Infrared radiance modelling and assimilation

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Radiative transfer models

The exploitation of infrared satellite radiance data requires the use of an accurate radiative transfer (RT) model to simulate radiances from an input atmospheric profile.

There are two main types of RT models:

- Accurate but computationally expensive LBL models based on first principles.
- Look-up table based LBL models and fast RT models. These models are generally based on LBL models and use efficient parameterisations that allow the simulation of radiances at a fraction of the cost required by a LBL model.
Radiative transfer models

The current list of RT models include:

**LBL**

- LBLRTM (Clough et al. 2005)
- GENLN2 (Edwards 1992)
- KOPRA (Stiller et al. 2002)
- RFM (Dudhia 1997)
- STRANSAC (Scott, 1974)

**Look-up table based “LBL” models**

- 4A/OP (Scott and Chedin 1981)
- FORLI (Hurtmans et al. 2012)
- σ-IASI (Amato et al. 2002)
- kCARTA (deSouza-Machado et al. 1998)

**Fast models**

- RTTOV (Matricardi et al. 2004)
- CRTM (Kleespies et al. 2004)
- SARTA (Strow et al. 2003)
- OSS (Moncet et al. 2008)
- HT-FRTC (Havemann et al. 2014)
- PCRTM (Liu et al. 2006)
- PC_RTTOV (Matricardi 2010)
LBL models

The quality of the products retrieved from infrared spectra hinges on the accuracy of the forward calculations carried out in the algorithms used in the retrieval processes.

Accurate LBL computations require:

- State of the art models of the line shape
- The accurate specification of the spectroscopic parameters used as input to the LBL model
The basic line shape describes the effects of pressure (Lorentz profile) and Doppler (Gauss profile) line broadening.

The line shape commonly used in LBL models is the Voigt line shape (i.e. the convolution of the Lorentz and Gauss profiles).

- The simplified assumptions on which the Voigt line shape is based (e.g. the collisional parameters are independent on the velocity of the absorber) affect the accuracy of the simulated spectra.

There is the need for a better representation of the line shape than the Voigt profile (the IUPAC task group (Tennyson et al., 2016) recommends the adoption of the Hartmann-Tran profile).
In regions where absorption lines are closely spaced, line-mixing (or line-coupling) effects cause a departure from the Voigt line shape. This is especially true in the important CO$_2$ temperature sounding regions.

Line mixing effects in the P/Q/R Branches (Strow and Reuter 1998, Niro et al. 2005) of CO$_2$ are generally incorporated in LBL algorithms.

- CO$_2$ line mixing calculations should be based on the best available data (e.g. use as many lines as possible and include more parameters such as H$_2$O broadening parameters of CO$_2$).

In some models, half-width and line shift values used in line-mixing calculations are determined empirically. Ideally, experimental or calculated values should be used.
GENLN2 does not include CO$_2$ P/R branch line mixing
Line mixing effects have also been observed for CH$_4$ (Tran et al. 2006), N$_2$O (Rachet et al. 1995) and even H$_2$O (Brown et al. 2004).

Some LBL models include line-mixing effects in the $\nu$3 (3000 cm$^{-1}$) and $\nu$2 (1300 cm$^{-1}$) absorption bands of CH$_4$.

Further work is needed towards the introduction of N$_2$O, and to a lesser extend H$_2$O, line-mixing effects in LBL models.
The difficulty of achieving good measurements of water vapour amounts in the atmosphere and in the laboratory is still hindering progress in the development of improved water vapour line shapes further from line centres where a slowly varying continuum absorption is observed.

The MT_CKD (Clough et al. 2005) model has been used successfully for many years in atmospheric RT codes, and is capable of reproducing many of the observed water vapour features in the mid-infrared spectral region. Some issues, however, still remain:

- The temperature dependence of the MT_CKD continuum has been found not be well captured when compared to recent laboratory data.
- The MT_CKD model also appears to underestimate the strength of the continuum in some high transmittance atmospheric windows.
IASI band 3: Observations minus simulations

Tropics

Continuum model
Uncertainties in line parameters (e.g. line position, line intensity, line width and temperature dependence, pressure shift) can have significant effects on the forward calculations.

- Improvements can be achieved through better experimental techniques and more sophisticated and robust theoretical models.

For large polyatomic molecules line data are generally not available or incomplete. For these molecules infrared cross-sections are used instead.

- It is important to characterise cross sections for a wide range of pressures and temperatures.
H$_2$O line intensities are difficult to measure but experimental techniques and theoretical methods have greatly improved (e.g. measurements by Coudert et al. (2008) and calculations by Martin et al. (2013))

- There is evidence that the widths and the temperature exponent of some lines are underestimated

For CO$_2$, important progress has been made by using improved effective Hamiltonian and effective dipole models to re-calculate line parameters throughout the CO$_2$ range (Tashkun et al. 2003).
Line parameters used in LBL computations are mainly obtained from the HITRAN (Rothman et al. (2013) and GEISA databases (Husson et al. 2011).

In many instances, HITRAN and GEISA use similar sources.

However, the data that enter the two databases go through different processes (e.g. different quality control, include calculations instead of measurements, re-calculate some parameters etc.)

Should we consider assessing the relative merits of the two databases?
Accuracy of line intensity and half-width in the HITRAN database
Brightness temperature signal associated with HITRAN uncertainties

Figures courtesy of Sergio DeSouza-Machado, UBMC

- Line centre
  - $H_2O$  
  - $O_3$  
  - $N_2O$  
  - $CO$  
  - $CH_4$  
  - $SO_2$  
  - $HNO_3$

- Pressure shift
  - $H_2O$  
  - $O_3$  
  - $N_2O$  
  - $CO$  
  - $CH_4$  
  - $SO_2$  
  - $HNO_3$

- Broadening parameters
  - $H_2O$  
  - $O_3$  
  - $N_2O$  
  - $CO$  
  - $CH_4$  
  - $SO_2$  
  - $HNO_3$

- Line intensity
  - $H_2O$  
  - $O_3$  
  - $N_2O$  
  - $CO$  
  - $CH_4$  
  - $SO_2$  
  - $HNO_3$
Difference between LBLRTM_v_11.1 and LBLRTM_v12.3 spectra for a dataset of 5190 profiles

The red curve is the standard deviation of the difference
The black curve is the mean value of the difference

Changes in O$_3$ spectroscopy

Changes in CO$_2$ spectroscopy and line mixing (Tashkun et al. 2003, Lamoroux et al. 2010)

Changes in CO$_2$ spectroscopy and line mixing (Tashkun et al. 2003, Lamoroux et al. 2010)

Changes in H$_2$O and CO$_2$ continuum

Changes in H$_2$O spectroscopy (Coudert et al. 2008)
IASI: global observations minus simulations (ECMWF first guess fields)

Note the inconsistency of the residuals in the CO$_2$ $v_2$ and $v_3$ bands

Note the consistency of the residuals in the CO$_2$ $v_2$ and $v_3$ bands

Smaller residuals in the O$_3$ band

Smaller residuals in the H$_2$O band

More realistic CO profiles
IASI: global observations minus simulations (ECMWF first guess fields)

Tropics

LBLRTM_11_1 + old spectroscopy

LBLRTM_12_2 + new spectroscopy
IASI: global observations minus simulations
GRUAN: MANUS island

- LBLRTM_12_2 + new spectroscopy
- Water vapour continuum?

Radiosondes
ECMWF forecasts
LBL models: accounting for accurate isotopic ratios

LBL models compute the absorption due to minor isotopologues using fixed fractional abundances relative to the major isotopologue.

- The isotopic ratios of water vapour isotopologues can exhibit significant variations in space (horizontally and vertically) and time.
- The HDO case is a specially important one because HDO/H$_2$O ratios can provide crucial insight into water vapour processes in the atmosphere.

In order to improve the accuracy of the radiance simulation, LBL models should allow for vertically varying isotopic ratios, at least for water vapour isotopologues.
Fast radiative transfer models

Fast RT model errors are dominated by two main components:

a) The errors associated with the parameterisation used for the radiance simulation (e.g. the transmittance model).

b) The errors associated to the line-by-line models on which fast RT models are generally based.

Parameterisation errors typically represent a small fraction of the total error budget.
RTTOV (Saunders et al. 2017) is a \textit{regression based fast model} that computes channel-integrated layer optical depths using profile dependent predictors that are functions of temperature, absorber amount, pressure and viewing angle.

In RTTOV, the atmosphere is divided into $N$ homogeneous layers bounded by $N+1$ fixed pressure levels. The channel-integrated optical depth for layer $j$ is written as:

$$\hat{\tau}_{j,v^*} = \sum_{k=1}^{M} a_{j,k,v^*} X_{k,j}$$

where $M$ is the number of predictors and the functions $X_{k,j}$ constitute the profile-dependent predictors of the fast transmittance model. The expansion coefficients $a_{j,k,v^*}$ are computed by fitting the model optical depths to a data set of LBL optical depths.
Fast radiative transfer models: RTTOV

RTTOV features three sets of predictors:

i) ‘v7’: H$_2$O, O$_3$ variable

ii) ‘v8’: H$_2$O, O$_3$, CO$_2$ variable

iii ‘v9’: H$_2$O, O$_3$, CO$_2$, CO, N$_2$O, CH$_4$, SO$_2$ variable

Fit to LBL radiances over land and sea surfaces for a dataset of 12000 atmospheric profiles independent of the regression coefficients, v9 predictors with constant SO$_2$. 
Fit to LBL radiances over land and sea surfaces for a dataset of 12000 atmospheric situations independent of the regression coefficients.
ECMWF is planning the implementation of all-sky assimilation (i.e. clear and cloudy conditions) of infrared radiances (Geer et al. 2017).

The computational efficiency of a fast radiative transfer model can be seriously degraded if explicit calculations of multiple scattering are introduced.

RTTOV uses a parameterization for scattering by aerosols and clouds (scaling approximation, Chou et al 1999, Matricardi 2005) that allows to write the radiative transfer equation in a form that is identical to that in clear sky conditions.

In the scaling approximation the absorption optical depth, $\tau_a$, is replaced by an effective extinction optical depth, $\tilde{\tau}_e$, defined as: $\tilde{\tau}_e = \tau_a + b \tau_s$
where $b$ is the fraction of back-scattered radiation and $\tau_s$ is scattering optical depth.
RTTOV calculates multi-layer cloudy radiances by dividing the atmosphere into a number of homogeneous columns using the maximum overlap assumption.

Each column contains either cloud-free layers or totally cloudy layers.

Once the top of the atmosphere radiance has been computed for each homogeneous column, the cloudy radiance is computed as the sum of all the single column radiances weighted by the column fractional coverage.
The black line denotes the difference between clear sky and full scattering computations (i.e. adding-doubling) performed introducing water and ice clouds.

The red line denotes the difference between approximate (RTTOV) and exact scattering computations.

Scattering simulations in RTTOV

Cumulus (Continental clean) – Height of cloud = 6km
Tropical profile – Single layer

Cirrus – Height of cloud = 12km
Tropical profile – Single layer

Double layer

Double layer

Wave number (cm\(^{-1}\))

Brightness temperature difference (K)
The accuracy of scattering computations can be significantly affected by errors and uncertainties in the optical properties of the scattering particles.

Several methods exist to compute the optical properties of spherical and non-spherical particles (e.g. Baran 2012).

- An outstanding issue is represented by the representation of the optical properties of an ensemble of scattering ice particles of different sizes and different habits.
- Microphysical and sub-grid assumptions should be made compatible with the NWP model physics.
Importance of non-LTE processes in the short wave

- If not accounted for, non-LTE processes in the short wave can have a large impact on the accuracy of the radiance simulations.

- Parameterisations of non-LTE processes have been developed by deSouza-Machado et al. (2007), Chen et al. (2013), Matricardi et al. (2018).

Surface radiation

To improve the remote sensing of the atmosphere in the lowest 1 to 3 kilometres we need an improved modelling of the surface radiation in RT models.

For instance, a 2% error in the knowledge of the surface emissivity can result to a 1K error in the derived surface temperature.

The radiative transfer modelling of the surface is limited by the accuracy and the availability of laboratory measurements of terrestrial surface types.

Residuals obtained using emissivity values from the land emissivity atlas by Borbas et al. (2007).

Residuals obtained using a constant emissivity value (i.e.0.98).