Study on Upper Troposphere / Lower Stratosphere Sounding

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Executive Summary

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1 Overview

The upper troposphere/lower stratosphere (UTLS) region is a major focus of interest for atmospheric research at present, and is expected to remain so during the coming decade due, for example, to the importance of this region to climate radiative forcing, stratosphere/troposphere exchange, stratospheric ozone depletion and tropospheric chemistry. Although sensors to fly on Envisat and METOP have potential to sound this region, it is anticipated that the attributes of millimetre-wave limb-sounding should be especially well-suited to the task. As a consequence, the Millimetre-wave Acquisitions for Stratosphere Troposphere Exchange Research (MASTER) instrument was conceived by ESA as the core instrument for a future Atmospheric Chemistry Explorer mission, to be complemented by METOP nadir-sounders and possibly also IR and other instruments on a dedicated platform.

The objective of MASTER is to provide innovative, global measurements of atmospheric composition in the UTLS with which to improve knowledge of: atmospheric dynamics, especially stratosphere/troposphere exchange; radiative forcing of climate; tropospheric chemistry and stratospheric ozone depletion. This is to be achieved, firstly, through making simultaneous limb-measurements of H_2O, O_3 and CO in the upper troposphere and lower stratosphere at higher vertical resolution than can be achieved through nadir-sounding and, secondly, by measuring height-resolved distributions of a suite of stratospheric species, (primarily BrO, ClO N_2O, HNO_3 and CH_3Cl). It is further anticipated that assimilation of high-quality H_2O and O_3 UTLS measurements by forecast models could have potential benefits for numerical weather prediction.

To achieve its objective, MASTER is configured to limb-scan the troposphere and stratosphere in the orbit plane, sampling at 1 km in tangent-height and $\leq$100 km along-track in five broad frequency bands. The designation of bands and principal target species is:

A 200 GHz − mid-tropospheric H_2O

B 300 GHz − O_3 and O_2 (pointing/temperature)

C 325 GHz − H_2O

D 345 GHz − CO and HNO_3

E 500 GHz − stratospheric ClO, BrO, N_2O and CH_3Cl.

The purpose of the *Study on Upper Troposphere / Lower Stratosphere Sounding* (ESA contract 12053/97/NL/CN) was to examine and optimise the MASTER instrument specification to meet its objective, and to establish its measurement capabilities as core instrument in a future *Atmospheric Chemistry Explorer* mission. In order to undertake this study, a consortium was assembled comprising Serco Europe Ltd. (prime contractor), Rutherford Appleton Laboratory (RAL, technical co-ordinator), University of Bremen (IFE), University of Bern (IAP) and University of Bonn (MI Bonn)[1]. The three main elements of the study and the institutes primarily responsible were as follows:

- I - Instrument Parameters and Cloud-Free Measurement Capabilities (RAL)
- II - Upper Troposphere Humidity Retrieval from the Millimetre-wave Atmospheric Sounder (IAP)
- III - Sensitivity to Cloud (IFE/MI Bonn)

[1] University of Oxford also participated in an initial radiative transfer model intercomparison exercise.

The starting point for the study was MASTER Requirements Document Version 2 (D. Lamarre, 1997), which specified key instrumental parameters. The bulk of the study employed the methodology of "retrieval simulation", whereby measurements were synthesised using a "forward model", comprising an atmospheric radiative transfer model and an instrument model, and then inverted using a "retrieval model". The "optimal estimation" retrieval approach was employed for the most part, and a variety of retrieval diagnostics were examined to assess and optimise MASTER's performance to retrieve constituent profiles (single-scan precision, vertical resolution etc.). As a pre-cursor to the main study, the forward and retrieval models of participating groups were intercompared.

In general, instrument-induced errors were evaluated through "linear mapping", although iterative, non-linear retrievals were also conducted, where necessary. From the individual profile errors, indicative random and systematic error budgets were generated for a mid-latitude scenario.

An important additional component of the study was to simulate upper troposphere humidity (UTH) retrievals in the presence of horizontal structure in the flight direction (ie in the limb-viewing plane). In this exercise, measurements were synthesised rigorously, but a "spherically-symmetric" atmosphere was assumed in the retrieval of each individual profile.

The study of UTH retrieval from MAS flight data was conducted in parallel to the MASTER retrieval simulation study, providing a complementary insight into the practicalities of upper troposphere limb-sounding.

The investigation of cloud sensitivity involved four components: firstly, a review of upper tropospheric cloud occurrence (principally from SAGE II observations); secondly, the adaptation and integration with a line-by-line radiative transfer code of a state-of-the-art multiple-scattering model to synthesise measurements in the presence of cloud; thirdly, retrieval simulations for five representative cirrus clouds and, fourthly, an assessment of the impact of crystal shape on the millimetre-wave radiation field in the presence of cirrus.

2 Instrument Parameters and Cloud-Free Measurement Capabilities (RAL)

2.1 Forward and Retrieval Models and Approach to Error Analysis

Four existing radiative transfer models to simulate limb-emission spectra were modified specifically for MASTER simulations by RAL, IFE, IAP and Oxford University and intercompared. While certain discrepancies were found, their causes were understood and the accuracy of the RAL model (as used in most cloud-free simulations in the MASTER study) was demonstrated to be sufficient for the task. Optimal Estimation retrieval models were developed by RAL and IFE and diagnostics from basic retrieval simulations for the principal target species in each Band were intercompared. Only minor anomalies were found. Two further modifications were then made to both RAL and IFE schemes:

1. Joint retrieval with target species of "continuum coefficient" profiles at the low- and high-frequency ends of each Band, in anticipation of the need to accommodate a continuum of unspecified frequency dependence in the study of cloud sensitivity, and to make provision for possible error in the specified frequency dependences of the "dry air" and/or "anomalous water vapour" continua, as might prove necessary in a scheme to be applied to real flight data.

2. Provision for retrieval of the temperature profile and two pointing offset parameters from each limb-scan.

In regard to (1), attribution of "out-of-band" H_2O lines was an issue. It was decided to attribute them to H_2O for Bands A, C and E, for which there is an "in-band" H_2O line, so that H_2O is a retrieved species. (The impact of attributing them instead to the "continuum" was demonstrated for Bands A and C and found to be insignificant to retrieval of H_2O in both cases.[2]) As a consequence, the modelled frequency dependence of the "continuum" was close to linear in all five Bands, consistent with the adopted approach to continuum coefficient retrieval.

An extensive programming effort was needed to ensure that all potentially retrievable species in each Band could be handled (ie not only the principal species originally designated as target species) at adequate vertical resolution and with frequency sampling equivalent to the maximum (3 MHz) attainable. Considerable further effort was expended to optimise retrieval level spacings and *a priori* uncertainties for each species and Band individually. The issue of *a priori* uncertainty can be significant for optimal estimation retrievals. In certain specific cases, to confirm results from standard optimal estimation retrievals, these were repeated either with a much larger *a priori* uncertainty or with the "global fit" formulation, (effectively setting *a priori* uncertainty to infinity).

The relationship between limb brightness temperature and retrieved variables is not always linear, especially at low altitudes, meaning that a non-linear, iterative formulation of the retrieval equations would have to be implemented for inversion of real measurements made by MASTER. However, matrix algebra permits system noise on synthetic, measured spectra to be mapped directly onto the retrieved error covariance matrix. Since most other instrumental errors to be investigated were expected to cause relatively small perturbations on nominal spectra, "linear mapping" was adopted as a general philosophy for the study. Since the computational requirements for non-linear, iterative retrievals would have been prohibitive for a comprehensive study of instrument parameters, linear mapping offered the only practicable approach in any case. In the relatively few cases for which "linear mapping" was judged to be inappropriate, non-linear, iterative retrievals were performed in addition[3].

2.2 Instrument Specification

2.2.1 Spectral Parameters

The spectral coverage of MASTER has been examined in depth in terms of spectral resolution, the bandwidth of each receiver and the relative value of each Band to each retrieved quantity. It has been demonstrated that, although high (3 MHz) spectral resolution is needed to resolve weak lines in the upper stratosphere (eg ClO and BrO), 50 MHz is more than adequate for sounding the UTLS region (ie <20 km), and that 100 MHz would almost certainly suffice. To optimise information on measurable species, it is recommended that the following bandwidths be used for Bands A, B, C, D and E, respectively: 200.5–209.0, 294.0–305.5, 316.5–325.5, 342.25–348.75 and 497.0–506.0 GHz. In the case of Band B, this represents a significant increase in bandwidth over that originally specified. This is needed to target HNO_3 and BrO in addition to the previously designated target species for that Band. For both species, Band B measurements offer major benefits, allowing information from other Bands to be increased in precision and to be extended to lower altitudes.

Because antenna main-beam width is $\approx 1.5\times$ larger at 200 GHz than at 300 GHz, simulations showed the measurements in Band A to be generally inferior to those in other Bands for all constituents. Only for H_2O around $6-8$ km does Band A offer a worthwhile contribution, by adding height-resolved H_2O information below the range (<8 km) covered adequately by Band C. In the presence of significant high-altitude cloud, the lower sensitivity to cirrus of Band A would be a further advantage. However, a substantial (factor ≈ 2) decrease in beamwidth would be needed for Band

[2]In the case of Band E, the contribution to emission below 14km from out-of-band H_2O lines was both spectrally non-linear and large in relation to that from the weak in-band line. So, attributing out-of-band lines to H_2O did substantially improve the H_2O retrieval below 14km.

[3]Eg simulation of Band B pointing retrieval in the presence of a large (2 km) imposed bias and Band C H_2O retrieval sensitivity in the upper troposphere to various instrumental errors.

A to achieve 2 km vertical resolution in the troposphere. The use of the 203.3 GHz isotopic ($H_2{}^{18}O$) line further depends upon the assumption that the relative abundances of this and the main isotope ($H_2{}^{16}O$) are fixed, which needs to be verified.

Moreover, operational nadir-sounders (eg MHS, IASI) are expected to be able to sound H_2O in the middle and lower troposphere with vertical resolution and precision comparable to or better than that of Band A (ie < 2 km, <30 %).

2.2.2 Antenna

Sensitivity to a number of antenna parameters has been examined using a set of patterns supplied by ESTEC with diverse main-beam, near- and far-wing combinations, along with different assumptions concerning errors in measurement of the pattern and distortion after measurement. The study has clearly demonstrated that, to achieve its principal objective of retrieving high-quality information on H_2O, O_3 and CO in the upper troposphere as well as the lower stratosphere, no significant increase could be tolerated over the nominal main-beam width (achieved with the nominal antenna of 2.2 m height) and, rather, that highly desirable improvements in quality could come from decreasing main-beam width substantially. This might be achieved by a change in antenna pattern to produce a narrower main-beam width at the expense of increased side-lobes. However, although sensitivity to near- and far-wings of the antenna pattern has been shown to be low, if these are known perfectly, *knowledge* of the antenna pattern has been shown to be *vitally important* for UT sounding, resulting in stringent requirements being placed on the accuracy with which it is characterised pre-launch and on its stability. In terms of the systematic error budgets on retrieved species, the scenario of -35 dB noise and up to -20 dB non-linearity on antenna measurement was found to be unacceptable, but that of -45 dB noise and up to -30 dB non-linearity was found to be tolerable. Distortion occurring after measurement of the antenna pattern was found to be unacceptable at the 20μm RMS level, but to be tolerable once resulting errors were decreased by a factor four.

2.2.3 Pointing

Along with the antenna pattern, instrument pointing was anticipated to be a crucial issue for measurement quality in the upper troposphere where humidity, and hence limb brightness temperatures, increase very rapidly with decreasing tangent-height. Although random errors due to compression/expansion of the effective beamwidth by "pointing jitter" were found to be negligible, this expectation was fully borne out in the case of random fluctuations in tangent-height error between adjacent limb-views. It was shown that Gaussian fluctuations in pointing error with RMS as low as 100 m would still dominate over system noise in the random error budgets of key species in the UTLS, thereby prejudicing several measurement objectives. However, it was found that when random pointing jitter was filtered with a 6 km FWHM filter, preserving an RMS of 200 m on the filtered values, random errors on those UTLS profiles retrieved at high resolution (ie $\leq$2 km) from a single scan were substantially lower than for the Gaussian 100 m RMS case. Although species (principally ClO and BrO) retrieved at low resolution (ie $>$2 km) were adversely affected by filtering, the resultant errors still had an RMS substantially below that that due to system noise on an individual scan and varied randomly from one scan to the next, so would therefore be reduced by averaging over a number of scans (as required anyway for BrO to achieve worthwhile precision).

On the other hand, it was demonstrated that a comparatively large pointing bias (2 km) and drift (0.5 km) could be retrieved with rather high precision. It is therefore recommended that the control mechanism for the MASTER antenna be designed to minimise pointing jitter (ie maximise stability) at the expense of pointing accuracy, since the latter can be recovered in retrievals whereas the former cannot.

2.2.4 Radiometry

Sensitivity to a number of radiometric errors has been investigated (ie frequency-independent offsets and random noise on space and black-body views, non-linearity in radiometric gain, image side-band contribution, discontinuities at boundaries between acousto-optical spectrometers (AOSs), baseline ripples). The most significant errors were found to arise from 1 K frequency-independent offsets on space and black-body views, especially at low retrieval altitudes. Although these errors were to some extent absorbed into the retrieved continuum coefficients, they were nonetheless found to contribute substantially to systematic error budgets (nb H_2O and O_3 in the UTLS region). While it might not be feasible to impose a more stringent requirement on absolute radiometric accuracy, it is recommended that the utmost attention be given to this issue in the design of the MASTER optics and onboard calibration system, with a view to reducing radiometric offset errors below 1 K.

Certain other errors were found to be significant in specific cases, eg image side-band errors for BrO and ClO and AOS discontinuities for CO, and it should be borne in mind that results are only *indicative*[4]. However, with the exception of radiometric offset, it does not appear from the study to be necessary to increase the stringency of radiometric requirements. In the case of image-side band rejection, it was shown that some relaxation would be acceptable for current LO selections; moving from a uniform -30 dB rejection to a linear variation from -20 dB to -30 dB from lowest to highest IF frequency.

It was also demonstrated that, provided integration times for space and black-body views were at least 4$\times$ longer than for atmospheric views, the correlated noise from calibration views would not add significantly to system noise on individual limb-views.

2.3 Single-Scan Measurement Capabilities

2.3.1 Assumptions

Having investigated retrieval sensitivity to instrument parameters and having optimised key instrument parameters, measurement capabilities were assessed on the basis of the following assumptions, except where stated otherwise:

1. Contiguous spectral sampling over each recommended bandwidth at 50 MHz resolution[5].

2. Noise equivalent brightness temperature of 1K in a 50 MHz spectral interval sampled in 0.3s (equivalent to 4000 K single side-band system noise temperature) in every Band.

3. Nominal antenna pattern for each band (half-power beamwidths of 3.3, 2.3 and 1.65km in the 200, 300/325/345 and 500 GHz bands, respectively) and nominal limb-scan, from -2 km to 50 km, sampling at 1 km.

2.3.2 Pointing and Temperature Profile Retrieval

It was demonstrated through iterative, non-linear Band B retrievals that, in the absence of pointing jitter, a 2 km pointing bias could be recovered with high precision [6], a finding of major importance to

[4]Although the amplitudes of simulated errors conform with current expectations, in some cases frequency dependencies can be highly variable and it was only feasible to simulate a small set of cases within the scope of the study. (Eg the error pattern due to an incorrectly-specified image side-band contribution would change if the the LO frequency is changed; baseline ripples can take a variety of forms, comprising more than one sinusoidal component.)

[5]6 MHz was employed for Band E ClO and BrO to characterise errors for their weak, narrow lines adequately in the middle and upper stratosphere

[6]Upper and lower pointing offsets were both recovered to within $\approx$10 m, well within their estimated uncertainties of $\approx$50 m

the study. The impact of pointing jitter was found to markedly degrade the precision with which bias and drift could be retrieved when the jitter is filtered; to ≈90 m and ≈500 m, respectively, cf ≈30 m and ≈80 m in the absence of jitter and ≈80 m and ≈160 m when the jitter is unfiltered (200 m RMS). A significant contribution to the Band B pointing offsets retrieval and a substantial contribution to the temperature retrieval was discovered to come from spectral features other than the isotopic O_2 line near 298 GHz targeted for these purposes (ie from non-uniformly mixed species). However, in simulations in which tangent-heights were restricted to ≥10km and spectral coverage was restricted to 297.5−299.25 GHz, ie mainly to the O_2 line, pointing bias and drift were still retrieved with estimated uncertainties of <100 m and <300 m, respectively[7].

Taking into account also the systematic errors on pointing retrieval, 100 m and 500 m were concluded to be conservative estimates of the accuracy with which pointing bias and drift, respectively, could be recovered from Band B, provided that antenna pattern measurement errors can be controlled to the necessary degree. So these were the estimates carried forward into error budget calculations for temperature and constituent profile retrievals. It was also shown that, by exploiting the fact that all Bands contain strong O_3 lines, co-registration errors with respect to Band B could be retrieved from all other Bands from a single-scan with (system noise-induced) precision equivalent to ≤35 m on bias and ≤100 m on drift. Although full analysis of random and systematic errors was beyond the scope of this study.

For a retrieval level spacing of 3 km, the system noise on Band B retrieved temperature was found to be <2 K up to 30 km. If tangent-heights were restricted to ≥10 km and spectral coverage was restricted to 297.5−299.25 GHz, this was degraded to 3 K. Furthermore, the RMS random error on *standard* Band B retrieved temperature associated with filtered pointing jitter was 3–4 K. Systematic errors were found to vary from ≤2 K to ≤4 K, depending on assumptions about antenna pattern measurement error.

Although useful for the purpose of MASTER constituent retrievals, temperature information of this quality would be unlikely to compete with that from IR limb- and nadir-sounders flying concurrently (eg IASI on METOP). In fact, it is likely that Band B temperature retrievals would offer only a modest (if any) improvement on the quality of *a priori* temperature information available from these other sources. Arguably the *best* temperature information from MASTER was shown to come from O_3 and other lines in Band E and Band C, for which uncertainty induced by system noise was shown to <1.5 K up to 30 km. However, a full random and systematic error analysis on temperature profiles retrieved from Bands other than B was beyond the scope of this study.

2.3.3 Constituent Profile Retrieval

Retrieval diagnostics from mid-latitude simulations for individual Bands have been examined in depth. The principal differences at equatorial and polar latitudes are the penetration depths into the troposphere of H_2O, O_3 and CO retrievals, which are controlled by the geographical pattern of upper troposphere humidity. In terms of geometric height, retrievals of a given precision occur several km nearer to the ground at polar latitudes but several km further from the ground at the equator. Other features reflect changes in profile shape on moving away from mid-latitudes. The most dramatic difference occurs in the case of ClO at polar latitude, for which “chemically enhanced” springtime conditions radically increase single-scan precision below 30 km (to <10% at 3 km resolution around 20 km).

Indicative random and systematic error budgets for mid-latitude conditions have been compiled for each target species and Band. On the assumption that scan motion would be damped such that the filtered pointing jitter with 200 m RMS is representative, system noise dominates random error

[7] In this simulation, contamination of the O_2 line by several weak O_3 lines is no longer characterised by measurement of adjacent, strong O_3 lines, which adversely effects precision estimates for pointing (and temperature).

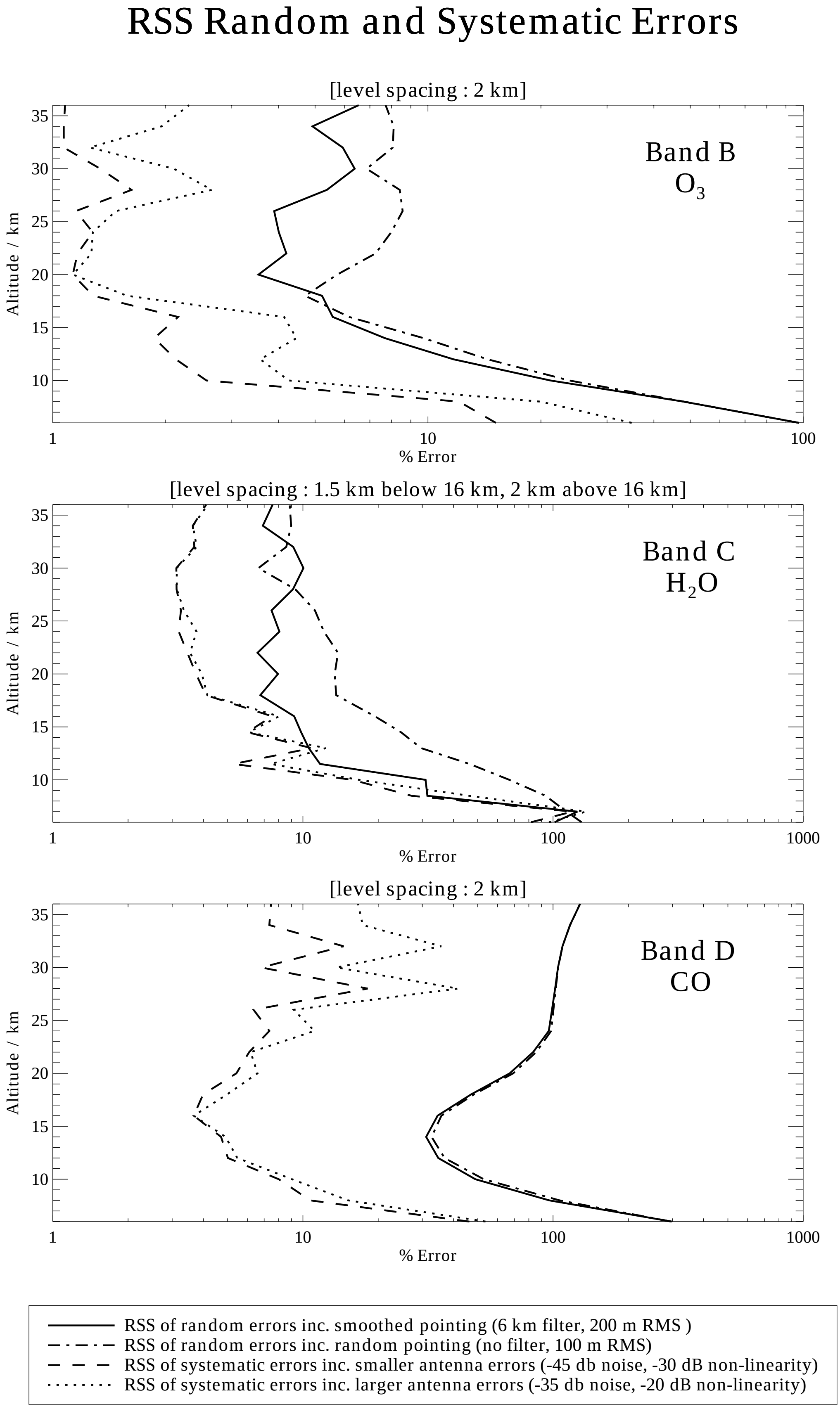

Figure 1: Curves of root-sum-squares (RSS) of random and systematic error budgets for O_3 retrieved from Band B, H_2O retrieved from Band C and CO retrieved from Band D.

budgets in most cases, although filtered pointing jitter is larger in the cases of: Band A H_2O <7 km; Band C H_2O <34 km; Band B O_3 >16 km and Band E O_3 >26 km. Useful precision (10's%) from an individual limb-scan is attainable on H_2O (at 1.5 km resolution), O_3 and CO (at 2 km resolution) in the upper troposphere from Bands C, B and D, respectively (Fig.1). Useful single-scan precision is also obtained on these three species throughout the stratosphere and on N_2O, HNO_3, (CH_3Cl) and ClO in different height regions within the stratosphere. The quality of lower stratospheric O_3 retrievals was demonstrated to be impressively high for Band E: $<15\%$ precision at 1km resolution between 18 and 26 km. Although the single-scan precision on BrO (and HOCl) is comparatively poor, useful precision would be obtained on daily zonal-mean stratospheric profiles sampled at 10° latitude: 20% (and 30%) at 4 km resolution between 24 km and 36 km (26 km and 34 km).

Systematic errors have been examined carefully, especially in regard to upper tropospheric retrievals of H_2O, O_3 and CO (Fig.1) and stratospheric retrievals of ClO and BrO. The factors which generally limit systematic errors on these and other constituents are: antenna pattern measurement; radiometric zero and gain offsets; pointing bias and drift. For all Bands except E[8], antenna pattern measurement errors are critical and two cases have been considered for error budget purposes: one in which measurement noise and non-linearity are, respectively, -35 dB and -20 dB and the other in which they are 10 dB lower. For all Bands except B[9], errors on pointing bias and drift are important, and conservative values of 100 m and 500 m, respectively, have been used for constituent error budget calculations. Radiometric zero and gain offsets are important in most cases. For error budget purposes, offsets equivalent to 0.5 K on both zero and black-body views have been used, in line with the 1 K requirement on absolute radiometric accuracy specified in the Requirements Document. In all cases, systematic errors exclusive of antenna pattern measurement have been combined in an RSS way. The "high" and "low" cases of antenna pattern measurement error have been included into the RSS to generate two estimates of total systematic error. With the exception of Band C H_2O ≤ 16 km, RSS systematic errors in the height ranges of importance were found to be $\leq 10\%$ for the "low" case.

2.3.4 Multi-band Retrievals

For species measured in common by more than one Band, the incremental improvement to precision from adding other Bands to the primary Band has been gauged by using the retrieved error covariance matrix from the first Band as *a priori* for the second, and so on. While for CO (Band D only), ClO (Band E primarily) and HOCl (Band C primarily) the improvements from adding additional Bands were negligible, for all other species (H_2O, O_3, N_2O, HNO_3, CH_3Cl and BrO) the improvements were significant in at least part of the height range.

2.4 Measurement of Horizontal Structure in Upper Troposphere Humidity

A series of simulations have been performed to investigate how well horizontal as well as vertical structure in the orbit plane (ie line-of-sight plane) can be recovered in the presence of a tropopause fold. The Band C retrieval scheme was able to capture most important structure in the H_2O cross-section down to $\approx$250 ppmv (the $\log_{10} = -3.6$ contour in Fig.2). Results obtained using an identical approach for Band A were less satisfactory. There are several ways in which the state-of-the-art Band C simulations performed in this study could be further improved, but they have clearly demonstrated MASTER's capability to resolve horizontal structure on a scale of several 100's km in the along-track direction. Horizontal structure in the across-track direction is determined by inter-orbit spacing ($\sim$1400 km at the equator) though. This asymmetry between along- and across-track sampling could, in principle, be reduced by viewing at several azimuth directions with multiple receivers.

[8] Main beam width is substantially narrower for Band E.

[9] Pointing offsets (and temperature) have been retrieved jointly with constituents in Band B.

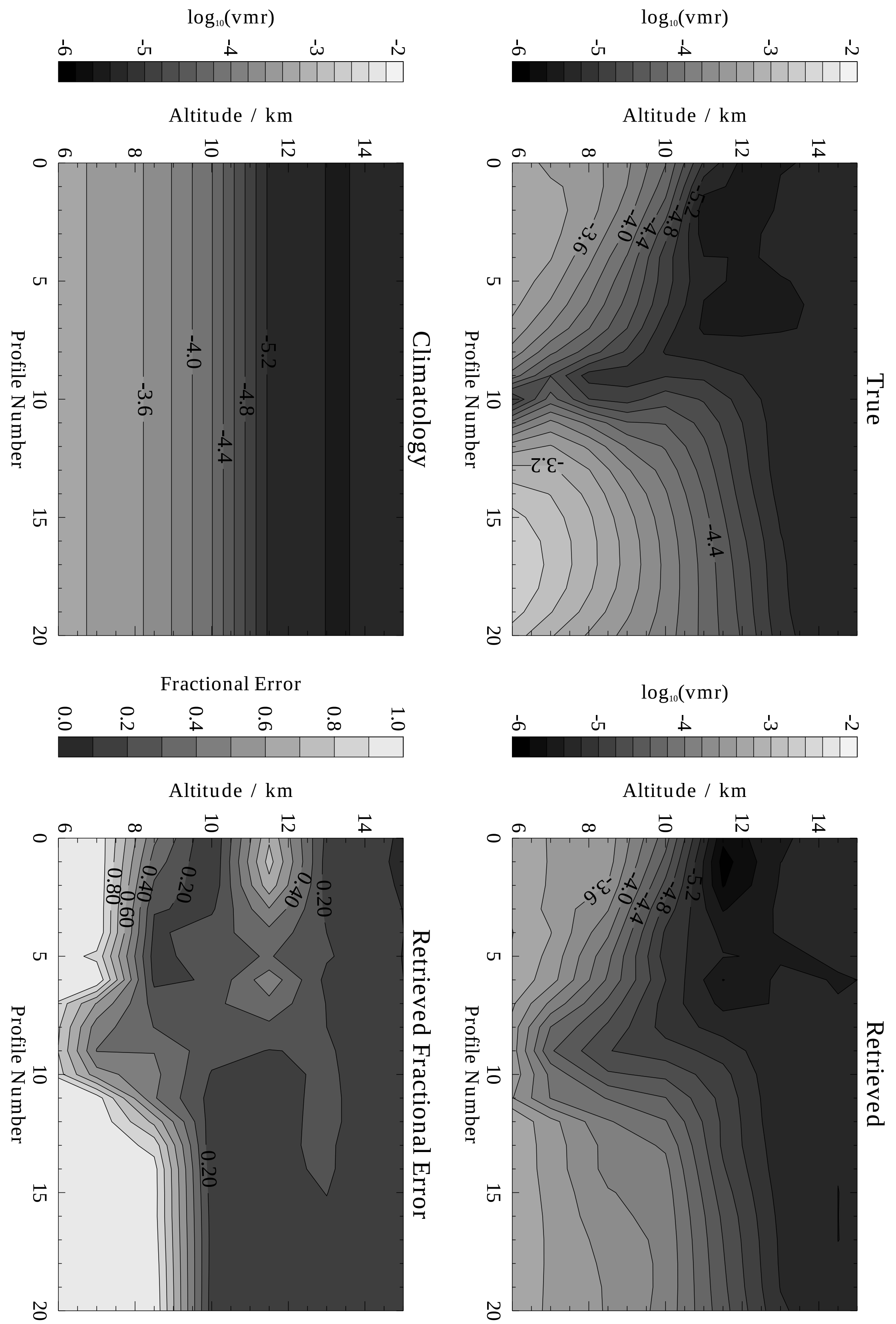

Figure 2: Band C 2-D cross-section retrieval. True and retrieved H_2O fields (in log of mixing ratio) are shown, as well as the climatology used as a first guess and the fractional retrieved errors.

3 Upper Troposphere Humidity Retrieval from the Millimetre-wave Atmospheric Sounder (IAP)

Although the Millimetre-wave Atmospheric Sounder (MAS) was not designed to measure at low altitudes, many limb-scans recorded during three ATLAS missions on the space-shuttle extended down to 5 km. Atmospheric limb-opacity remained semi-transparent down to this tangent-altitude across the 400 MHz widths of both side-bands (centred at 201.95 and 204.35 GHz) of the receiver designated for stratospheric ClO measurements.

Double side-band measurements near 204 GHz by the Microwave Limb Sounder on UARS had been found to contain information on the distribution of upper tropospheric humidity (UTH), arising from emission in the wing of the strong H_2O 183 GHz line and the H_2O continuum. The intention of this study was to determine the extent to which this might also be possible for MAS.

Simulated retrievals showed considerable promise, in terms of both the accuracy and vertical resolution achievable. However, in the lower stratosphere, where the radiance contribution from H_2O should be much smaller than that due to dry air, measured radiances showed a large excess over predicted radiances. In order to compensate, retrieved water vapour at these altitudes would have been unrealistically large (several orders of magnitude larger than expected), and this precluded the retrieval of reliable UTH values.

Although no single factor could be identified to explain the discrepancy, it was concluded that a combination of uncertainties in several key instrumental parameters was probably to blame. Inadequate knowledge of the antenna pattern and absolute pointing were identified as likely candidates, although uncertainty in the dry air continuum could also have contributed. The need for highly accurate knowledge of antenna pattern and pointing confirmed two of the main findings from the MASTER retrieval simulation study.

Measuring over a 400 MHz bandwidth in double side-band mode did not allow MAS to discriminate between 183 GHz line wing and continuum emission, making retrieval of UTH very sensitive to errors in knowledge of continua of all types (instrumental, dry-air and H_2O). This finding from MAS provides support for the MASTER approach of single side-band measurements over broad ($\sim$10 GHz) bandwidths, to minimize sensitivity to continua.

4 Sensitivity to Cloud (IFE/MI Bonn)

The first part of this investigation was a review based on climatological cloud statistics of SAGE II and the International Satellite Cloud Climatology Project with respect to cloud coverage and altitude as well as cloud vertical and horizontal extent. The published data allowed an estimation of the abundance of cirrus clouds. According to SAGE II climatology, in the altitude range targetted by MASTER (i.e. $>$6 km), the abundance of subvisual clouds is around 20 % at mid-latitudes and around 45 % in the tropics. The abundance of optically thick cirrus clouds is around 15 % at its maximum in the tropics.

The results of a number of field campaigns with respect to the microphysical properties of different types of cirrus clouds were summarised. This allowed a representative set of typical cirrus clouds to be identified for use in retrieval simulations. All five investigated cirrus clouds belong to the type defined by SAGE II as optically thick cirrus, subvisual clouds showed no impact upon the MASTER measurements.

The state-of-the-art multiple-scattering radiative transfer model SHDOM was adapted and integrated with the present IFE radiative transfer model to allow realistic simulations of cloud effects to be performed for the MASTER spectral range and measurement geometry. The newly-developed model was shown to be consistent with the IFE standard forward model in the clear sky case.

Radiative transfer in the presence of clouds was validated in up-looking geometry against the MWMOD multiple-scattering model of the University of Bonn and against the BEAM model of the University of Berne. The agreement with MWMOD was very good, although BEAM yielded slightly lower brightness temperatures. This was attributed to the fact that the BEAM model included extinction, but not scattering into the beam.

Broadband calculations for limb-geometry with the cloud radiative transfer model showed that, because scattering predominates over absorption for cirrus, brightness temperatures can either be raised or lowered by a cirrus cloud, depending on cloud altitude and size distribution. Even at the same altitude, brightness temperatures were raised by one cloud and lowered by another. The most important parameters to characterise the cloud were found to be ice mass content and median mass equivalent sphere radius. The width of the cloud particle size distribution (α parameter) was found to be relatively unimportant.

The cloud radiative model based on SHDOM was used to synthesise measurements for a set of five test cases. These were then used to perform retrievals. Retrievals of upper troposphere target species were affected by clouds with a median mass equivalent sphere radius $\geq 80\,\mu$m and ice mass content $\geq 20\,\mathrm{mg\,m^{-3}}$. It was not possible to pinpoint thresholds on cloud properties more precisely from the limited number of simulations performed here, since the effect of cirrus on MASTER measurements depends upon a combination of the ice mass content, the median mass equivalent sphere radius and the altitude of the cloud. The H_2O retrieval in Band A is somewhat less affected by a given cloud than that in Band C, due to differencies in the optical properties of both water vapour and cirrus in the two bands.

The retrieval of an absorption coefficient offset was not able to compensate for the effect of cirrus clouds on gaseous retrievals for two reasons. Firstly, scattering is sufficiently strong to make the treatment of the cloud as a “grey absorber” inadequate. Secondly, the cloud introduces a horizontal inhomogeneity which cannot be ignored. It was concluded that a single-scattering representation of cirrus within the retrieval model might offer more promise, in regard to retrieval of gaseous constituents. Although, concerning the possibility of retrieving accurate information about cirrus clouds themselves, it was concluded that this would be difficult from limb measurements.

The cloud radiative transfer model used in this study was limited to spherical particles. An assessment of the influence of particle shape on the modelled brightness temperatures was performed by MI Bonn. The conclusions were that crystal shape and orientation were important to both the intensity and polarisation of the radiation field, and that the assumption of spherical particles was an important limitation of the cloud model used in the main study. Nevertheless, that model, which coupled multiple-scattering to limb-viewing geometry for the first time, allowed a valuable first assessment to be made of cirrus cloud impact on MASTER.

5 Conclusions

1. The MASTER instrument parameters have been investigated and optimised to sound UTLS composition, and its measurement capabilities have been demonstrated in an extensive set of retrieval simulations.

2. Penetration into the troposphere is governed by H_2O and is therefore dependent *inter alia* upon latitude and season. For the cases simulated, the lower limit was $\approx$6 km at mid-latitude, and several km higher and lower at equatorial and polar latitudes, respectively.

3. The vertical resolution, precision and accuracy with which H_2O, O_3 and CO could potentially be retrieved in the upper troposphere and stratosphere from individual limb-scans has been

demonstrated, and also for retrievals of stratospheric N_2O, HNO_3, ClO and BrO. For the assumed instrumental errors, single-scan[10] precision was found to be several 10's% in the UT for retrieval of H_2O at 1.5 km resolution and O_3 and CO at 2 km resolution, while systematic errors were found to be somewhat lower ($\leq$ 10% for O_3 an CO). So it is anticipated that single-scan retrievals would allow MASTER to meet its scientific objectives for all target species except BrO, for which daily zonal averaging would be needed to obtain adequate precision.

4. The capability to resolve horizontal structure in the UTH field has been demonstrated through retrieval simulations in the presence of a tropopause fold.

5. The critical importance of the antenna has been confirmed. It has been shown that knowledge of the antenna pattern is especially vital and that a factor 2 decrease in main-beam width would be very desirable for UT measurements. This could perhaps be obtained at the expense of increased side-lobes, provided these could be characterised with sufficient accuracy.

6. Pointing jitter has been found to be critical to the precision on profiles retrieved at high vertical resolution in the UTLS region. It has been shown that pointing accuracy can be sacrificed if necessary to maximise stability, since it should be recoverable *a posteriori* through retrieval of pointing bias and drift to accuracies of $<$100 m and $<$500 m, respectively.

7. The 200 GHz receiver is significant only to mid-tropospheric H_2O retrieval. It potentially extends downwards by several km the height range over which the H_2O profile can be retrieved from the 325 GHz receiver alone and also has a higher tolerance to cirrus.

8. From the investigation of MAS 204 GHz data, it was concluded: (i) that UTH retrievals are very sensitive to knowledge of certain instrumental parameters, particularly the antenna pattern and pointing, corroborating two of the principal findings of the MASTER simulation study, and (ii) that these parameters are not known well enough to allow meaningful UTH retrievals from MAS 204 GHz data.

9. MAS double side-band measurements over 400 MHz were also shown to be sensitive to continua (nb that due to dry air), confirming the benefit of the approach adopted for MASTER: to measure in single side-band over broad ($\approx$10GHz) bandwiths, in order to minimize sensitivity to continua.

10. A multiple-scattering model (SHDOM) with the unique capability to simulate limb-viewing geometry was adapted and implemented within the MASTER study to synthesise measurements in the presence of cirrus cloud.

11. Simulations were performed for five cirrus clouds of 2 km vertical thickness and 75 km horizontal extent, typical of those detected by SAGE II. Those with ice mass content $\geq$0.02 g m^{-3} were found to have a significant impact on UT retrievals.

12. In the height-range targeted by MASTER, the frequency of occurrence of clouds classified by SAGE as "optically thick" is $<$15%, except in the tropics (where it peaks at $\approx$15% near 12 km) and at northern latitudes around 60° (where it approaches 20% $\leq$7 km). But, taking into account the size distributions of cirrus detected in mid-latitude field campaigns, the frequency of occurrence of cirrus clouds *which would have a significant impact on MASTER UT retrievals* appears to be comparatively low ($<$10%) at all latitudes.

[10]The time taken for a single scan spanning the troposphere and stratosphere is commensurate with an along-track spacing of $\approx$100 km between scans. A scan range more restricted to the UTLS would permit closer along-track spacing.

13. Cirrus scattering was found to predominate over absorption, so that limb brightness temperatures could either be elevated or depressed by cirrus, depending on circumstances, and cirrus could not be handled simply as a *grey absorber*. Moreover, for clouds of opacity sufficient to perturb limb brightness temperatures, multiple scattering was found to be significant. However, the frequency-dependencies of multiple- and single-scattering were found to be linear within each MASTER band, suggesting that joint retrieval of cirrus parameters using a single-scattering treatment might allow a further reduction in the range of clouds to which gaseous retrievals are sensitive[11].

14. The complicated relationships between limb brightness temperature and cloud properties would make it difficult to retrieve quantitative information about cirrus itself. In addition to the location, ice water content and particle size distribution of a cloud, crystal shape and orientation were also found to impact significantly upon both the intensity and polarisation of millimetre-wave radiation viewed at near-limb geometry in the presence of cirrus. It is therefore concluded that nadir-geometry is preferable for cloud observations.

6 Further Work

In this study, MASTER's potential measurement capabilities have been examined in considerable detail, to a depth unprecedented for a space instrument prior to launch. Recommendations for further work arising from this study fall into three categories: (i) scientific studies; (ii) technology development and (iii) development and deployment of a MASTER airborne simulator. The major recommendations for further scientific studies are:

1. Refine UT retrieval scheme, to seek to improve H_2O retrieval quality at the lowest altitudes.
2. Account explicitly for horizontal gradients in the forward and retrieval models used in 2-D cross-section simulations, and extend to other cases.
3. Compare MASTER's UTLS retrieval capabilities with those of METOP nadir-sounders and limb-sounders in other planned missions.
4. Perform detailed error analyses on temperature profiles retrieved from non-uniformly mixed gases (nb O_3).
5. Investigate whether the impact of (multiply-scattering) clouds on retrieval of gases could be reduced by using a single-scattering cloud model and joint retrieval of appropriate cloud parameters.
6. Establish more precisely the range of conditions in which sensitivity to cirrus is significant.

The major technical issues arising from this study are:

1. The extent to which main-beam width could be reduced to increase vertical resolution, in conjunction with the accuracy with which the antenna pattern could be characterised prior to launch and subsequently maintained.
2. The potential impact of relaxation from 50 to 100 MHz resolution on selection of spectrometer-type, power and mass.

[11]While allowing the radiation field to be simulated adequately, cirrus parameters retrieved using a single-scattering treatment might not necessarily give an accurate representation of the cloud physical properties.

3. Design of the instrument and on-board calibration system to meet the challenging requirement of 1K absolute radiometric accuracy.
4. Possible use of MMIC technology for multiple receivers to measure simultaneously in several azimuth directions.

Arguably the most important next step for MASTER will be the development and deployment of an airborne simulator to evaluate the UTLS measurement capabilities of a broad-band, millimetre-wave limb-sounder in the field.