FAST RT MODELS FOR RADIANCE ASSIMILATION; ISSUES FOR THE NEXT MILLENNIUM

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1. INTRODUCTION

The direct assimilation of ATOVS radiances in variational data assimilation systems is now well established with several major NWP centres all adopting this approach for the definition of the initial atmospheric state for operational weather forecasts. A major component of the observation operator for satellite radiances is the radiative transfer (RT) model which given a first guess profile of temperature, water vapour (and optionally ozone, other minor gases and cloud water/ice concentrations) plus several surface variables enables a vector of radiances to be computed which correspond to those measured. These RT models must be flexible to cope with all the different types of satellite radiances and fast to enable both the simulated radiances and, for a given profile, their gradient with respect to the profile variables to be computed rapidly.

Over the past decade several fast RT models have been under development and at least two (RTTOV and OPTRAN) have been used in an operational environment where speed of execution is critical. The current status of these fast models is given in the following references: *Saunders et. al.* (1999a), *Saunders et. al.* (1999b) for RTTOV; *McMillin et. al.* (1995) for OPTRAN. The various fast models are now being compared with each other and line-by-line models for HIRS channel 12 (*Soden et. al.,* 1999) and for several other HIRS and AMSU channels (*Garand,* 1999). These comparisons show there is still room for improvement in several aspects of these fast RT models and this paper attempts to highlight the main areas where developments are underway or could be made. Future developments in fast models for the high resolution infra-red sounders are described in *Matricardi and Saunders* (1999).

2. APPLICATIONS OF FAST RT MODELS

There are several applications for fast RT models related to NWP briefly mentioned below. The primary application is for radiance assimilation which requires not only the forward model $y_i = H_i(x)$ where y_i is a radiance vector of i channels computed from a state vector x of j elements, but also the Jacobian matrix $H_{ij}'(x)$ defined for element i,j as:

$$H_{ij}'(x) = \partial H_i(x) / \partial x_j$$

Note the observation and forward model error covariance matrix is also required. A second activity, which is crucial for the first, is to monitor the difference between the radiance observations and the corresponding simulated observations from the NWP model fields. If the mean difference or the standard deviation of the mean difference changes suddenly this is indicative of a problem with either the instrument or the model fields. A third application is to use climate model fields to compute top of atmosphere radiances over a long time scale and compare these with the measured radiances (e.g. MSU-2) as a validation of the climate model.

Recently forecasters have begun to simulate satellite imagery from the regional NWP model fields using fast RT models. Comparisons with the real imagery can quickly highlight errors in the model forecast fields. Finally fast RT models are used for simulating future instrument datasets (e.g. IASI) which can be used for Observing System Simulation Experiments.

3. POTENTIAL IMPROVEMENTS FOR FAST RT MODELS

There are several categories of improvements that are itemised below. Firstly there are those related to the properties of the dependent set of line-by-line transmittances on which the fast models are 'trained'. Secondly the discrete representation of the profile variables (and hence transmittances) in terms of layer values needs to be addressed. Thirdly the actual prediction of optical depth from profile variables, which is the core of the fast model, should be evaluated in terms of accuracy of reproducing the line-by-line values. Fourthly the enhancement of the current fast model to include more variable gases and/or cloud/aerosol profiles, fast surface emissivity models and more channels, to allow the advanced infra-red sounders to be simulated, are underway. Finally there is an additional class of improvements, not addressed here, related to improved user interface (e.g. to allow access to more of the internal arrays) and optimisation in terms of speed of execution, memory allocation, etc., in a MPP computer environment.

3.1 Line by line model transmittance profile datasets

This item concerns the models and databases used to generate the spectral transmittances on which the fast model is based. There are several issues to consider which are summarised here. The first assumption that has to be made is to decide which gases are assumed fixed and globally uniform in concentration and which are assumed to be variable. Water vapour and ozone are typically in the latter class whereas carbon dioxide and oxygen are normally in the former. Gases such as methane, nitrous oxide and carbon monoxide are variable but for NWP assimilation they are assumed to be constant to simplify the calculations but with the result that channels affected by these gases will have a larger fast model error due to this unaccounted for variability. For instance these minor constituent gases do influence the transmittance of several HIRS channels.

The spectral transmittances are computed either using a line-by-line (LbL) model (e.g. GENLN2, *Edwards* (1992); MPM89, *Liebe* (1989)) or using a spectral database (e.g. 4A, *Tournier et. al.* (1995); kCARTA *Strow et. al.* (1998)) to compute the absorption due to both lines and continuum absorption. The latter includes the contribution far from the line centres ideally defined in a consistent way with the lines and is particularly important in the millimetre and 10-12μm atmospheric windows due to water vapour continuum absorption. Various versions of the CKD formulation (*Clough et. al.* 1995) are normally used to parameterise the continuum. In addition to their treatment of the continuum, other issues for each LbL model are, (i) how line mixing is treated, which is important for the long-wave HIRS channels which peak in the stratosphere and (ii) treatment of complex molecular absorption (e.g. CFCs) which can affect the mid-infrared window channels. Differences are seen between LbL models for the same atmospheric profile due to differences in spectral line datasets and modelling the various absorption mechanisms. A good summary of the various models/datasets used for the current and past generation of fast RT models is given in *Soden et. al.* (1999).

The other main ingredient required for LbL transmittances is a set of diverse atmospheric profiles. These can be either from a radiosonde profile dataset such as TIGR-2 (*Escobar-Munoz,* 1993) or from a NWP model set of fields (*Chevallier,* 1999). The former samples the real atmosphere but only at point locations and the measurements include instrument errors particularly for the humidity data (e.g. lag in response). The latter samples the simulated atmosphere at all locations (providing more extremes) but is limited by the realism of the model analysed fields. For the infra-red region only a limited number of profiles (~100) can be realistically considered as the LbL model calculations are computationally expensive. Microwave LbL models are much faster to run and so can compute transmittances from a larger sample of profiles if required. The radiosonde or model profiles both have to be interpolated on to the fast model pressure levels and often extrapolated above the last measured layer up to 0.1hPa (although note the latest version of the ECMWF model now goes up to this level). This extrapolation can introduce discontinuities into the profile set and will rely on climatology where no measurements are available. Finally it is important to define the upper and lower limits for each profile variable outside which the transmittance calculations are no longer accurate. Experiments with RTTOV have shown the limits are at least 5% beyond the max/min values of the dependent set of profiles.

3.2 Discretisation of the Radiative Transfer Equation

There are several instances where the accuracy of the RT model has to be compromised due to the necessity to divide both the spectra and profile into discrete intervals/layers. The spectral sampling is defined by the LbL model. The need to sample adequately the spectral lines should be taken into account to obtain the most accurate computed spectrum but if the spectral width of the instrument response function is wide (>10cm^{-1}) some of the errors introduced by inadequate sampling can average out. In practice recent datasets have been produced with future high spectral resolution instruments in mind and the corresponding spectral sampling required has been shown to be 0.001cm^{-1} in order not to introduce significant errors. This level of sampling produces large datasets when the whole mid-infra-red spectrum is simulated. In the microwave region the sampling is normally not so critical as the radiometer pass-bands usually straddle the line centre so that the centre is not required to be sampled. An exception to this is the SSM/I 22 GHz channel which includes the 22.2 GHz water vapour line centre within the pass-band. In this case the sampling must be higher in order not to compute anomalously low transmittances in the stratosphere.

The division of the profile into discrete layers needs to be considered. Current fast models range from 40 to 100 levels. For the ATOVS radiometers around 40-50 layers is thought to be sufficient as the weighting functions are broad for these channels. For the future high-resolution sounders though, more levels will be required to represent accurately their narrower weighting functions. A related issue is the computation of the layer mean profile temperatures. There are several possibilities ranging from a simple average of the level values adjacent to the layer to employing a full Curtis-Godson computation of the layer mean temperatures for well mixed gases, water vapour and ozone. The difference between these two extremes in terms of layer mean computed temperature is shown in Figure 1 for two profiles where values up to ±1K are possible.

3.3 Development of fast transmittance models

Several approaches for rapid computations of transmittances have been adopted. The fixed pressure level linear regression scheme (*McMillin et. al.* 1979) has been adopted by several models (e.g. RTTOV) and has been in use operationally for many years now. However this approach still leads to significant errors (greater than instrument noise) for the computation of the water vapour channel radiances. More recently similar models but working on layers of constant absorber amount for fixed and each variable gas have been developed (e.g. OPTRAN) which have improved the simulation of water vapour channel radiances. Other approaches under development are the 'radiance sampling' approach (*Tjemkes and Schmetz,* 1997) which give more accurate radiances than the regression techniques but at an increased computational cost, and more physically based models (*Garand et. al.* 1999). Finally work is underway to investigate the use of neural networks for fast transmittance and radiance models (*Aires et. al.* 1999).

The need to develop a unified transmittance model for ***all*** radiometer channels, both infra-red and microwave, and in the infra-red for the new high resolution spectra from spectrometers and interferometers provides a challenge to encompass all possibilities within one model. For instance there are good reasons why water vapour channels in the infra-red spectrum behave differently from those in the microwave spectrum and this can have an influence in the form of the optimal fast model predictors. The move to high spectral resolution with many thousands of channels can also influence the design of the code relative to the current ATOVS 40 channel fast models.

3.4 Instrument spectral responses

There is now a requirement, for the applications mentioned above, for fast RT models to be able to simulate a range of different radiometers. These include: *(A)TOVS, AVHRR, VTPR, Geostationary imager and sounder data (e.g. MVIRI, SEVIRI, GOES imager and sounder, GMS imager), SSM/I, AIRS, MODIS and IASI* for which there is an interest within the NWP radiance assimilation community. An example of the performance of the RTTOV model in terms of transmittance for the proposed SEVIRI imager on MSG-1 is shown in Figure 2. For all these instruments the RT model relies on the instrument spectral response function (i.e. filter response for radiometers) being known in the space environment to within a few percent. There have been clear examples in the past (e.g. comparisons of GOES-8 and GOES-10 radiances) which have shown that filter responses have not been accurately known. Pre-launch calibration of the instruments is important to verify the spectral responses are correct. For the advanced sounder interferometer data decisions have to be made as to whether to simulate apodised or unapodised spectra. Current fast models for IASI simulate the former but this implies a non-diagonal observation error covariance matrix.

3.5 Additional state vector variables

The basic elements of the state vector for a fast RT model are profiles of temperature and water vapour and surface skin temperature but more recently ozone profiles and more surface parameters have been added. However as the demands for fast models to simulate more atmospheric situations increase additional variables have to be included in the state vector. For instance surface emissivity is important to model accurately for the window and lower sounding channels. At infra-red wavelengths the tables published by *Masuda et. al.* (1988) are now used for the ocean surface and at microwave wavelengths the FASTEM model (*English and Hewison,* 1998) is used. These models are being used as the basis for parameterisations which are now being included within fast RT models. For the former the surface emissivity varies with wind speed and angle but for the latter the sea surface temperature is an additional variable. Over land there is a much larger uncertainty in surface emissivity but atlases are now being compiled as the first step to improving the NWP model's representation of land surface emissivity. The impetus is to be able to assimilate some of the sounder channel radiances over land which have already been shown to have a positive impact on forecast skill.

Secondly including clouds in the state vector is an important addition in preparation for assimilation of cloudy radiances. In the infra-red clouds are currently treated as grey bodies emitting at the level of the specified cloud top. In the microwave cloud liquid water concentration profiles can be treated assuming Rayleigh scattering is negligible and only emission/absorption is considered. At both wavelengths ice cloud is less well modelled and more work on the parameterisation of cirrus cloud transmittances is needed.

Of less importance, but still significant for the short-wave infra-red, is scattering due to tropospheric and stratospheric aerosols and inclusion of a solar reflection term for high albedo surfaces. There is evidence in NWP model radiance bias statistics that the HIRS short-wave channels are affected by these factors.

3.6 RT model validation

There are several different levels of fast model validation:

- Validate fast model transmittances with corresponding line-by-line values for both dependent and independent profile set. This measures the ability of the fast model to reproduce the line-by-line model on which it is based as demonstrated in Figure 2.
- Compare different line-by-line models and measurements which can provide a measure of the uncertainty of our current knowledge of the spectroscopy for atmospheric gases. The Intercomparison of Transmittance and Radiance Algorithms (ITRA) has made such comparisons in the past and EUMETSAT are co-ordinating such a comparison for IASI line-by-line model simulations.

- Fast model comparisons which compare the accuracy of different fast models both in terms of the simulated radiances and their Jacobians. The Jacobian comparisons can show anomalies in fast models not evident in the forward model comparisons and these can be important for radiance assimilation. A fast model comparison for a selection of ATOVS channels is reported in the paper by *Garand* (1999) in these proceedings.
- Comparison of observations with simulations from NWP model fields. Similar channels should have similar biases and rms. differences and the biases should on average be less than 1K.

These validation steps can provide an estimate of the forward model error covariance which must be assumed in the radiance assimilation process.

3.7 Technical issues

The final category is classed as more technical and includes a number of minor issues. The fundamental constants and 'channel constants' used by the RT model should be the same as those used in the calibration of the instrument. Currently there are small differences between the constants used for calibration and RT modelling. Another important consideration is that the code is portable but also runs fast on MPP supercomputers. These constraints can be incompatible unless careful compromises are made. Another issue is how often to call the fast RT model during the minimisation process. Current wisdom suggests the tangent linear assumption for the temperature sounding channels is a sufficiently good approximation to the full non-linear model that only a single call to the RT model is needed. For the water vapour and ozone channels however 2-3 calls are needed, as there are significant non-linearities in the radiances with respect to water vapour and ozone amounts.

4. SUMMARY

The main issues related to fast RT model development are summarised above. Distilling the above information the following general points can be made:

- Creation of a line-by-line model profile dataset is a large undertaking both in terms of computational resources and data storage. The current ECMWF GENLN2 transmittance dataset occupies almost a Tbyte of disk space. Therefore the creation of large line-by-line model transmittance databases should be co-ordinated.
- Diverse forecast model profile datasets are now available as a new resource for fast model developments.
- Improved knowledge of the instrument spectral responses are required from the space agencies.
- The accuracy of the model simulated radiances and Jacobians is still in need of improvement for some channels/profile variables.
- Surface emissivity and modelling of cloud should be included within the fast model.
- Unify fast models for all instruments within an NWP model (challenge for AIRS/IASI).
- Validate fast models through occasional comparisons with other fast and line-by-line models.

The development of fast RT models is co-ordinated in a number of different fora. The International TOVS Study Conference has a fast model technical sub-group which reviews progress in fast RT models once every 2 years. Recently EUMETSAT have formed a NWP Satellite Application Facility and one of its tasks is to develop fast RT models within European Met. Services.

As satellite radiances are now increasingly being used within NWP models, and have clearly shown benefits to the forecast skill (see other papers in these proceedings), the need to optimise the fast RT models is gaining more importance. Consideration of the points raised in this paper will be important in achieving the goal of better fast RT models.

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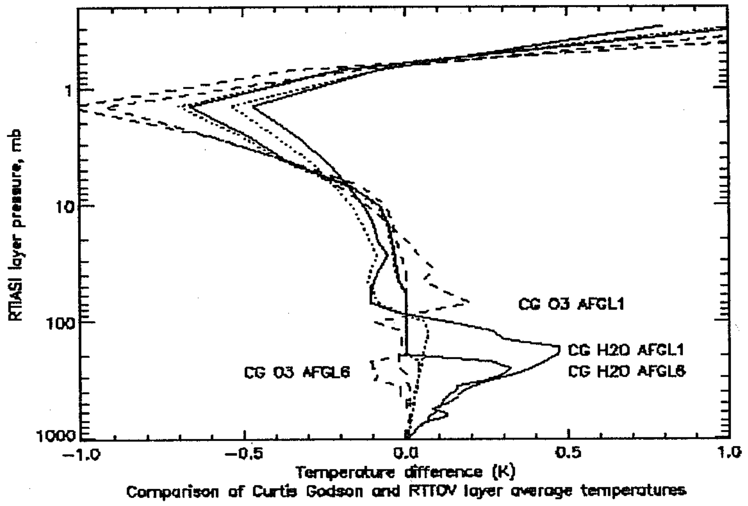

Figure 1. Differences between Curtis-Godson absorber weighted layer averaged temperatures and RTTOV layer averaged temperatures. Differences are illustrated for 2 atmospheres (AFGL1; tropical and AFGL6; U.S. Standard) and three absorbing gases: water vapour (solid line), carbon dioxide (dotted line) and ozone (dashed line).

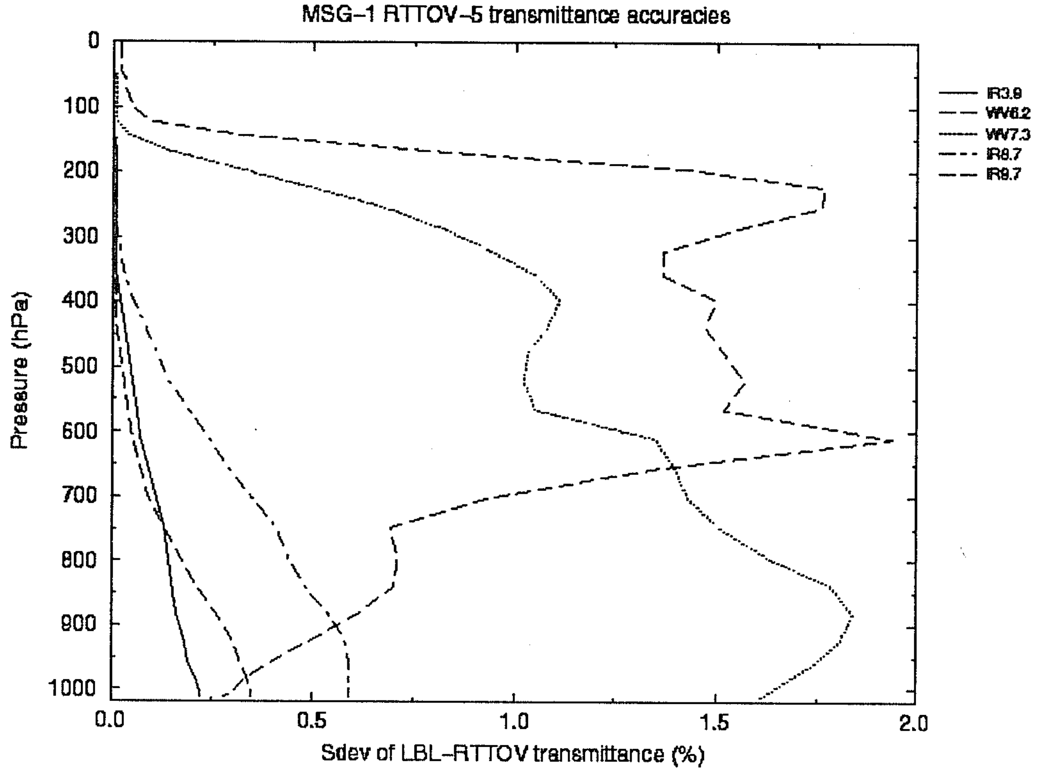

Figure 2. Standard deviation of difference between GENLN2 and RTTOV-5 computed MSG-1 SEVIRI transmittances for the dependent 43 profile dataset for all viewing angles. The differences are expressed as a percentage of unit transmittance.