ASSIMILATION OF IASI AND AIRS DATA: FORWARD MODELLING

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SUMMARY

This paper describes the current status of radiative transfer models specifically for the new generation of advanced infrared sounders that will start providing data within the next few years. All the components of the forward model necessary for radiance assimilation within a numerical weather prediction model are addressed. The instruments themselves are first briefly described. The current developments in fast radiative transfer models for infrared sounders are described together with their associated error characteristics. The status of diverse profile datasets and accurate line-by-line radiative transfer models which are necessary ingredients for the fast model development are reviewed. Finally a list of recommendations where further work is required is given. A companion paper in these proceedings by Collard gives details on how the forward model described here and its gradient are used within a variational assimilation system.

1. INTRODUCTION

One of the primary tasks of operational Numerical Weather Prediction (NWP) centres and an important aim of the World Climate Research Programme (WCRP) is to improve our representation of the atmospheric and surface hydrological cycle in global NWP and climate models. The former is needed to improve the short to medium term weather forecasts from the more accurate analyses produced. An additional requirement of the climate change community is to monitor the concentrations of the atmospheric minor constituents consistently over a long (>10 years) period of time.

One way of contributing to these objectives is to make more comprehensive and accurate measurements from a satellite of the upwelling infrared radiance emitted by the Earth's atmosphere and surface. A step in this direction will be the launch of high resolution infrared sounders on meteorological polar orbiting satellites which will have the potential to provide temperature and constituent profiles at a higher accuracy and with higher vertical resolution than the existing filter wheel infrared radiometers that have been flown since the early 1970s. They will provide the capability of more accurate temperature retrievals (i.e. in the free troposphere and lower stratosphere to 1K and vertical resolution of 1 km) and water vapour retrievals to an accuracy of 10% in relative humidity and vertical resolution of 1km in the low troposphere. They will also allow ozone and other minor constituent concentrations (e.g. N_2O. CO, CH_4 and others) to be estimated. Figure 1 shows a comparison of a radiance spectrum that will be measured by an advanced sounder with the filter responses of the current operational infrared sounder HIRS (High-resolution Infra-red Radiation Sounder) overlain. This illustrates how much the current filter wheel radiometers integrate over the infrared spectrum smearing out all the details. It is the finer spectral resolution along with the number of channels sampling the entire spectrum which provides a wider range of sharper weighting functions resulting in better vertical resolution of the retrieved profiles.

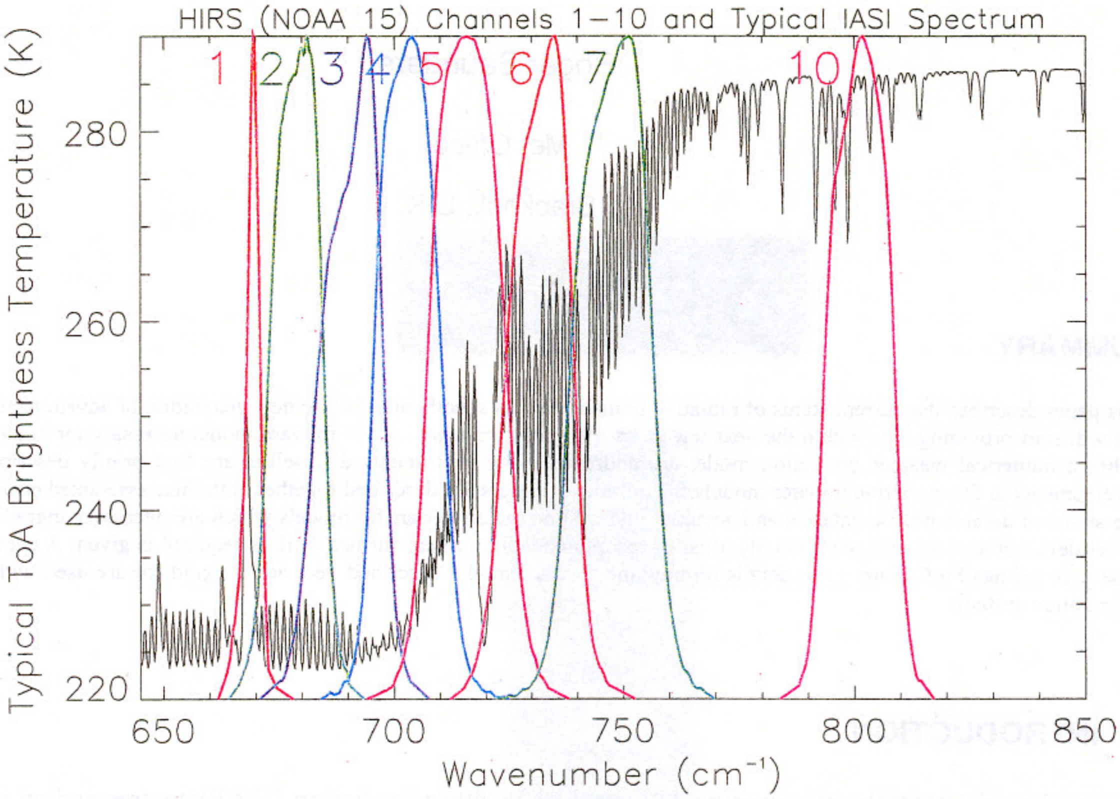

Figure 1 Simulated IASI spectrum with HIRS/3 (NOAA-15) channel filter responses overlain.

In recent years operational NWP centres (e.g. ECMWF *Andersson et. al.,* 1994, NCEP, *Derber and Wu,* 1998, Met Office, *English et. al.,* 2000) have moved from using retrieved temperature and humidity profiles from the TIROS-N Operational Vertical Sounder (TOVS) to assimilating the radiances directly into their models using a variational analysis scheme. For example 1D-Var is described by *Eyre et al.* (1993) for a single profile retrieval or 3/4D-Var is described by *McNally et. al.,* (2000) and *Rabier et al.* (2000) for direct assimilation of radiances in a global NWP analysis. A prerequisite for exploiting these radiance data in a NWP model using the variational analysis scheme is the development of an observation operator which includes a fast radiative transfer (RT) model to accurately compute the top of atmosphere radiances given first guess model fields of the atmospheric state. These include profiles of temperature, water vapour, other constituents, surface parameters and later cloud. This fast RT model has to simulate the radiance spectrum for each observation point to give the model equivalent of the observation with which each measurement is compared. A key requirement is it must be fast enough to cope with the processing of observations in near real-time.

In addition to radiance assimilation fast RT models also have a number of other related applications at NWP centres:

- Real time instrument monitoring through global/regional biases and standard deviations of observed minus simulated radiances
- Validation studies of NWP model (e.g. compare model simulated cloudy radiances with measured radiances)

- Pre-launch studies to assess the information content of a new instrument in an NWP context.
- Generation of a simulated observation dataset for observing simulated system experiments

This paper is aimed at those who want to learn more about forward modelling for advanced infrared sounders but does not go into detail on any particular aspect. For those who want to learn more, a comprehensive list of references is provided. An overview of the planned instruments is provided in section 2, a description of the methodology of fast RT models together with the status of line-by-line RT models and profile datasets is provided in section 3 and a summary with recommendations for future work in section 4.

2. ADVANCED INFRARED SOUNDERS

The first advanced infrared sounder IRIS (InfraRed Interferometer Spectrometer) was launched on NIMBUS-3 on 14 April 1969. It was an interferometer which provided spectra in the range 5-25μm at a resolution of 2.8cm^{-1} and provided a new insight into the atmospheric thermal emission as seen from space (*Hanel et. al.,* 1971). Another IRIS instrument was launched on NIMBUS-4 in 1970 but since then it was not until 1996 when IMG (Interferometric Monitor for Greenhouse gases) was launched on ADEOS that a nadir viewing high spectral resolution infrared instrument was once again in Earth orbit (*Kobayashi et. al.,* 1999). This was a much higher resolution instrument (0.1cm^{-1} apodised) but still only viewed close to nadir.

With operational NWP in mind, to obtain global coverage, several high-resolution infrared sounders are planned to be launched in the next few years. Table 1 lists their respective attributes. The Atmospheric InfraRed Sounder, AIRS, will be the first instrument to be launched on the NASA Aqua polar orbiting platform (*Aumann and Pagano,* 1994). It is a grating spectrometer with 2378 discrete spectral channels which views a swath of the Earth centred at nadir. A combination of band-pass filters and grating dispersion produce the radiance spectrum at a spectral resolution of $\nu/2400$ cm^{-1} where ν is the frequency. AIRS will fly with the Advanced Microwave Sounding Unit, AMSU-A, and Humidity Sounder Brazil, HSB (the latter is similar to AMSU-B) and the MODerate resolution Imaging Spectroradiometer, MODIS, imager.

The Infrared Atmospheric Sounding Interferometer (IASI) has been designed as an advanced infrared sounder on the new generation of European operational meteorological polar orbiters (*Cayla,* 1993). The IASI instrument is a Fourier-Transform Spectrometer (FTS). The design of the interferometer is based on a classical Michelson instrument with a -2 to +2 cm optical path difference (OPD) range. IASI has a constant spectral sampling interval of 0.25 cm^{-1} and it will cover the spectral range from the CH_4 absorption band at 3.62μm (2760 cm^{-1}) to the CO_2 absorption band at 15.5μm (645 cm^{-1}) with an unapodised spectral resolution between 0.35 and 0.5 cm^{-1}. IASI will fly in combination with the Advanced Microwave Sounding Unit, AMSU-A, the Microwave Humidity Sounder, MHS, and the Advanced Very High Resolution Radiometer (AVHRR/3).

Parameter	Advanced Sounder		
	AIRS	IASI	CrIS
Instrument type	Grating Spectrometer	Interferometer	Interferometer
Satellite Agency	NASA/JPL	EUMETSAT/CNES	NOAA IPO
Spectral range (cm^{-1})	649-1135; 1217-1613; 2169-2674	Contiguous 645-2940	650-1095; 1210-1750; 2155-2550
Number of channels	2378	8461	~1300
Unapodised spectral resolving power/spectral sampling (cm^{-1})	1000-1400 ~ν/2400	2000-4000 0.25 cm^{-1}	900-1800 0.625/1.25/2.5 cm^{-1}
Spatial footprint (km)	13	12	14
Nominal Altitude (km)	705	833	824
Sampling density per 50km^2	9	4	9
Power (W)	225	200	86
Mass (kg)	140	230	81
Platform	Aqua	Metop-1	NPP and NPOESS
Nominal launch date	May 2001	2005	2006(NPP), 2009(NPOESS)
Primary Advantages	Lowest noise esp. for shortwave	Most versatile spectral coverage and best resolution	Smallest sensor

Table 1 Summary of instrument characteristics (note the CrIS values are provisional)

The Cross-track Interferometric Sounder (CrIS) is scheduled to fly on the NPOESS (National Polar-orbiting Operational Environmental Satellite System) Preparatory Program (NPP) satellite in a similar timeframe to IASI and also on the NPOESS satellites themselves at the end of the decade. Unlike IASI it does not sample the entire spectrum but 3 parts as defined in Table 1 and the spectral sampling and resolution for CrIS is lower than for AIRS and IASI. It is intended that CrIS will be the prototype of the operational infrared sounder on the future NPOESS platforms.

Finally the prospect of an advanced sounder in geostationary orbit may become a reality in the near future. The U.S. has tentatively approved the Geostationary Imaging Fourier Transform Spectrometer (GIFTS) as a proof-of-concept demonstration under the NASA New Millennium Program, planned for launch in 2003. GIFTS will cover the spectral range 800-2400 cm^{-1} at 0.3 cm^{-1} nominal resolution, coupled with a visible imager for coincident imaging. It is planned to be located first over the American continent and later over the Indian Ocean.

3. FAST RADIATIVE TRANSFER MODELS

3.1 Introduction

For radiance assimilation in an operational NWP model the top of atmosphere radiance measurements made by an advanced sounder must be computed rapidly from the model fields (i.e. < 1s per field of view) in order to produce an atmospheric analysis using these and all other observations in a timely manner. To meet this requirement fast RT models have been developed and the methodology adopted is given below.

The basis of variational assimilation is to minimise a cost function J which is a function of the atmospheric state vector $\mathbf{x}$:

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{y}^o - \mathbf{H}(\mathbf{x}))\mathbf{R}^{-1}(\mathbf{y}^o - \mathbf{H}(\mathbf{x}))^T + \frac{1}{2}(\mathbf{x} - \mathbf{x}^b)\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b)^T \tag{1}$$

Where $\mathbf{y}^o$ are the observed radiances; $\mathbf{x}^b$ is the first guess atmospheric state (normally from a short range forecast); $\mathbf{H(x)}$ is the observation operator for radiances (see below); $\mathbf{R}$ is the sum of the observation and forward model error covariance matrices; $\mathbf{B}$ is the error covariance matrix of the first guess and ^{T} denotes matrix transpose and $^{-1}$ matrix inverse. The fast RT model is part of $\mathbf{H(x)}$ which given an atmospheric profile interpolated to the observation point from the model grid computes the model equivalent of $\mathbf{y}^o$. The interpolation from model fields to observation point is also part of the $\mathbf{H(x)}$ operator but this will not be addressed further in this paper. Note an estimate of the error covariance matrix of the fast RT model is required (as part of $\mathbf{R}$) and this is discussed below in sec. 3.5.2.

To simulate the top of atmosphere radiance measured by a satellite, the transmittance of the atmosphere, the radiance emitted and reflected from the surface and/or clouds all have to be calculated rapidly and then input to the radiative transfer equation. The top of the atmosphere upwelling radiance, $L(\nu,\theta)$, at a frequency ν and viewing angle θ from zenith at the surface, neglecting scattering effects, can be written as:

$$L(\nu,\theta) = (1-N)L^{Clr}(\nu,\theta) + NL^{Cld}(\nu,\theta) \tag{2}$$

where $L^{Clr}(\nu,\theta)$ and $L^{Cld}(\nu,\theta)$ are the clear sky and fully cloudy top of atmosphere upwelling radiances and N is the fractional cloud cover. The second term related to cloud is considered later in sec. 3.4. For clear sky radiance, $L^{Clr}(\nu,\theta)$ can be written as:

$$L^{Clr}(\nu,\theta) = \tau_s(\nu,\theta)\varepsilon_s(\nu,\theta)B(\nu,T_s) + \int_{\tau_s}^{1} B(\nu,T)d\tau + (1-\varepsilon_s(\nu,\theta))\tau_s^2(\nu,\theta)\int_{\tau_s}^{1} \frac{B(\nu,T)}{\tau^2}d\tau \tag{3}$$

where the first and third terms on the RHS of equation 2 are the radiance from the surface (emitted and reflected assuming specular reflection) and the second term is the radiance emitted by the atmosphere where $B(\nu,T)$ is the Planck radiance for a scene temperature T, $\tau_s(\nu,\theta)$ is the surface to space transmittance, τ the layer to space transmittance, $\varepsilon_s(\nu,\theta)$ the surface emissivity, T is the layer mean temperature and T_s, the surface radiative temperature.

For convenience the different components of fast models: the clear sky atmospheric transmittance, surface and cloud emissivity computations are described separately below. In addition there are several components not addressed further here. Aerosol scattering should be included in future models but for typical cases is only significant for the shorter infrared wavelengths measured by advanced sounders. Similarly the contribution from solar reflected radiance does affect the shorter wavelengths during the day and should be included in fast RT models

3.2 Clear Sky Atmospheric Transmittance

There are several types of fast radiative transfer models in use or under development which are relevant to advanced sounder radiance assimilation. These models compute transmittance or layer optical depths from the profile variables (e.g. $T(p)$, $H_2O(p)$, $O_3(p)$, $sec(\theta)$, where p is the pressure) for each 'active' gas in the model. To date only water vapour and ozone are considered as variable gases with the remaining gases, assumed to have a constant mass mixing ratio, referred to as mixed gases. The various models can be categorised into regression models on pressure levels or levels of equal absorber amount (strictly overburden), physical models, and neural net based models. These different models are described briefly below but the interested reader should refer to the references given.

A model used operationally at ECMWF and other NWP centres, to simulate radiance measurements from the HIRS and the Advanced Microwave Sounding Unit (AMSU) on the National Oceanic and Atmospheric Administration (NOAA) satellites is the Radiative Transfer for Tiros Operational Vertical Sounder (RTTOV) (*Eyre,* 1991; *Saunders et al.* 1999a; *Saunders et al.* 1999b and the web site at: *http://www.met-office.gov.uk/sec5/NWP/NWPSAF/rtm*). The basis of the method is through linear regression to predict a layer optical depth to space, d_j, for mixed gases and separately for variable gases (e.g. water vapour and ozone) from a set of predictors computed from the input profile variables (e.g. temperature, constituent mixing ratios, viewing angle, etc):

$$d_j = d_{j-1} + \sum_{k=1}^{M} a_{k,j} X_{k,j} \tag{4}$$

where j is the pressure level (typically up to 100), M is the number of predictors (typically 10-15) and the functions $X_{k,j}$ constitute the profile dependent predictors of the fast transmittance model. To compute the regression coefficients $a_{k,j}$ the set of diverse atmospheric profiles (see sec. 3.2.2) is used to compute, for each profile and for several viewing angles, accurate line-by-line (LbL) transmittances (see sec. 3.2.1) for each layer. The layer LbL transmittances, integrated over the radiometer channel spectral response function, are then used to compute the coefficients by linear regression after conversion to layer optical depth which was found to give better results than using the transmittances directly (*Eyre and Woolf,* 1988). These regression coefficients can then be used by the fast transmittance model to compute optical depths given any other input profile. As the channel transmittances are not monochromatic it is not strictly valid to multiply the transmittances of the mixed and variable gases together to compute the total layer to space transmittance. A better approximation (*McMillin et al,* 1995) is to multiply the mixed gas channel transmittance with the total channel transmittance divided by the transmittance of mixed gases plus other variable gas transmittances, for example:

$$\tau_j^{tot} = \tau_j^{mix} \cdot \frac{\tau_j^{mix+wv}}{\tau_j^{mix}} \cdot \frac{\tau_j^{mix+wv+oz}}{\tau_j^{mix+wv}} \qquad (5)$$

where the superscripts denote what selection of gases were included in the line-by-line monochromatic transmittance calculations. The superscripts are defined as *mix* for those gases assumed to have fixed mass mixing ratios, *wv* for water vapour and *oz* for ozone. The fast model predicts the three terms on the right hand side of equation 5 separately and then combines them to give a total layer transmittance. In the future when more variable gases are included in the fast models this approach will need to be reconsidered. This parametrisation of the transmittances makes the model computationally efficient and in principle should not add significantly to the errors generated by uncertainties in the spectroscopic data used by the LbL model.

The fast RT model developed at ECMWF for exploiting IASI radiances, RTIASI (*Matricardi and Saunders*, 1999), is based on the approach followed by RTTOV. It comprises a fast model of the transmittances of the atmospheric gases that is generated from accurate line-by-line transmittances for a set of diverse atmospheric profiles over the IASI wavenumber range. The monochromatic layer-to-space transmittances are integrated over the appropriate IASI Instrument Spectral Response Function (ISRF) and used to compute channel-specific regression coefficients by using a selected set of predictors.

A similar approach known as the Optical Path Transmittance (OPTRAN) method has been developed (*McMillin et al.*, 1979; *McMillin et al.*, 1995) and implemented for operational radiance assimilation at the National Center for Environmental Prediction (NCEP). This is similar to the fixed pressure level grid adopted by RTTOV but uses layers of equal absorber amount instead. This can be advantageous for gases like water vapour where the path absorber amounts are not simple functions of pressure. OPTRAN has been shown to be superior to RTTOV for water vapour affected infrared channels (*Soden et. al.* 2000; *Garand et. al.*, 2001).

A more physical approach to fast RT modelling has recently been developed by *Garand et. al.* (1999) and demonstrated for HIRS radiance assimilation. This approach averages the spectroscopic parameters for each channel and uses these to compute layer optical depths. All the gaseous absorbers are treated separately. A correction factor is applied to ensure a close fit to a LbL model. The advantages of this approach are: (i) more accurate computation for some gases (cf. regression methods), (ii) any vertical co-ordinate grid can be used and (iii) it is easy to modify if the spectroscopic parameters change (e.g. when the line databases are updated). However to date these physical models are a factor of 2-5 slower than the regression based models which is significant for radiance assimilation purposes.

A semi-fast model, SYNSATRAD, being used for METEOSAT simulations (*Tjemkes and Schmetz*, 1997) uses precomputed tables of mean optical depths which sample the spectral range for the channel of interest.

This has proven to be very accurate for infrared filter radiometer channels but is an order of magnitude slower than regression models. The size of the tables may become prohibitive for advanced sounders.

Models using neural nets are under development (*Schwander et. al.* 2000) and may provide an even faster means to compute the radiances and this has been demonstrated for forward model calculations (e.g. *Chevallier and Mahfouf*, 2000). However the gradient versions of the model to compute the Jacobians (see below) are proving more difficult to develop using neural nets at the present time and more work is needed before operational centres can consider using these techniques for advanced sounder radiance assimilation.

3.2.1 Line by Line Models

The database of 'true' atmospheric infrared transmittances, on which the fast RT models are based, is calculated using a line-by-line atmospheric transmittance model. The atmosphere is subdivided into a number of layers within which the gas is considered homogeneous and is represented by appropriately weighted mean layer parameters. Mean temperature, pressure and gas amount are defined for each gas along the actual ray trajectory within the layer (gas path) and, since within a path the gas is considered homogeneous, the line-by-line computation of the transmittance proceeds for each gas path at each point of the frequency (wavenumber) grid. To evaluate the path optical depth, the absorption contributions from all the molecular spectral lines in the spectral range of interest must be considered. For each spectral line the parameters required are obtained from a spectral line database such as the High-resolution Transmission (HITRAN) molecular database (*Rothman et. al.* 1998). The 1996 edition contains almost 1,000,000 spectral lines for 35 different molecules. In addition to the molecular database there are extensive infrared cross-sections at different pressures and temperature, for some more exotic gases (e.g. CFCs). A similar database, GEISA, is also available (*Jacquinet-Husson et. al.* 1999) for LbL calculations.

Several LbL models exist, for example GENLN2 (*Edwards,* 1992), and LBLRTM (*Clough et. al.*, 1992). The basic input to these models is the atmospheric profile that defines the gas conditions, the gases that are spectroscopically active over the spectral region relevant to the user, the spectral sampling interval and range, molecular spectral line data and choice of line shape. The line strengths and half-widths are calculated at the path pressure and temperature. The Voigt (*Armstrong,* 1967) line shape is often adopted for most gases to include the effects of both pressure and Doppler line broadening. Line coupling (interactions between closely spaced vibrational-rotational lines) and non-Lorentzian line wing effects should also be taken into account as the effects caused by line coupling, can produce large differences in very localised spectral regions. Line coupling coefficients (*Strow et. al.,* 1994) are available to compute the CO_2 modified line shape.

In addition to line absorption, the continuum absorption of certain molecules must also be taken into account. This is the additional absorption observed in excess of the line absorption. The exact mechanism for the continuum absorption is still a matter of debate but it is now generally accepted that the main reason is due to an inadequate description of the line shape well away from the line centres. In particular the water vapour continuum is important in the infrared and is responsible for most of the absorption in the 'atmospheric windows' around 4μm and at 8-12μm. Laboratory and field measurements have measured the excess absorption and empirical relationships have been derived. In GENLN2 and LBLRTM the water vapour continuum absorption is parameterised using the semi-empirical approach of *Clough et. al.,* (1989) and *Clough* (1995). In addition CO_2, N_2 and O_2 continua should also be included. Finally to model the heavy molecules (e.g. CFC11 and CFC12) high-resolution cross-section data are used.

To date fast models have only assumed water vapour and ozone are variable gases. This leaves fixed gases defined as CO_2, N_2O, CO, N_2, CH_4, O_2, CFC11 and CFC12 in the fast RT model. The transmittance spectra for all these gases are computed over the required spectral range (e.g. from 500 cm^{-1} to 3000 cm^{-1}) at wavenumbers pre-determined by a specified wavenumber grid the spacing of which defines the resolution of the calculation. The resolution used in the line-by-line spectral computation is determined by studying how the point spacing of the full resolution spectra affects the convolved radiance of the instrument being considered. IASI records atmospheric spectra the natural resolution of which is much higher than the instrument resolution. It has been shown (*Matricardi and Saunders,* 1999) that a sampling of 0.001 cm^{-1} is a sufficient resolution for IASI simulations. The sampling in the vertical pressure level space also has to be considered. The AIRS science team has chosen 101 levels for their AIRS RT calculations. This number of levels may be too high for radiance assimilation and it is likely that a number between this and the current 43 levels used for ATOVS will be adopted. Research is underway to determine the optimum number of levels for advanced sounder RT models.

Transmittance spectra, at this resolution, for fixed gases, water vapour and ozone are then computed for each level to space, for a range of viewing angles for each atmospheric profile. This computation is expensive both in CPU and disk space. Efforts to alleviate this have been made by compressing the transmittances by a factor of 100 in disk space, using singular value decomposition, to produce the kCARTA dataset (i.e. *Strow et. al.* 1998). A similar approach has been adopted in the 4A model (Automatized Atmospheric Absorption Atlas, *Scott and Chedin,* 1981, *Cheruy et. al.,* 1995) where monochromatic layer transmittances are stored for a wide range of different atmospheric conditions. Given an atmospheric profile, the model then allows the most appropriate transmittances to be extracted from the database without the need for a full LbL computation.

Errors in LbL models can be difficult to assess statistically as it is expensive to compute many spectra but comparisons with specific observational radiance datasets with a good characterisation of the atmospheric state, particularly the humidity profile, are being made (*Tjemkes et. al.,* 2001) and also comparisons between the LbL models themselves (*Garand*, 1999 and *Garand et. al.,* 2001). These show the errors in brightness temperature are in most cases less than 0.25K. Remaining uncertainties include accurate parameterisations of line mixing effects in the carbon dioxide absorption bands and accurate modelling of the water vapour continuum absorption. In addition improved spectral line parameters are providing a better fit of the LbL model output to the measured data. Inclusion of all the radiatively active gases (e.g. CFCs) is also a prerequisite for reducing the measured minus LbL model differences. Finally in certain parts of the spectrum (e.g. the CO_2 band at 4.3μm) with strong absorption bands the assumption of LTE (Local Thermodynamic Equilibrium), where the energy levels are populated according to the Boltzmann distribution, breaks down and allowance should be made for this in the LbL calculations (*Rodgers et. al.,* 1992). This only applies to channels which sense the upper stratosphere and mesosphere.

3.2.2 Profile datasets

To develop a fast RT model for top of atmosphere radiance measurements a dataset of 'true' atmospheric transmittance profiles has to be generated on which to train a fast model. This dataset is obtained by running a LbL RT model on a set of diverse atmospheric profiles. These can be either from a radiosonde dataset such as TIGR (*Escobar-Munoz,* 1993) or from a NWP model set of fields (*Chevallier et. al.,* 2000). 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, poor absolute accuracy below –25°C). The latter has the potential to sample the simulated atmosphere at all locations (providing more extremes) but is limited by the realism of the model analysed fields. For the infrared region only a limited number of profiles (~100) can be realistically considered as the LbL model calculations are computationally expensive. The radiosonde or model profiles both have to be interpolated on to the required RT model pressure levels and often extrapolated above the last measured layer up to 0.1hPa (although the latest version of the ECMWF forecast model now includes this level). This extrapolation can introduce discontinuities into the profile set and will rely on climatology where no measurements are available. The profile dataset will define the upper and lower limits for each profile variable outside which the fast model transmittance calculations are no longer as reliable.

The profiles used to compute the database of line-by-line transmittances are chosen to represent the range of variations in temperature and absorber amount (for variable gases) found in the real atmosphere. Only a few atmospheric gases are allowed to vary, the others are held constant and will be referred to as fixed gases and it is assumed that spatial and temporal variations of their concentrations do not contribute significantly to the observed radiance variations. To date only H_2O and O_3 are considered as variable gases although in localised spectral regions gases such as CO, N_2O and CH_4 should also be considered variable.

For the TIGR radiosonde profile set currently used for fast RT model training each profile has data for temperature and absorber amount that cover the whole range of pressure values used in the radiative transfer computations. However, the quality of the radiosonde stratospheric humidity measurements in the TIGR data set is a matter of concern. Within the framework of a regression-based fast RT model, the provision of some kind of variability to the stratospheric water vapour is desirable. To provide such variability a compilation has been made of 32 diverse HALOE (Halogen Occultation Experiment) water vapour profiles as a subset of the dataset produced by *Harries et al.* (1996) for the stratosphere. To optimise the training set of the LbL transmittances it is desirable that at each pressure level the profile variables are distributed as uniformly as possible across the range spanned by the temperature and water vapour/ozone mixing ratio values at that level.

3.3 Surface Emissivity Models

For the channels in 'atmospheric windows' (i.e. where the atmospheric absorption is low) the top of atmosphere radiance is dominated by the emitted and reflected radiance from the surface and so for these channels it is important to accurately model the surface emissivity, $\varepsilon_s(v,\theta)$, in equation 3. At infrared wavelengths the sea surface emissivity is close to unity but does vary with wavelength, viewing angle and surface wind speed. Early versions of fast models just assumed a unit emissivity over the oceans, relying on the radiance tuning to correct any biases introduced through this assumption. Recently more accurate fast sea surface models have been developed (e.g. *Watts et. al.,* 1996; *Sherlock,* 1999) that parameterise the emissivity based on the model of *Masuda et. al.* (1988) in terms of wavelength, viewing angle and in some cases wind speed. These parameterised emissivity values are accurate to 0.0002 as shown in Figure 2 for the ISEM-6 model developed by *Sherlock* (1999).

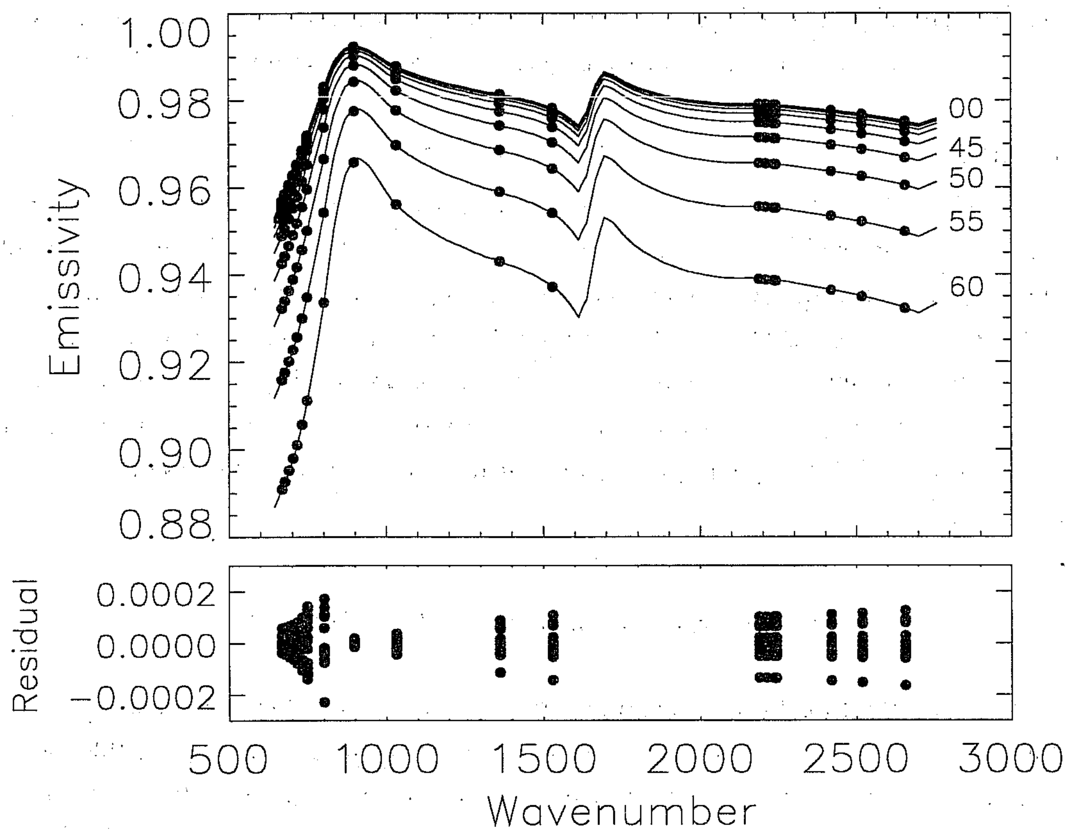

Figure 2 Top panel shows parametrised sea surface emissivities for several viewing angles with HIRS channel positions marked as dots. Bottom panel shows differènce between parametrised model and Masuda values for HIRS channels.

Over land and sea-ice the surface emissivity departs further from unity and is variable on small spatial scales and so inferring an emissivity which is representative of the mean value integrated over a sounder field of view is more difficult. The absolute value of emissivity is not as important to know as the spectral dependence of emissivity so that channels in different wavelength regions can be used together. The surface emissivity can vary with underlying soil type, vegetation cover, age and type, soil moisture and viewing angle. Work is underway to better define the surface emissivity for a variety of different generic surface types (e.g. *Snyder et. al.* 1998) which could form the basis of improved emissivity simulations over land/ice.

In parallel NWP models need to include a better representation of different surface types within their model grid squares. Assimilating radiance data over land has been shown to be beneficial (*English et. al.*, 2000) to Northern Hemisphere forecasts and so this is an important development to facilitate using advanced sounder radiance data over land.

For all surface types where the emissivity departs from unity consideration has to be given to the modelling of the downwelling component of the radiation which is reflected by the surface. Equation 3 assumes specular reflection (i.e. the reflected ray has the same surface incidence angle as the downwelling emitted ray) but in some cases this approximation is inadequate and surface emissivity schemes are now starting to take this into account. This is more important at microwave frequencies where the surface emissivities can be much lower. Reflection of solar radiation also becomes significant for the shorter wavelengths (<5μm).

3.4 Cloud models

At infrared wavelengths, to date radiance assimilation has been restricted to fields of view not affected by cloud (i.e. $L^{Cld}(\nu,\theta)$ is assumed zero in equation 2. However this results in typically 80% of the fields of view being excluded from the assimilation and so there is increasing interest in trying to assimilate cloudy infrared radiances. It has also been suggested (*McNally*, 2000) that the key sensitive areas where advanced sounder data will have the most impact on the medium-range forecast are nearly always covered with low cloud. Water cloud tops are good grey bodies (uniform emissivity with wavelength) at the mid-infrared wavelengths (10-15μm) and if they uniformly fill the field of view at a known pressure height then they can easily be modelled:

$$L^{Cld}(\nu,\theta)=\tau_{Cld}(\nu,\theta)\,B(\nu,T_{Cld})+\int_{\tau_{Cld}}^{1}B(\nu,T)d\tau \qquad (6)$$

where $\tau_{Cld}(\nu,\theta)$ is the cloud top to space transmittance and T_{Cld} the cloud top temperature, and the emissivity of the cloud top is assumed to be unity, which is a tolerable assumption for optically thick water cloud, at infrared radiances. The problems come when there is broken cloud within the field of view and multi-layer cloud and/or ice cloud is present which can have an emissivity significantly less than unity. For the former cloud overlap assumptions have to be invoked which are widely used in NWP model radiation schemes (*Hogan and Illingworth,* 2000). For the latter our knowledge of the radiative properties of ice cloud is still limited. However data are now available and work is in progress using complex scattering models (e.g. *Baran et. al.* 2000) to develop fast parametrisation schemes and then to fit them to the measured data.

The accuracy of the NWP model's representation of clouds still leaves a lot to be desired and so the sounder data itself will define the cloud cover within its field of view with no or little reliance on the model background. As the models improve through better cloud physics schemes and higher resolution (vertically and horizontally) assimilation of at least simple cloud affected radiances (e.g. uniform low water cloud) will become possible.

3.5 Issues for radiance assimilation

3.5.1 Gradient of the radiative transfer model

For variational data assimilation the gradient or derivative of the forward model is required in addition to the forward model itself to compute changes of radiance with respect to the profile variables about the first guess profile $\mathbf{x}_0$. To minimise equation 1, assuming the observations $\mathbf{y}^o$ to be linearly related to $\mathbf{x}$ then the minimum value for $J(\mathbf{x})$ is when:

$$\mathbf{x} = \mathbf{x}^b + \mathbf{B}.\mathbf{H}'^T \cdot (\mathbf{H}'.\mathbf{B}.\mathbf{H}'^T + \mathbf{R})^{-1} \cdot (\mathbf{y}^o - \mathbf{H}(\mathbf{x}^b)) \tag{7}$$

where $\mathbf{H}'$ is the derivative of $\mathbf{H}$ often referred to as the *Jacobian matrix* which simply gives the change in radiance $\boldsymbol{\delta}\mathbf{y}$ for a change in the state vector $\boldsymbol{\delta}\mathbf{x}$ for a given atmospheric state $\mathbf{x}_0$:

$$\boldsymbol{\delta}\mathbf{y} = \mathbf{H}'(\mathbf{x}_0)\boldsymbol{\delta}\mathbf{x} \tag{8}$$

The elements of the Jacobian matrix contain the partial derivatives $\partial y_i/\partial x_j$ where the subscript i refers to channel number and j to position in state vector. The Jacobian gives the contributions to the top of atmosphere radiance change for each channel from *each level* in the profile. It shows clearly, for a given profile, which levels in the atmosphere are most sensitive to changes in temperature and 'active gas' concentrations for each channel. Jacobians from different LbL and fast RT models have recently been compared for the first time (*Garand et. al.,* 2001) and some models were found in some cases to have spurious spikes or unphysical gradients which would be damaging to the radiance assimilation process. *Sherlock* (2000) has attempted to quantify how errors in Jacobians can affect the 1DVar retrievals and for one model (RTIASI) the poor water vapour Jacobians significantly reduced the accuracy of the simulated retrieved temperature profiles from IASI. Therefore a good fast RT model not only has to be able to model the radiances accurately but also the Jacobians at least for radiance assimilation or 1DVar retrievals. More details on how the RT model and its gradient are used in radiance assimilation can be found in the companion paper by *Collard* (2001).

3.5.2 Errors of fast radiative transfer models

In order to correctly weight the radiance observations in a minimum variance solution the observation $\mathbf{E}$ and forward model $\mathbf{F}$ error covariances matrices must be estimated and combined (i.e. $\mathbf{R}=\mathbf{E}+\mathbf{F}$ from equation 1). Here only the component of forward model error covariance $\mathbf{F}$ is considered which should include all errors arising due to the simulation of radiances from the model fields. This includes errors due to the fast model parameterisation of transmittance, errors due to the LbL model on which the fast model is based, errors due to interpolation of the model fields and representativity error. One way of estimating at least the first of these is to compare the simulated radiances with the corresponding LbL model radiances for a set of diverse profiles which are independent from the set used to compute the fast model regression coefficients. This computation has been made to evaluate the errors of the RTIASI fast model (*Sherlock,* 2000) and the standard deviation of the errors along the diagonal are plotted in Figure 3 along with estimates of the IASI instrumental noise $\mathbf{E}$. The errors are expressed in units of normalised brightness temperature difference for a scene temperature of 280K. The fast model error is, in most cases, less than the IASI instrumental noise which it should be in order for the radiance data not to be down-weighted in the assimilation due to forward model errors. Note the errors in Figure 3 do not include errors due to the LbL model itself which can be significant in certain spectral regions and also residual undetected cloud. Persistent airmass dependent biases in forward models are corrected for in radiance bias correction schemes (e.g. *Eyre,* 1992; *Harris and Kelly,* 2001) usually by considering the mean bias over a period greater than 2 weeks and correlating it with model variables or other observations.

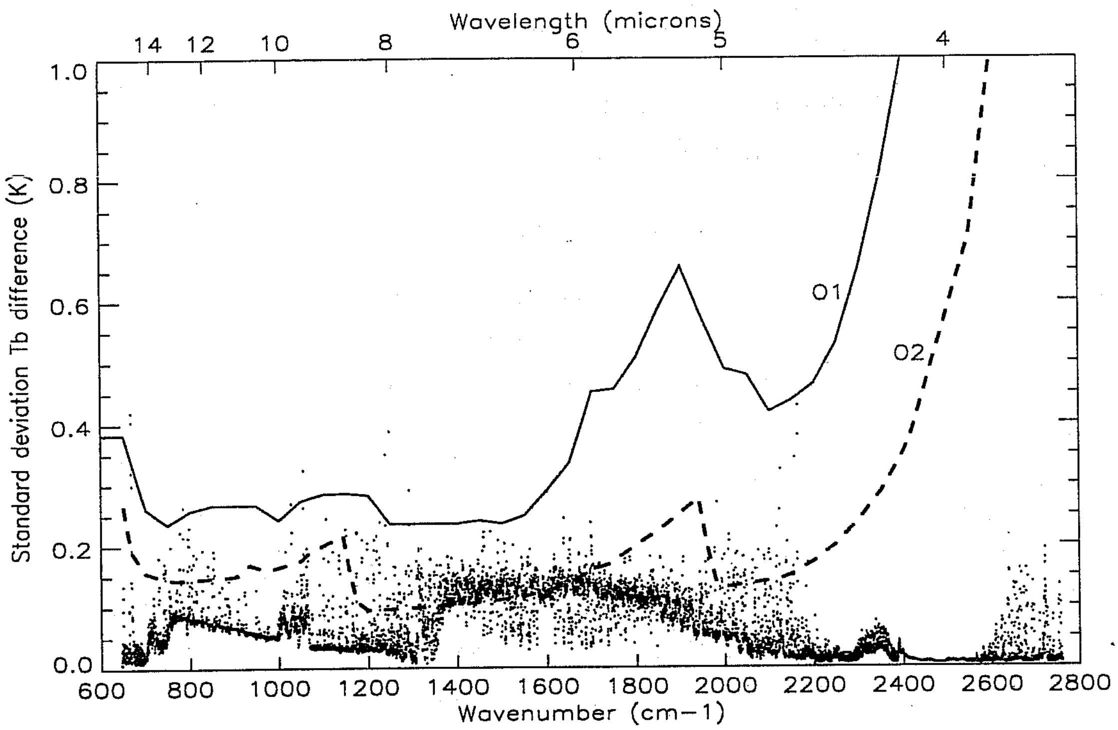

Figure 3 Standard deviation of errors for the RTIASI version 1 with 3 predictor sets for water vapour. Units are equivalent brightness temperature differences for a scene temperature of 280K. The statistics are derived by comparing the fast model radiances with those computed from a LbL model for 117 diverse profiles. The solid curve is the noise specification for IASI and the dashed curve is the estimate based on measurements of the pre-flight model.

To date the off-diagonal terms of the **F** matrix have been assumed to be zero (i.e. zero correlation between channels). However for infrared sounders, which sample several parts of the infrared spectrum, errors in absorption bands of the same gas or in window regions may well be correlated. The correlation matrix, for the component of fast model error due to parametrisation of the transmittances, has been computed for RTIASI (Sherlock, 2000) and is shown in Figure 4. It clearly shows correlations between carbon dioxide bands (at 15 and 4.3 microns) and within the 15 micron band and also high correlations between and within the window regions. Finally there is a high correlation within the water vapour ν_2 band. These results demonstrate that the assumption of a diagonal matrix for forward model errors is not a good one. The impact of assuming a diagonal matrix relative to a full covariance matrix has been assessed for 1DVar retrievals (Sherlock, 2000). The diagonal approximation leads to a small degradation in retrieval accuracy, showing that at least for a preliminary radiance assimilation system a diagonal F matrix may be a tolerable assumption for advanced sounders. Sherlock (2000) shows if the covariance matrix is simplified into a block diagonal matrix then all the important correlations can be captured and retrievals can still be performed without the need to store the full matrix.

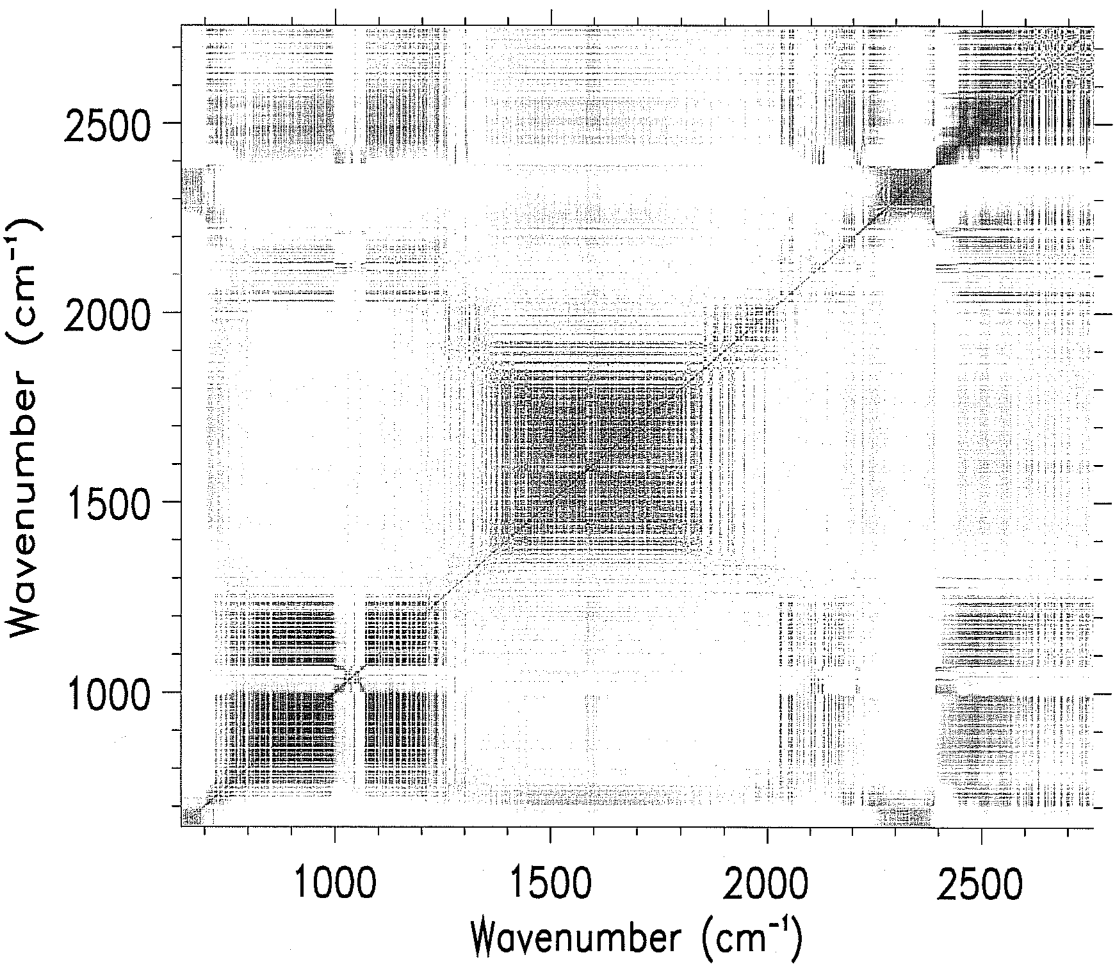

Figure 4 Forward model error correlation matrix for the RTIASI model with one water vapour predictor set. High correlations are black, low correlations are white, anti-correlations are not shown.

3.5.3 Non-linearity of forward model

In data assimilation systems if the observation operator (i.e. forward model) is linear or close to linear then the gradient of the model (i.e. Jacobian) only needs to be computed once during the minimisation process. If however there is a high non-linearity between the profile variables and the observations then the gradients have to be recomputed regularly during the minimisation process. This was investigated for RTTOV by *Saunders* (1996) who showed that for temperature retrievals the forward model was almost completely linear but for water vapour and ozone retrievals it was non-linear and a few recomputations of the gradient are required during the minimisation. This increases the cost of the assimilation significantly but is necessary in order to obtain accurate water vapour and ozone fields. The forward modelling of cloudy radiances is highly non-linear especially for medium to high level clouds.

There is always a trade-off between the accuracy and the computational cost of running the forward and gradient versions of the model and how many times the model is called during the minimisation process. More accurate models will run slower and as a result limit the number of channels that can be assimilated whereas faster models can allow more channels to be used but with a larger forward model error. Experiments are required to determine the correct balance for advanced sounders where >1000 channels are potentially available. Of course the information content of each channel relative to those already included also needs to be considered.

4. SUMMARY AND OPEN ISSUES FOR RESEARCH

This paper attempts to document the current status of forward modelling for the new generation of advanced infrared sounders that are planned to be launched in the next five years. In order to exploit the valuable measurements from these new instruments within a NWP data assimilation system a fast RT model is required to rapidly simulate the observations. The development of these fast models relies on LbL model transmittances computed from a diverse set of profiles for each active gas to be modelled. Currently only well mixed gases, water vapour and ozone transmittances are considered but in the future more of the fixed gases will be considered variable. LbL models are in general accurate enough for radiance assimilation purposes as their uncertainties in most parts of the spectrum are below the instrument noise. However there are still a few regions that would benefit from improved spectroscopic parameters. Diverse profile datasets used as input to the LbL model calculations are being improved through the use of NWP model sampled profiles making it easier to obtain realistic profiles of temperature, water vapour and ozone from the surface to 0.1hPa. However we still need accurate observations for water vapour (upper troposphere/lower stratosphere) and ozone plus any other trace gases included in the state vector.

Fast models are currently being used operationally for the assimilation of ATOVS radiances (maximum of 40 channels) but there is now a challenge to increase the number of channels by an order of magnitude and still allow a significant number of observations to be assimilated. Currently the methodology employed for ATOVS fast models is being applied to fast RT models for advanced sounders although research into neural nets is underway. Not only the forward model, but also the differential of the model with respect to the state vector is required for radiance assimilation or 1DVar retrievals.

For the future the following issues need to be considered:

- An accurate measurement and characterisation of the instrument response function and/or apodising function is a necessary requirement for accurate forward modelling.
- The number of profile levels (in pressure or absorber space) required for a fast RT model. 43 levels are used for ATOVS but this is recognised to be insufficient for the advanced sounders.
- Accurate cloud detection and characterisation is assumed for the measured data.
- Improve accuracy of fast model radiances *and* Jacobians for water vapour channels.

- How best to allow for fast model error correlations.
- Improve surface emissivity models over land and the representation of land surfaces in NWP models.
- Consider what radiance bias tuning is required for advanced sounder data (difficult to do until real data is available).
- Data compression (channel selection, empirical orthogonal functions, etc)
- Continue validation of fast RT models through:
    - Comparison with independent LbL model radiances
    - Comparisons with other models
    - Comparisons with measured radiances from satellites and aircraft where the atmospheric state is known accurately
    - Studying the global or regional mean bias and standard deviation of the difference between observations and simulated observations from NWP model profiles.

5. ACKNOWLEDGEMENTS

Vanessa Sherlock, Andrew Collard and Peter Rayer (Met Office), Marco Matricardi and Frederic Chevallier (ECMWF) provided some of the material for this paper and their assistance and comments are gratefully acknowledged. I also thank John Eyre (Met Office) for useful comments of an early draft of this paper.

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