

## 4A/OP Operational release for 4A (Automatized Atmospheric Absorption Atlas)

4A, stands for Automatized Atmospheric Absorption Atlas is a fast and accurate line-by-line radiative transfer model developed and validated at LMD for the computation of transmittances, radiances and jacobians. It is a particularly efficient tool in terms of accuracy and computation time.

Within this frame, and with the support of the CNES (the French Space Agency), NOVELTIS has created an operational version of this code called 4A/OP. 4A/OP is a user-friendly software for various scientific applications, co-developed with the LMD, easily and freely distributed to registered users. This code is regularly updated and improved by the LMD, NOVELTIS and CNES.

The 4A/OP software is used by several research groups and can be integrated in operational processing chains including inverse problems processing. In particular, 4A/OP has been chosen as reference RT code for CNES missions such as IASI, MicroCarb or IASI-NG.

4A allows the fast computation of the transmittances and the radiances with the same precision of a classic line-by-line algorithm from NIR to LWIR wavelengths at high spectral resolution. The 4A calculation relies in particular on a multi-dimensional interpolation using a pre-built optical thickness database called "Atlases" [1].

The Atlases are built for up to 53 atmospheric molecular species, 12 nominal atmospheres, 44 pressure levels, for a  $5 \times 10^{-4}$  cm<sup>-1</sup> nominal spectral step (compressed in wave numbers / layer / temperature). The atlases are created by using the line-by-line and layer-by-layer model, STRANSAC [2], with state-of-the-art physics and up-to-date spectroscopy from the latest edition of the GEISA spectroscopic catalogue [3] and also <http://ether.ipsl.jussieu.fr>

4A interpolates in the Atlases to get the optical thickness profile for any given atmospheric condition. 4A returns the high spectral resolution spectra (nominal spectral resolution: 5.10-4 cm<sup>-1</sup>) or the convolved spectra with various types of instrument functions and provides jacobians on user-defined layers.

### MAIN FEATURES

- ✓ Spherical atmosphere
- ✓ Zenith, nadir or limb observations
- ✓ Usual spectral domain: [600 - 13300] cm<sup>-1</sup>
- ✓ Wide variety of surface: numerous typical spectral emissivities, surface albedo, multiple BRDF/BPDF models (via VLIDORT)
- ✓ Solar contribution: any available solar spectrum, including Doppler shift of solar lines
- ✓ Scattering: by molecule (Rayleigh) and aerosols/cirrus (coupled with DISORT, LIDORT, VLIDORT), including jacobian calculation
- ✓ Polarization with VLIDORT

### What is 4A/OP?

#### SOFTWARE PACKAGE FEATURES

The current operational version 4AOP2012v1.0 (03/2012) includes:

- Regular updating and improvements
- Graphical User Interface (GUI)
- Reference Documentation [4] and quick Start Guide
- Website including an on-line registration form: <http://4aop.noveltis.com>
- Distribution with maintenance and assistance; the full software package is available as a freeware product for academic and scientific research

#### SOFTWARE FEATURES

GUI: create a basic input file by selecting values with buttons, pull-down menus, and text fields.

Portable: 4A/OP runs on any platform with several Fortran 90 compilers (PGI, intel, GNU) and has been tested on Sun and Linux PC.

Running time: 4A/OP is 100 times faster than a classical "line by line" for an equivalent precision.

#### SUCCESS STORY

##### TIR domain

- ✓ IASI: RT model for level 1 Cal/Val
- ✓ IASI: Metop-A & Metop-B: level 1 operational processing at CNES (Technical Expertise Center) for the monitoring of the IASI data

##### SWIR domain

- ✓ MicroCarb: preliminary design studies (CNES)
- ✓ MicroCarb: chosen by the PI as reference code
- ✓ Merlin: Validation of the spectroscopy (CH<sub>4</sub>)
- ✓ GOSAT: retrievals /spectral calibration

##### Cal/Val activities for Metop-A & B

- ✓ Spectral calibration for IASI/A and inter-calibration of IASI/A & IASI/B
- ✓ Daily collocations (clear scenes) with ECMWF analyses
- ✓ Statistics (Calc-Obs.) on 4 months in 2013 as a function of: time, viewing angle, wavenumber...

##### Main conclusions for the inter-calibration campaign:

- ✓ [645- 2760 cm<sup>-1</sup>):  
→ IASI/A-IASI/B < 0.1 K
- ✓ For all viewing angles:  
→ IASI/A - IASI/B < 0.15 K

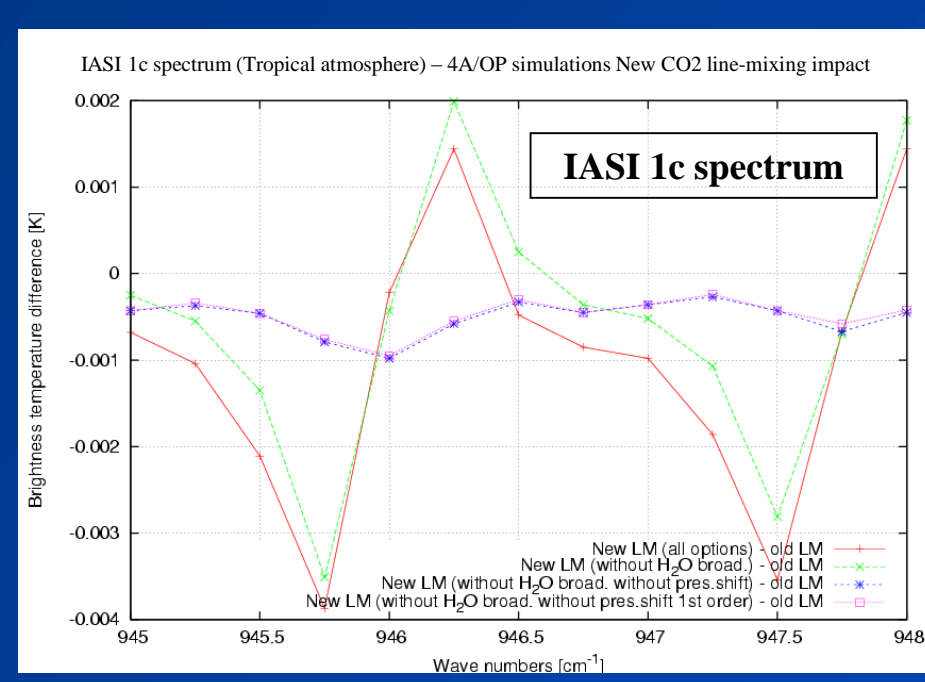
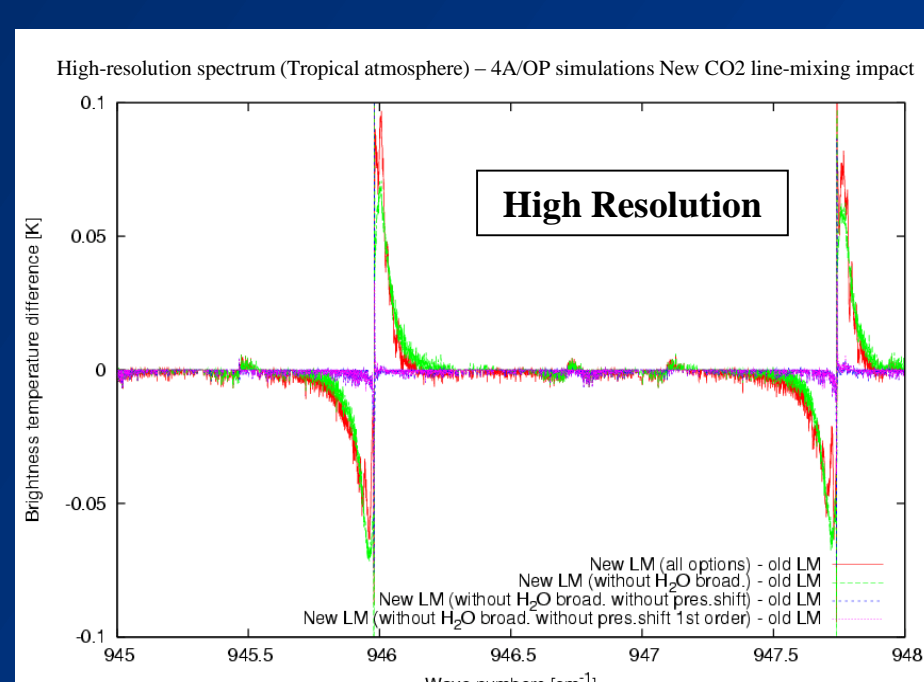
## Spectroscopic features

The 4A/OP software includes the up-to-date physics from the most advanced spectroscopic characteristic of the main molecules in the TIR and SWIR spectral domains.

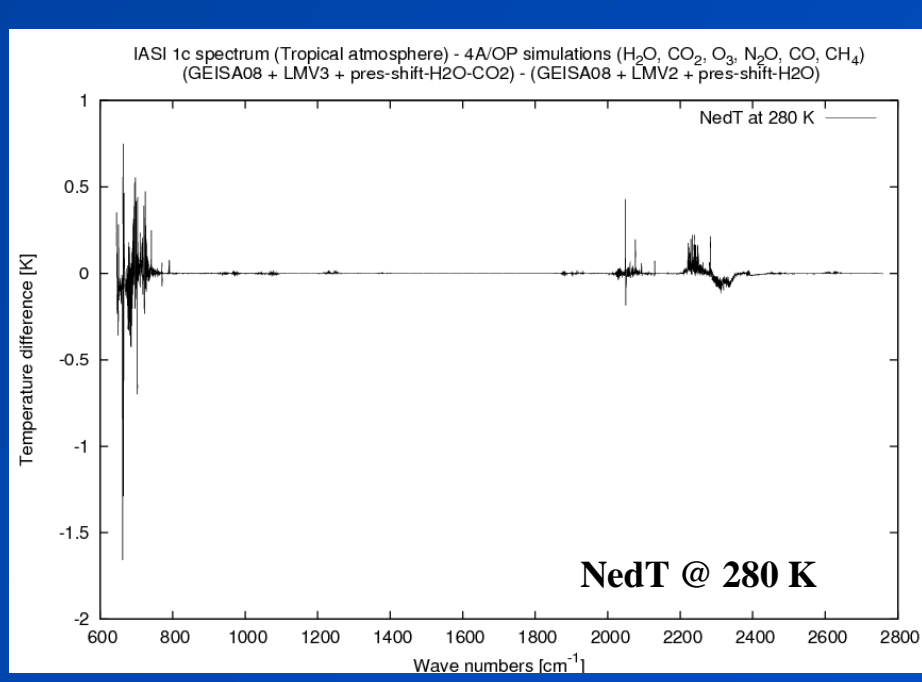
### CO<sub>2</sub> LINE-MIXING

- ✓ Complete matrix formulation for the calculation of the absorption coefficient: from Lamouroux *et al.*, 2010
- ✓ Spectroscopic parameters from HITRAN 2008 completed with database of CDS-296 (Tashkun *et al.*, 2006) and CDS-1000 (Tashkun *et al.*, 2003)
- ✓ Includes the pressure-shift for each CO<sub>2</sub> line: from the empirical formulation developed by Hartmann (2009)
- ✓ Foreign-broadening by H<sub>2</sub>O: from Sung *et al.*, 2009

#### Impact of the new line-mixing including PS and H<sub>2</sub>O broadening



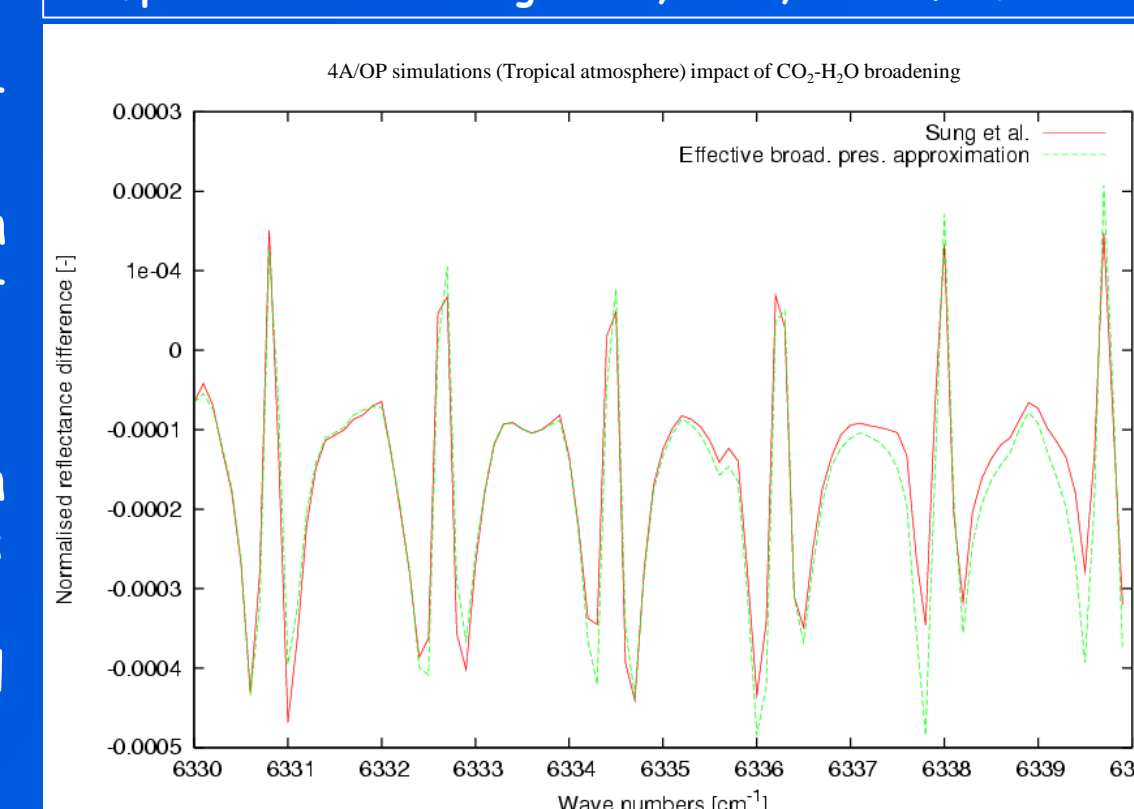
#### IASI 1c spectrum: H<sub>2</sub>O, O<sub>3</sub>, N<sub>2</sub>O, CO, CH<sub>4</sub>



### CO<sub>2</sub> - H<sub>2</sub>O FOREIGN BROADENING

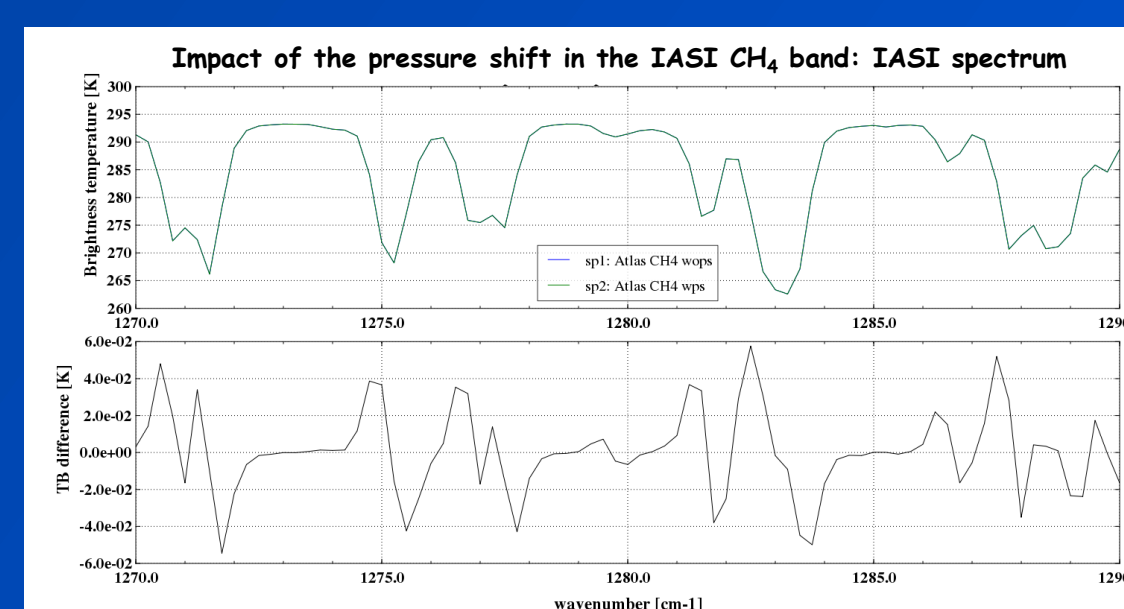
- ✓ Very important impact on the spectra regarding the high requirements on the CO<sub>2</sub> mission
- ✓ Complex to directly include in the atlas: fixed profile of H<sub>2</sub>O and no linear dependence with H<sub>2</sub>O profile
- ✓ Approximation that allows the calculation in 4A: take into account the H<sub>2</sub>O user profile
- ✓ "Effective broadening pressure approximation": determination of an effective pressure (P<sub>EFF</sub>) depending on the H<sub>2</sub>O content (X<sub>H2O</sub>): P<sub>EFF</sub> = P(1+0.835 X<sub>H2O</sub>) with P = the real pressure
- ✓ Get the CO<sub>2</sub> optical thickness at P<sub>EFF</sub> in the Atlases
- ✓ Impact of this approximation compared to the exact formulation (Sung *et al.*, 2009): example in the UVNS bands (see figure): relative error of 5/10000 : 2<sup>nd</sup> order
- ✓ Approximation developed and validated for the SWIR spectral domain
- ✓ Need consolidation in the TIR region: work in progress

#### "Effective broadening pressure approximation" at 1.6 μm: comparison with the Sung *et al.*, 2009, exact formulation



### Pressure Shift

- ✓ Take into account of the PS for H<sub>2</sub>O, CO<sub>2</sub>, N<sub>2</sub>O and CH<sub>4</sub>: included in the Atlases
- ✓ Spectroscopic coefficients from GEISA are used



## Solar Band Application (1)

### Polarization study from IASI-NG measurements

#### OBJECTIVES

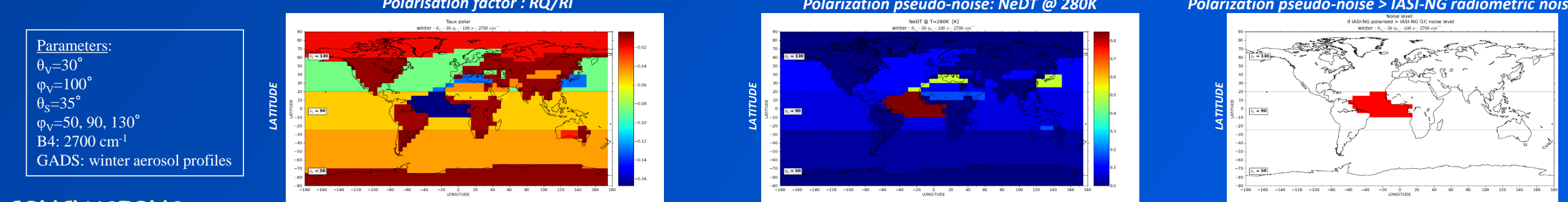
- ✓ Analysis of atmospheric polarization signal at high spectral resolution of IASI-NG measurements (Thermal infrared domain) from 4A/OP simulated IASI-NG polarized spectra based on a climatological aerosol distribution (GADS database)
- ✓ Establish recommendations for the IASI-NG instrument design

#### METHOD

- ✓ Qualitative sensitivity analysis : definition of typical and extreme observation cases
- ✓ Statistical analysis : definition of an ensemble of typical IASI-NG atmospheric scenes based on realistic aerosol distributions set-up using GADS
- 696 surface/atmospheric scenarios
- ✓ Calculation of the 2 polarization components (I, Q) and the polarization rate (Q/I) using 4A/OP + VLIDORT
- ✓ Radiometric analysis : definition of an "equivalent polarization pseudo-noise" due to atmospheric polarization : NeDT = ΔL / (ΔL/ΔT)<sub>TREF</sub> with ΔL = √[RI - (RI<sup>2</sup>+RQ<sup>2</sup>)]
- comparison to the IASI-NG radiometric noise specifications: definition of a flag → UPPER or LOWER the IASI-NG radiometric noise

#### RESULTS

- ✓ 99.5% of the scenarios are lower than the IASI-NG radiometric noise specification
- ✓ 3 scenarios over 174 in IASI-NG spectral band B4 show a "polarization pseudo-noise" greater than the IASI-NG radiometric noise: illumination and observation geometries are close to an aerosol backscattering situation (characterized by θ<sub>v</sub>=30° and 45°, φ<sub>v</sub>=100°, aerosol profile includes MITR)
- ✓ 4% of the scenarios in spectral band B4 have a relative error < 50%



#### CONCLUSIONS

- ✓ From a climatological point of view, IASI-NG is mostly not affected by aerosol polarization
- ✓ Critical geometrical/geophysical parameters : anti-solar direction, backscattering situation, mineral transported aerosol
- ✓ Future work : Extension of the geophysical scenarios to cirrus clouds and polarizing surfaces (BPDF)

### Distinguishing HDO from its H<sub>2</sub>O main isotope in the 4A/OP radiative transfer modelling from the GEISA-2015 spectroscopic database

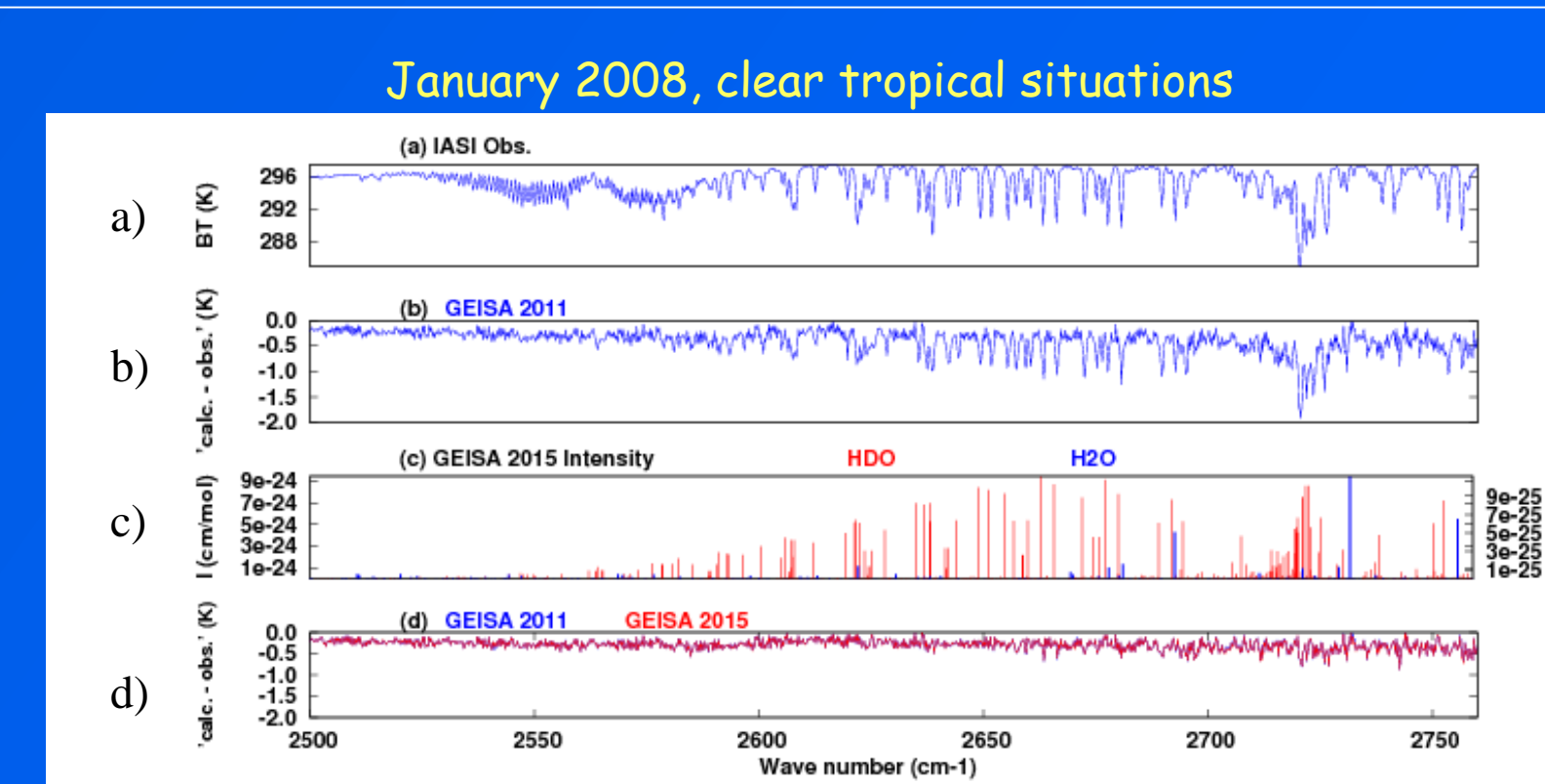
- ✓ Statement: Important biases observed (figure b) in the "calc-obs" chain developed at LMD in the region 2500-2760 cm<sup>-1</sup> which have been attributed to HDO lines (figure c).

- ✓ Introduction of HDO as an independent molecule in the radiative transfer modelling of 4A/OP from data in GEISA database in order to possibly use different concentration profiles for H<sub>2</sub>O and HDO

- ✓ Validation made at LMD: "calc-obs" considerably improved (figure d)

#### "calc-obs" between 4A/OP and IASI observation time and space collocated with radiosoundings from the ARSA database

- a) IASI observation
- b) « calc-obs » with the same concentration profile for H<sub>2</sub>O and HDO
- c) H<sub>2</sub>O and HDO line intensities



- More details in Armante *et al.* (2016, submitted) at Special Issue of J. Mos. Spectr. on « Spectroscopic databases »

## Solar Band Application (2)

### The BRDF effect in the IASI solar band B3

#### Statement:

GSICS, 2013: the calibration error between GOES-14 and IASI in the band 3 where the solar influence is not negligible is probably due to the BRDF effect (X. Wu *et al.*, 2009)

#### Objectives:

Show how to improve the simulations in the MWIR by taking into account the directional effect of the incident solar radiation reflection at the surface considering a BRDF

#### Method:

- ✓ Implementation of a BRDF model in the 4A/OP software
- ✓ Cox and Munk model: glitter simulation
- ✓ Comparison between the simulation and the observation

#### Preliminary results:

- ✓ Qualitative validation: simulation of a IASI orbit and comparison to the measurements on some spectra (approximation of the atmosphere and surface states by considering standard values)
- ✓ Improvements of ≈20K of the difference Simulation-Measurement

#### Future:

- ✓ Quantitative validation by the "calc-obs" at the LMD
- ✓ Official implementation in the 4A/OP software

## References

- [1] Scott, N.A. and A. Chedin, 1981: A fast line-by-line method for atmospheric absorption computations: The Automatized Atmospheric Absorption Atlas. J. Appl. Meteor., 20,802-812.
- [2] Scott, N.A., 1974: A direct method of computation of transmission function of an inhomogeneous gaseous medium: description of the method and influence of various factors. J. Quant. Spectrosc. Radiat. Transfer, 14, 691-707.
- [3] Jacquinet-Husson, N. et al., 2011: The 2009 edition of the GEISA spectroscopic database. J. Quant. Spectrosc. Radiat. Transfer, 112, 2395-2445.
- [4] L. Chaumat, C. Standfuss, B. Tournier, E. Bernard, R. Armante and N.A. Scott, 2012: 4A/OP Reference Documentation, NOV-3049-NT-1178-v4.3, NOVELTIS, LMD/CNRS, CNES, 315 pp.
- [5] IASI-NG: sensibilité des spectres atmosphériques à la polarisation TIR: étude 2, Rapport final NOV-FE-0277-NT-001\_version2