Instrumental Requirements for a Submillimeter-Wave Limb Sounder

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International Workshop on Submillimeter-wave Observation of Earth's Atmosphere from Space, Tokyo, January 27–29, 1999

The Institute of Remote Sensing has recently completed a study on the retrieval of data from sub-millimeter limb sounding. The study was financed by the European Space Research and Technology Center (ESTEC) and was conducted in collaboration with the Rutherford Appleton Laboratory, UK, and the Institute of Applied Physics, University of Bern, Switzerland. The results can be found in the extensive final report *Bühler et al.* [1999], which will be available from ESTEC shortly. A major part of the work was a comprehensive assessment of the impact of instrumental parameters and *uncertainties* in instrumental parameters on the quality of the retrieved data. Those findings that should be of general interest are reported here. The emphasis is put on those findings that are of particular significance for the JEM/SMILES instrument.

1 The SOPRANO Instrument

SOPRANO is planned to be a Submillimeter limb sounder dedicated to the measurement of trace gas species that take part in the ozone cycle. Seven bands are currently investigated (Table 1), but the actual instrument will probably have only three, the Bands A, B, and F. The instrument is in many ways similar to JEM/SMILES, as can be seen from the comparison of instrumental parameters in Table 2. The platform altitude of SOPRANO is almost twice that of JEM/SMILES, requiring a considerably narrower viewing angle—and hence larger antenna—to achieve the same width of the field of view at the

Table 1: SOPRANO frequency bands and main target species. The core instrument as currently planned consists of Bands A, B1/B2, and F.

Band	**f [GHz]**	**Species**
A	497.5 – 504.75	$\mathbf{O_3}$, **ClO**, $\mathbf{CH_3Cl}$, (**BrO**), N_2O, H_2O, (HNO_3), (COF_2)
B1	624.6 – 626.5	**HCl**, O_3, HOCl, (HNO_3), (BrO), (HO_2)
B2	627.95 – 628.95	**HOCl**, O_3, HNO_3, (COF_2)
C1	635.6 – 637.4	$\mathbf{CH_3Cl}$, O_3, HNO_3, HOCl, HO_2
C2	648.0 – 652.0	**ClO**, $\mathbf{O_3}$, N_2O, HNO_3, (H_2CO), (HOCl), (HO_2), (NO_2), (BrO)
D	730.8 – 732.25	**T**, O_3, Scan, $\mathbf{HNO_3}$, (CH_3Cl), (HO_2)
E	851.5 – 852.5	**NO**, O_3, N_2O, (HNO_3), (NO_2), (H_2O_2)
F	952.0 – 955.0	**NO**, **T**, Scan, O_3, N_2O, (HO_2), (HNO_3), (CH_3Cl), (NO_2)
G1	685.5 – 687.2	**ClO**, O_3, (HNO_3), (HOCl), (H_2O_2), (COF_2), (NO_2)
G2	688.5 – 692.0	**CO**, $\mathbf{CH_3Cl}$, ClO, O_3, HNO_3, (HO_2), (HOCl), (HCN), (NO_2), (H_2O)

Table 2: Instrument specifications for JEM/SMILES and SOPRANO. The former are taken from *Masuko et al.* [1997] and the NASDA/CRL leaflet, the latter are taken from *Lamarre* [1997].

	JEM/SMILES	SOPRANO
Spectral resolution	1.4 MHz	3 MHz
Platform altitude	400 km	800 km
Nominal scan range	10–60 km	10–50 km
Antenna size	0.6 m	1.0 m
-3 dB beam width at tan. point	2 km	2.7 km
System noise temperature	700 K	2372–11384 K

tangent point. In fact, if one compares the antenna diameters of 1.0 and 0.6 m with the platform altitudes of 800 and 400 km, and assumes that the antenna efficiency stays the same, it turns out that the field of view should be about 12 % narrower for JEM/SMILES than for SOPRANO. How the calculation is done explicitly is described in *Bühler* [1999].

The—by far—most significant difference between the two instruments is that JEM/SMILES will have a much lower noise temperature than SOPRANO because it will use the SIS receiver technique. Because the measurement noise for JEM/SMILES is so much lower, systematic errors which may be introduced by imperfectly known instrumental parameters can play an even greater role than in the case of SOPRANO. What is *not* expected to change, however, is the *relative* impact of the different instrumental parameters. In other words, instrumental parameters that are critical for SOPRANO are likely to be also critical for JEM/SMILES and parameters that are uncritical for SOPRANO are likely to be uncritical for JEM/SMILES.

2 The Linear Mapping Method

The impact of different instrumental parameters on the retrieval was investigated by *linear mapping* of error terms. This method makes use of the measurement contribution function matrix

$$\mathbf{D} = \partial\hat{\mathbf{x}}/\partial\mathbf{y} \tag{1}$$

where $\hat{\mathbf{x}}$ is the retrieval estimate of the state vector (i.e., the retrieved atmospheric profile) and $\mathbf{y}$ is the measured spectrum. The contribution function matrix is calculated once within the retrieval model, which is based on the optimal estimation method as described by *Rodgers* [1990], using logarithmic VMR coordinates and a diagonal a priori error covariance matrix with all diagonal elements equal to one. (Roughly equivalent to 100 % a priori error.) Different spectral error terms $\Delta\mathbf{y}$ can be mapped onto retrieval error patterns $\Delta\hat{\mathbf{x}}$ according to

$$\Delta\hat{\mathbf{x}} = \mathbf{D}\Delta\mathbf{y}. \tag{2}$$

For some of the investigated errors, such as the impact of the unwanted sideband, there is only one spectral error pattern $\Delta\mathbf{y}$ which is then mapped onto a retrieval error pattern $\Delta\hat{\mathbf{x}}$. For other error terms the spectral error $\Delta\mathbf{y}$ has to be regarded as statistically distributed. An example is the pointing uncertainty. For these errors, a set of 100 spectral error patterns $\Delta\mathbf{y}_i$ was generated and mapped onto retrieval error patterns $\Delta\hat{\mathbf{x}}_i$. From this set of error patterns root mean square (RMS) errors were computed. The assumed spectral noise is that of a single scan. Except where stated otherwise the retrieval altitude resolution is 2 km. Because this method makes a linear approximation, the errors can be very easily scaled to slightly different values of the instrumental parameters.

3 Investigated Parameters and Results

3.1 Antenna

3.1.1 Antenna Efficiency

Antenna patterns with different near and far wing contributions were investigated under the assumption that the antenna pattern is perfectly known in the simulated measurement and in the retrieval. Investigated were near wing contributions from 1 to 10 % and far wing contributions from 0 to 4 %. The nominal case for SOPRANO is 4 % near wing and 1 % far wing.

The result is that the actual shape of the antenna pattern is relatively uncritical, if the following three conditions are true: Firstly, the shape is well known, secondly, the FHHM stays the same, and thirdly, the scan goes all the way down into the opaque region of the atmosphere.

3.1.2 Far Wing Knowledge

The knowledge of the antenna pattern is of critical importance for accurate retrievals. However, the actual antenna pattern is known only to a certain extent. This was simulated by using antenna patterns which had been degenerated by added noise. The noise on the antenna measurement is critical, because it limits the sensitivity of the antenna pattern measurement, and hence the angular range where the pattern can be determined. Also simulated was the effect of an antenna distortion. Investigated were the cases of -35 and -45 dB noise on the antenna measurement and of 2.5 and 10 μm antenna distortion.

The sensitivity of the antenna measurement turns out to be one of the most critical parameters. If there exists a significant far wing it must be covered by the pre-launch antenna measurement. If one assumes 0 % contribution from the far wing, then -35 dB sensitivity of the antenna measurement is good enough, but for the nominal case of 1 % far wing, the -35 dB sensitivity already has a significant impact on the retrieval, whereas the -45 dB case shows no impact.

The antenna distortion of 10 μm, on the other hand, is tolerable.

3.2 Pointing

Limb sounding instruments are very sensitive to uncertainties in the tangent altitude. The tangent altitude information provided by the satellites attitude control system is generally not accurate enough, therefore a tangent altitude offset is introduced in the retrieval.

3.2.1 Pointing Accuracy

Varying errors in the pointing direction during the limb scan will lead to errors in the tangent altitude associated with individual spectra. This may have a critical impact on the retrieval of trace gases from the limb measurement. Two cases were studied, firstly, the case of ± 200 m random pointing offsets, and secondly, the case of correlated random pointing with 200 m RMS. The latter can be achieved technically by an increased delay in the antenna control loop. It was simulated by convolving the first case with a filter of 6 km full width at half maximum (FWHM) and then scaling the result to 200 m RMS). The retrieval altitude grid is important for the impact of this parameter, therefore two different cases, 2 and 4 km grid, were investigated.

This is the the most critical parameter in most investigated cases. The case of ± 200 m random pointing offsets leads to intolerable errors for the 2 km grid retrieval. At least, both increasing the delay in the antenna control loop and degrading the retrieval grid to 4 km brought a significant improvement. However, combining these two options gave no further improvement, on the contrary, errors in the 4 km grid retrieval sometimes even got worse for the correlated pointing errors.

The conclusion is that the pointing error should be significantly smaller than 200 m for each individual spectrum. If this is technically not feasible, a smoothing of the pointing error distribution by increasing the delay in the antenna control loop should be considered. The size of the necessary delay depends on the retrieval altitude grid.

3.2.2 Pointing Stability

It is assumed, that the SOPRANO instrument scans continuously over an altitude range of 1 km within 0.3 seconds during its nominal scan. This is simulated in the forward calculations by a convolution of the nominal antenna pattern with a boxcar function with 1 km width. Irregularities in the scan or pointing instability will lead to expanded or compressed effective antenna patterns, which can be simulated by doing the convolution with wider or smaller boxcar functions. Investigated was the effect of random variations of $\pm$ 200 m, which turns out to be a tolerable value.

3.2.3 Coregistration Error

Due to the coregistration error the scan offsets can be different for different bands. If the scan offset is solely determined in bands with temperature and pressure retrieval and then applied to other bands, this may lead to a scan offset error in the other bands. Investigated was the effect of 200 m scan offset, with and without a simultaneous scan offset fit. Without the scan offset fit, the 200 m offset has a large impact, but it is suppressed to a large degree if the scan offset fit is included. The conclusion is that this is also not a critical parameter.

3.3 Radiometric Errors

3.3.1 Baseline Ripples

Instrument non-linearities, imperfect calibration processes, and other unknown effects usually cause remaining structures on the spectral baseline, so called 'baseline ripples'. This was simulated by adding to the spectra sinusoidal offsets with an amplitude of 0.1 K and periods of 100 and 400 MHz. Depending on what causes the baseline ripple, the phase can either be assumed as constant during a single scan, or as randomly distributed during a single scan. Both cases were studied.

It turns out that the ripples with 400 MHz period have a larger impact than those with 200 MHz period, but the impact of both is rather uncritical. However, it has to be pointed out that 0.1 K amplitude of the ripples represents already quite a good suppression of baseline structure.

3.3.2 Baseline Discontinuities

Current technology does not allow to construct AOS that cover a bandwidth of more than 2 GHz with the desired resolution. The spectrometer for wider bands therefore has to consist of two or more adjacent AOS modules, which may lead to discontinuities in the spectral baseline. This was simulated by a sawtooth function from -0.2 K to +0.2 K every 2 GHz. Since this parameter will be a fixed property of the instrument, the RMS error for a large ensemble is not meaningful. Therefore, only 20 cases, with each phase shifted by 100 MHz, were investigated.

The investigation shows that the impact is stronger for weak spectral lines, as could be expected, and that the worst case is represented by discontinuities near the center of the line of interest. Hence, the impact of discontinuities can easily be minimized by an appropriate placement of the AOS modules.

3.3.3 Impact of Unwanted Sideband

The SOPRANO instrument is designed as a single sideband receiver. Nevertheless, the rejection of the unwanted sideband can never be perfect, which means that the unwanted sideband will still appear to some degree in the measured spectrum. Investigated was the nominal case of 20 dB rejection. This means that a 200 K line in the unwanted sideband will still appear with 2 K in the measured spectrum.

The impact of the unwanted sideband depends very strongly on the LO frequency, therefore, results can be only indicative. In cases where the unwanted sideband contains strong spectral lines the impact can be quite severe. If possible, the LO frequencies should be optimized so that the unwanted sideband contains no strong spectral features. If both sidebands should be used alternatively for measurements this is not possible, so in that case a sideband suppression of significantly better than 20 dB (e.g., 30 dB) is necessary.

The spectrum in the unwanted sideband can be included in the modelling, therefore a very high sideband suppression is not strictly necessary. However, in that case the crucial parameter becomes the *knowledge* of the sideband ratio. A sideband suppression of less than 20 dB is acceptable, if the sideband ratio knowledge is 30 dB.

3.3.4 Calibration Errors

Errors in the determination of the calibration load temperature and instrument non-linearities will lead to incorrect scaling, offsets, and non-linearities in the atmospheric spectra. Three cases were studied, firstly, a 1 K error at 300 K (incorrect scaling), secondly, a 1 K offset, and thirdly, a quadratic error of 0.2 K at 150 K.

It turns out that the 1 K offset can introduce a significant error in the retrieved VMR profile. The error intoduced by the 0.2 K quadratic error, on the other hand, is small (partly because its 0.2 K magnitude is small).

3.3.5 Correlated Noise

The hot and cold calibration measurements themselves will also contain noise. This noise will result in correlated noise patterns on the calibrated spectra during one atmospheric scan. Assumed was an integration time of 2 seconds for the calibration measurements, corresponding to 10× the atmospheric integration time. Under these conditions, the error introduced by correlated noise is comparable in magnitude to the error introduced by direct measurement noise. Although this is quite significant, the correlated noise error was not judged as critical, because it is of a statistical nature and will decrease in the same way as the direct noise error when data is averaged.

3.4 Temperature Uncertainty

Although this is not an instrumental parameter, it was also investigated how errors in the assumed atmospheric temperature affect the retrieval. Because weighting fuctions with respect to temperature were already available, the temperature error could be evaluated directly, without using the linear mapping method. Two cases were studied, firstly, 3 K uncorrelated temperature error, sencondly, a 3 K temperature offset (corresponding to the first case with 100 % correlation). If the atmospheric temperature is treated in this way, it has quite a significant impact on the retrieval accuracies. However, it is expected that the impact of temperature uncertainties can be minimized by simultaneous temperature retrieval within each band. This topic is currently under further investigation.

4 Summary and Conclusions

Summary plots make it possible to directly compare all significant instrument parameter errors. Two examples are given in Figure 1 and Figure 2. From these summary plots, together with the investigations described in the last section, we can rate the instrumental parameters in the categories ‘most critical’, ‘slightly less critical’, and ‘relatively uncritical’, as follows:

4.1 Most Critical Parameters

- Antenna pattern knowledge (far wing must be covered, requires −35 dB noise or better)
- Pointing accuracy (should be better than 200 m, increased delay in antenna control loop helps)
- Unwanted sideband (the suppression should be significantly better than 20 dB if there are strong lines in the sideband)

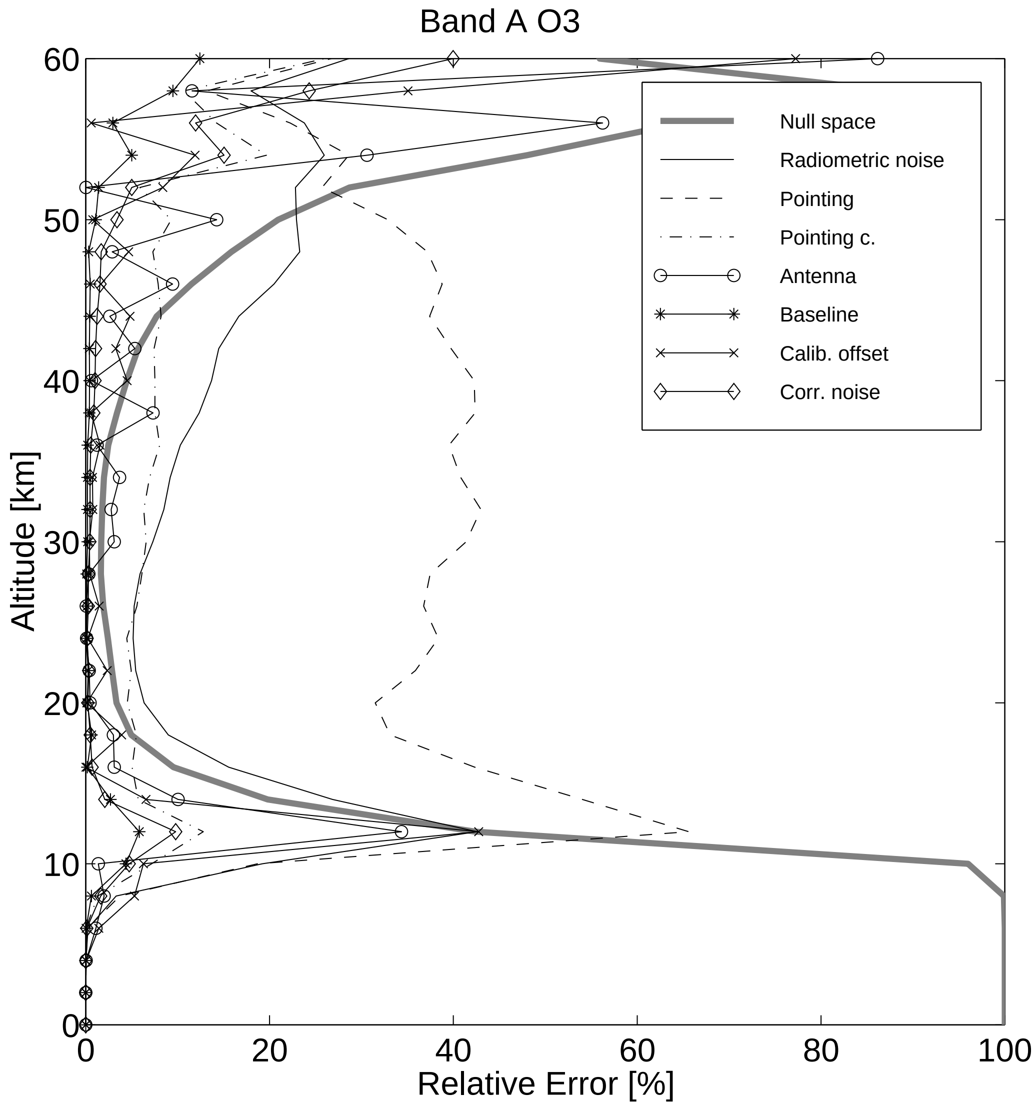

Figure 1: Error summary for the retrieval of O_3 near 500 GHz. By far the most critical parameter is the pointing accuracy (dashed line). Its impact is drastically reduced by increasing the delay in the antenna control loop, resulting in a correlated pointing accuracy (dashed-dotted line).

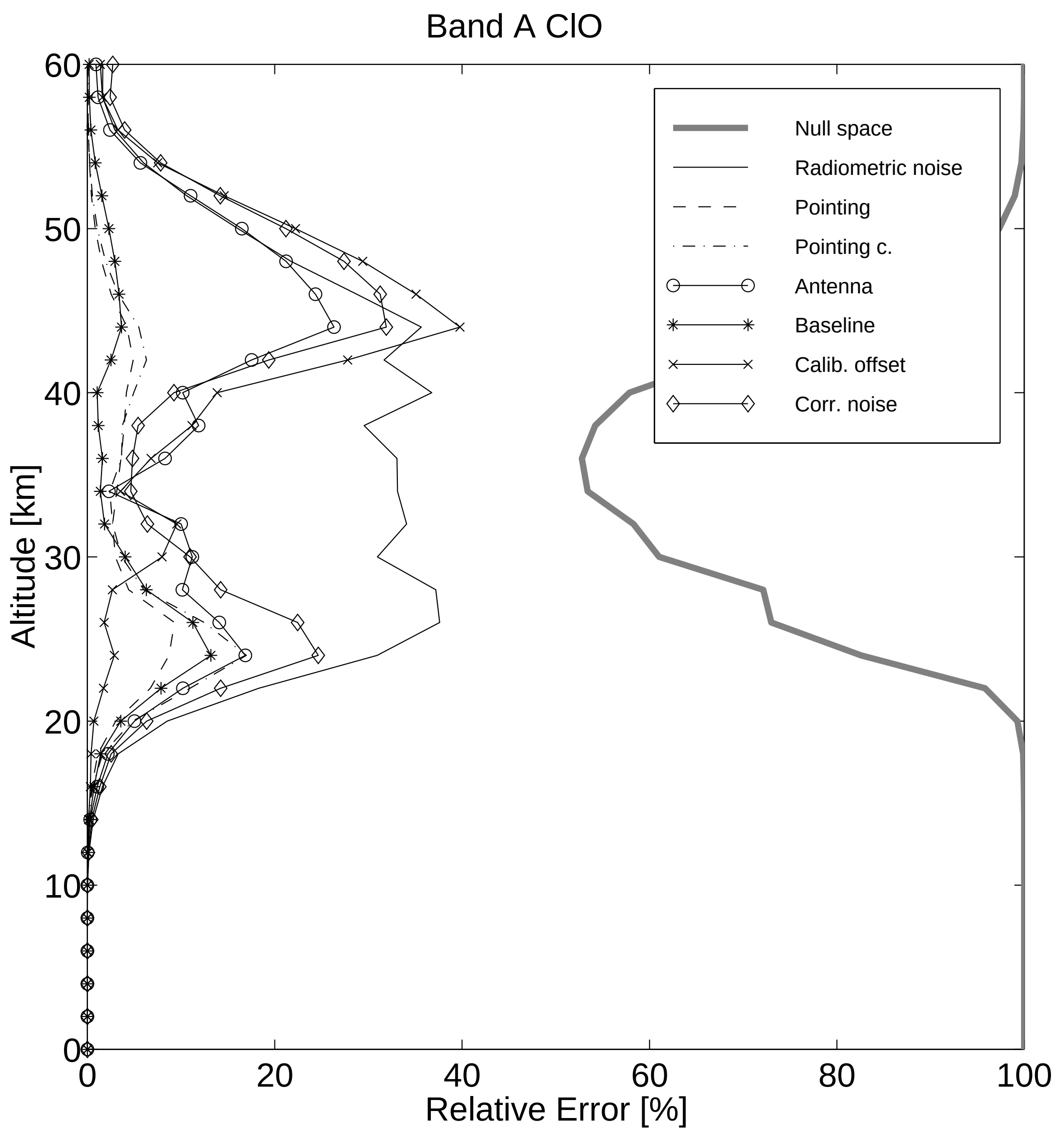

Figure 2: Error summary for the retrieval of ClO near 500 GHz. All of the plotted parameters have a significant impact.

  - Can be optimized if other sideband is not used for measurements

- Atmospheric temperature uncertainty

  - Temperature retrieval schemes are currently investigated

4.2 Slightly Less Critical Parameters

- Baseline ripples
- Calibration errors

But SOPRANO radiometric requirements are stringent (one could also say optimistic):

- 0.1 K amplitude of baseline ripples
- 1 K hot and cold load temperature errors
- 0.2 K non-linearity

Radiometric requirements are even more significant for SMILES because radiometric noise is lower. From all our practical experience, baseline ripples are likely to be a problem with the actual instrument.

4.3 Relatively Uncritical Parameters

- Actual shape of antenna pattern (investigated 1–10 % near wing, 0–4 % far wing)

  - provided it is well known
  - provided FWHM stays the same
  - provided the scan goes down into the opaque region

- Pointing stability

  - Leads to slightly increased width of effective antenna pattern
  - $\pm$ 200 m is tolerable

- Baseline discontinuities (0.4 K every 2 GHz is tolerable)

  - Can be optimized (discontinuities not on line centers)

- Correlated noise
  - Same order of magnitude as measurement noise (for integration time $10\times$ atmospheric)
  - Statistical error, i.e., goes down when data is averaged

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