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Evaluation of hyperspectral MW observations for global NWP: Simulation framework consolidation

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Abstract

The advent of space-borne hyperspectral microwave (MW) instruments brings a major change to MW sensor technology that has been relatively stable for many years. The present project develops for the first time the use of hyperspectral MW data in a global Numerical Weather Prediction (NWP) system, and the expected impact will be assessed using the Ensemble of Data Assimilations (EDA) method. This report considers necessary assimilation choices and outlines characteristics of the instrument to be used. One-dimensional information content studies have previously shown that a hyperspectral MW instrument has the potential to exceed the benefit in clear and cloudy temperature and humidity retrievals relative to its traditional counterpart. The wide frequency band and fine spectral sampling result in a diverse vertical sensitivity and exploitation of novel parts of the MW spectrum including the ability to probe narrow features in the oxygen absorption band around 50-60 GHz. To manage the large data volumes in assimilation, forming a channel subset will be required and an approach guided by the current strategy for hyperspectral infrared instruments is proposed. After initial removal of channels e.g. through quality control, channel selection following an information content-based approach may be employed. The Hyperspectral MW Sounder (HyMS) developed by Spire Global Inc. (Spire) and Rutherford Appleton Laboratory Space (RAL Space) will form the basis of the instrument to be evaluated. This covers a temperature (49.42-57.75 GHz) and humidity band (182.31–190.31 GHz) in addition to a window channel at 89 GHz. The fine spectral sampling means that individual channels have relatively high instrument noise, which needs to be compensated for by using a larger number of channels and, in some limited cases, averaging neighbouring frequencies to form a low-noise super channel. Adaptations in the all-sky MW assimilation strategy for HyMS are considered which include restriction of surface-sensitive channels over land/sea-ice and frequency selection for quality control procedures. The all-sky observation error model also requires modification to choose suitable indicators to estimate the presence of cloud and account for inter-channel error correlations.

1 Introduction

Microwave (MW) sounding instruments currently provide the largest benefit to global Numerical Weather Prediction (NWP) in the ECMWF system (Bormann et al., 2019). A valuable capability is the provision of temperature and humidity information in cloudy as well as clear sky situations (Geer et al., 2017). Microwave instruments have a long heritage spanning decades but the underlying technology and number of channels (typically less than 40 different frequencies sampled) has not greatly evolved. Furthermore, the vertical sampling of the atmosphere has also changed little, with a modest and reasonably stable set of relatively broad passband channels sampling an oxygen absorption band 50-60 GHz and a water vapour line around 183.31 GHz.

Recent technological advances have made it feasible to develop space-borne hyperspectral MW instruments, in particular the capability to process an ultra-wide bandwidth at hyperspectral resolution while remaining cost effective and within practical size and power limits (Gambacorta et al., 2023; Kummerow et al., 2022). Additionally, the advent of small satellites provides the opportunity to accelerate the development and demonstration of new hyperspectral MW instruments in space. While the first space-borne platform is yet to be launched, there have been recent demonstrations of the technology on aircraft (Henry et al., 2023; Liu et al., 2025). The Hyperspectral Microwave Sounder (HyMS) instrument developed by Spire Global Inc. (Spire) and Rutherford Appleton Laboratory Space (RAL Space) (Henry et al., 2023) is expected to the be first space-borne hyperspectral MW mission and is currently scheduled for launch towards the end of 2025. Theoretical studies have highlighted the potential benefit of hyperspectral MW measurements over conventional MW sounders, using 1-dimensional information content approaches (e.g. (Aires et al., 2015; Maddy et al., 2024), and these will be further discussed below. However, the expected impact on global NWP has not yet been assessed. Consequently, in this study we aim to evaluate the benefit of a hyperspectral MW sounder to global NWP in order to support refining requirements and future deployment options for the MW sounding constellation.

The evaluation of the benefit of a hyperspectral instrument in NWP will be carried out using the Ensemble of Data Assimilations (EDA) method. Here we build on the experience gained in earlier studies using this technique to assess aspects of the future MW constellation (Lean et al., 2023, 2025). The EDA method uses a Monte Carlo approach to estimate reductions in analysis or forecast uncertainty and can be applied to both simulated and real observations (Lean et al., 2025; Harnisch et al., 2013; Tan et al., 2007). The EDA consists of an ensemble of 4D-Var assimilation systems where the initial conditions (observations, forecast model and sea surface temperature) are perturbed. The reduction in EDA spread – the variation of the members about the ensemble mean – forms the key measure of benefit. In this study, observations from a potential future hyperspectral MW instrument will be simulated and assimilated with EDA experiments. Benefits as measured by EDA spread diagnostics can be put into context by comparing to impacts from existing MW sounders as well as using results from the earlier MW constellation studies.

Reliable impact evaluation in the EDA requires an appropriate strategy to simulate and assimilate the new observations, as well as an adequate representation of expected uncertainties. For hyperspectral MW observations, it is particularly necessary to develop approaches to assimilate the large number of channels available, combined with much larger instrument noise compared to heritage instruments. Hyperspectral infrared (IR) instruments are well established and extremely valuable in the NWP system with a heritage reaching back decades to the Atmospheric Infrared Sounder (AIRS) instruments. Experience can be drawn from the processing techniques both in the reduction of data volume such as channel selection strategies and assimilation. However, there are different strengths between the IR and MW that must be accounted for. In particular, the number of spectral features differs greatly with many more distinct absorption lines available in the IR part of the spectrum but hyperspectral IR instruments are not yet assimilated in an all-sky framework so the ability to probe cloudy conditions with MW observations is an important advantage. In moving to hyperspectral technology, a substantial additional positive impact was achieved for the IR instruments e.g. (Hilton et al., 2009) however the fundamental differences to MW assimilation means that a comparable increase is not guaranteed.

In this first work package report, we focus on a review of the hyperspectral MW technology and propose plans to address challenges in the assimilation approach. Future reporting will detail final assimilation settings and the EDA evaluation. Section 2 provides a brief overview of the MW spectral features and a literature review of the results of studying hyperspectral MW instruments. Section 3 presents key details of the HyMS instrument which forms the basis of the hyperspectral instrument characteristics to be used for evaluation in this study. The techniques for handling the huge array of frequencies and forming a channel subset for assimilation are discussed in section 4 while section 5 outlines plans and highlights challenges for the assimilation strategy. Finally, section 6 provides a summary and discussion of the next steps in this study.

2 Prospects for Hyperspectral MW instruments

To support the launch of future hyperspectral MW instruments, 1-dimensional information content studies have suggested benefit and new insights beyond the capabilities of the current MW constellation. In this section, first the relation of the finer spectral sampling to MW spectral features is briefly discussed, highlighting differences to spectral features sampled by hyperspectral IR instruments. Secondly, some of the key findings are summarised from literature exploring the potential of hyperspectral MW instruments.

2.1 MW spectral features

The region of the spectrum typically covered by IR instruments is very rich in distinct spectral lines. Therefore, the fine sampling produces diverse weighting functions peaking at a range of altitudes, leading to the capability to capture vertical structures in higher vertical resolution. Additionally, these IR instruments provide vital information on atmospheric composition with sensitivity to many trace gases. In contrast to the multitude of IR spectral lines, current MW instruments primarily sample an oxygen absorption line and water vapour absorption at around 60 and 183 GHz respectively.

While there are fewer spectral lines in the MW part of the spectrum compared to the IR, there are nevertheless fine scale structures of the order of a few MHz around the oxygen absorption line which can be resolved due to pressure broadening. Figure 1 illustrates the small structures in the transmittance at different pressure levels with increased broadening effects as the pressure increases. For the current MW instruments, the frequency width and location of the channels is a trade-off between achieving lower noise through a wider passband while sampling a part of the spectrum that is relatively flat in variation with transmission i.e. to achieve a narrower weighting function/Jacobian. The locations of these heritage channels in the MW spectrum are selected to adequately sample specific altitudes in the vertical. The low noise performance is key for the current generation of MW temperature sounders (Lean et al., 2023), as instrument noise is the dominant error source for these channels. Hyperspectral MW instruments in contrast cover a broad MW band continuously with very narrow passbands. This allows sampling of small spectral features, resulting in an increased diversity of weighting functions, albeit at the expense of larger instrument noise for individual channels. In any applications of the data, the latter will need to be compensated for by using an increased number of channels, in order to reduce the effective noise through repetitive measurements. Additionally, hyperspectral MW instruments sample spectral regions between heritage channels that are currently not sampled, which may help to reduce the effective noise. The potential benefits of hyperspectral MW sounders hence arise from two aspects: A greater diversity of weighting functions, and sampling of parts of the spectrum that are currently not sampled. The former is key for achieving a higher vertical resolution, whereas the latter may enable improving the effective noise performance, provided the used part of the spectrum can be increased compared to heritage sensors.

2.2 Potential for hyperspectral MW

Several studies have used 1-dimensional information content techniques to explore the potential of hyperspectral MW instruments with promising results. In information content studies, the uncertainty in atmospheric 1D retrievals is considered (Rodgers, 1990) and can be used to estimate the impact of new satellite concepts on such retrievals. Different hyperspectral MW instruments have been proposed and assessed in these studies, typically covering the 50 and 183 GHz bands, with spectral resolutions ranging from 10 to 100 MHz and 40-400 MHz respectively. In this section we summarise some of the key themes in supporting hyperspectral MW instruments.

In clear-sky conditions, using hyperspectral MW instruments results in a strong performance in improving temperature and humidity fields. Furthermore, the estimated impact is shown to exceed the benefit from non-hyperspectral MW instruments. Aires et al. (2015) and Mahfouf et al. (2015), for example, suggest the temperature retrieval improvement is around double the impact of the combined three MW instruments on the future Metop-SG. Meanwhile a hyperspectral instrument is also shown to perform better than Advanced Technology Microwave Sounder (ATMS) (Kummerow et al., 2022). Note that these information content studies will significantly depend on the assumptions made regarding the observation errors, including both the instrument noise as well as representation errors. The instrument noise is typ-

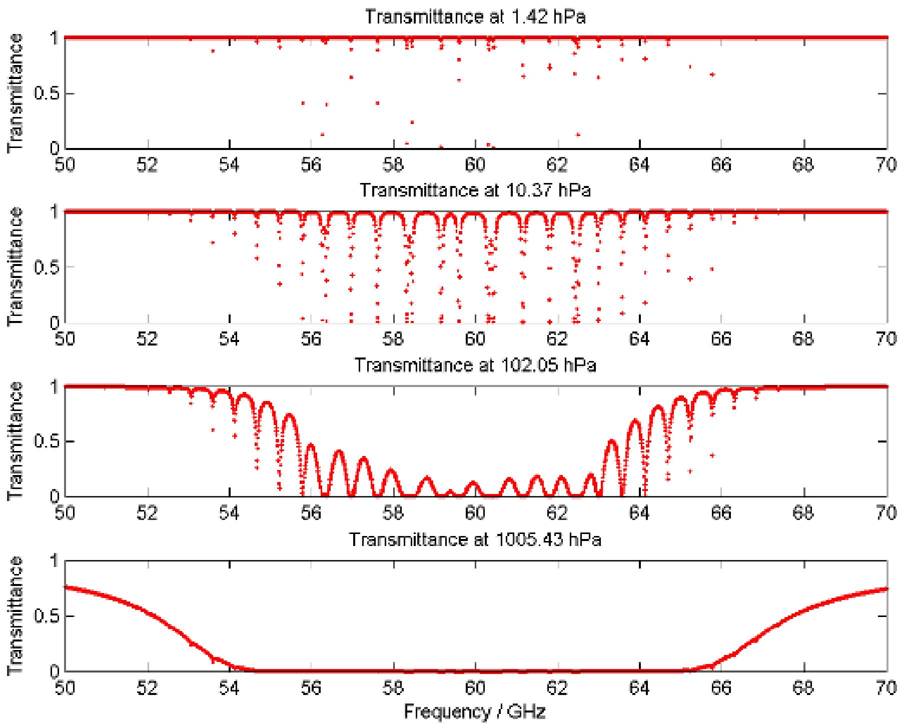

Figure 1: Transmittance from a selection of pressure levels to top of atmosphere generated using the Liebe Millimetre-wave Propagation Model (MPM) 92 model (Liebe, 1989) for the frequency range 50-70 GHz. This figure has been directly reproduced from recent ECMWF training course material on "Measurement, modelling and information content" of the MW spectrum (`https://events.ecmwf.int/event/375/contributions/4249/attachments/2308/4037/microwave1_2024.pdf`, accessed Feb, 2025).

ically assumed to be diagonal, whereas an attempt to account for spectrally correlated radiative transfer error has been included in Aires et al. (2015). Other aspects of representation error are not usually taken into account.

Many of the studies focus on clear-sky conditions, in part because constructing a reliable measure of improvement is more difficult in cloudy situations (Aires et al., 2019). Nevertheless, hyperspectral MW instruments are also demonstrated to provide valuable information on cloudy and precipitating scenes e.g. Boukabara and Garrett (2011); Aires et al. (2019); Maddy et al. (2024). This improvement includes better characterisation of hydrometeors and retrieval of cloud microphysical properties. Aires et al. (2019) also shows that the benefit in cloudy situations is greater than the combined MW instruments on Metop-SG, particularly regarding the temperature retrievals.

The analyses discussed here in some cases use all the available channels on their respective proposed instruments while others make use of a channel selection strategy to create a subset of channels. Aires et al. (2015) and Mahfouf et al. (2015) are parallel studies that demonstrated that use of the full 276 channels available on the instrument versus 110 channels respectively yielded similar retrieval statistics. Maddy et al. (2024) also investigated the influence of spectral resolution in their channel selection using four resolutions ranging from 1 to 50 MHz and 10 to 100 MHz in the temperature and humidity-sounding bands respectively. They suggested that to construct a set of maximum 200 channels for each frequency band regardless of resolution, the increase in total information content became minimal for the temperature-sounding channels when reducing from 10 to 1 MHz. For humidity-sounding, where the spectrum does not have the fine features as discussed for the oxygen band, 50 MHz showed little improvement over 100 MHz. Aires et al. (2015) also considered reducing the spectral resolution from 100 to 10 MHz and 400 to 40 MHz for the temperature and humidity-sounding bands respectively. Advantages from such a fine resolution were primarily noted for temperature in the stratosphere, as a result of better capturing the fine spectral structure in the oxygen band. Investigation by Spire also compared using fine sampling (4.8 MHz) throughout the oxygen band with retaining the high frequency sampling only close to absorption features while using lower spectral resolution (57.6 GHz) elsewhere. Comparable performance was found at higher pressures but finer sampling throughout the band resulted in more improvement to temperature errors in the upper troposphere/lower stratosphere (pers. comm. M. Belal (Spire), 7 Nov 2024).

Across these studies, the impact, spanning from near surface to stratosphere, is thought to originate in particular from:

- Greater diversity in the peaks of the weighting functions for individual channels in the temperature-sounding band, as the finer sampling is able to better probe the smaller structures in the oxygen absorption line (as discussed in section 2.1).
- Measuring in previously unsampled parts of the spectrum, including the wings of the absorption line, with benefits for the effective noise performance when all channels are considered together.

Regarding the last point, some studies particularly highlight the improved skill at sensing the lower troposphere/planetary boundary layer (PBL) (Gambacorta et al., 2023; Maddy et al., 2024) facilitated by the dense sampling at frequencies with greater surface sensitivity. Gambacorta et al. (2023) suggest that the substantial increase in window channels would help to better understand the PBL. Additionally, the potential near surface impact on temperature and water vapour is estimated as significantly greater (up to 40% improved) than ATMS. Boukabara and Garrett (2011) goes further to suggest that a hyperspectral MW instrument could also be beneficial for retrieval of surface properties including over snow/sea ice. Whether these theoretical benefits are achievable in practice will highly depend on how well the surface characteristics can be modelled. For current NWP applications, the use of surface-sensitive channels over land and sea-ice still suffers considerable errors from the description of the surface contributions, so achieving the theoretical benefits for sensing the PBL may require considerable development.

The overall improvement to temperature and humidity retrievals in both clear and cloudy situations is expected to be beneficial to global NWP but could also benefit climate applications and the prediction of extreme weather conditions such as tropical cyclones e.g. Gambacorta et al. (2023). Kummerow et al. (2022) further highlight the potential to use hyperspectral MW instruments for calibration activities, citing their flexibility in frequency response functions as a key feature. The literature also emphasises the advantages of hyperspectral MW instruments for improved Radio Frequency Interference (RFI) detection e.g. Misra et al. (2009); Kummerow et al. (2022); Maddy et al. (2024). Hyperspectral MW instruments allow greater cross-checking of spectral consistency to identify RFI, and subsequently the removal of isolated parts of the spectrum that are affected. The focus of work so far is largely on lower frequency channels, such as around 23 GHz which will not be included in our study. However, Maddy et al. (2024) point out that evolving telecommunications strategies may lead to RFI affecting frequencies around the 60 GHz absorption line in the future so efficient detection and mitigation may become more critical.

3 Characteristics of Hyperspectral Microwave Sounder (HyMS)

The HyMS instrument, developed by Spire and RAL Space, will be used in this study as the basis for our hypothetical hyperspectral MW instrument. It is expected to be launched as the first instrument of this type on a space-borne platform towards the end of 2025 (pers. comm. M. Henry (Spire), 15 Jan 2024). Earlier development has been conducted using an airborne demonstrator which is based on an ultra-wideband high-resolution Fast Fourier Transform digital spectrometer (Henry et al., 2023). While the airborne simulator was successful in demonstrating the technology, comparisons to simulations showed some spectral bias features which required further investigation. Spire expect to launch the space-borne demonstrator into a local equator crossing time (LECT) of 1700 which provides a useful complement to the Metop and JPSS missions that currently populate orbits with 0930 and 1300 LECT respectively. The instrument is cross-track scanning with 45 fields of view on each scan line at 18 km spacing which results in contiguous coverage for the 89 and 183 GHz frequencies while oversampling for the temperature-sounding band. Figure 2 provides an example of the typical coverage over a 6-hour period. These are based on simulations of the geographical sampling kindly provided for the present study by Jörg Ackermann (EUMETSAT).

The HyMS instrument covers two finely sampled frequency bands, 49.42 – 57.75 GHz and 183.13-191.55 GHz, plus a broad passband window channel at 89 GHz. Unlike many current MW instruments, there is no equivalent channel at 150 GHz and no low frequency channels are accommodated. Table 1 summarises the key characteristics of the HyMS space demonstrator which will be used in this study and provides details of ATMS for reference. Note that for the 183 GHz channels, Spire have already applied a pre-processing step where blocks of 8 neighbouring channels have been averaged together throughout the frequency band.

Coefficients to provide clear-sky simulations for the HyMS space-borne demonstrator have been obtained from the NWP SAF, and these can be used to investigate the sensitivity of the various channels to the atmosphere. Jacobians for each of the HyMS channels provide information about the contribution of each atmospheric layer to the radiances measured by each channel i.e. the vertical sensitivity of the instrument. Figure 3 illustrates the temperature Jacobians for all the temperature-sounding channels with figure 4 focusing on the stratosphere. The temperature-sounding channels exhibit very dense vertical

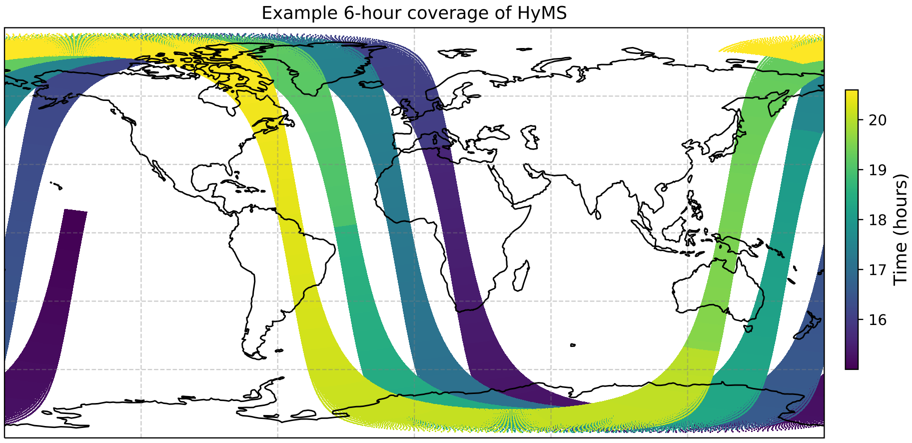

Figure 2: Typical coverage for HyMS for a 6-hour timeslot. Colours represent the hour of the day of the simulated observation location.

coverage at all pressure levels and many channels with high surface sensitivity i.e. smaller Jacobian values showing less response to variation of temperature in the atmosphere. The appearance of a smooth bumpy structure where peaks are formed from particularly dense groups of frequencies with similar sensitivity corresponds to the areas of relatively flat changes in transmission in the spectrum (highlighted in figure 1) and locations of channels on conventional MW sensors. Figure 5 and 6 show the humidity and temperature Jacobians respectively for the 183 GHz channels. The humidity-sounding channels have sensitivity to vertical variations in both temperature and water vapour. For humidity, sensitivity is greatest between around 250-600 hPa while for temperature is it slightly lower in height, around 300-700 hPa. However, as the peaks are relatively broad, there is some substantial sensitivity outside of this pressure range.

Spire have also provided instrument noise characteristics for the instrument – both NEDT (Noise Equivalent Delta Temperature) values and the inter-channel correlation information from prelaunch testing. Here the sample NEDT values are given which correspond to scaled values of the 3 dB Field of View (FOV) NEDT, accounting for the sampling interval of the instrument (Atkinson, 2015). For channels in the 50-60 GHz band, NEDT is given as 1.53 K for each channel while for the binned 183 GHz, NEDT is 1.63 K. For comparison, sample NEDT values for similar channels on the ATMS instrument are of order 0.25 K and 0.4 K, respectively, albeit of course for channels with much broader band-width. Higher values for HyMS are expected due to the narrower spectral bands, and it is clear that a larger number of channels compared to heritage sensors needs to be used to achieve a similar effective noise performance. For individual channels, it is worth recalling that errors in the background temperature fields are of the order 0.1 K (Bell et al., 2008). Using 940 channels sampled at 10 MHz, Aires et al. (2015) demonstrated benefit with similarly high noise values (starting at 1.26 K). Their study indicated low sensitivity to increases in the noise, especially in the lower/mid troposphere, though likely at least partly due to assuming sizeable radiative transfer errors. For hyperspectral MW instruments, lower effective noise performance is achieved through repetitive sampling of similar atmospheric layers through several individual channels

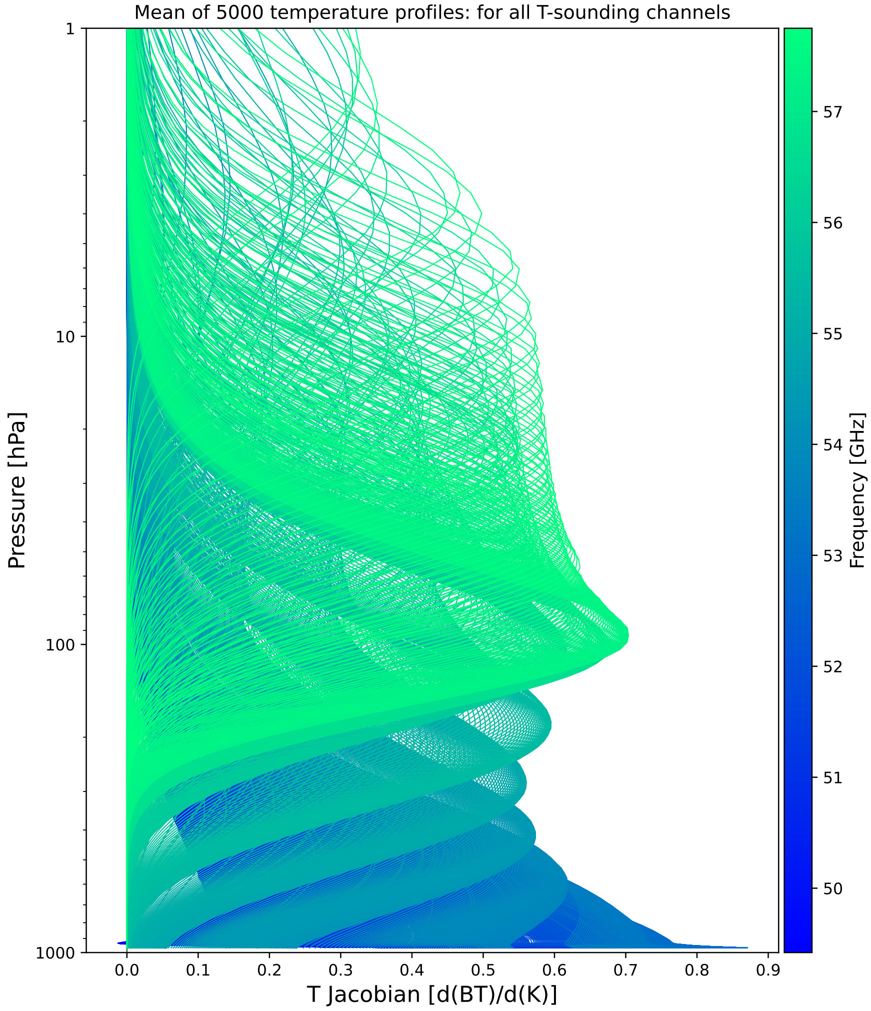

Figure 3: Temperature Jacobians for the HyMS temperature-sounding channels. Data have been generated by a radiance simulator employing RTTOV (https://nwp-saf.eumetsat.int/site/software/radiance-simulator/) on 5000 variable atmospheric temperature profiles. The average profile is shown here. Jacobian values have been normalised by the corresponding log of the model layer depth in pressure units.

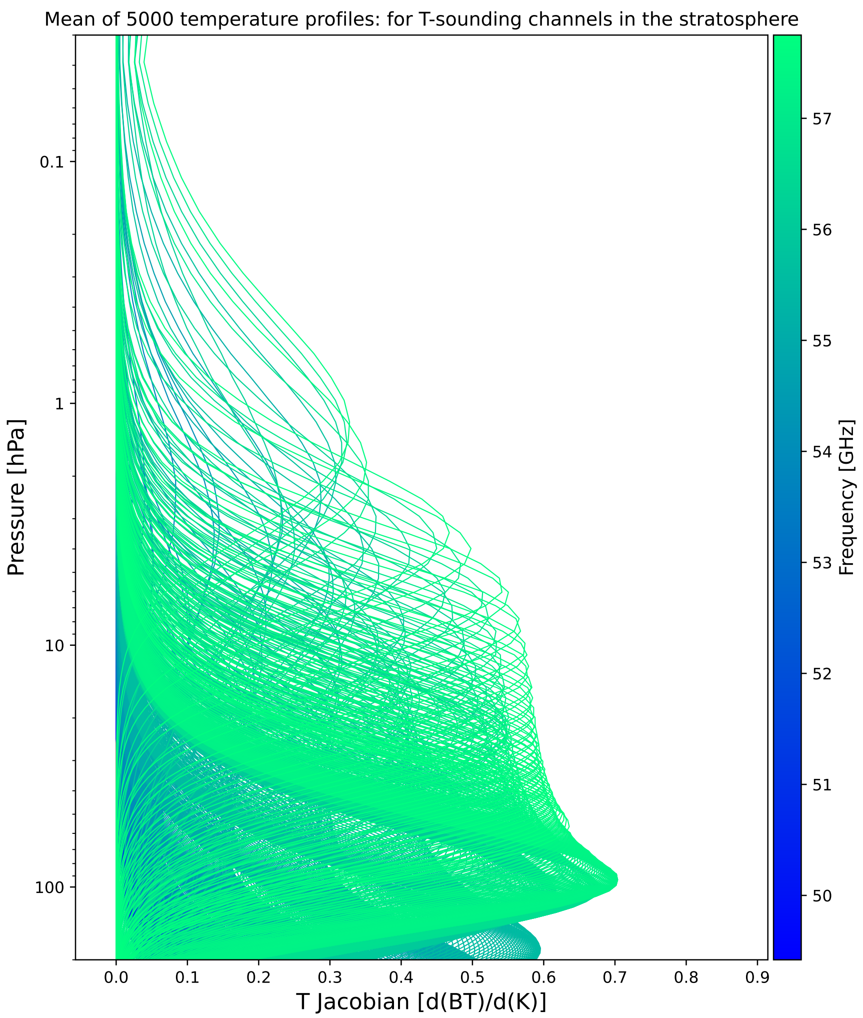

Figure 4: As for figure 3 but focusing on stratospheric pressures.

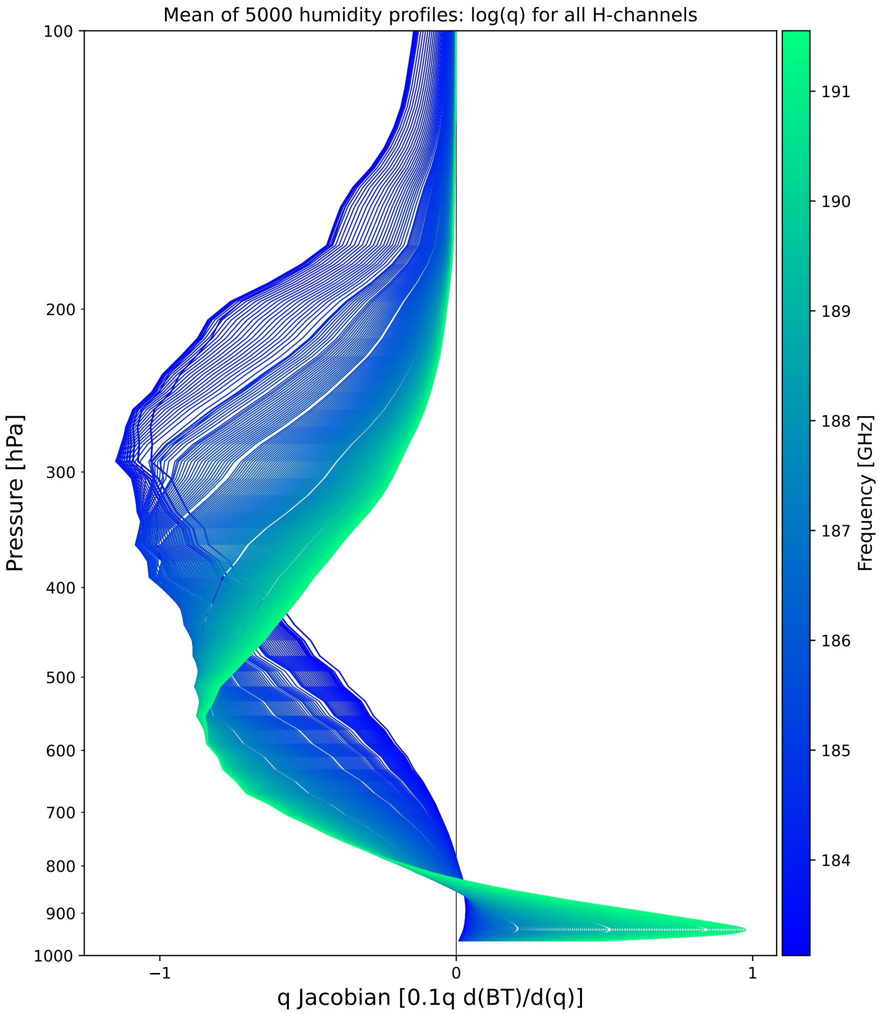

Figure 5: Humidity Jacobians with a 10% perturbation in humidity for the HyMS humidity-sounding at tropospheric pressures. Data have been generated by a radiance simulator employing RTTOV on 5000 variable atmospheric humidity profiles. Note that the average profile is shown here but variations in humidity content will affect the Jacobian height. Jacobian values have been normalised by the corresponding log of the model layer depth in pressure units.

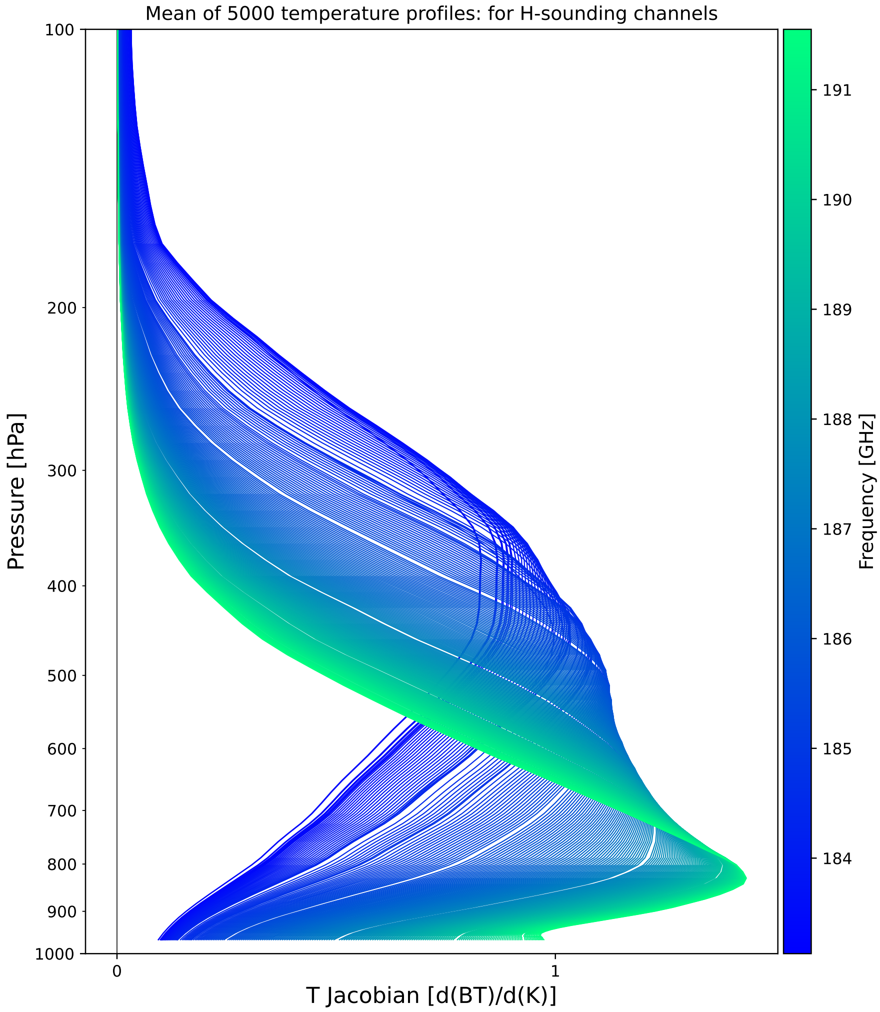

Figure 6: Temperature Jacobians for the HyMS humidity-sounding channels at tropospheric pressures. Data have been generated by a radiance simulator employing RTTOV on 5000 variable atmospheric temperature profiles. The average profile is shown here. Jacobian values have been normalised by the corresponding log of the model layer depth in pressure units.

Table 1: Summary of key information for the HyMS instrument (kindly provided courtesy of Spire). *Channels in the 183 GHz band have already been combined into bins of 8 neighbouring channels.

Instrument characteristic	HyMS	ATMS
Number of channels	1689 channels 49.42-57.75 GHz, 1 x 89 GHz and 212* x 183.13-191.55 GHz	13 channels 50.3 – 57.62 GHz, 5 channels 182.31–190.31 GHz, 1 x 23.8, 31.4, 88.2, 165.5 GHz
Channel bandwidths	6.34 MHz for 50-60 GHz, 40 MHz for 183 GHz	155-400 MHz for tropospheric 50 GHz, 500-2000 MHz for 183 GHz
Polarisation	50 GHz: vertical, 183 GHz: Horizontal	Horizontal for all 50 and 183 GHz channels
Number of pixels per scan line	45	96
Maximum scan angle	45 deg	52.7 deg
Scan duration	2.55 s	8/3 s
Local equator crossing time	1700	1330
Orbit height	500 km	824 km
Footprint size	33 km at 50 GHz band, 18 km at 183 GHz	32 km at 50 GHz 16 km at 183 GHz

with vertical overlap (Maddy et al., 2024). The noise has been reported to have Gaussian characteristics (pers. comm. M. Henry (Spire), 30 Apr 2025) which should allow for better effective noise reduction when averaging observations.

Spire also provided information on the inter-channel correlations of the NEDT for HyMS. Non-zero noise correlations are mostly confined to immediately adjacent channels, and they are negligible for frequencies further apart. For the temperature-sounding band, neighbouring frequencies have a correlation of around 0.45 and less than 0.05 between channels that are not immediately adjacent. For the humidity-sounding channels which are binned into groups of eight channels, the correlation between these neighbouring groups is only around 0.05.

4 Approaches to assimilate hyperspectral radiances

While hyperspectral IR instruments have thousands of channels available, in practice a much smaller subset of channels is assimilated – typically around 200-400. This is largely motivated by computational expense in assimilation but also many frequencies are currently manually removed by users e.g. to avoid signals from poorly characterised variable trace gases or other poorly modelled parts of the spectrum (Collard, 2007). However, ad hoc removal of the IR channels still results in a large number of frequencies remaining. Furthermore, as IR instruments become more advanced, the practicalities and expense of data transfer also become important factors. To achieve manageable data volumes for assimilation and data dissemination, three strategies applied to IR data are outlined here followed by the proposed strategy for

HyMS.

4.1 Assimilation of selected raw radiances

The operational assimilation of hyperspectral IR instruments at ECMWF and all other operational centres is based on selecting a set of raw radiances, typically of the order of 300-400. The channel selection at ECMWF is based on an information content method first implemented with the IASI instrument (Collard, 2007). It is applied to raw radiances and takes into account the channel characteristics to select a set of channels that optimise a figure of merit. Figures of merit which broadly measure the reduction in uncertainty in the analysis include the Degrees of Freedom for Signal (DFS), entropy reduction (Rodgers, 2000) and Channel Score Index e.g. Noh et al. (2021). On the basis of findings by Rabier et al. (2002) which evaluated different information content techniques, the DFS formulation based on information theory was used at ECMWF to estimate the value of assimilated channels. This technique has been adopted more widely for subsequent hyperspectral IR instruments and iterations in channel selection e.g. Coopmann et al. (2020); Carminati (2022). The DFS takes into account the channel characteristics through the Jacobians, as well as the uncertainty in the background and the observations. Assuming Gaussian error characteristics, the DFS is defined as:

$$DFS = Tr(I – AB^{-1}) \tag{1}$$

Where I is the identity matrix and A and B are the analysis and background error covariance matrices respectively. The analysis matrix can be further written as:

$$A = (B^{-1} + H^T R^{-1} H)^{-1} \tag{2}$$

Where H is the Jacobians, giving the derivatives of each channel radiance with respect to the state vector parameters and R is the observation error covariance matrix. This means that for the DFS calculation, sensible estimates of the observation error are required as well as representative background errors. Further details can be found in Collard (2007).

The DFS is calculated using a selection of input atmospheric profiles which are typically a small set broadly representing different geographical areas. For IR instruments, temperature, humidity, ozone and surface parameters are usually considered and channel selections are optimised for clear-sky conditions. The channel selection is performed in an iterative approach. In the first processing step, the DFS is calculated for each channel separately and the most valuable channel is selected as determined by the highest DFS value. The second step finds the next channel that adds the most value when combined with the first and so this process continues of finding the next channel in combination with those already selected. A cut off is required where it is determined that the increment in benefit of an additional channel is negligible. This threshold is empirically set by the user. In addition to the use of DFS, the method allows a large degree of flexibility in additional channel exclusion, for example, for IR instruments, channels sampling spectral lines of traces gases that are poorly modelled are rejected prior to the DFS calculation (Collard, 2007).

While channel selections based on information content are well-established for hyperspectral IR instruments, the selections also have their short-comings and limitations. The resulting channel selection will be highly sensitive to the estimates of the observation and background error covariance matrices used, which may be considerably simplified. Coopmann et al. (2020) also show that considering the optimisation of all variables of interest simultaneously could be an advantage over treating them separately in DFS calculations. A simultaneous channel selection will, however, rely even more strongly on the adequacy of the assumed background error statistics, as these will be influential in separating ambiguous radiance signals into geophysical variables. In this context it is worth noting that Vittorioso et al. (2021) validate their channel selection by comparison with a random channel selection of the same number of channels and show that with a reasonable distribution across the full spectrum it is possible to still achieve good impact of a similar order as with a more carefully constructed selection. The DFS produces better results overall, particularly above 400 hPa, but in the mid-troposphere the benefit is comparable. This implies that although there is sensitivity to the method, simplifying assumptions in the DFS construction can still result in a satisfactory channel subset.

4.2 Assimilation of selected reconstructed radiances

Observations from hyperspectral instruments form very large data volumes making transmission and computational costs more expensive. One method to represent most of the information through smaller data volumes is to use Principal Component (PC) compression. Here, the spectra are projected onto the eigenvectors (i.e. the PCs) of the climatological covariance matrix of the data, resulting in a set of so-called PC scores. The PC scores of the leading eigenvectors capture the majority of the information of the spectrum, whereas the trailing eigenvectors tend to capture the instrument noise contributions. Compression is achieved by retaining the scores for the leading PCs (in the case of IASI typically a few hundreds) and discarding the rest. Depending on the number of retained PC scores, PC compression results in high compression rates while preserving most of the thermodynamic information (Lupu et al., 2021). Radiances can be reconstructed from the retained PC scores by projecting back into radiance space. The reconstructed radiances can be treated with similar techniques as the original radiances such as bias correction and channel screening for quality control. A channel selection based on techniques outlined in section 4.1 is still subsequently required to achieve manageable data volume prior to assimilation. However, for a given number of selected channels, reconstructed radiances will contain more of the information of the full spectrum than raw radiances.

Taking full advantage of the higher information content represented in reconstructed radiances, however, requires careful treatment of the resulting observation errors, and benefits in terms of impact in NWP have so far been limited. While the instrument noise in the reconstructed radiances is smaller, the process of generating the reconstructed radiances introduces strong noise correlations which pose additional challenges in data assimilation. Furthermore, signals in the true spectrum can be lost if these are not represented in the sample used to generate the PCs, leading to additional errors that ideally should be accounted for during the radiative transfer modelling. Results aimed at demonstrating that the assimilation of reconstructed radiances for hyperspectral IR instruments leads to better impact compared to using raw radiances have been mixed so far, and no operational NWP centre has moved to the assimilation of reconstructed radiances. For the present study, we hence will not consider the use of reconstructed radiances.

4.3 Direct assimilation of principal component scores

Rather than using reconstructed radiances, it is also possible to directly assimilate the PC scores from the eigenvector decomposition of the raw radiances (Matricardi and McNally, 2014), using only the scores from the leading eigenvectors. This results in information from all of the channels being incorporated and therefore covers all the spectral regions being sampled. This can lower computational costs for data dissemination and assimilation and may increase the information content presented to the assimilation system (Matricardi and McNally, 2014). An adapted version of the radiative transfer model to process PCs is required. While a version of the radiative transfer model employed at ECMWF, PC-RTTOV (Matricardi, 2010), is mature for the IR, the use of PCs in the MW part of the spectrum has not been evaluated yet. Furthermore, the use of PCs brings challenges in finding alternative methods of e.g. bias correction and screening which relies on information from specific individual channels. While promising results have been achieved in research experiments, no NWP centre currently assimilates principal component scores operationally for any of the hyperspectral IR instruments. Overall, we consider the assimilation of principal component scores not sufficiently mature to be applied for a first assimilation of hyperspectral MW radiances.

4.4 Proposed assimilation approach for hyperspectral MW

Following the above considerations, the approach for assimilating hyperspectral MW data in the present study will be based on assimilating a set of selected raw radiances. This is closest to established practices for hyperspectral IR instruments as well as heritage MW sounders, and should hence be the most tractable approach. While the use of reconstructed radiances or PC scores has theoretical advantages, in practice these have not yet been demonstrated for hyperspectral IR instruments. Additional uncertainties that are introduced e.g. through the correlated errors in reconstruction are hard to quantify, and the process of using PC analysis and reconstructed radiances introduces unnecessary extra complications at this stage in a new instrument evaluation. The choice could be revisited in the future, once further experience has been gained with the use of hyperspectral MW data.

Prior to applying any more sophisticated channel selection, a manual removal or superobbing of parts of the frequency spectrum will be considered. There are two aspects to this:

- Where channels have higher surface sensitivity it may be possible to average neighbouring frequencies to create lower noise “super channels” .
- Frequency ranges could be excluded from the channel selection procedure where they are rejected from assimilation due to quality control choices e.g. restrictive use of surface sensitive channels (further detailed in section 5.2). Furthermore, we may wish to remove channels that could be at high risk of contamination by RFI.

Channels with higher surface sensitivity are more challenging to use so their assimilation currently tends to be much more restricted. In some cases, it may be beneficial to consider producing super channels that reduce the noise through averaging groups of frequencies with very similar surface sensitivity. By careful study of the spectrum, Jacobians and with guidance from the location from the channels on existing MW instruments, this selection could be manually achieved. Regarding RFI, currently there is only a small frequency range in the HyMS temperature-sounding band completely protected for passive MW Earth Observation (50.2-50.4 and 52.6 – 54.25 GHz). However, there is a large portion allotted to passive MW observation activities above 54.25 GHz that this shared with other applications that should not theoretically cause too much degradation (Radio Regulations, 2024 Edition). Conversely, in some unprotected ranges such as 51.4-52.6 GHz there is considerable risk of RFI issues and therefore it would be sensible to remove these channels.

Ultimately, it is desirable to use as much of the frequency spectrum as possible to exploit new parts not currently covered by conventional MW sensors and acquire a higher diverse vertical sampling. The use of many channels should also help to reduce high instrument noise levels. This noise limitation is not a factor in the current hyperspectral IR channel choice. Different findings regarding the benefit of higher sampling are likely the result of different assumptions for observation errors. For the present study, we will initially aim to keep the high spectral sampling, based on Spire's results, but this could be revisited in the future. Computational constraints must be kept in mind, but it is reasonable to expect that a few hundred channels could be a plausible proposal. With the manual removal and averaging of parts of the spectrum, it may even be possible to achieve this without the use of a more formal channel selection strategy such as using the DFS iterative method.

5 Assimilation challenges for HyMS

The HyMS instrument will follow as closely as possible the current all-sky assimilation strategy of MW sounders. The data will first be simulated using ECMWF high resolution NWP analyses where model variables are converted to brightness temperatures with application of RTTOV-SCATT[1] (Saunders et al., 2020; Geer et al., 2021). Perturbations will be added to the observations reflecting the NEDT values and inter-channel instrument noise correlations provided by Spire (discussed in section 3). A channel selection will be applied and appropriate spatial/temporal thinning strategies employed to mitigate spatially correlated observation errors. In following similar all-sky processing to the current MW sensors, there are three key features – the emissivity calculation, quality control and observation error modelling - that will need adaptation for HyMS. Here we discuss the challenges and outline potential solutions.

5.1 Radiative transfer modelling

Radiative transfer modelling for HyMS will be performed with RTTOV-SCATT. Coefficients for the clear-sky radiative transfer have been obtained from the NWP SAF. HyMS will test the fine spectral detail of the under-lying line-by-line calculations, but no particular technical challenges in performing the radiative transfer are expected. For the representation of cloud-scattering, enhancements to the RTTOV-SCATT capabilities may be needed, and these are currently under investigation.

Ocean surface emissivity modelling will be performed with SURFEM (Kilic et al., 2022), the new fast ocean surface emissivity model included in RTTOV. Given the relatively smooth behaviour of surface emissivity over the MW spectrum, no particular additional challenges for ocean-surface emissivity modelling for HyMS are expected.

Over land and sea-ice surfaces, the surface emissivity is dynamically retrieved in the current assimilation of MW radiances, using pre-defined window channels (Baordo and Geer, 2016). Over all land surfaces, 50.3 GHz is employed for the temperature-sounding channels while 89 GHz and 150 GHz are used over snow-free land and snow/sea-ice surfaces respectively for the humidity-sounding channels. For temperature-sounding channels, the use of a single HyMS channel around 50.3 GHz would not be appropriate due to the high NEDT which would lead to poorer retrieved emissivity values. Meanwhile for humidity-sounding channels, HyMs does not have an equivalent 150 GHz channel.

To limit the complexity, the initial focus will be on assimilating channels over sea and surface-insensitive channels over land. This could be done for example, by placing a threshold on the surface transmittance which is a method used for the assimilation of channels with higher surface sensitivity on SAPHIR, which does not have any window channels (Chambon and Geer, 2017). Alternatively, a frequency cut-off could be explored, guided by the frequency use on current MW instruments and HyMS channel

[1]RTTOV = Radiative Transfer for TOVS, TOVS = TIROS Operational Vertical Sounder, TIROS = Television Infrared Observation Satellite

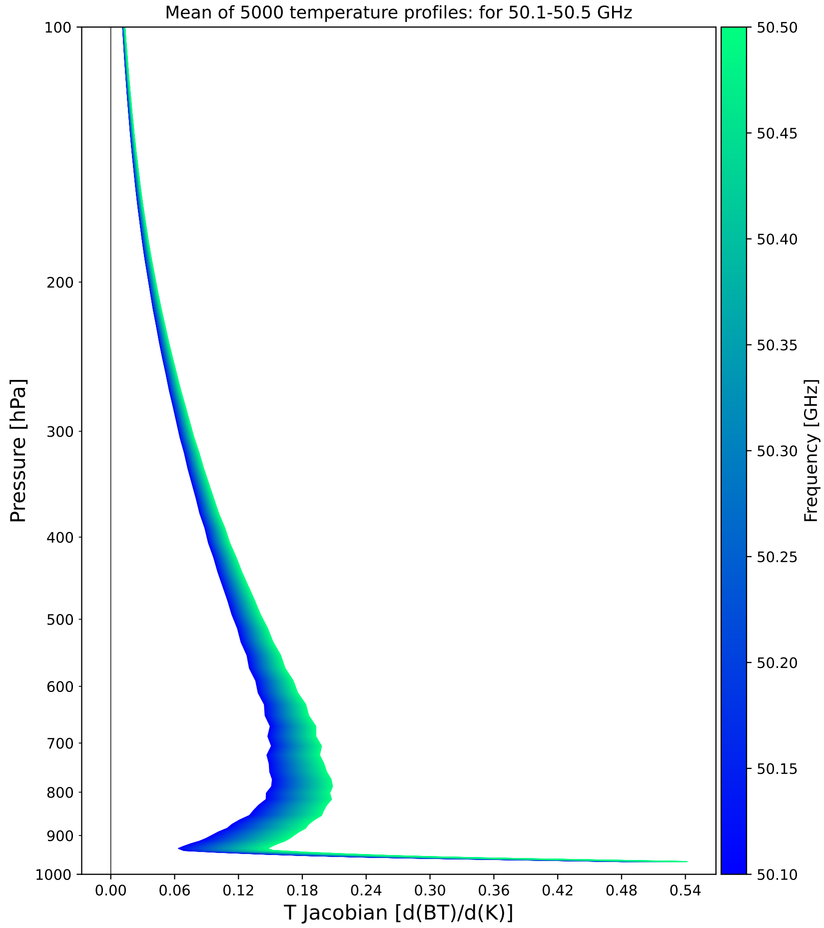

Figure 7: Temperature Jacobian for the HyMS temperature-sounding channels as in figure 3 but covering only the frequency range 50.1 – 50.5 GHz.

vertical sensitivity. Adding surface-sensitive channels over land/sea-ice could be considered later if the activity can be accommodated within the project timeframes. To address the use of temperature-sounding channels, it could be envisaged that a group of neighbouring channels centred around 50.3 GHz could be averaged together to create a lower noise "super channel" equivalent for use in the retrieval process. Figure 7 shows that the group of HyMS channels around the region of AMSU-A channel 3 (central frequency 50.3 GHz, passband width 180 MHz) have very similar Jacobians and little sensitivity to the changes in atmospheric temperature characteristic of window channels. Relatively large sensitivity to skin temperature would be expected for these channels.

For the humidity-sounding channels, the broadband 89 GHz channel on HyMS can be used for emissivity retrievals over snow-free land as in the current approach. For emissivity retrieval over snow/sea-ice surfaces, there is no straightforward substitute for the 150 GHz channel normally used for this purpose but it may be possible to use a super channel approach with frequencies in the wings of the 183 GHz band. A pragmatic approach may be to continue to screen humidity-sounding channels with high surface sensitivity over these snow/sea-ice surfaces.

Table 2: Summary of key quality control choices made in the assimilation of MW radiances on existing MW sounders requiring adaptation to the fine spectral sampling of HyMS.

Assimilation choice	Application to all-sky MW
Tropics (<30° N/S) orography rejection	53.246 and 53.596 GHz height < 1000m, 54.4 GHz height < 2000m
Extratropics orography rejection	53.246 and 53.596 GHz height < 500m, 54.4 GHz height < 1500m
Polar regions (>60° N/S)	53.246, 183±7 and 183±4.5 GHz rejected over all surfaces, 53.596 GHz rejected over land/sea ice in Antarctic region only
Coast	53.246, 53.596, 54.4, 183±7 and 183±4.5 GHz rejected
Snow/sea-ice	53.246, 183±7 and 183±4.5 GHz rejected
Surface sensitive channel rejection over land	50.3, 52.8, 89 GHz not directly assimilated (but used e.g. in emissivity and observation error calculation)

By screening these low peaking channels over land surfaces, the impact of the data would likely be underestimated in these regions. For fairness, in any evaluation of the HyMS impact relative to a real MW instrument, a similar screening strategy would be applied to the real observations during assimilation. Developments are ongoing at ECMWF to better constrain the surface emissivity, particularly with use of low frequency channels on MW instruments. With a more accurate model emissivity available, instruments without key window channels should not have to rely on these dynamic retrievals in the future.

5.2 Quality control

Quality control measures will be applied to HyMS following examples of current MW data use. Table 2 summarises the rejection choices that will need to be considered for HyMS. Complete details of the all-sky treatment of temperature and humidity sounding instruments in assimilation can be found in Duncan et al. (2022) and Geer et al. (2022) respectively. The main challenge is defining equivalent frequency bounds on the more continuous spectral sampling of HyMS. These limits will be influenced by careful study of the Jacobians, spectral features and inspection of geophysical structures once observations have been simulated in the next stage of the project. Note that some screening steps will remove frequencies that will also feature in restrictions introduced through a simplistic approach to the emissivity described earlier (where the focus will be on using surface insensitive channels over land/sea-ice). The removal of channels from the assimilation as part of these quality control measures will also be incorporated into the HyMS channel selection, noting e.g. that some surface sensitive channels will still be required as part of emissivity or observation error model calculations.

5.3 Observation error

Observation error modelling for HyMS is expected to largely follow established procedures used at ECMWF for all-sky assimilation of MW radiances. This takes into account contributions from the instrument noise, as well as situation-dependent contributions from representation error such as resulting from the representation of clouds, spatial mis-match, or radiative transfer. The latter contributions tend to increase in cloudy situations, and this is taken into account on the basis of a symmetric cloud indicator, indicating the presence of cloudy signal from either the observation or model (Geer and Bauer, 2011). The assigned observation errors influence the weighting of the observations in the assimilation, as well as the perturbations added to the observations to generate the ensemble members in the EDA. Realistic spread changes are therefore dependent on realism of the observation error definition and future activity to investigate the sensitivity is planned in a later work package in this study. Here we briefly discuss two important factors for the construction of the error model for HyMS which will be expanded and carefully tested as part of a later phase of this project:

- Defining suitable indicators of cloud to estimate the cloud presence so that higher observation errors can be assigned when there is a greater amount of cloud detected in the observations or model.
- Treatment of inter-channel error correlations. While information provided by Spire suggests that the instrument noise for HyMS is largely uncorrelated (except for neighbouring temperature-sounding channels), inter-channel error correlations can arise from representation error, and these may need to be taken into account.

Regarding the choice of cloud indicator, the unavailability of key frequencies on HyMS that are part of the calculations for current MW instruments (low frequencies for temperature sounding (Bennartz et al., 2002; Grody et al., 2001) and the 150 GHz channel for humidity-sounding (Geer et al., 2014)) means that different indicators will be needed. The approach for temperature-sounding channels can be based on earlier work assessing small satellites which utilises an estimate of cloud effect around 52.8 GHz (Lean et al., 2021). The relatively large instrument noise on individual HyMS channels would lead to less reliable estimates of the cloud presence. Similar to the temperature-sounding emissivity retrieval strategy outlined earlier, creation of an equivalent low noise "super channel" around this frequency by averaging neighbouring channels with very similar vertical sensitivity may provide a suitable alternative. For the humidity-sounding channels, current MW instruments use a scattering index based on differences between the 89 and 150 GHz channels. As there is no 150 GHz equivalent on HyMS, a new cloud indicator will need to be developed for these channels. A good starting point will be to use information in the low peaking 183 GHz channels, extracting the cloud effect in a similar way to the temperature-sounding indicator. A similar strategy has been used to assimilate 183 GHz channels on SAPHIR (Chambon and Geer, 2017).

Experience with hyperspectral IR instruments shows that taking into account inter-channel error correlations in clear-sky conditions results in significant additional positive impact e.g. Weston et al. (2014); Bormann et al. (2016); Campbell et al. (2017). For the IR instruments, the error correlations are thought to primarily arise as a result of cloud screening, spatial representativeness and surface contributions. Taking the error correlations into account avoids over-weighting of the observations in the assimilation. Inflation of error variances can be used to avoid such over-weighting, but explicitly including the correlations is shown to be more beneficial.

It is unclear to what extent the experience with hyperspectral IR instruments is applicable to the assimilation of the HyMS instrument. The relevance of inter-channel error correlations will depend on the size of the contribution from correlated representation errors relative to the instrument noise, which is comparatively large for individual channels on HyMS. For clear-sky regions, the instrument noise is hence expected to dominate. However, representation errors due to clouds are expected to be larger than the instrument noise, and this aspect likely needs to be taken into account when considering hundreds of HyMS channels, to avoid an overly optimistic estimate of the impact.

The current all-sky MW data assimilation does not take any inter-channel correlations into account, but the technical capability has been developed and is currently undergoing scientific testing. The specification and treatment of potentially correlated observation errors will form an important part in considering appropriate choices for the EDA experimentation.

6 Summary

MW instruments are a well-established and critical component of the observing system but the underlying instrument technology has been relatively stable for many years. The recent maturation of hyperspectral MW instruments for space-borne platforms presents an exciting new avenue for exploring what additional impact can be realised from observing the MW spectrum. In particular, the increased spectral sampling should better capture the fine features present around the oxygen absorption line. There are opportunities therefore for more diverse vertical sampling of the atmosphere and the ability to cover more of the spectrum including new parts unexplored by conventional MW sensors. Information content studies have shown very encouraging results supporting the use of hyperspectral MW instruments. Key themes from the literature include:

- Improved retrieval of temperature and humidity profiles also exceeding impact from heritage MW instruments in both clear and cloudy conditions.
- Advantages in Radio Frequency Interference (RFI) detection.
- Better sensing of lower troposphere/PBL and improved characterisation of hydrometeors/cloud parameters.

The studies also concluded that the performance of hyperspectral MW instruments have the potential to exceed the benefit of current MW sensors. The dependence on spectral resolution was not particularly significant in the configurations trialled with most benefit of using high resolution (around 10 MHz) seen at low pressures in temperature retrievals, linked to the better sampling of the fine spectral features in the 50-60 GHz band.

A future space-borne hyperspectral MW instrument, HyMS, developed by Spire and RAL, forms the basis of the instrument we will evaluate in this study. It covers finely sampled temperature (49.92-57.75 GHz, passband size 6.24 MHz) and humidity (183.31-190.31 GHz, passband size 40 MHz) bands in addition to broad passband window channel at 89 GHz. The channels present very dense coverage vertically for temperature sounding and a broad range of tropospheric pressures around 250-600hPa with high humidity sensitivity. The instrument noise values are relatively high, as expected in the trade-off with narrower channels. Use of many frequencies with overlapping vertical sensitivity should help to effectively reduce this noise. Inter-channel correlations in the instrument noise are only relevant for directly adjacent channels and will be accounted for in the subsequent observation simulation and corresponding observation error construction.

Large volumes of channels bring computational challenges for assimilation so we draw on the experience of hyperspectral IR instruments to propose a channel selection strategy. In the first instance channels will be removed that would be screened out by quality control measures, such as some of the surface sensitive channels. Parts of the frequency spectrum at high risk of RFI contamination in the future will also be excluded. Ideally, it would be preferred to retain a high number of channels to get the best vertical distribution and sampling of novel parts of the spectrum but also for noise reduction, which is a less critical consideration for hyperspectral IR. However, a formal channel selection using the DFS, such as employed for the hyperspectral IR instruments, may be required to create a frequency subset balancing information content with practicalities of assimilation.

In addition to handling a large number of channels, there are challenges in following similar processing routes as current MW instruments in the assimilation. Three areas have been highlighted where a different strategy will be needed. A dynamic retrieval of emissivity, usually from key window channels, is difficult due to a combination of the high noise on single channels and the unavailability of a 150 GHz channel. As a more conservative first attempt, frequencies with high surface sensitivity will be screened over land/sea-ice surfaces. Time permitting, a more sophisticated solution may be developed later. Screening may come from a threshold on transmittance or a limit on the frequency range. Further frequency selection will need to be considered as part of quality control measures, for example where additional channels on current MW instruments are removed over high orography. Careful study of the frequency spectrum, Jacobians and geophysical features from simulated observations will support the choices. Finally, appropriate modifications to the all-sky observation error model will be needed. This involves developing suitable cloud indicators which can be formed from super channels – groups of neighbouring frequencies averaged to give a single lower noise channel. Accounting for inter-channel error correlations may also need to be considered.

The next phase of this project will be a technical step to implement the observation simulation and assimilation using the characteristics of HyMS. Where possible, this will build on the existing framework developed in earlier EDA studies (Lean et al., 2025). Initial simulations of the observations will be produced to explore the geophysical structures which will help to inform assimilation choices and creating an appropriate channel subset. Developing the representation of the observational uncertainties is also a key activity before we can finalise settings and conduct the EDA experiments for impact evaluation. Accurate estimates of the uncertainties are important for obtaining reliable forecast impact estimates. Firstly, simulated data will need to be perturbed to represent instrument noise. Additionally, an appropriate observation error model is necessary which will influence the weighting of the observations in assimilation but also the perturbations added in the EDA to represent observation uncertainties and generate the ensemble members. As discussed earlier, key aspects will be the choice of suitable cloud indicators and the treatment of inter-channel error correlations.

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