Use of Spectral Information at Microwave Region for Numerical Weather Prediction

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Executive summary

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In the context of satellite remote sensing, “hyper-spectral” is a generic term that means that “many channels” are observed. For InfraRed (IR) instruments, this term is associated with thousands channels, but for the MicroWave (MW) domain, an instrument with hundred of channels is already considered to be hyper-spectral. There are two main alternative concepts in using hyper-spectral information in MW:

1. Hyper-spectral observations can consist in observing given absorption bands with a very high spectral resolution. The current operational MW instruments only provide observations in a few channels in each absorption band, and a continuous sampling within those bands with much finer spectral resolution deserves investigation. Following the ESA instructions, it is this concept that has been examined here.
2. Hyper-spectral observations can also be interpreted as a continuous sweep of a large frequency domain. In the MW, it could mean systematic observations from 20 to 800 GHz, with a spectral resolution of the order of 1 GHz. This option has not been considered in this study, following the ESA instructions. However, its interest for the scientific community will be discussed in the perspectives section.

This study investigated the benefits of a satellite HYper-spectral Microwave Sensor (HYMS) for the retrieval of atmospheric temperature, humidity and hydrometeor profiles, in the context of Numerical Weather Prediction (NWP), for the troposphere and the lower stratosphere. Both clear and cloudy conditions have been considered. We focused on the potential of the high spectral resolution in the O_2 and H_2O absorption bands between 20 and 800 GHz.

First, it is important to note that despite their lower data volume, assimilation of MW satellite observations in NWP systems are as beneficial (and even more) than the assimilation of the IR satellite observations. In addition, even under clear sky conditions with instruments such as IASI and MHS, it has been shown that it is possible to exploit the synergy between IR and MW observations (Aires et al. 2011, 2012). With a better MW instrument (HYMS concept), the synergy would even be better. Furthermore, IR is much more sensitive to the presence of clouds. This means that an atmospheric situation considered to be cloudy for the IR could still be treated as clear for the MW. Since cloudy cases are much more difficult to deal with than clear-sky cases, the use of MW observations would be a strong advantage to NWP centres.

Methodology

In agreement with the NWP practices, we used in this study the traditional Information Content Analysis (ICA) to measure the impact of the MW hyper-spectral observations. This technique requires various components that need to be as realistic as possible:

(1) A large and diverse set of atmospheric situations needs to be gathered. It should be representative of the possible cases encountered in nature. This is easier for the clear-sky case where the community has already invested time in the elaboration of such database. It is more complex for cloudy conditions (hypothesis for hydrometeors, multiple parameters that need to be described such as liquid, ice, snow and rain contents, each one being linked to the others). Two databases have been constructed for this study, one for the clear-sky case, the other one for the cloudy-sky case.

(2) Another very important element of this ICA is the background (*a priori*) information. In the NWP context, this background information represents the model forecast and the

satellite observations are added in the assimilation scheme to correct this forecast. We used state-of-the-art background information from the ECMWF NWP centre for the clear-sky case. For the cloudy case, background information has been provided from ECMWF, but it was rapidly judged not realistic and unusable. We had to develop an innovative model (Gaussian background errors with correlations among the vertical layers).

(3) Realistic instrument noise has to be estimated. An extensive work as been done to define it, based on instrument expertise.

(4) The selected Radiative Transfer (RT) model is the Atmospheric Radiative Transfer Simulator (ARTS) (Eriksson et al., 2011). This code had to be optimized for the instrumental configuration considered in this study. The cloudy cases represented a very high computational burden (several months on large computing facilities).

(5) The RT error is a key element in the ICA analysis and it dominates the error budget, especially under cloudy conditions. A model to estimate these RT errors has been developed for this study.

These 5 elements of the ICA are essential. The results of the ICA are highly dependent on the assumptions. In this study, special emphasis has been put on the realism of the different hypothesis. We cannot stress enough that the information carried by hyper-spectral MW observation can highly be overestimated if the chosen assumptions are too simplistic.

Results of the study

Clear-sky conditions

An information content analysis has been conducted to assess the impact of hyper-spectral microwave measurements in the absorption bands, on the retrieval of temperature (T) and water vapour (q) profiles under clear-sky conditions. As already mentioned, it uses RT simulations over a large variety of atmospheric situations. It accounts for realistic noise and background information assumptions, compatible with NWP practices. The additional information provided by a HYMS instrument on temperature and water vapour retrievals has been clearly demonstrated. Three aspects have been examined:

1. *Comparison of the current and planed instruments with an instrument with an increased number of spectral channels in oxygen and water vapour absorption lines in the MW*: The estimated retrieval performances of the hyper-spectral instrument are compared with those of the MW instruments to be on board the future generation of European operational meteorological satellites (MetOp-SG). The results confirm the positive impact of a hyper-spectral instrument on the atmospheric profiling capabilities compared to MetOp-SG (Aires et al. 2015, Mahfouf et al. 2015), see Fig. 1. The reduction in retrieval uncertainty, compared to background information, goes from 2 to 10 %, depending on the atmospheric layers, and is more than twice what will be obtained with MetOp-SG. Improvements compared to background for humidity sounding can reach 30 %, a significant benefit as compared to MetOp-SG results, especially up to 250 hPa. Therefore, there is a clear benefit, in terms of information content, in having more channels in the 55 GHz O_2 and 183 GHz H_2O absorption lines with respect to current and future instruments.

2. *Evaluation of the interest of a very high spectral resolution in the oxygen and water vapour absorption lines in the MW*: The study of Aires et al. (2015a) has also revealed that there is no clear benefit in increasing the number of channels from hundred to

thousands with narrower bandwidths in individual spectral lines, except for the temperature in the 55 GHz band for the high atmosphere (Fig. 1). This is due to the corresponding increase in radiometric noise and also to the less complex shapes of absorption lines in the other bands of the microwave spectrum, especially when compared to the infrared spectrum. For temperature estimation at high altitudes, very high spectral resolution (10 MHz) in the 55 GHz would increase the retrieval accuracy. However, note that this study focussed on the troposphere and the lower stratosphere and that the Zeeman effect has not been simulated: as a consequence, definitive conclusions cannot be drawn for the temperature profiling at high altitudes.

3. *Evaluation of the interest of additional channels at higher frequencies (above 60 GHz for the O_2 bands and above 200 GHz for the H_2O bands)*: It has also been shown that the impact for temperature and humidity retrieval is less significant when adding new channels at higher frequencies compared to the 55 and 183 GHz regions. However, if possible, these other bands can be independent measurements (compared to the 55 and 183 GHz bands) and this can help limit the negative effects of the instrumental and RT errors, reducing the retrieval uncertainties.

The results are not very sensitive to the instrument noise, under our assumptions. The results are presented over ocean at nadir, but similar conclusions have been obtained for other incidence angles and over land.

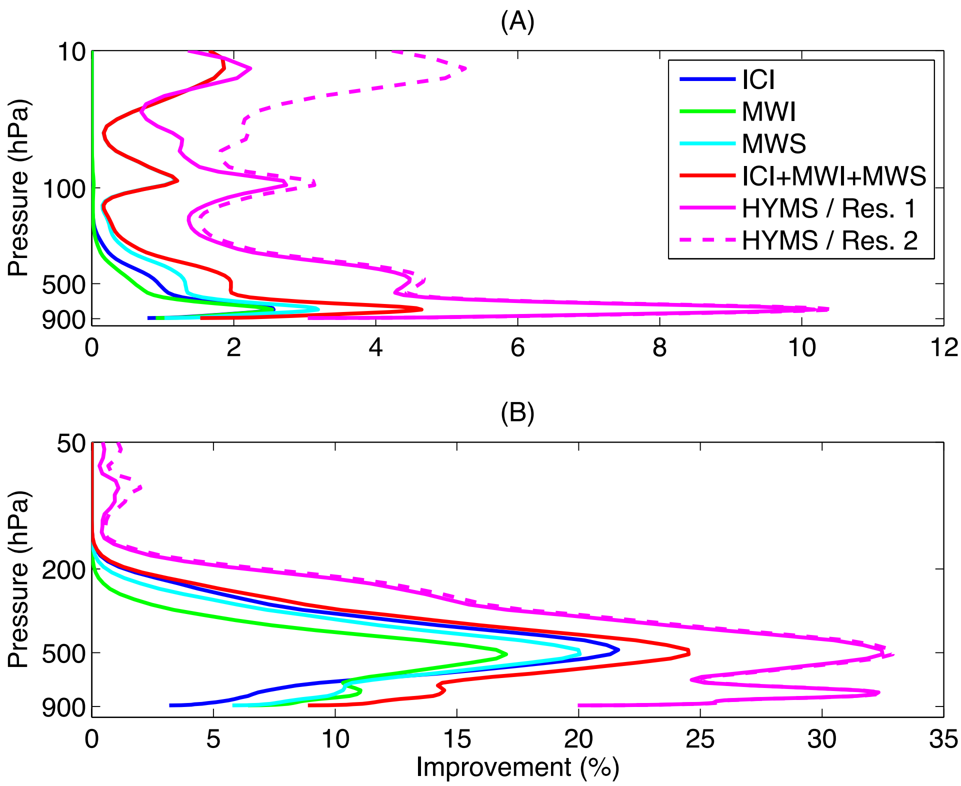

Figure 1: Estimation of the retrieval statistics in terms of relative improvement in % as compared to the *a priori*. Statistics are provided for temperature (top) and humidity (bottom), for the HYMS instrument with spectral resolution 1 (spectral resolution of 100 MHz for T and 400 MHz for q, solid line) and 2 (spectral resolution of 10 MHz for T and 40 MHz for q, dashed line) as well as for the MetOp-SG microwave instruments, separately and jointly.

Cloudy-sky conditions

A similar analysis has been conducted under cloudy-sky conditions. RT calculations have been performed over a variety of cloudy and precipitating situations. A representative database of cloudy atmospheric profiles is selected. Associated background error covariance matrices have been modelled. RT simulations have been performed on this dataset (the radiances as well as the Jacobians), with careful selection of the hydrometeor hypotheses. Note that the results provided in this study are very dependent upon the hypothesis on the hydrometeor optical properties. These properties have been selected as closely as possible to what is adopted at ECMWF so far (Geers and Baordo, 2014). Different assumptions have been tested for the estimation of the instrument and RT noises. An Information Content Analysis has allowed drawing the following conclusions:

1. The impact of the hyper-spectral observations on the retrieval of the temperature (T) and humidity (q) profiles under cloudy conditions is first investigated. Again, the interest for a hyper-spectral microwave instrument is shown when compared to MetOp-SG MW suite (Fig. 2). The benefits are more important at higher atmospheric levels, particularly over the clouds. Impact is important for T compared to MetOp-SG, and significant for q above 500 hPa.

2. Going from a few hundred to a few thousand channels (HYMS spectral resolution increased by a factor 10) has only a limited impact. The information content on T and q would not be significantly higher when increasing the number of channels in the O_2 and H_2O absorption lines, except above the clouds (Fig. 2), in agreement with the clear-sky case.

3. The addition of the 118, 183, 325, 420 and 448 GHz bands provides a good improvement compared to the use of hyper-spectral only at 60 GHz band, even for the T retrieval (Fig. 3).

4. The ICAs was performed as well on the Cloud Liquid Water (CLW), Cloud Ice Water (CIW), Rain Water Content (RWC) and Snow Water Content (SWC). Results confirmed that the future microwave instruments (MWS, MWI, ICI) on board MetOp-SG will bring information on CLW, RWC, and SWC with respect to the background information (more than 10 % improvement). However, the HYMS instrument does not bring any additional information compared to the instruments planned on MetOp-SG in terms of hydrometeor profiling, with our hypotheses on hydrometeor parameters.

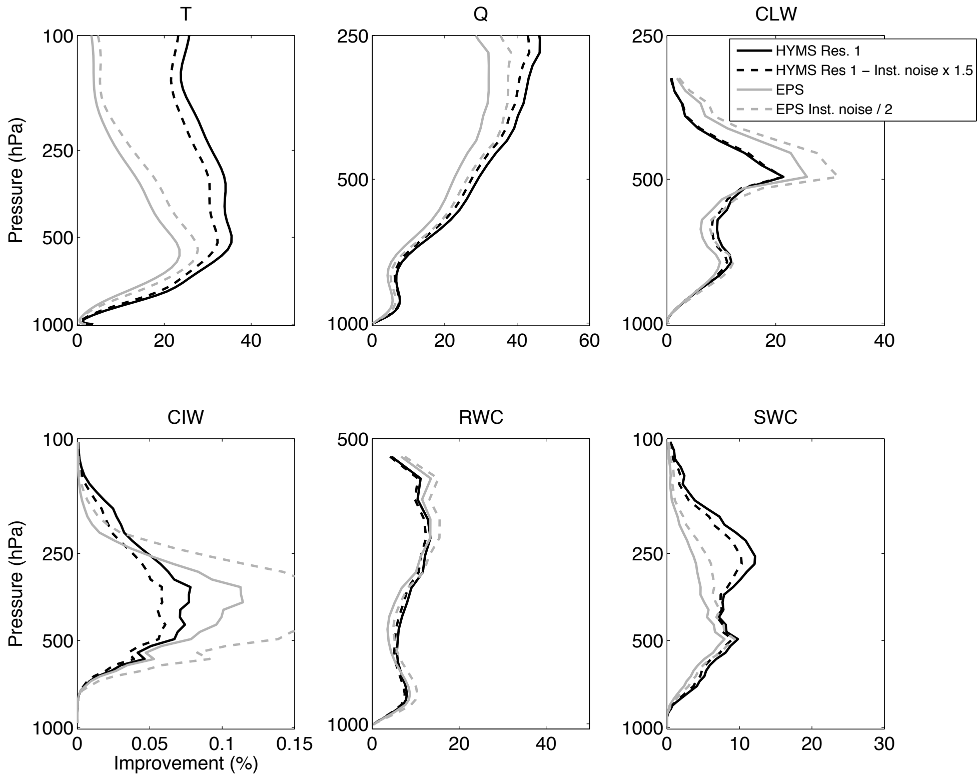

Figure 2: Improvement of the performance compared to the background, for the retrieval of T, q, Cloud Liquid Water, Cloud Ice Water, Rain Water Content, and Snow Water Content, from top to bottom and from left to right. Results are presented for HYMS with the initial noise, for HYMS with a 50% noise increase, and for MetOp-SG microwave suite (MWS, MWI, and ICI) with currently planed and divided-by-two noise levels.

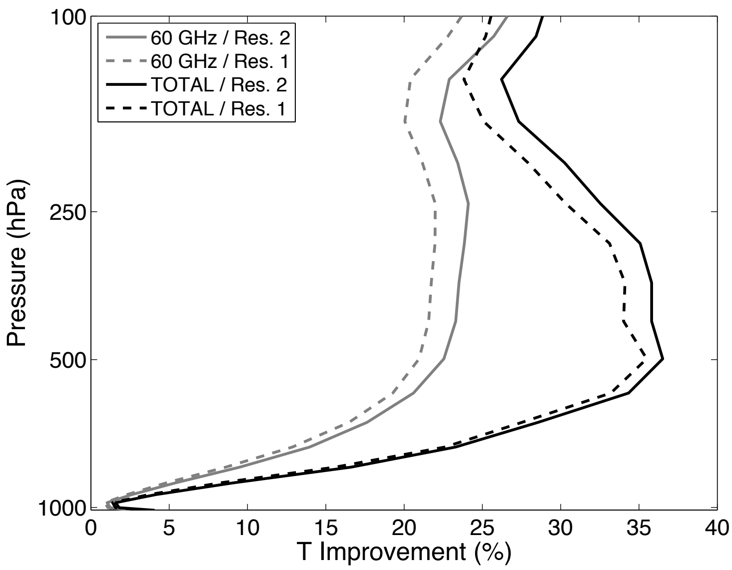

Figure 3: Improvement of the T retrieval, for the HYMS instrument, at high spectral resolution (100 MHz - dashed line) and very high (10 MHz – continuous line) spectral resolutions, for the 60 GHz band only, or the all bands together (60, 118, 183, 325, 420, 448 GHz).

Regarding cloudy and rainy atmospheres, it is important to stress that the assimilation of cloudy and rainy radiances is still a research area in current NWP centres, and that it is only at ECMWF that satellite radiances are assimilated operationally under such conditions.

Conclusion on a hyper-spectral instrument in absorption band as compared to MetOp-SG

The overall conclusion of this study is that a hyper-spectral instrument would be an improvement over the MetOp-SG suite for the retrieval of both T and q atmospheric profiles, under clear and cloudy conditions. A very high spectral resolution would benefit the T retrieval only for the 60 GHz band and on the upper layers of the atmosphere. The 60 GHz is the only band with complex absorption structures in the MW spectrum where reducing channel bandwidth slightly reduces the vertical spread of channel Jacobians, and therefore increases vertical resolution and reduces retrieval errors.

Frequency band priority

Our analysis confirms that hyper-spectral observations are first interesting in the O_2 spectral band at 60 GHz. This is a complex band of spin-rotation lines with fine structures that can only be captured with high spectral resolution. The current instruments already partly explore this fine structure with the help of channels with optimized double and quadruple structures. The MWS instrument on board MetOp-SG will include additional channels for a better exploration of this structure, as suggested by Sreerekha et al. (2007). However, we showed here that hyper-spectral exploration every 100 MHz in the O_2 band provides an improvement over the MetOp-SG suite (Aires et al. 2015, Mahfouf 2015).

The H_2O line at 183 GHz holds key information about the water vapour profile in the atmosphere, but is also very sensitive to the temperature in the lower atmospheric layers. This is obviously related to its water vapour sensitivity and the relationship between the water vapour emission and the temperature. In classic information content analysis, the sensitivity of the water vapour line to the temperature is commonly bypassed, because of its excessively high sensitivity to water vapour. However, in assimilation / retrieval that simultaneously estimates water and temperature, the use of hyper-spectral information at 183 GHz is efficient, for both water vapour and temperature profiling.

Hyper-spectral information in the other spectral bands has less interest. Compared to the 60 GHz band, the simple structure of the 118 GHz O_2 line does not justify hyper-spectral observations. The O_2 and H_2O isolated lines above 200 GHz do not deserve hyper-spectral observations either for temperature and water vapour profiling, as they add limited information as compared to the information already provided by the lower frequencies and because of their high sensitivity to the presence of clouds. This has been confirmed by the ICA. For cloud characterization and profiling, the hyper-spectral information in the absorption band has been shown to bring very limited additional information and thus the hyper spectral information in the high frequencies cannot help, despite their high sensitivity to the clouds.

Possible compression of data volume

Hyper-spectral measurements at higher frequencies bring T and q information with independent RT and instrumental errors, and this can be exploited by the retrieval (see Fig. 3). However, using hundred or even thousands of channels in the 60, 118, 183, 325, 420 and 448 GHz will introduce a volume of data that is extremely costly for the transmission, storage or retrieval. Nevertheless, it would be possible to optimize their use through data reduction techniques (compression or channel selection, as in the infrared community). For instance, the information carried by 276 channels in our HYMS instrument can be reproduced using only about 100 channels (Mahfouf et al. 2015) when considering the retrieval of T and q profiles under clear-sky case. An even better compression rate could be expected if about 2500 channels were originally measured (i.e. higher spectral resolution in our experiments). In (Aires et al. 2015b, Pellet et al. 2015), this result was confirmed and an innovative data dimension tool was introduced, the Bottleneck Channel. It is a compromise between the compression techniques that reduce the observation noise in data, and the channel selection techniques that preserve the physical meaning of the measurements. This type of technique would make possible the use of an HYMS instrument.

Spectral and radiometric requirements for a HYMS instrument

The suggested instrument characteristics for hyper-spectral observations in the 60 GHz O_2 band and in the 183 GHz H_2O line are summarized in Table 1. They satisfy the conditions derived from both clear-sky and cloudy-sky information content analysis. For the 60 GHz O_2 band, hyper-spectral observations from 52.600 to 57.300 GHz and from 63.300 to 67.900 GHz are suggested, with a spectral resolution of 100 MHz. Note that parts of the spectrum from 55.780 to 57.300 GHz and from 65.000 to 66.000 GHz are not protected. It is shared with fixed services, with threshold defined. For potential aircraft operation of a hyper-spectral demonstrator, this can be problematic and will have to be accounted for. Urban areas might have to be avoided in order to prevent serious Radio Frequency Interferences (RFI). For the H_2O 183 GHz line, the frequency domain between 173.300 to 193.300 GHz could be explored, with a spectral resolution of 400 MHz. For an aircraft demonstrator, the instrument incidence angle, polarization, and spatial resolution will be selected as close as possible to other potential microwave instruments on the platform, for optimal comparison.

Tableau 1: Specification of a hyper-spectral instrument HYMS in the O_2 band around 60 GHz, and in the H_2O 183 GHz line.

Spectral band	Frequency coverage (GHz)	Bandwidth per channel (MHz)	NeDT (K)
O_2 around 60 GHz	from 52.600 to 57.300 GHz and from 63.300 to 67.900 GHz	100	0.4
H_2O at 183 GHz	from 173.300 to 193.300 GHz	400	0.4

Perspectives

Methodological improvements

In this project, various methodological difficulties have been faced, particularly for the cloudy case. These aspects should be considered carefully for future analyses, not only for the hyper-spectral, but for the optimization of next generations of satellite instruments in general:

1. It is important to have a large and representative dataset of atmospheric situations for such analysis. The ECMWF dataset used for the clear-sky case is the standard in the NWP community, but it is biased towards polar situations, located over elevated surfaces. A better sampling procedure to build such a dataset should be considered in the future (e.g. Paul and Aires, 2014). Furthermore, the cloudy dataset including 25 atmospheric atmospheres is not enough to consider all the variability, and complex links between all the hydrometeor parameters.
2. Information content analysis is based on simple hypotheses (i.e., Gaussian character of random variables or linearization of the RT). Retrieval tests could provide a better

picture of what can be accomplished with the MW hyper-spectral observations. For such retrieval tests, again, a large and representative dataset of atmospheric situations would be required.

3. A fast RT model is essential to provide the radiances corresponding to the atmospheric situations. The computational time has been a strong limitation in this study. A line-by-line model could be used to calibrate a fast RT model (this is the strategy of RTTOV). Such a RT model would allow even more ambitious studies, including realistic retrieval tests. A difficulty comes from the fact that RT simulations for cloud properties are based on hydrometeor assumptions which are not yet well mastered.

4. The Zeeman effect was not included in our radiative transfer simulations. There has been some recent work to add this effect in the community models, but more efforts have to be conducted for its accurate simulation and for its evaluation.

5. Results of the information content analysis are very much dependent on the underlying assumptions (either for information content or retrieval). For instance, the RT errors are a very important piece of information. No RT code today provides uncertainty estimates. In our study, the RT noise has been modelled but feedbacks from the NWP community should be gathered to obtain an agreement for a standard procedure. The estimation of the background information uncertainty is more mature, under clear sky conditions. NWP centres have been working on the clear sky case for decades, but the cloudy case is not satisfactory yet and strong efforts should be dedicated towards a solution. Again, a procedure has been suggested in this study to obtain a reasonable background uncertainty characterization, but the community should converge to a standard procedure. The correlation on background uncertainty between the geophysical variables is rarely considered even under clear sky conditions (e.g. link between temperature and water vapour). It would be even more important to consider the link between the hydrometeor properties but, again, this is impossible without a very large dataset of cloudy situations.

6. If an innovative instrument for operation on board an aircraft is scheduled, it is essential at the same time, to develop further the information content and retrieval methodologies presented in this study. Forward RT simulations compared to airborne measurements will not be enough to assess the ability of hyper-spectral observations to retrieve atmospheric variables under clear and cloudy conditions. These observations are indeed sensitive to atmospheric variables (temperature, humidity or hydrometeor properties) but only realistic retrieval tests can quantify their ability for retrievals, not forward RT simulations.

It is extremely easy to over-estimate the quality of the retrieval results if the above-mentioned points are not carefully considered. For instance, we showed that when performing independently the retrieval of the cloudy profiles, results are much better than when considering the contamination effects and ambiguities related to more realistic conditions where all cloudy variables are retrieved simultaneously. As a consequence, we cannot stress enough the need to develop new and more sophisticated methodological approaches for forthcoming studies of this nature.

Other applications of the hyper-spectral MW observations in absorption bands

The following applications of the hyper-spectral information in the microwave have not been explored during this study but are also directly relevant for NWP applications.

***Mitigation of RFI*:** Mitigation of the RFI has not been analysed here, but this is also of key interest for the use of hyper-spectral instrument in the future. The International Telecommunication Union regulates the use of the MW frequencies. Passive MW observations should be limited to protected bands, but RFI can occur despite the regulations. There are two main types of RFI: pulsed, wide bandwidth signals and continuous narrow band signals. The first type of RFI can be detected by analysing the measured signal in the time-domain, and by searching for energy outliers; while the second RFI type can be detected by inspecting the signal in the frequency-domain and searching for anomalies in the spectrum. RFI detection and mitigation algorithms rely on some common features of anthropogenic signal that make them distinguishable from natural emission. These features include differences in the spectral shape and in polarization, and directional anisotropy. High spectral resolution can be very beneficial in detecting and mitigating narrow band RFI using spectral algorithms. The availability of multiple correlated channels allows the rejection of individual contaminated channels without suffering significant information content loss. This is vey important as more and more emitters up to 100 GHz are emerging with W-Band links envisioned for Low Earth Orbits (Dainelli et al., 2005) with ground-based and satellite instruments already suffering from contamination. Regarding pulsed RFI signals, the availability of hyper-spectral information will be of minor interest. For such kind of RFI, the energy peak is shared among a large number of frequencies, affecting to a lesser extent the measured spectrum. Mitigation of pulsed RFI is more effective analysing the signal in the time-domain.

***Improving spectroscopic information*:** There are still uncertainties in the description of the complex 50-60 GHz O_2 band despite the intensive use of this spectral band by the NWP community. The line width, the temperature dependence of the line width, and the line coupling parameters are still debated (e.g., Tretyako et al., 2005; Payne et al., 2011), with impact on the accuracy of the temperature (Caddedu et al., 2007). In addition, questions are also raised about spectroscopic information in the 183 GHz H_2O line (e.g., Payne et al., 2011). Systematic differences were noted between observations and simulations, with increasing amplitude further from the line centre (Clain et al., 2014). Uncertainties could be related to line width and strength as well as to the parameterization of the continuum absorption. High spectral resolution over broad bands can help improve the knowledge of spectroscopic parameters (line width and strength, line coupling) because stronger constraints in inter-comparison studies can be made as shown for IR spectrometers. Better spectroscopic parameters would be very valuable for existing operational NWP models, especially in the 50-60 GHz O_2 band and in the 183 GHz line. Hyper-spectral measurement will also help improve the description of the far wings of the water vapour absorption lines. Discrepancies among different water vapour continuum parameterizations and between models and measurements are still reported for both foreign- and self-broadened water vapour continuum absorptions (e.g., Turner et al., 2009; Payne et al., 2011). Brightness temperature measured at a high spectral resolution over a wide range of temperatures and precipitable water vapour amounts could help validate and improve continuum parameterizations. Furthermore, investigation of signature of other trace gases in the MW spectrum could give information on the total column of the gas or, if its vertical distribution is known, add information to the T profile retrieval.

A hyper-spectral instrument demonstrator on an aircraft?

Digital spectrometers have been developed in Europe under ESA contracts. Operation of an airborne hyper-spectral instrument around the 60 GHz band would make it possible to test the technical concept as well as its scientific potential. Natural aircraft candidates for such an instrument would be the FAAM aircraft of the UK Met Office or the German HALO. This instrument could be for instance mounted in one of the three boxes that have already been certified for flights in the HALO aircraft. Both aircrafts are already equipped with MW instruments and are used by the NWP community. Key campaign programs are underway that would benefit from improved T profiling, especially under cloudy conditions. This is the case for example for the NAWDEX flight campaigns with the objective to better understand and forecast the development of frontal systems (www.wmo.int/pages/prog/arep/wwrp/new/documents/T-NAWDEX.pdf).

Interest of systematic spectral sampling of the microwave domain up to 800 GHz

In this project, the use of hyper-spectral information in specific absorption bands has been investigated. This is technically possible and an aircraft demonstrator could be developed. Systematic exploration of the full microwave to sub-millimeter domain has not been considered in this study. Note that this interpretation of the hyper-spectral concept corresponds better to a IASI-like instrument, where the full infrared spectrum is systematically observed. In the microwave, it could mean systematic observations from 20 to 800 GHz, with a spectral resolution of the order of 1 GHz. The scientific community has already shown its interest for this systematic analysis of the MW spectrum (Boukabara and Garret, 2011), under cloudy sky condition, for temperature, humidity and hydrometeor profiling (performances of an instrument from 1 to 330 GHz with a 100 MHz resolution was studied). Simulations are also underway at the University of Hamburg, to assess the interest of systematic measurements from 150 to 800 GHz every 1 GHz, for cloud profiling. So far, passive MW observations from satellite for meteorological applications are based on receivers at room temperature. At the beginning of this project, a review of the different instrumental solutions had been presented by LERMA, and it included cooled receivers. These solutions were disregarded at this point, as too complex for operational applications. However, they might be worth revisiting, with the recent technological progresses achieved with cooled bolometer-type detectors. With cryogenic Kinetic Inductance Detectors (KIDs), it is now possible to build large arrays of detectors, with high spectral resolution and low noise, with detection time of a few microseconds (communication from P. Hargrave, Cardiff University). These detectors are very flexible in terms of spectral bands and spectral resolution: the full spectrum can be explored or part of it. These new possibilities should be explored in the future.

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