Sources of Biases in Microwave Radiative Transfer Modelling

Peter Bauer

ECMWF
Shinfield Park, Reading, RG2 9AX, UK
peter.bauer@ecmwf.int

1. Introduction

Microwave satellite observations represent the most important information source for atmospheric temperature and temperature distributions in most current operational numerical weather prediction systems. At ECMWF, most data from the Advanced Microwave Sounding Unit (AMSU) instruments A and B are assimilated from four different satellites of the National Oceanic and Atmospheric Administration (NOAA) polar orbiting series (NOAA-15, 16, (17,) 18) as well as from National Aeronautic and Space NASA's Aqua satellite. Microwave imager measurements are sensitive to integrated atmospheric moisture, surface properties as well as clouds and precipitation. While advanced infrared sounders offer better vertical resolution for sounding applications, microwave data is less affected by cloud contamination and therefore provides better data coverage.

At ECMWF, microwave sounder data is operationally assimilated since 1992 (Eyre et al. 1993) and imager data (Special Sensor Microwave / Imager, SSM/I) since 1999 (Phalippou 1996, Gérard and Saunders 1999). Initially, the assimilation was performed through a 1D-Var retrieval of geophysical variables such as temperature profile or integrated moisture that were then assimilated in the global system as pseudo-observations. This procedure was later replaced by the direct assimilation of radiances in the 4D-Var system (McNally et al. 2000, Bauer et al. 2002). The radiative transfer (RT) modeling was aimed at the Tiros Operational Vertical Sounder (TOVS) data modeling (RTTOV, Eyre 1991) that developed into a general RT modeling tool-kit applicable to most available satellite sensors (Saunders et al. 2005).

The sources of biases and random errors due to radiative transfer modelling are not easily separable. This is because only few reference measurements exist with which an absolute error can be estimated. In Numerical Weather Prediction (NWP) data monitoring systems, biases and error can be derived from comparison of observed and modeled radiances; however, the error estimation is usually based on the assumption that the model is unbiased, that the model error are known and that the observations are uncorrelated. The impact of these assumptions is quite substantial but there are no alternative solutions available at present. In the following, we will therefore refer to errors rather than biases unless there is evidence that biases can be actually separated from random errors.

Figure 1 shows the components that are involved in microwave radiative transfer modeling and that therefore contribute to modeling errors and biases. In most operational NWP applications where data is sensitive to surface emission and reflection, only ocean surfaces are regarded because sea-surface emissivity can be more accurately modeled. For temperature and moisture sounding, atmospheric emission due to dry and moist air continuum effects as well as oxygen and water vapour molecular line absorption are the only physical processes to be modeled. The accuracy of the radiative transfer model depends on the employed numerical approximations that are mainly introduced to enhance computational efficiency. If clouds and precipitation are regarded, many more effects have to be included that are single particle and multiple scattering as well as cloud geometry effects. For spatially inhomogeneous scenes even the radiometer imaging properties (antenna pattern) may become important.

Recently, the status of microwave radiative transfer modeling has been summarized by Mätzler et al. (2006). Many of the accuracy figures cited in the text were taken from this reference.

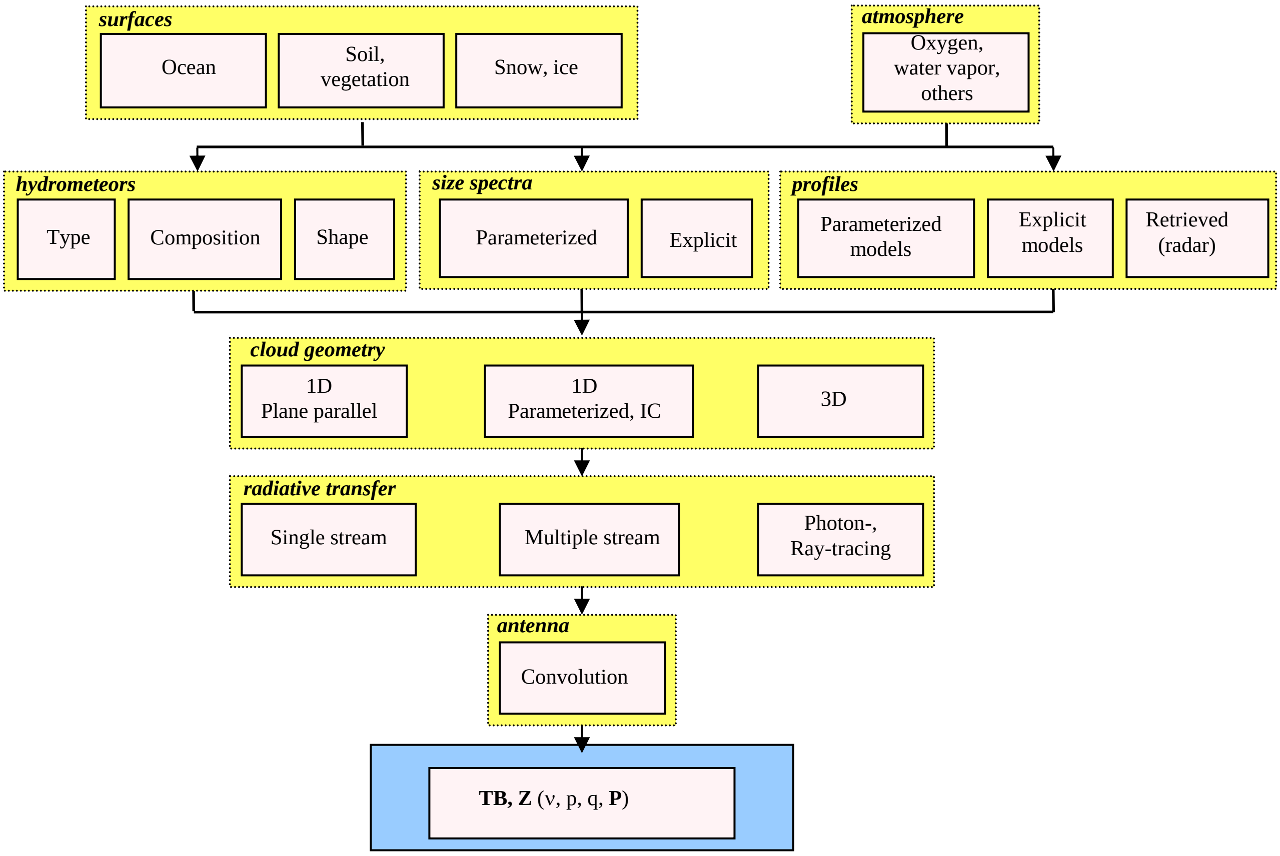

Figure 1: Components of microwave radiative transfer modeling.

2. Absorption

2.1. LBL models

The modeling of atmospheric absorption represents the key to the utilization of sounding instruments in NWP data assimilation systems. Therefore, a substantial effort has been made to develop reference databases of atmospheric absorption from continuum and line effects over the desired wavelength (frequency) range. These line-by-line (LBL) models are derived from laboratory and field measurements and are constantly updated (see International TOVS Working Group: www.cimss.wisc.edu/itwg/rtwg.html.).

Line absorption is defined by natural broadening, pressure broadening (at higher pressure, mainly in troposphere) and Doppler broadening (at lower pressures) and is a function of temperature and pressure. Depending on the molecule, line position, line strength and shape are modeled. The latter also determines line interaction at wavelengths off the line centers. For the largest part of the microwave spectrum, the inclusion of oxygen and water vapour line absorption contributions suffices. However, John and Buehler (2004) found that ozone line absorption contributes significantly at AMSU-B frequencies near 183 GHz.

Continuum absorption (mainly water vapour at microwaves) is produced to a small degree by photo-ionization and photo-dissociation. The origin of the bulk of continuum absorption is not fully understood but absorption by molecular clusters with complex structures and far wing absorption from lines at high frequencies are considered. The modeling of continuum absorption represents one of the weaker parts of microwave modeling and becomes in particular important at so-called window frequencies, i.e. frequencies that are the least affected by line absorption.

LBL models and databases are too comprehensive to be used in NWP systems as such. Absorption is modeled by parameterized models that represent an optimal trade-off between computational cost and accuracy. The accuracy of the parameterized models depends on the approximation to LBL absorption, in terms of regressions with atmospheric variables as predictors, and the atmospheric profile dataset used for calibrating the regression coefficients.

Mätzler et al. (2006) state that between different LBL models, line frequencies are accurate to within 0.1 kHz, line intensities agree within 1%, the modelling of line widths/shifts agrees with measurements to within a few %. The water vapour continuum modelling is the most controversial component and modelled values agree with measurements to within 10-20 %. All the above are functions of molecule and frequency.

a)

AMSU-A		**RTTOV-8 117 independent set**		
Channel #	NeDT degK	Mean bias degK	St.dev. degK	Max diff degK
1	0.20	0.00	0.01	0.04
2	0.24	-0.01	0.02	0.12
3	0.19	-0.02	0.03	0.18
4	0.13	0.01	0.01	0.07
5	0.13	0.02	0.01	0.08
6	0.11	0.01	0.01	0.06
7	0.12	0.00	0.01	0.03
8	0.13	0.00	0.00	0.01
9	0.15	-0.01	0.01	0.07
10	0.19	0.19	0.16	0.39
11	0.20	0.00	0.04	0.27
12	0.31	-0.02	0.07	0.44
13	0.42	-0.05	0.09	0.58
14	0.70	-0.04	0.06	0.41
15	0.10	0.07	0.10	0.34

b)

AMSU-B		**RTTOV-8 117 independent set**		
Channel #	NeDT degK	Mean bias degK	St.dev. degK	Max diff degK
1	0.32	0.07	0.10	0.33
2	0.71	-0.02	0.08	0.73
3	1.05	-0.01	0.07	0.74
4	0.69	-0.01	0.04	0.44
5	0.57	0.00	0.05	0.40

c)

Model	**AMSU-06**		**AMSU-10**		**AMSU-14**		**AMSU-18**	
	std	bias	std	bias	std	bias	std	bias
RTTOV-7/8	0.04	-0.06	0.15	0.25	**1.36**	0.90	**0.35**	-0.39
Optran	0.09	0.00	0.05	-0.04	**0.73**	-1.97	0.10	0.00
AER_OSS	0.06	0.13	0.04	0.03	0.09	0.14	0.14	-0.16
MIT	0.01	0.00	0.04	-0.04	0.08	-0.09	0.19	-0.40
RAYTHEON	**0.42**	-0.57	0.17	0.24	0.20	0.60	**0.50**	-0.07
AER_LBL	0.06	0.13	0.05	0.03	0.09	0.16	0.14	-0.15
MSCMWLBL	0.03	0.05	0.03	0.04	0.20	0.51	**0.32**	-0.36
ATM	0.19	0.46	0.07	0.08	0.11	0.23	0.24	-0.28

Table 1: Statistics of parameterized model (RTTOV) vs. LBL model performance based on independent profile dataset testing for AMSU-A (a) and AMSU-B (b). Similar statistics between different models for selected AMSU channels (c). For details and information on individual models, see Saunders et al. (2005).

Tables 1a-b show a summary of biases and standard deviations between LBL and parameterized (fast) models for independent profile datasets and for channels of the AMSU-A/B radiometers (Saunders et al. 2005). In most cases, the standard deviations between models are well below the radiometer channel noise (often up to one order of magnitude) and biases are negligible. Given the range of channel sensitivity that is covered by these two instruments, this evaluation suggests that parameterized models are very accurate compared to the reference models as long as the model predictors and training datasets are carefully chosen. This means that excellent modelling accuracy and computational efficiency are achievable at the same time.

Between different reference and fast models, however, significant differences may be observed if they are applied to the same profile dataset (Table 1c). Model differences are of the order or larger than channel noise. Model biases are often of the same size as the standard deviations and they greatly vary between channels. This suggests systematic differences in the treatment of the absorption by individual atmospheric constituents.

2.2. Additional effects

Polarized radiation at low frequencies may be affected by Faraday rotation that is the rotation of polarization through the interaction of polarized light passing through a strong magnetic field (in ionosphere). The electromagnetic wave is split into two circularly polarized rays due to polarization dependent permeability (in form of a tensor) causing phase delay. This affects polarized light, i.e., radiation sensitive to surface emission and polarization caused by reflection. The rotation angle, β, can be approximated by $\beta \approx 17 / \nu^2$ (β in degrees, ν in GHz). Therefore, substantial modifications of polarized radiation measurements can be obtained that influence observations of, for example, the radiometer of the Soil Moisture Ocean Salinity (SMOS) mission, the Advanced Microwave Scanning Radiometer (AMSR) and the Windsat instrument. Measurements of the full Stokes vector are particularly concerned due to the small dynamic range of the signal.

Zeeman splitting is the splitting of O_2 absorption lines in the 55-60 GHz band and the 118.75 GHz line through interaction of O_2 electronic spin that carries a magnetic dipole moment with the Earth’s magnetic field. For the 118.75 GHz line three line centers are produced with a relative displacement of ~1 MHz. This means that the RT modeling of this effect is dependent on the Earth’s magnetic field orientation and that it is dependent on polarization. Only those instruments with channels sensitive to the upper stratosphere and mesosphere are affected, for example, the Special Sensor Microwave Imager Sounder (SSMIS) and the Microwave Limb Sounder (MLS).

3. Dielectric properties of condensed matter

The modelling of the interaction of microwave radiation with surfaces and clouds/precipitation in the atmosphere requires the modelling of the dielectric properties of condensed matter. The complexity and accuracy of the available models greatly depends on the surface or hydrometeor type. In many cases, models represent parameterizations and fits to observed data some of which sparsely covers the targeted frequency range and the variability of key parameters. The following compilation has been extracted from Mätzler et al. (2006).

Water permittivity models are based on Debye model and fits to observational datasets which basically span the frequency range of 3-20 and 30-100 GHz. No sea-water data is available above 105 GHz, only one dataset exists for 9.62 GHz and for super-cooled water (-18^{o} C). Fits are required to cover the desired range of temperatures ($T \in$ [250-300 K]) and frequency ($\nu \in$ [1, 1000 GHz]).

Solid ice permittivity models are mainly based on empirical fits to observational data. The real part of the complex permittivity is rather constant while the imaginary part is very uncertain.

Snow/ice permittivities are derived from mixing formulae based on air/water/ice mixtures and assumptions on inclusion shape/orientation.

Vegetation permittivity is mainly a function of water content but the complex organic structure limits applicability of conventional mixing theory (as for ice). Experimental (field) observations are available but their extrapolation to spatial scales observed by satellites and wide frequency ranges is difficult.

Soil permittivity is mainly a function of frequency, temperature, and salinity, volumetric water content, volume fraction of bound and free water related to the specific soil surface area, soil bulk material, and shape of the water inclusions. Again, some experimental (field) observations are available but their extrapolation to satellite scales and frequencies is difficult.

4. Surface emissivity

Given the difficulty of land surface and snow/ice permittivity modeling, most applications of RT modeling in NWP systems are limited to ocean surfaces. However, some simple attempts have been made to include microwave radiometer channel observations over land (Kelly and Bauer 2000, Prigent et al. 2004). The systematic assessment of model errors and biases is still an open issue.

Over water, plane surface emission and reflection is accurately modeled from the Fresnel equations (for the full Stokes vector) if the sea-water permittivity is known. For wind roughened ocean surfaces, the complex wave structure is usually modeled in different stages or scales. These are large-scale waves with wavelengths well above the radiation wavelength, gravity-capillary and capillary waves (wind speeds above 2 m/s), whitecaps (wind speeds above 7 m/s) and foam (wind speeds above 10-12 m/s). Most available parameterized models account for these effects (e.g. RTTOV with Fastem v2).

For the simulation of fully polarized observations (e.g. Windsat), directional wind roughened surface effects must be accounted for (e.g. RTTOV with Fastem v3). For the optimal range of wind speeds (8-12 m/s) these can be modeled to within 20% accuracy (English, pers. communication).

Model	**Bias (Obs.-Model), K**	**Standard deviation, K**
	Frequency 89 GHz	
RTTOV KS	-6.00	3..36
RTTOV FASTEM	-0.95 (-0.84)	2.37 (2.36)
	Frequency 157 GHz	
RTTOV KS	-5.04	1.68
RTTOV FASTEM	-0.13 (-0.15)	1.99 (2.36)
	Frequency 183± 7 GHz	
RTTOV KS	-0.92	0.99
RTTOV FASTEM	0.74 (0.74)	1.02 (1.02)

Table 2: Bias and standard deviations between modeled (RTTOV model with Klein and Swift (1977) vs. Fastem surface emissivity model) and observed AMSU-B radiances (Ellison et al. 2002).

A comparison between two different surface emissivity models was performed by Ellison et al. (2002) using global ECMWF model fields and observations with the AMSU-B radiometer (Table 2). The atmospheric radiative transfer calculations were carried out with the RTTOV model (v5) and surface emissivity was computed with the Klein and Swift (1977; KS) or the fast emissivity model (English and Hewison 1998; FASTEM), respectively. The difference in emissivity modeling accounts for most of the biases because standard deviations are quite similar and biases become similarly small with increasing optical depth of the atmosphere, i.e. less visibility of surface contributions.

Using the Met Office global model, Bell (pers. communication) found emissivity biases that accounted for differences up to 10 K between observed and modeled SSM/I radiances. These mainly occur at low temperatures and low moisture contents (total column water vapour less than 15 kg m^{-2}).

Another error source is the occurrence of sun-glint effects at microwaves that is the reflection of direct solar radiation into the satellite viewing direction. These errors are mainly manifested as biases if the sun-glint is not modeled and may amount to a few degrees K (e.g. at 18 GHz from AMSR observations; Bennartz, pers. communication).

5. Clouds and precipitation

As indicated in Figure 1, the calculation of radiative transfer for cloud and rain affected profiles may become rather complex. Single particle scattering property calculations require assumptions on particle composition, shape and size distribution. This and the modeling of cloud geometry account for the largest error and therefore bias contributions. However, in model vs. observation comparisons, these errors are difficult to separate from the primary errors of model hydrometeor contents.

In principle, multiple scattering modeling is very accurate (Smith et al. 2002) but errors larger than one order of magnitude with respect to clear-sky calculations can be produced by the above uncertainties. Recent comparisons of model calculations with SSM/I observations suggest, however, that biases are acceptable (Chevallier and Bauer 2003) and even allow the assimilation of cloud and rain affected observations in global NWP models (Bauer et al. 2006). Even for regional model scales (spatial resolution 5-10 km), the largest source of uncertainty seem to be the model fields themselves and not the radiative transfer modeling.

6. RFI

Radio frequency interference (RFI) has been observed near areas of high population and traffic density, even over oceans. The interference produces significant biases and requires the exclusion of the contaminated data from the analysis in most cases. RFI is observed in the AMSR C-band (6.75–7.1 GHz) and X-band (10.6–10.7 GHz) data. The C-band is unprotected by international frequency regulations but useful for sea surface temperature and soil moisture sensing. The X-band is protected between 10.68–10.7 GHz.

Strong RFI for geophysical algorithms can be identified and filtered by classification algorithms but weak RFI cannot reliably be separated from geophysical signals. C-band RFI is mostly observed in the U.S., Japan, Middle East, some in Europe, Asia, S. America, Africa. X-band RFI mostly affects measurements over Japan, England, Italy, and some parts of the U.S. The situation at C-band has worsened considerably since the Seasat and Nimbus-7 Scanning Multichannel Microwave Radiometer (SMMR) 1978-1987 (6.6 GHz). The Conical Microwave Imager Sounder (CMIS) that is planned for the National Polar-orbiting Observing Satellite System (NPOESS) also operates at C- and X-bands. Given the past development of RFI, a re-assessment of future radiometer designs is required.

7. Summary

Currently, microwave data from satellite remote sensing represents one of the most important contributions in operational NWP data analyses. It has been actively used in data assimilation for ~10 years and both national and international space agencies will maintain the currently existing sensors

The following table (Table 3) briefly summarizes the status of microwave radiative transfer modeling and identifies the largest sources of modeling errors and biases.

Contribution/Effect	Frequencies	Comments
Atmospheric absorption:		
Spectroscopy, LBL	All	H_2O continuum problematic
	183 GHz	O_3 line absorption missing
Parameterized models	all	very accurate relative to LBL models
Zeeman splitting	O_2 lines	limited applicability (<10 hPa), SSMIS, MLS
Faraday rotation	1.4 GHz	limited applicability, SMOS
Total	20-300 GHz	Clear-sky atmospheric TB's accurate within 1-3%
Surface emission:		
Sea surface		
Permittivity	all	1 K between 20-150 GHz
Polarimetry	10-37 GHz	10% for 4 m/s < SWS < 12 m/s
Land surfaces		
Soil, vegetation	all	uncertain
Snow/ice		
Type, age, etc.	all	uncertain
Cloud droplet emission:		
Permittivity	all	well modelled between 5-500 GHz and T>273 K
	5-500 GHz	for T < 273 K models differ by 20-30%
Precipitation emission/scattering:		
Size distribution, Permittivity, Shape	all	uncertain
Radiative transfer modelling:		
Clear-skies	all	biases up to 3 K due to layer integration, otherwise accurate
Clouds/precipitation		
Multiple scattering	all	biases < 0.5 K
Layer inhomogeneity	all	biases up to 5 K, can be parameterized

Table 3: Summary of error sources in microwave radiative transfer modeling.

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