, represented by one polynomial expansion of the same form as currently used for water vapour alone.

A.6 The new ozone model

Using the same symbols as in section 2.2, the original model of Weinreb et al (1981) can be written:

$$d_{ij}^O = -\ln \left\{ \sum_{k=1}^{L} \lambda_k \left( \beta_{ij} \right)^{1 + (\omega*\phi-1)} \sigma_{ik} \right\}$$

and so this allows us to use the same coefficients, $\sigma_{ik}$ and $\beta_{ij}$ as in the ITPP model. The two models will agree exactly at the two values of $\Omega$ used in calculating the coefficients (257 and 480 Dobson units). Elsewhere they will differ, but the maximum difference in transmittance is found to be ~0.001, which is probably much less than the error in either model.

These models are rather crude but probably adequate for all HIRS channels except channel 9 (9.7 μm).
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Edited by
W. P. Menzel

Cooperative Institute for Meteorological Satellite Studies
Space Science and Engineering Center
University of Wisconsin
1225 West Dayton Street
Madison, Wisconsin

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