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Importance of spectroscopy and radiative transfer for the use of IASI data

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Radiative transfer models

■ The exploitation of IASI 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 for IASI

● Accurate but computationally expensive LBL models based on first principles.

● Fast and hyper-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)

FAST

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

HYPER-FAST

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 IASI 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 (e.g. Ngo et al. 2013).

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- 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
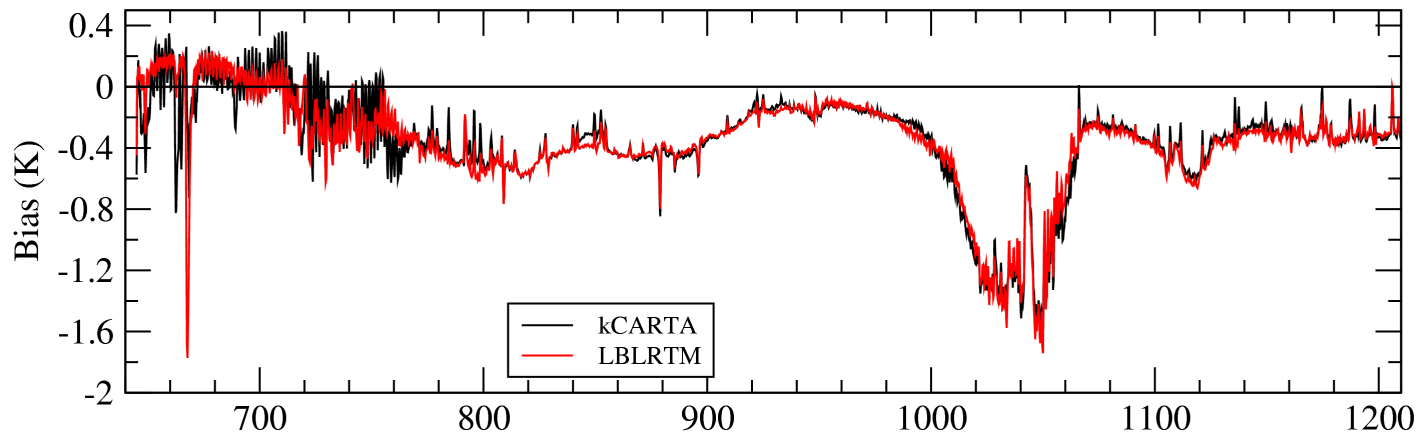
GENLN2 does not include CO_2 P/R branch line mixing
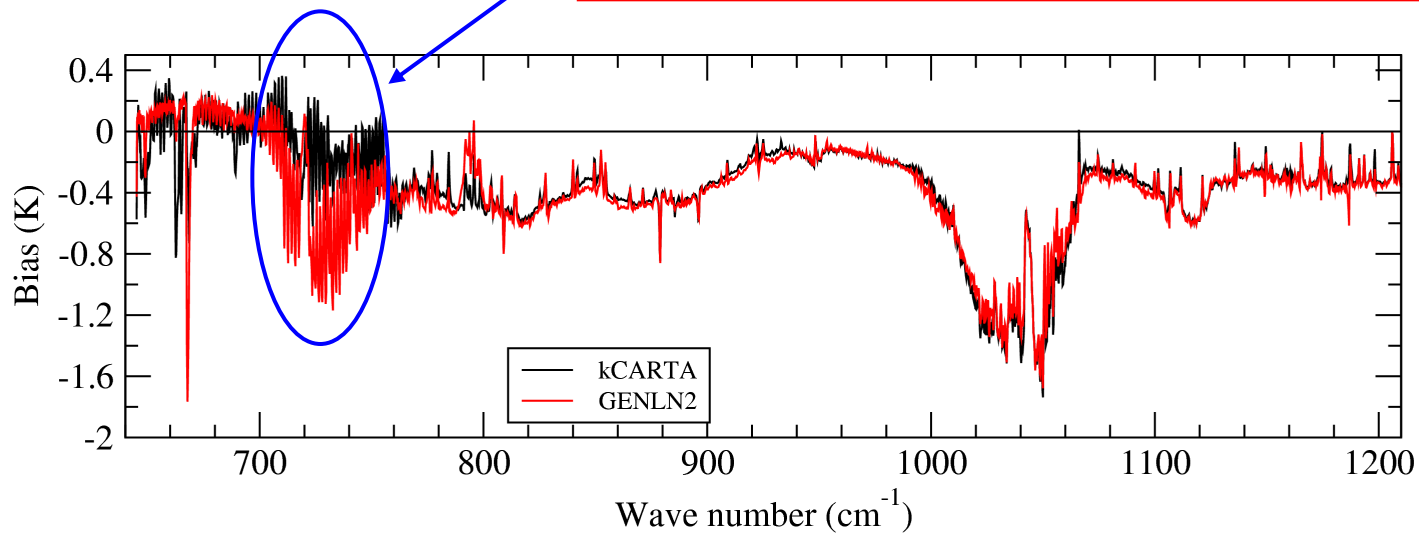
■ Line mixing effects have also been observed for CH_4 (Tran et al. 2006) , N_2O (Rachet et al. 1995) and even H_2O (Brown et al. 2004).

■ Some LBL models include line-mixing effects in the ν3 (3000 cm^{-1}) and ν2 (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 nature of water vapour continuum absorption and its effect on atmospheric radiance is an outstanding and unresolved issue.

- A unifying theory of the water continuum is still lacking, with competing formulations based on the far wing of allowed transitions of the water monomer (Ma et al. 2008) and on the existence of bound water complexes known as dimers (Ptashnik et al. 2011).

- Because of the uncertainty of the cause of the continuum, semi-empirical parameterisations have been developed based on laboratory and aircraft measurements.

- These parameterisations have evolved from the CKD model (Clough et al. 1989) to the MT_CKD model (Clough et al. 2005).

LBL models: Water vapour continuum absorption

The MT_CKD 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
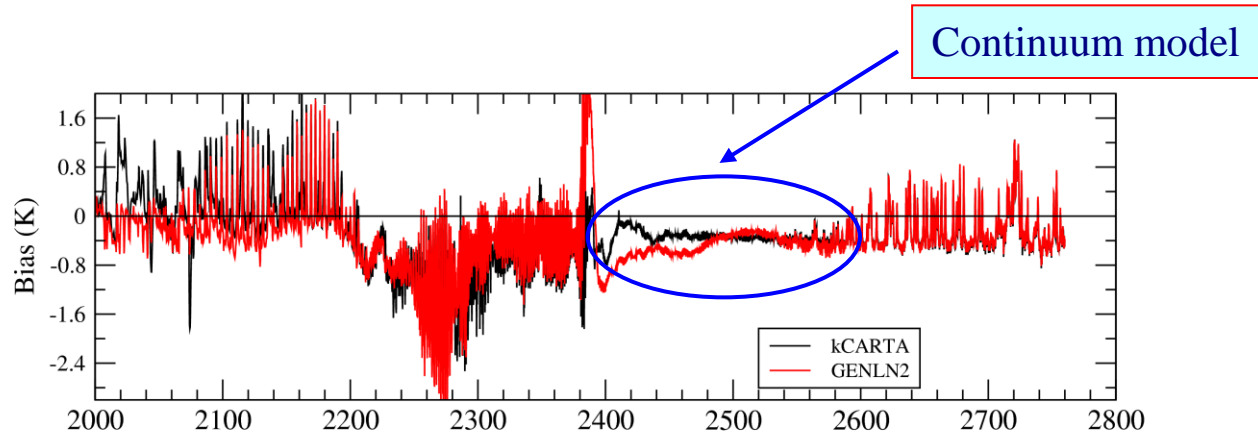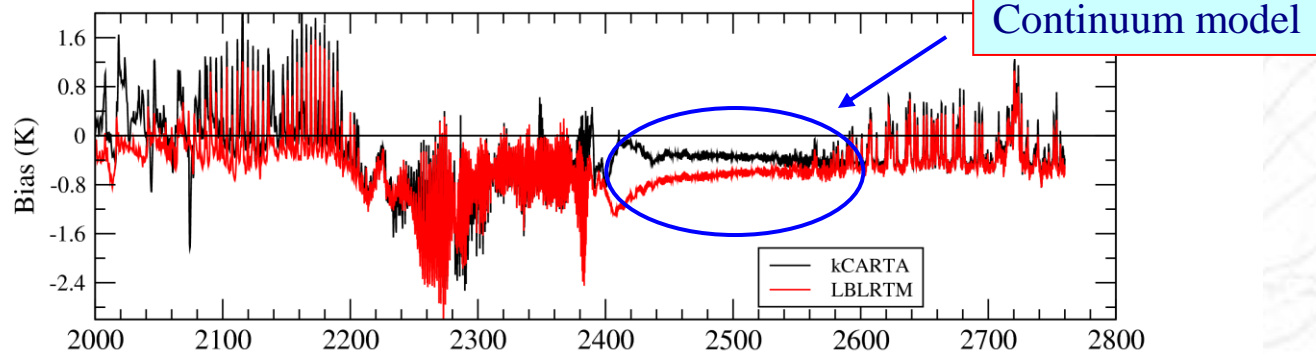
Continuum model

Do we need a physically based representation of the water vapour continuum in LBL models?

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.)

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)
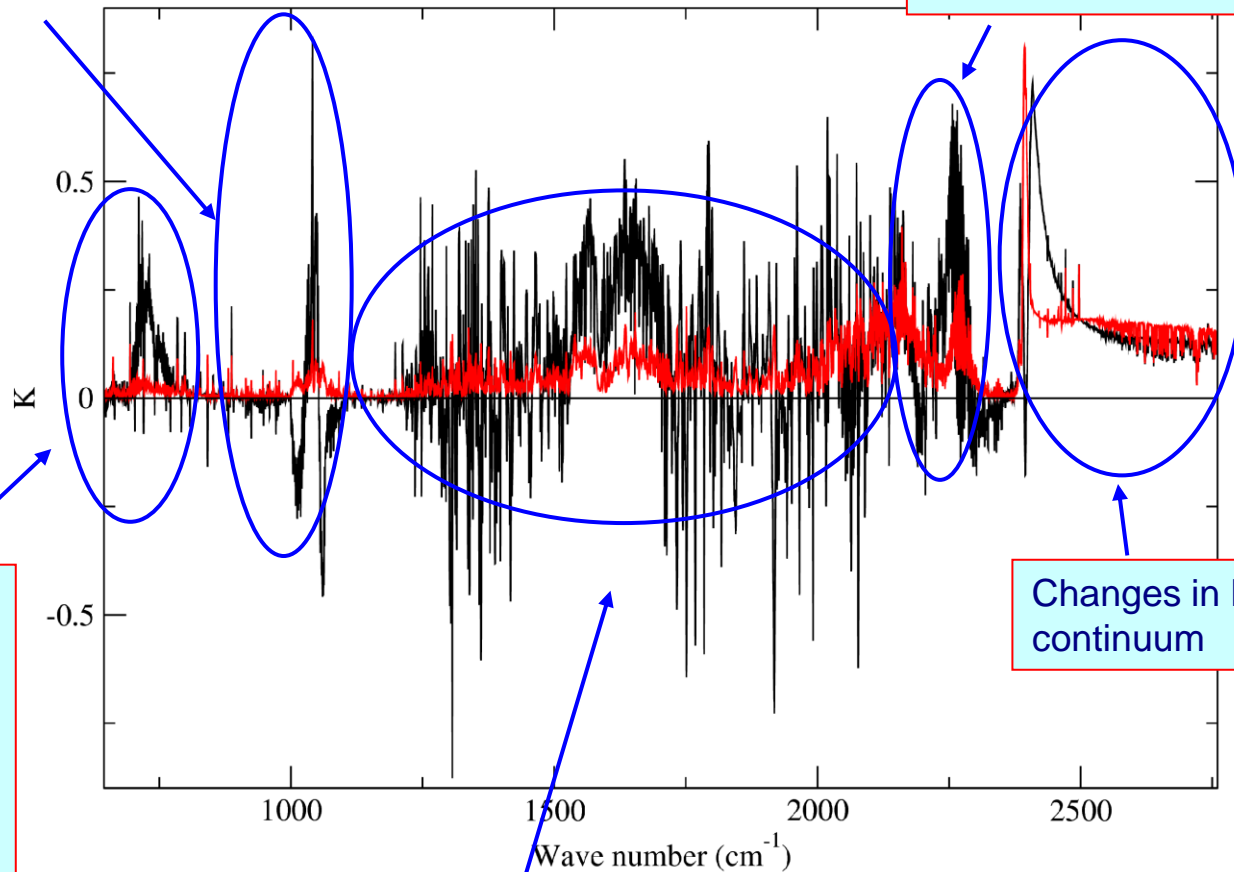
Changes in CO_2 spectroscopy and line mixing (Tashkun et al. 2003, Lamoroux et al. 2010)

Changes in H_2O and CO_2 continuum

Changes in H_2O spectroscopy (Coudert et al. 2008)

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IASI: global observations minus simulations

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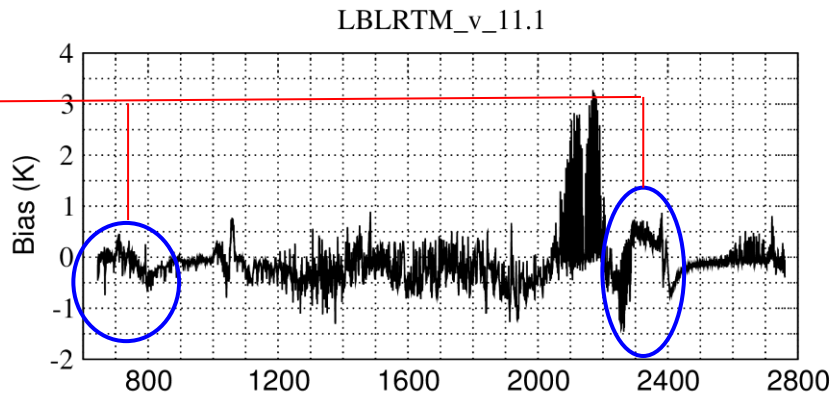
Note the consistency of the residuals in the CO_2 ν2 and ν3 bands

Smaller residuals in the O_3 band
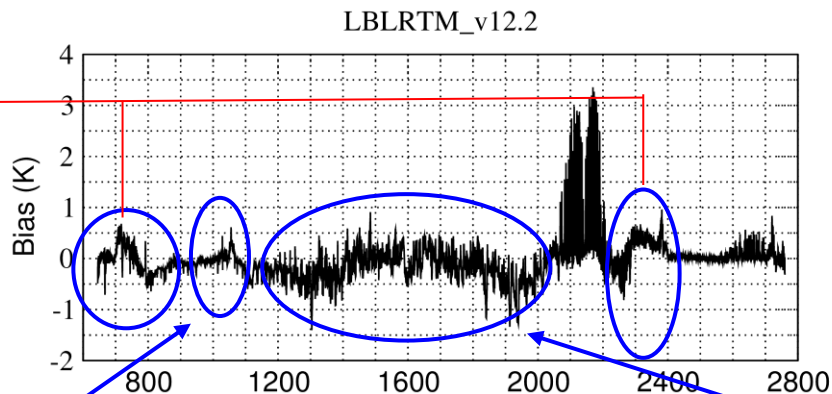
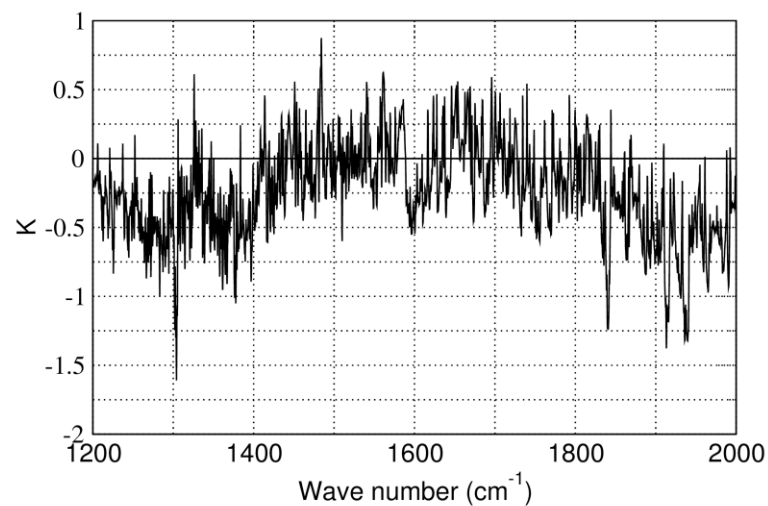Smaller residuals in the H_2O band
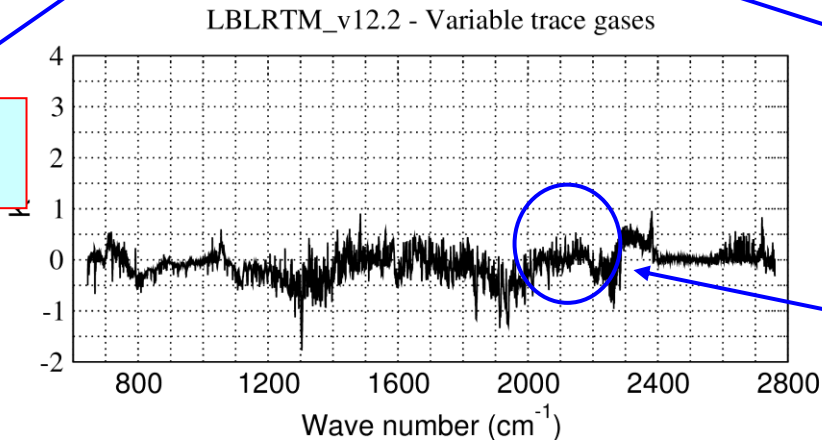
More realistic CO profiles

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IASI: global observations minus simulations
Tropics
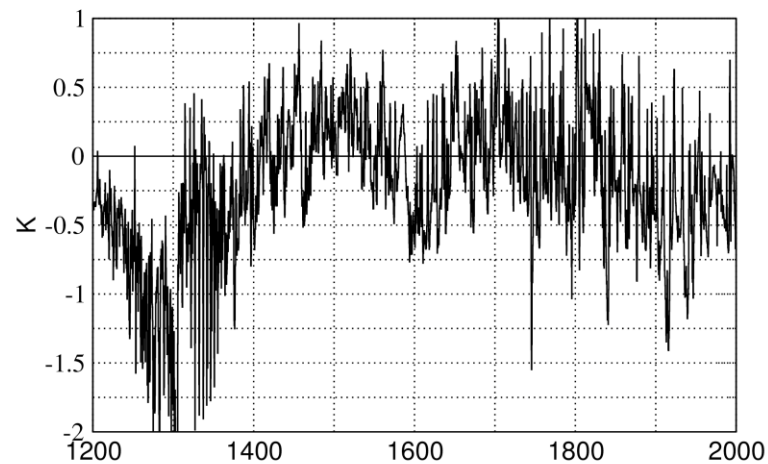
LBLRTM_11_1 + old
spectroscopy

LBLRTM_11_2 + new
spectroscopy

IASI: global observations minus simulations
MANUS island

Radiosondes

ECMWF forecasts
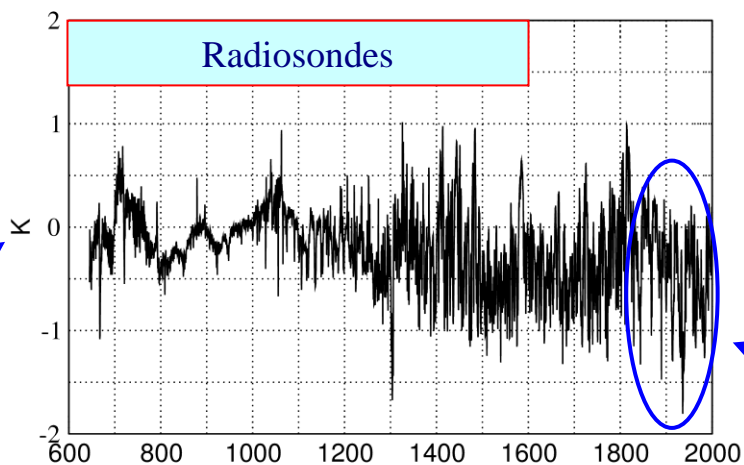
LBLRTM_12_2 + new spectroscopy

Water vapour continuum?

Wave number (cm^{-1})

LBL models: accounting for accurate isotopic ratios
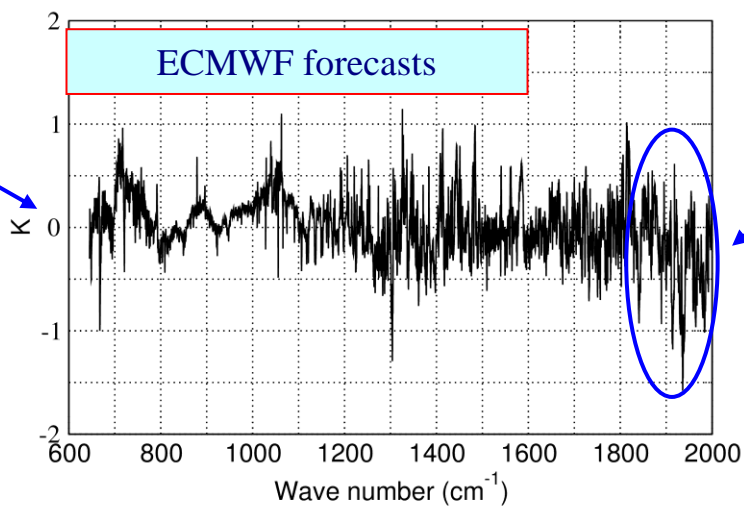
■ LBL models compute the absorption due to minor isotopologues using fixed fractional abundances relative to the major isotopologue.

● 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.

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.

Hyper-Fast radiative transfer models

- Hyper-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.

Hyper-Fast radiative transfer models

- Parameterisation errors have been further reduced following the development of Principal Component based hyper-fast RT models (e.g. PC_RTTOV, PCRTM, HT-FRTC)

The fit of the RTTOV model to the LBLRTM line-by-line model

Independent set : 5195 observations

5195 independent profiles

PC_RTTOV

Standard RTTOV
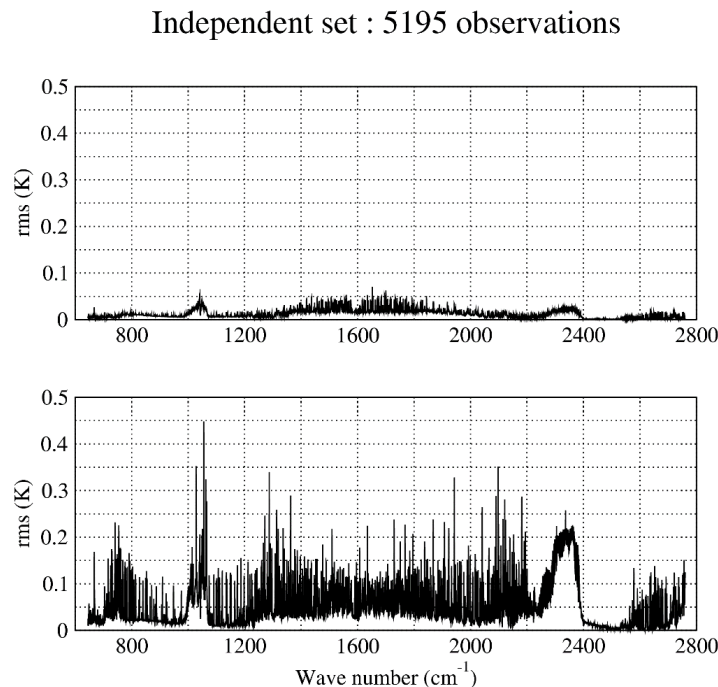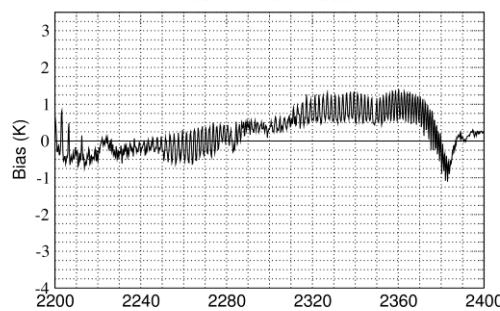
Importance of non-LTE processes in the short wave

■ 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 (2016).
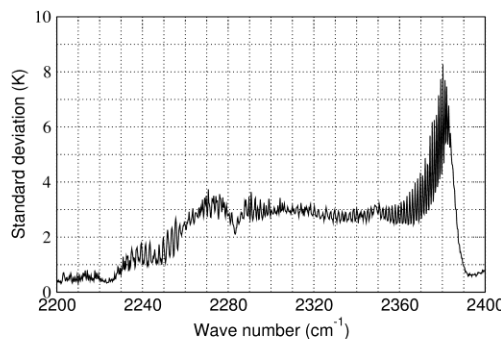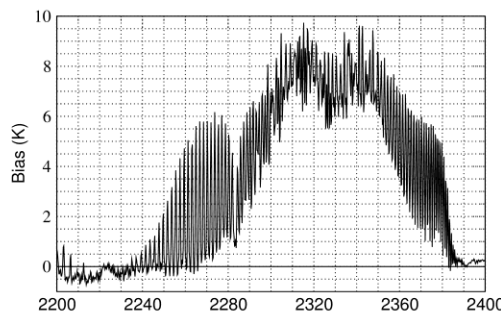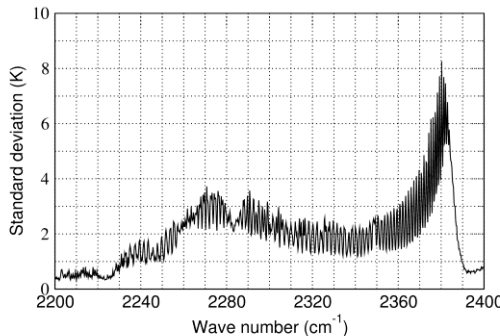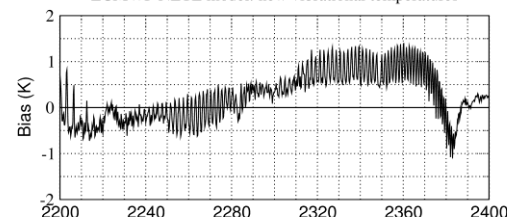

Vibrational temperatures from Funke et al. (2012)
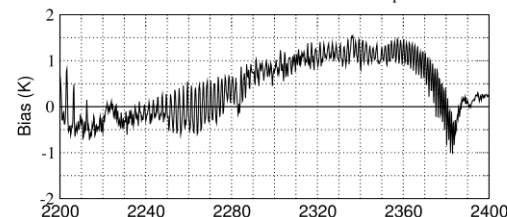
Vibrational temperatures from Funke et al. (2002)

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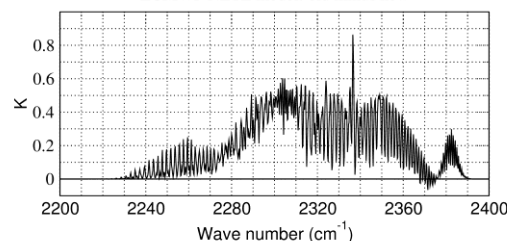
Surface radiation

- 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.

Difference between IASI observations and IASI simulations
Barren/desert land type
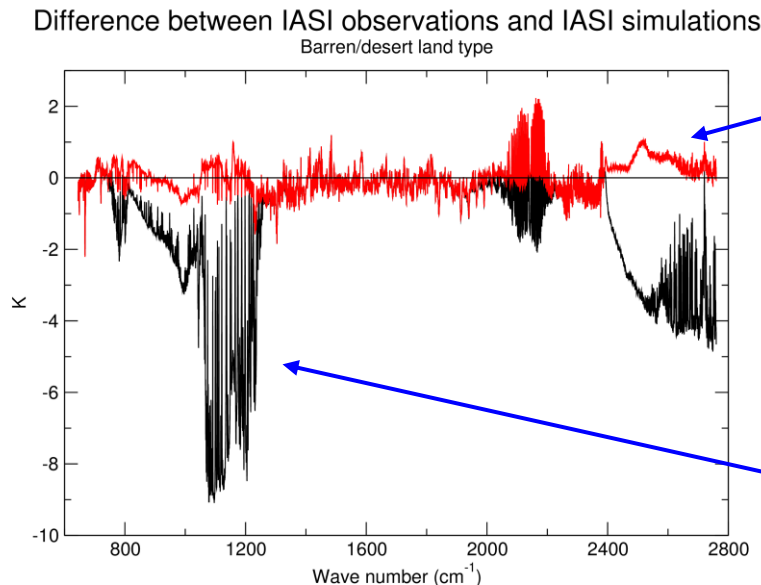
Residuals obtained using emissity values from the land emissivity atlas by Borbas et al. (2007).

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

- The scattering approximations used in fast/hyper-fast models should be properly validated against full scattering schemes and against observations through intercomparison/validation exercises.

- The effects of three-dimensional cloud structures should also be studied. Simplified methods like the one used in RTTOV (Matricardi 2005) can only provide a gross approximation of the inhomogeneity observed by satellite born instruments.

- For aerosol scattering computations more research is needed to characterise the regimes where fast approximate methods work better.

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.