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

LBL models: Voigt line shape

- 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 Voight 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).

LBL models: CO_2 line mixing

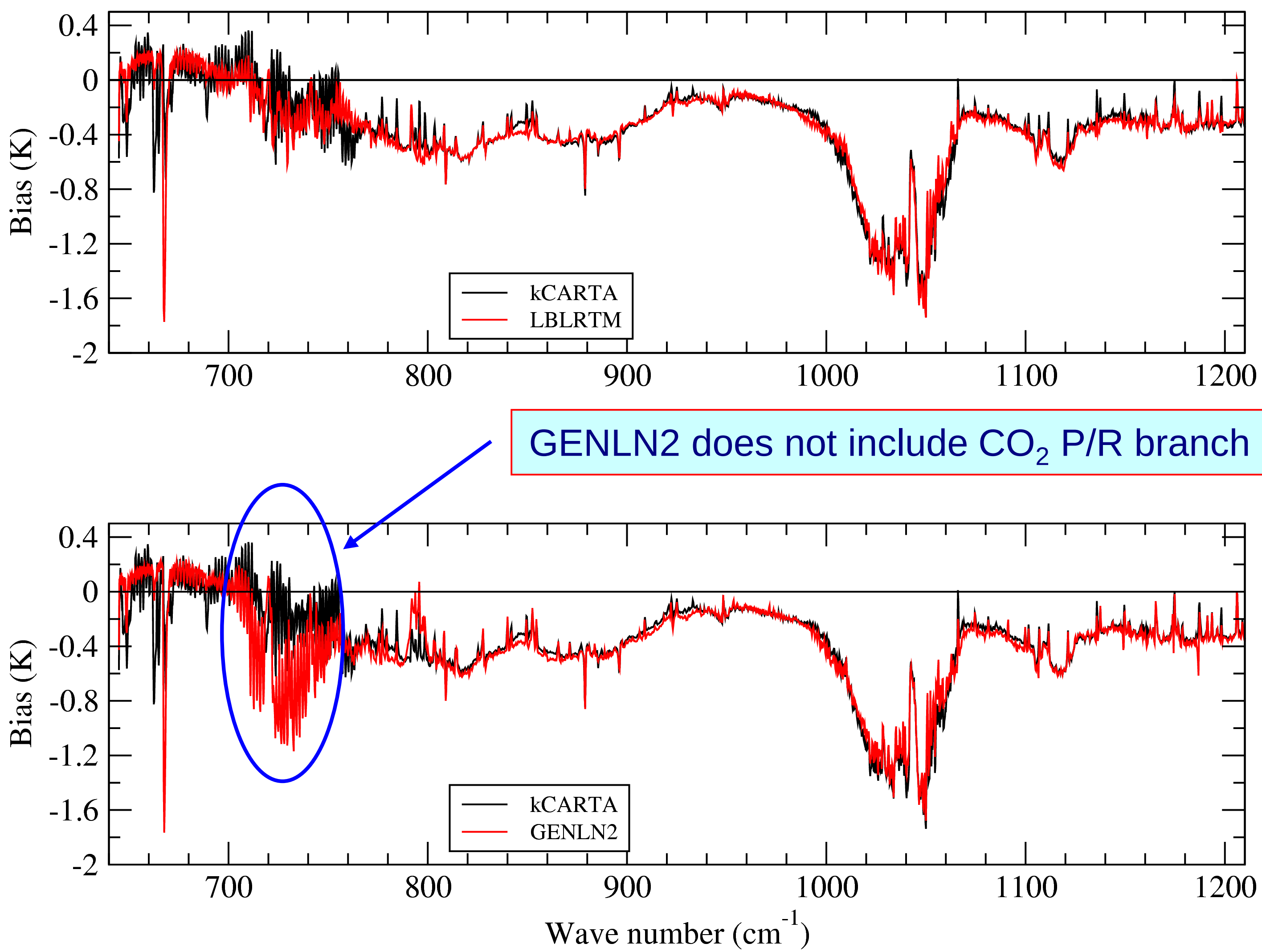
- In regions where absorption lines are closely spaced, line-mixing (or line-coupling) effects cause a departure from the Voigt line shape. This is especially true in the important CO_2 temperature sounding regions.

- 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_2O 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.

IASI band 1: observations minus simulations



LBL models: CH_4 and N_2O line mixing

- Line mixing effects have also been observed for CH_4 (Tran et al. 2006) , N_2O (Rachet et al. 1995) and even H_2O (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_2O, and to a lesser extend H_2O, line-mixing effects in LBL models.

LBL models: Water vapour continuum absorption

- 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.

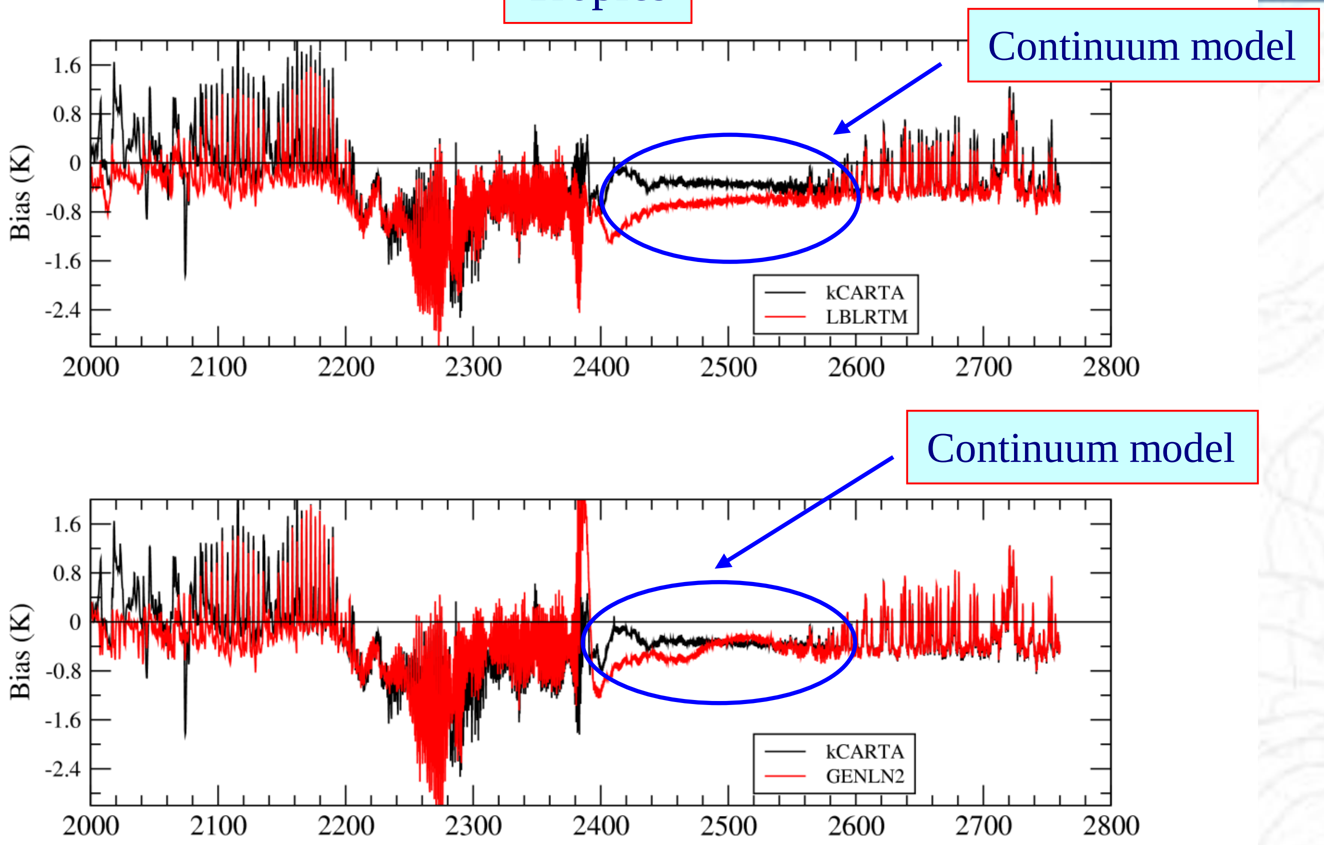
- The MT_CKD (Clough et al. 2005) model has been used successfully for many years in atmospheric RT codes, and is capable of reproducing many of the observed water vapour features in the mid-infrared spectral region. Some issues, however, still remain:

  - 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



LBL models: spectroscopic parameters

- 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.

LBL models: spectroscopic parameters

- H_2O 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).

LBL models: spectroscopic parameters

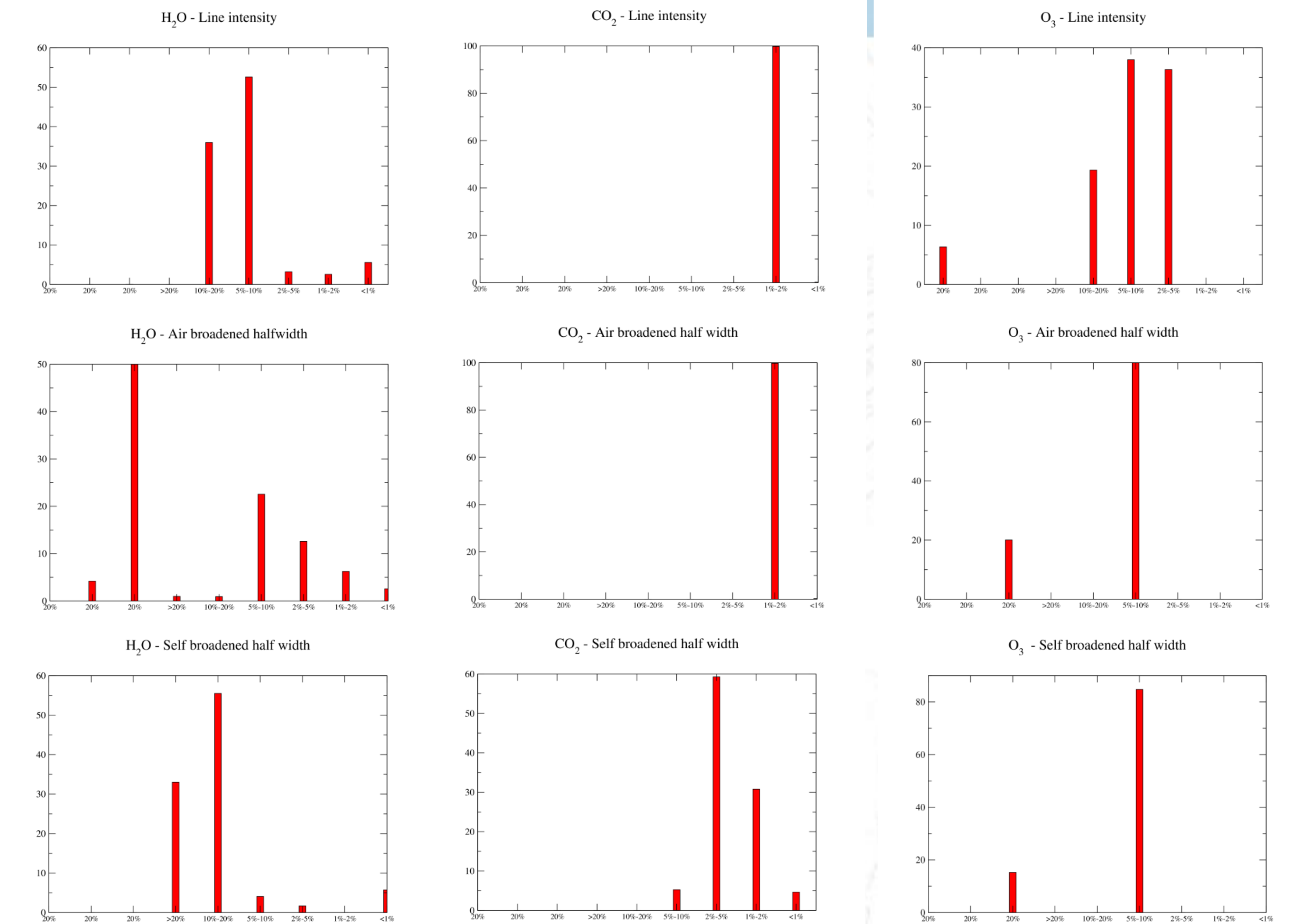
- Line parameters used in LBL computations are mainly obtained from the HITRAN (Rothman et al. (2013) and GEISA databases (Husson et al. 2011).

- 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?

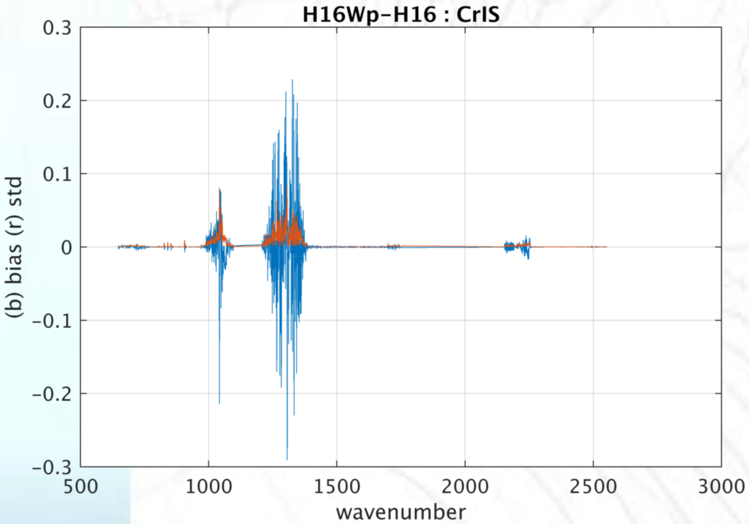
Accuracy of line intensity and half-width in the HITRAN database



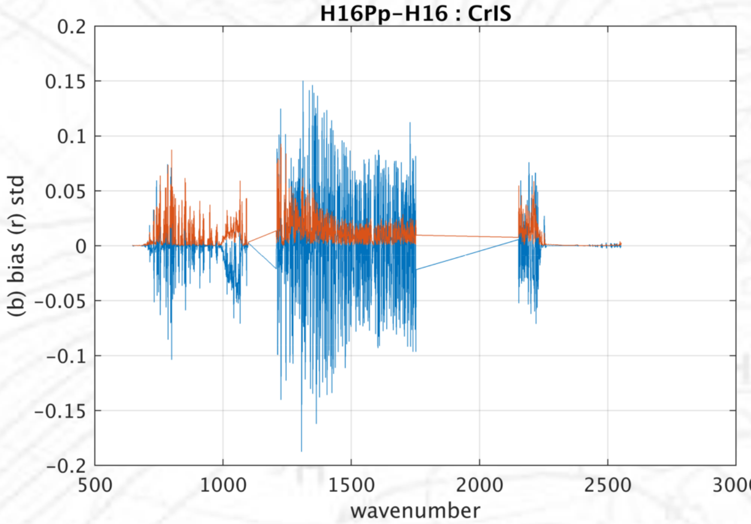
Brightness temperature signal associated with HITRAN uncertainties

Figures courtesy of Sergio DeSouza-Machado, UBMC

Line centre

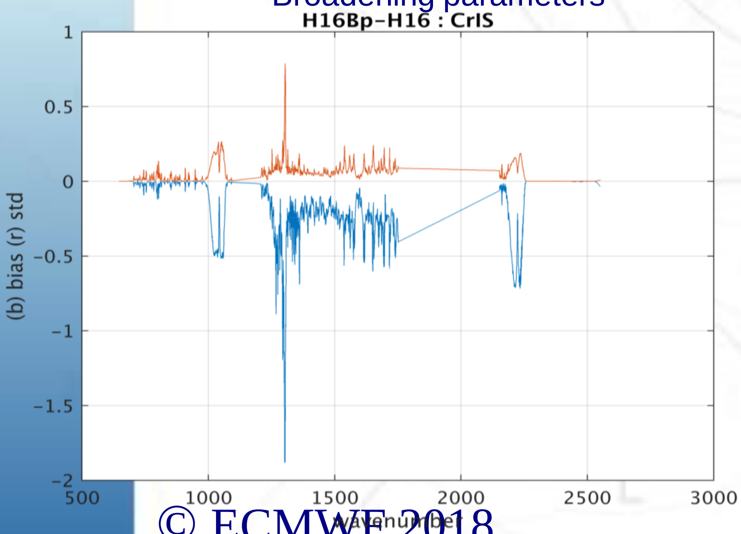


Pressure shift

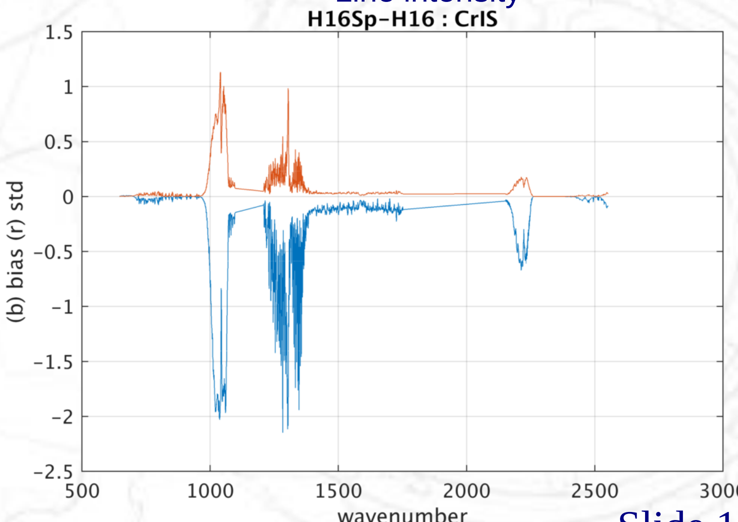


H_2O
O_3
N_2O
CO
CH_4
SO_2
HNO_3

Broadening parameters



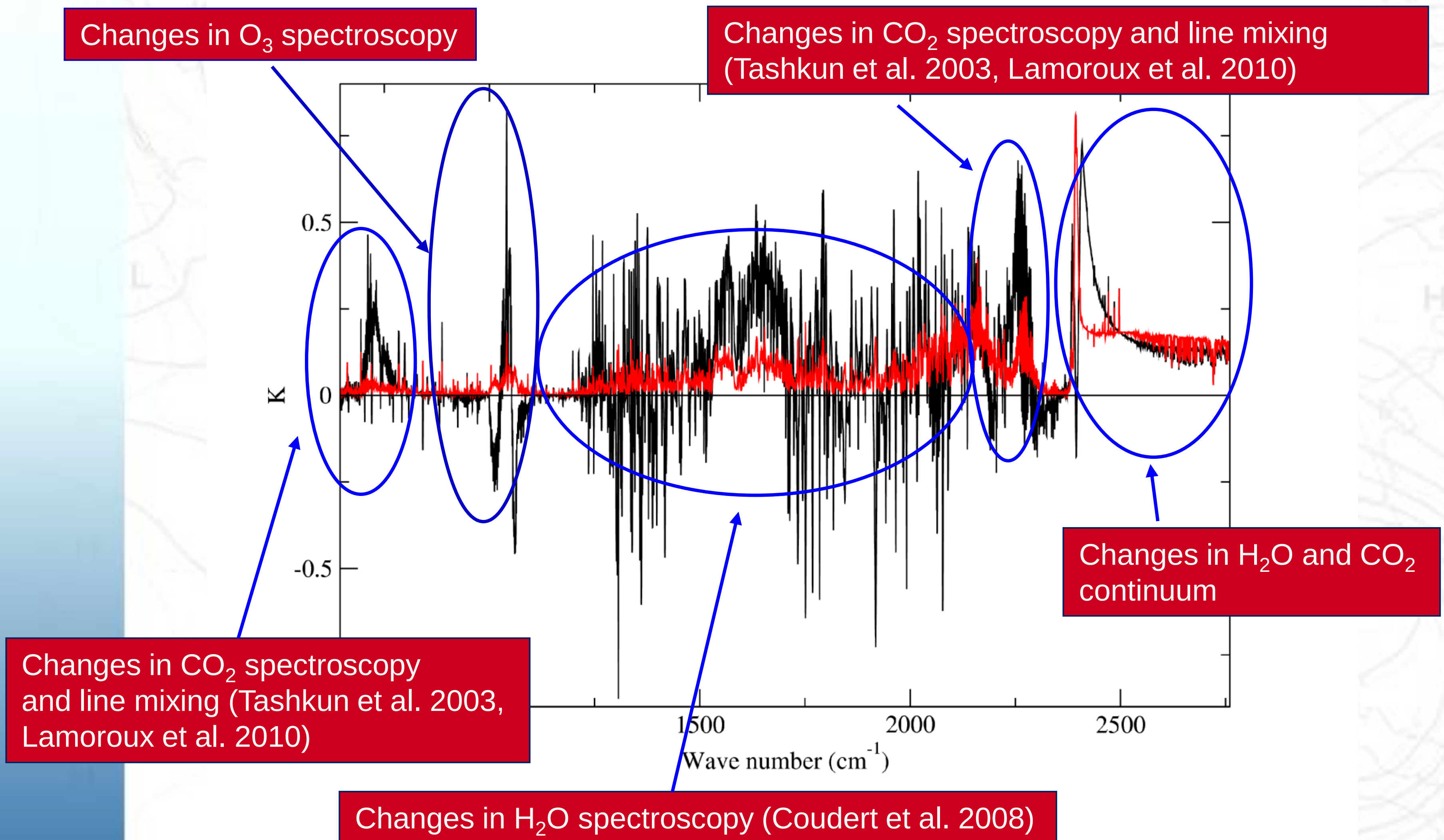
Line intensity



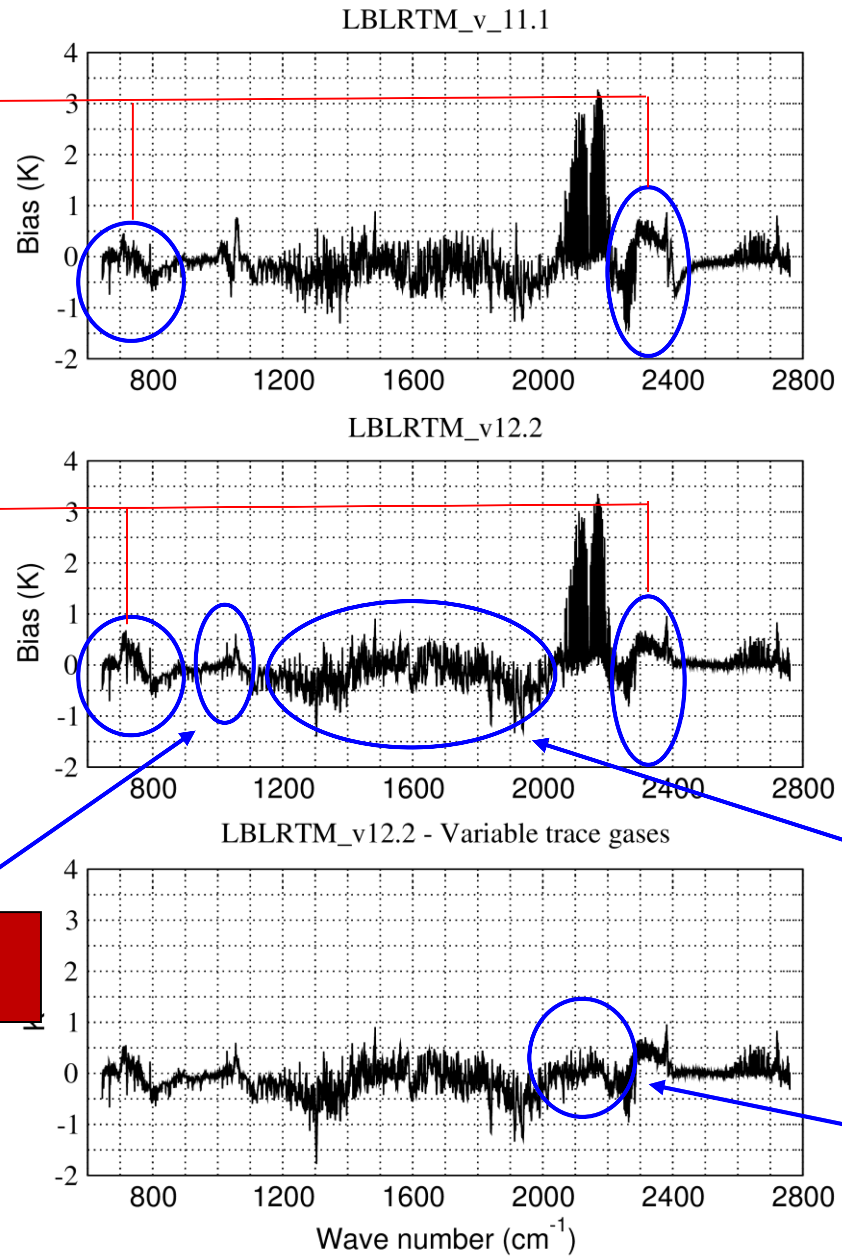
Difference between LBLRTM_v_11.1 and LBLRTM_v12.3 spectra for a dataset of 5190 profiles

The *red* curve is the standard deviation of the difference

The *black* curve is the mean value of the difference



IASI: global observations minus simulations (ECMWF first guess fields)



Note the inconsistency of the residuals in the CO_2 ν2 and ν3 bands

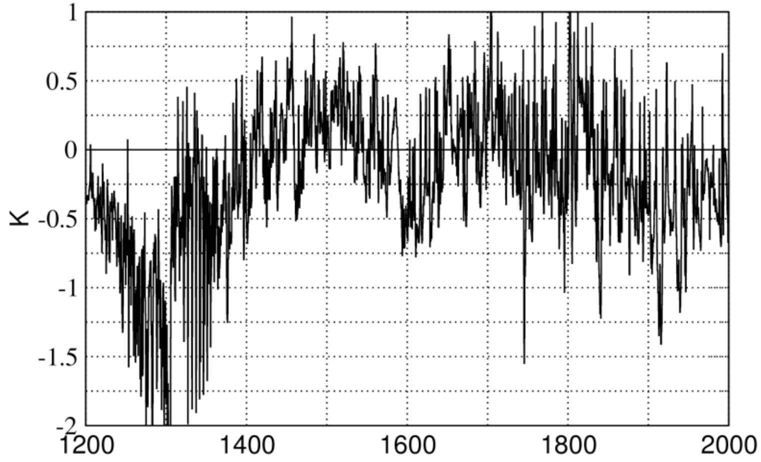
Note the consistency of the residuals in the CO_2 ν2 and ν3 bands

Smaller residuals in the O_3 band

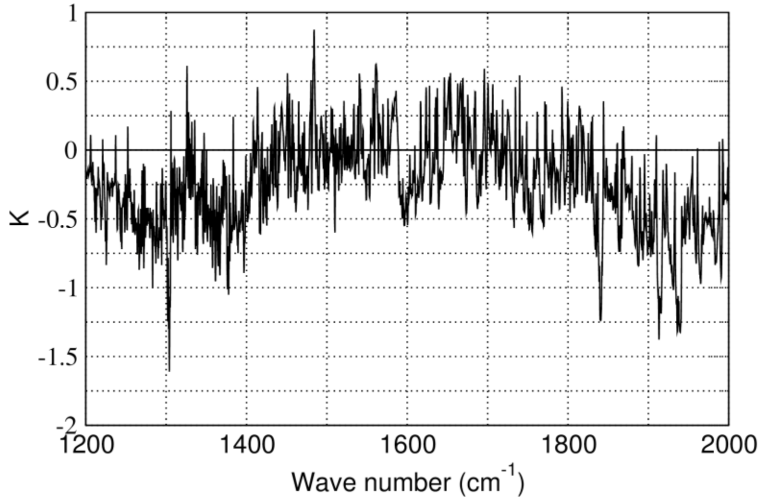
Smaller residuals in the H_2O band

More realistic CO profiles

IASI: global observations minus simulations (ECMWF first guess fields) Tropics



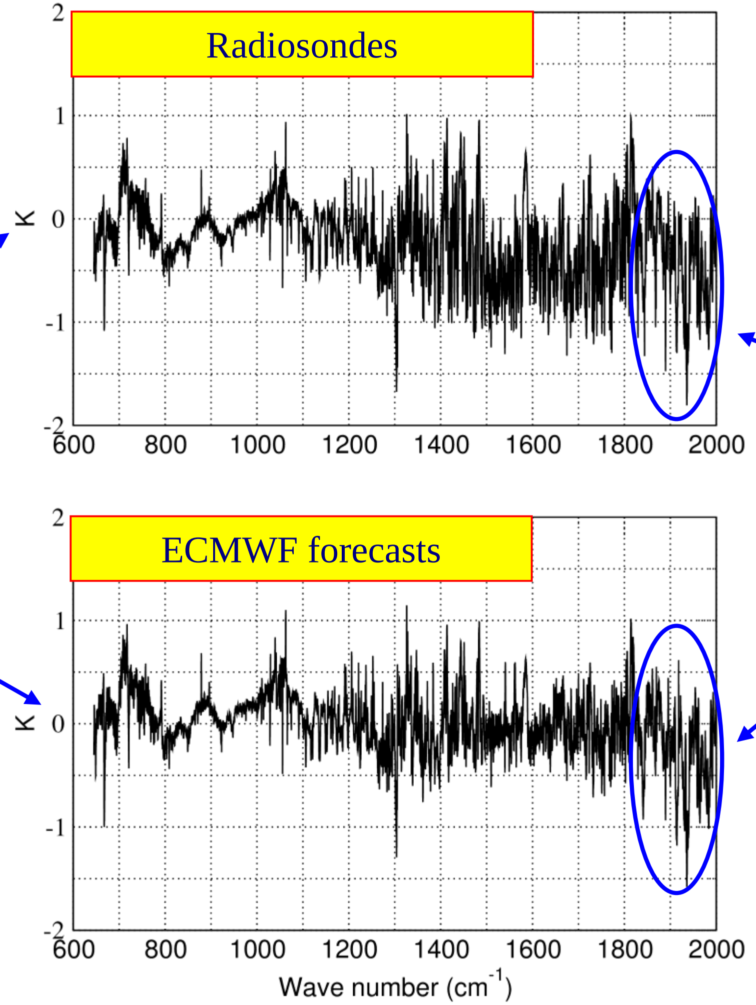
LBLRTM_11_1 + old spectroscopy



LBLRTM_12_2 + new spectroscopy

IASI: global observations minus simulations
GRUAN: MANUS island

LBLRTM_12_2 + new spectroscopy



Water vapour continuum?

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 is space (horizontally and vertically) and time.

  - The HDO case is a specially important one because HDO/H_2O 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 isotopolgues.

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.

Fast radiative transfer models: RTTOV

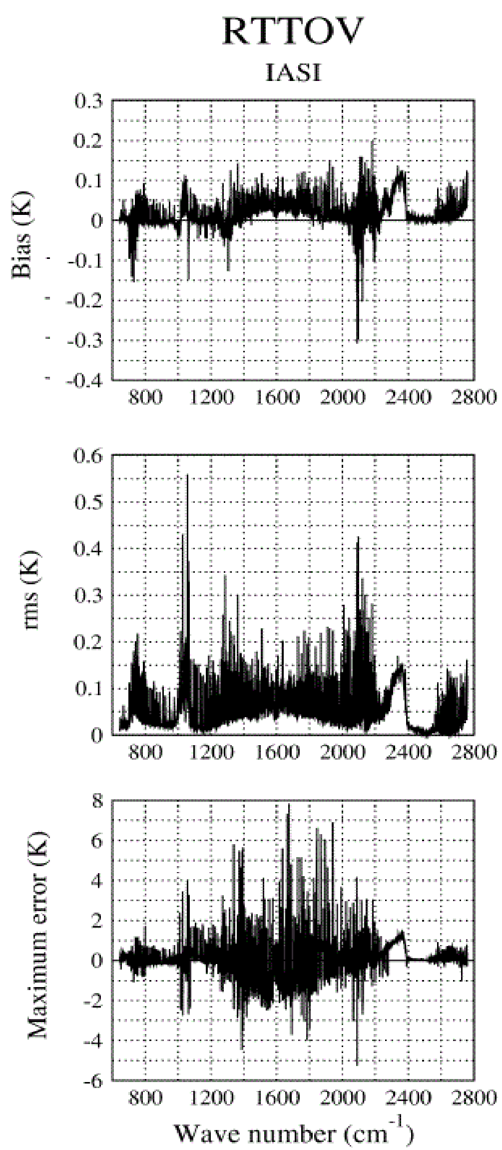
- RTTOV (Saunders et al. 2017) is a *regression based fast model* that computes channel-integrated layer optical depths using profile dependent predictors that are functions of temperature, absorber amount, pressure and viewing angle.

- 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:

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

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,ν^*} 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:

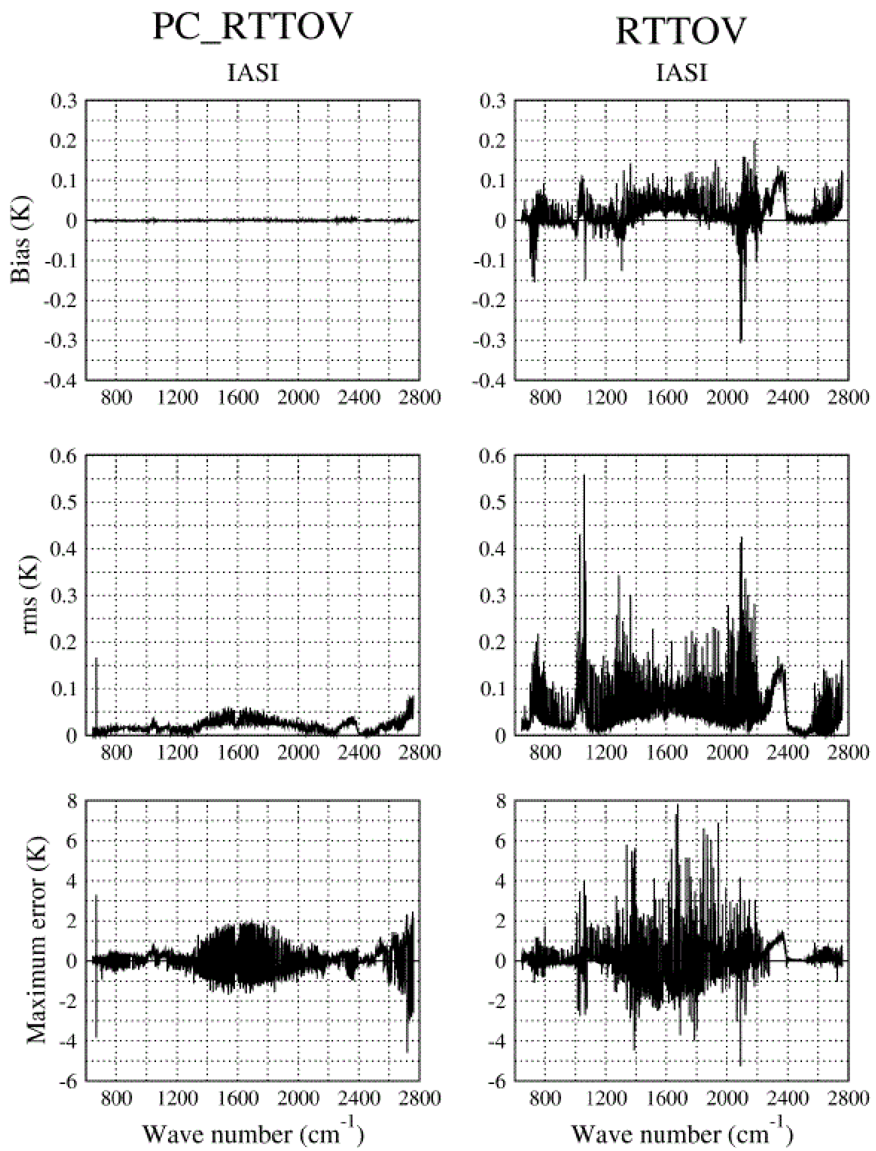
i) 'v7': H_2O, O_3 variable

ii) 'v8': H_2O, O_3, CO_2 variable

iii 'v9': H_2O, O_3, CO_2, CO, N_2O, 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 .

Principal component based RTTOV



Fit to LBL radiances over land and sea surfaces for a dataset of 12000 atmospheric situations independent of the regression coefficients.

Scattering simulations in RTTOV

- 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.

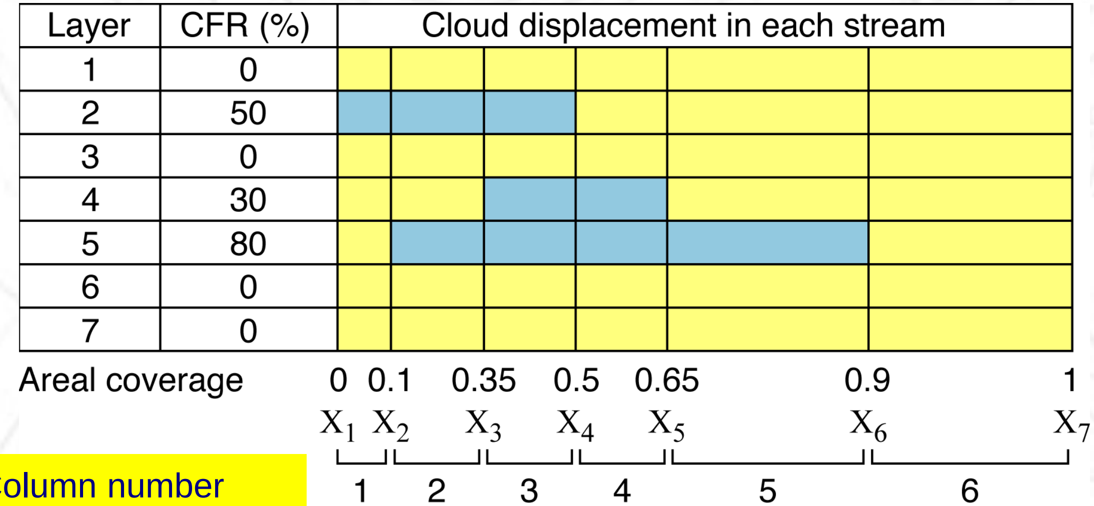
- In the scaling approximation the absorption optical depth, τ_a, is replaced by an effective extinction optical depth, $\tilde{\tau}_e$, defined as: $\tilde{\tau}_e = \tau_a + b\tau_s$ where b is the fraction of back-scattered radiation and τ_s is scattering optical depth.

Scattering simulations in RTTOV

- 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.

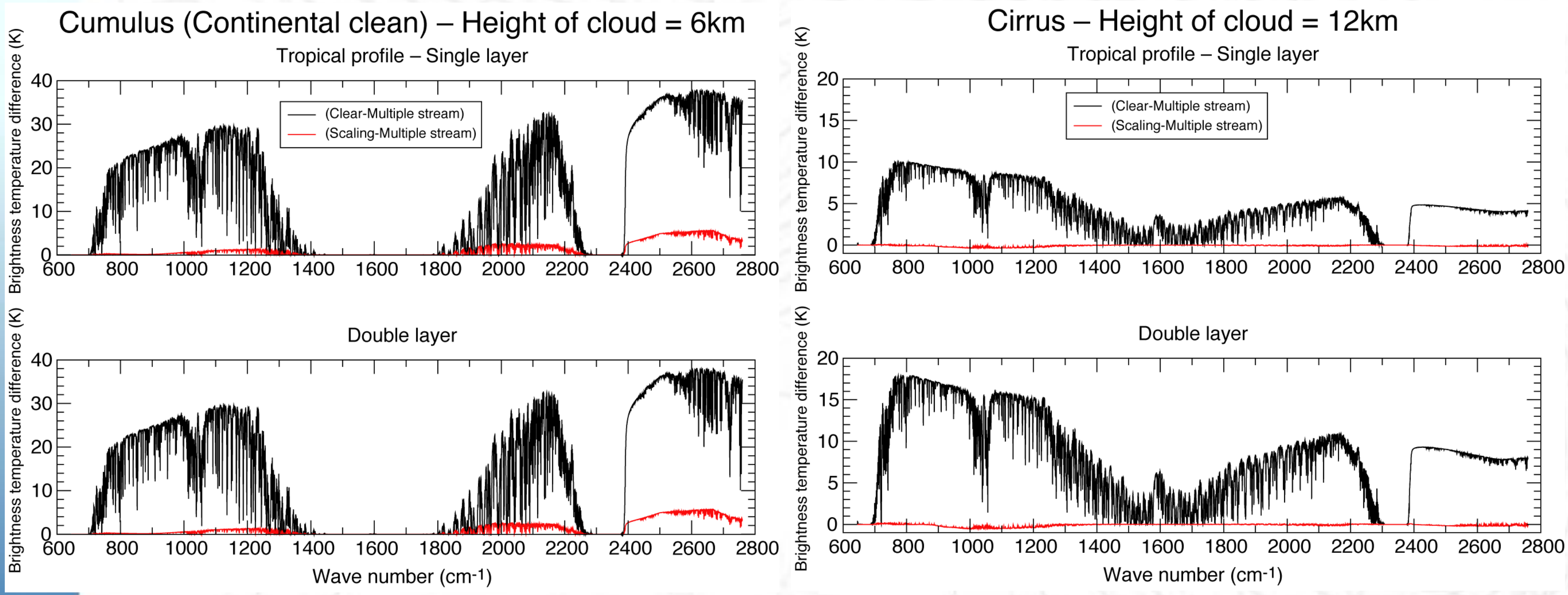
- Once the top of the atmosphere radiance has been computed for each homogeneous column, the cloudy radiance is computed as the sum of all the single column radiances weighted by the column fractional coverage.



Scattering simulations in RTTOV

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



Optical properties of clouds

- The accuracy of scattering computations can be significantly affected by errors and uncertainties in the optical properties of the scattering particles.

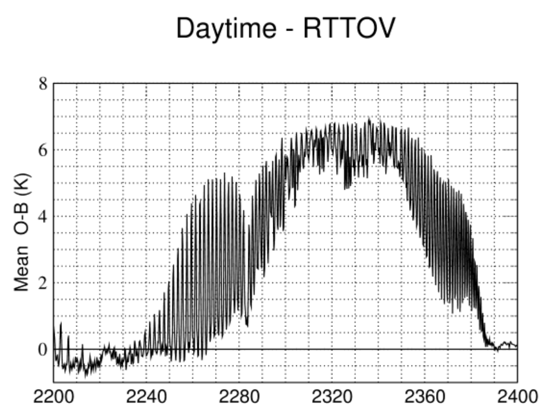
- Several methods exist to compute the optical properties of spherical and non-spherical particles (e.g. Baran 2012).

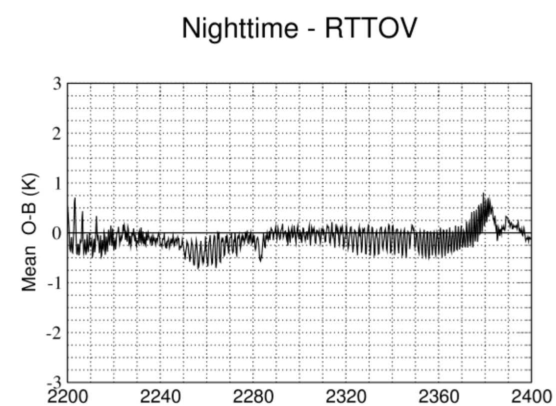
  - An outstanding issue is represented by the representation of the optical properties of an ensemble of scattering ice particles of different sizes and different habits.

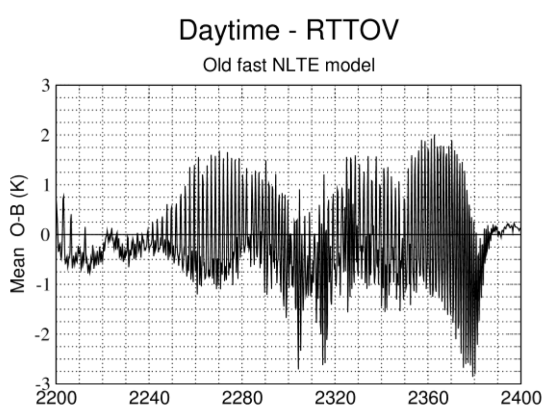
  - Microphysical and sub-grid assumptions should be made compatible with the NWP model physics.

Importance of non-LTE processes in the short wave

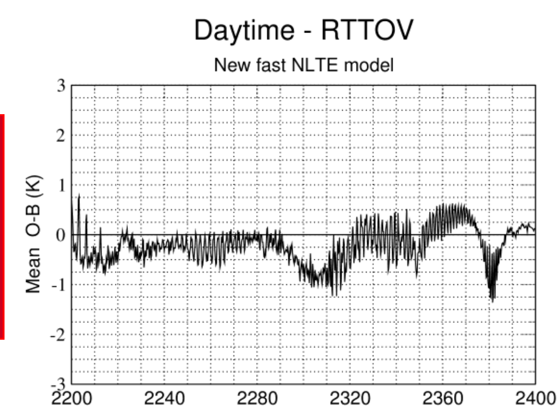
- If not accounted for, non-LTE processes in the short wave can have a large impact on the accuracy of the radiance simulations.
- Parameterisations of non-LTE processes have been developed by deSouza-Machado et al. (2007), Chen et al. (2013), Matricardi et al. (2018).







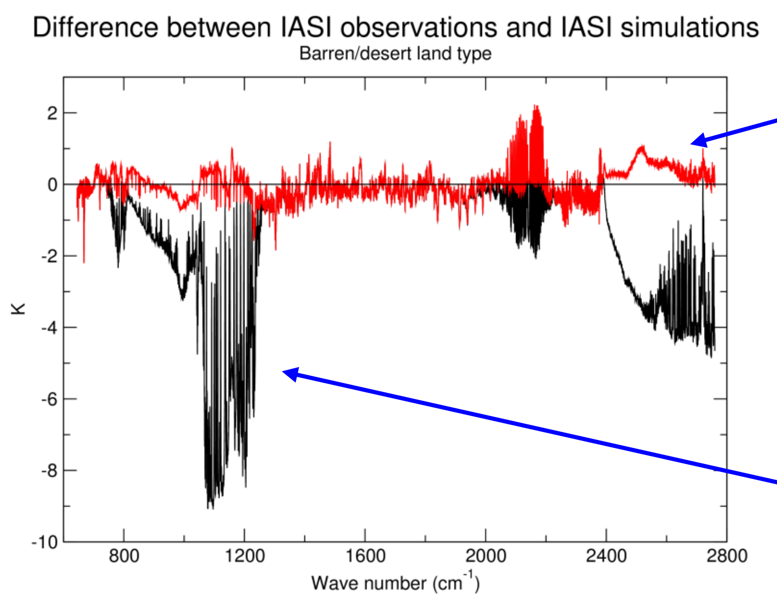
Old RTTOV fast NLTE model (Sauders et al. 2013). Vibrational temperatures from Funke et al. (2002)



New RTTOV fast NLTE model by Matricardi et al. (2018). Vibrational temperatures from Funke et al. (2012)

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 emissity values from the land emissivity atlas by Borbas et al. (2007).

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