Discussion on the spectroscopy

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Spectral bands covered by MTG-IRS

Band	Nominal extent (limits in cm^{-1})	Filter extent (limits in cm^{-1})	Main absorbers	Trace species + *weak contributors*
LWIR	700-1210	600-1300	**CO_2**, **H_2O**, O_3	CCl4,HCFC-22,HNO_3, CFC-12,CFC-11,NH_3,C_2H_4 SF_6,N_2O, HDO,CH_4,PAN + *SO_2, CH_3OH, HCOOH, other COVs…*
MWIR	1600-2175	1500-2250	**H_2O**, CO_2	CO, HNO_3, OCS, N_2O, + *NO_2, NO*

Basic L2 products
CO_2 → T(p)
H_2O → H_2O(p)

Important potential L2 products of MTG-IRS for tropospheric composition/chemistry: O_3, CO, NH_3
→ complement other infrared sounders (IASI, IASI-NG) for diurnal variations at high spatial resolution

Other interesting/important species could be envisioned at Day-2: PAN,SO_2, HNO_3

Consistency with other infrared sounders

- The NWP fast radiative transfer models (RTTOV,…) are generally based on LBLRTM (maintained by AER) and are using the successive versions of HITRAN complemented with dedicated AER spectroscopic data bases

- Several retrieval groups generating L2 products from L1 spectra (EUMETSAT, ULB/LATMOS, RAL, KIT, UniBas, BIRA-IASB, ACE-FTS, …) often use HITRAN as input of their forward radiative transfer model (LBLRTM, Atmosphit, FORLI, KOPRA, σ-IASI, ASIMUT, MUSICA, LARA, …)
  → last update HITRAN 2018

- GEISA and 4AOP are used by CNES for IASI and IASI-NG

Line-by-line parameters (1/2)

Line-by-line spectroscopic databases (for well identified lines, i.e. the ones confirmed by theoretical calculations and not just empirically measured/observed) are providing for a given molecular species and isotopologue (for example imol=1 for H_2O, with three isotopes of interest for the Earth's atmosphere i.e. iso=1 for $H_2{}^{18}O$, iso=2 for $H_2{}^{18}O$, iso=3 for $H_2{}^{17}O$ and iso=4 for HDO or imol=2 for CO_2, with 6 isotopic variants relevant for the Earth' atmosphere) the following spectroscopic parameters:

- Line position (at zero pressure) in cm^{-1}
- Line intensity $S(T_{ref})$ at T_{ref}=296 K in $cm^{-1}/(molecule\ cm^{-2})$
- Lower state energy E" in cm^{-1}
- Air-broadening coefficient $\gamma_{air}(T_{ref})$ in cm^{-1}/atm
- Exponent n_{air} of its temperature dependence $\gamma_{air}(T) = \gamma_{air}(T_{ref})(T_{ref}/T)^{nair}$
- Air-shifting coefficient $\delta_{air}(T_{ref})$ in cm^{-1}/atm (+ T dependence exponent)

For H_2O (a special case because of high tropospheric abundance in the lower layers)

- Self-broadening coefficient $\gamma_{H2O-H2O}(T_{ref})$ in cm^{-1}/atm
- Exponent n_{H2O} of its temperature dependence $\gamma_{H2O-H2O}(T) = \gamma_{H2O-H2O}(T_{ref})(T_{ref}/T)^{nH2O}$
- Self-shifting coefficient $\delta_{H2O-H2O}(T_{ref})$ in cm^{-1}/atm (+ T dependence exponent)

Line-by-line parameters (2/2)

Additional information is including:

- Quantum assignments (confirmed by analysis and theoretical modelling of laboratory spectra) including the symmetry of the upper and lower ro-vibrational levels involved in the transition
- Nuclear spin statistical weights (needed in the line mixing formalisms or for non-LTE)
- Quality indicators of the different line-by-line spectroscopic parameters
- Reference codes for the origin of these parameters
- Line-mixing (LM) indicator linking to another sub-table (when LM is important i.e CO_2)

As an example the current version of σ-IASI (UniBas) is using LBLRTM 12.1 combined with HITRAN2012 + AER v_3.2

C. Camy-Peyret, G. Liuzzi, G. Masiello, C. Serio, S. Venafra, S.A. Montzka (2017), Assessment of IASI capability for retrieving carbonyl sulphide (OCS). Journal of Quantitative Spectroscopy and Radiative Transfer 201, 197-208

Cross-sections

For the so-called "heavy molecules" for which a line-by-line description of their spectrum is not available (by theoretical calculations) or not feasible (by nature or because the number of lines is too large), the approach is to empirically measure the spectra of the absorbing species (pure and in mixture with air) at different temperature, pressure (and sometimes lengths for checking purposes).
One get then look-up-tables (LUT) providing the cross-section $\sigma(p_{air},T,wn)$ in unit of cm^2/molecule

p_{air} = air pressure (in atm or hPa) having a broadening effect on the spectral features (Q branches in particular)
T = temperature (in K)
wn = wavenumber (in cm^{-1})

Species relevant to IRS are HCFC-22 (821 cm^{-1}), CFC-11 (~850 cm^{-1}), CFC-12 (~922 cm^{-1}, ~1160 cm^{-1}), SF_6 (948 cm^{-1}), CCl_4 (~792 cm^{-1})

The corresponding data is available as a supplement to the successive HITRAN versions. New laboratory measurements by J.J. Harrison (Univ. Leicester)

A difficulty is usually the "purely experimental" data: what to do with the noise and/or negative transmittance?
Another one is the interpolation needed in p_{air} and T and the insufficient coverage

H_2O continuum

This is a very important issue for IRS (and for other TIR sounders like IASI, CrIS, AIRS, …).
The question is related to the description of the wings of H_2O lines: how far should one use the Voigt lineshape (or new line shape models) for individual water lines? What is the contribution of the far-wings when the standard line profile is cut at 25 cm^{-1} (the usual assumption). The remaining contribution is assigned to the "water vapour continuum". The "reference" model (almost used by everyone, but based on empirical measurements including satellite data) is MT-CKD v_2.5.2.

The absortion coefficient can be written in terms of a cross-section (in cm^2/molecule) as:

$\sigma_{H2O\text{-}continuum}(p_{air},p_{H2O},T,wn)$

p_{air} = air pressure (in atm or hPa)
p_{H2O}= water vapour partial pressure (in atm or hPa)
T = temperature (in K)
wn = wavenumber (in cm^{-1})

Distinction between foreign continuum and sef continuum → difference between tropics and poles

Very important topic of consistency beteween line parameters (Voigt + new line shape) and continuum parameters → the two sets of parameters have to consistently reproduce the existing experimental data (temperature and humidity dependence) on the continuum and the experimental/theoretical data on individual lines

A new H_2O line profile

- A new H_2O line profile is variously described as the partially-Correlated quadratic-Speed-Dependent Hard-Collision Profile (pCqSDHCP) or the partially-Correlated quadratic-Speed-Dependent Nelkin–Ghatak Profile (pCqSDNGP). This profile, and its computational implementation, is called the Hartmann–Tran profile (HTP)
- More work is needed to combine this new line profile with the existing experimental data on the water vapour continuum and the existing MT-CKD parameterization, to produce a new consistent representation of the contribution of the line core and near-wing (LBL) and of the continuum (cross-section)
- Is the ±25 cm^{-1} limit still a good choice? Is it valid everywhere and/or for every line?
- Is the HTP model valid over the full electromagnetic spectrum from the MW/sub-mm, FIR, LWIR, SWIR, VIS?

Outlook (1/2)

- Infrared spectroscopy, in the sense of availability of accurate and extensive spectroscopic data bases is a major input for all radiative transfer models, hence for all infrared sounders → need for coordinated efforts
- IRS is on the same footing as IASI, IASI-NG, CrIS, … and for consistency reasons within Europe (including ECMWF and EUMETSAT) one should try to use consistently similar/identical spectroscopic data bases
- HITRAN is well maintained and is benefiting from support within the USA for improving the laboratory and theoretical spectroscopic work for infrared remote sensing
- However, a recent focus has been on the SWIR region (OCO-2, GOSAT, S5P) rather than on the TIR
- Some support has been provided by ESA through ITTs on dedicated spectroscopic studies for S5P (SWIR)
- A new ITT has been launched by ESA for TIR studies (TIR/SWIR synergy)

Outlook (2/2)

- What could be the support of EUMETSAT for joint efforts on new and needed spectroscopic work related to IRS (and IASI/IASI-NG)?
- Certainly more work on the spectroscopy of H_2O (broadening coefficients and their temperature dependence, line shape, continuum)
- Is the new Hartmann and Tran line shape appropriate for both the core and the far wings i.e. for a consistent model of the H_2O lines and the continuum?
- Approach to identify where new spectroscopic effort is needed:
  - Examine spectral residuals (and ensemble means) after OEM retrievals $\rightarrow$ identify which species is responsible and which parameter to update/improve
  - Do this both for satellite spectra and for higher resolution spectra recored from the ground in solar absorption by FTS within the NDACC stations $\rightarrow$ example of the work on H_2O line intensity/width/shape by M. Schneider et al. from the Izana station