Submillimeter-wave spectroscopic performance of JEM/SMILES

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ABSTRACT

An acousto-optical spectrometer (AOS) is employed in order to meet scientific mission objectives of submillimeter-wave limb-emission sounder (SMILES) to be aboard the Japanese Experiment Module (JEM) of the International space station (ISS). The capability of multi channel detection with AOS is suitable for observing multi chemical species in a wide frequency region. Wide noise dynamic range enables us to obtain the spectra without unnecessary increase of system noise, suggesting a good combination of AOS with low noise front end system of SMILES. Several technical concerns relating to important instrumental characteristics of AOS are discussed and expected performance of the spectrometers to be used in the JEM/SMILES mission are overviewed.

Keywords: Limb-emission sounder, ISS, JEM/SMILES, spectrometer, AOS, noise dynamic range, differential non-linearity.

1. INTRODUCTION

Superconducting submillimeter-wave limb emission sounder (SMILES) is a mission to obtain global mappings of stratospheric trace gases such as ClO, HCl, HO\textsubscript{2}, HNO\textsubscript{3}, BrO and O\textsubscript{3} by observing them at the frequency band of 624.32 - 626.32 GHz and 649.12 - 650.32 GHz. It is scheduled to be launched in 2005 and operated on the Japanese Experimental Module (JEM, recently dubbed 'KIBO') at the International Space Station (ISS)\textsuperscript{1}. For achieving high-sensitive and multi-species observation of atmospheric emission aimed in our mission, it is desired to adopt low noise (near quantum noise-limit) receivers based on a super-conducting technology as well as multi-channel radiospectrometer capable of wide instantaneous observation band. In the JEM/SMILES, the use of Superconductor-Insulator-Superconductor (SIS) mixer operated at 4 K cooled by mechanical cooler fulfills our principal mission requirements\textsuperscript{2}. Selection of the radio-spectrometer, however, is also essential and should be paid attention to utilize high performance of the SIS mixer as much as possible.

Among spectrometers so far proposed and used for the backend of radiometers, filterbank(FB), autocorrelator(AC), and acoust-optical spectrometer(AOS) are three representatives. FB was widely used in the astronomical observation, but due to the complexity in increasing the number of detection channels, some FBs have been replaced by other spectrometers up to present. In an application of atmospheric observations, however, a dedicated FB can be a suitable choice for the spectrometer as we need only limited number of spectroscopic channels for retrieving height profile of the trace gas under investigation\textsuperscript{3}. Instrumental performance of AC is now improving in accordance with a recent innovation of digital

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technologies, but quantization noise of the state-of-the-art AC still cannot be neglected due to a small number of resolution bit. A large power consumption is another concern in wide band AC. On the contrary, AOS has a capability of multi-channel, and wide-band detection without additional noise. Power consumption and instrumental volume per single spectroscopic channel are small when compared to other spectrometers. We have concluded to adopt two AOSs for spectrometers of JEM/SMILES because of their advantageous points in resource consumption, available bandwidth, and noise performance. In the present paper, the technical concerns in specifying AOS instrumental characteristics are discussed, and expected spectroscopic performance of AOS to be used in JEM/SMILES is overviewed.

2. TECHNICAL CONCERNS IN SPECIFYING AOS INSTRUMENTAL PERFORMANCE

2-1. Working principle of AOS

The application of AOS and its usefulness was first demonstrated in the field of radio astronomy in 1970s\(^4,5\). Since then it has been recognized as one of the suitable spectrometers for analyzing a wide band and faint signal embedded in radiometric noise. The key component of AOS is Bragg cell, that is responsible for converting microwave signal to corresponding acoustic wave propagating in the crystal. If the monochromatic light is irradiated to the crystal, propagating acoustic wave generates a diffracted beam by Bragg diffraction. The diffraction angle of the impinged light is inversely proportional to the wavelength of acoustic wave, consequently the frequency domain spectra of input microwave signal appears at a focal plane of the deflected light. The detection will be achieved by putting one-dimensional light detector such as CCD at the position of the focal plane.

Development and sophistication of AOS have been mainly lead by two research groups in France and Germany\(^6,7\). They applied their spectrometers not only for radio-astronomy, but also for another field such as atmospheric science\(^8\). From instrumental point of view, state-of-the-art AOS has been passed space qualification and its capability has been demonstrated in the sub millimeter-wave observation satellites\(^9,10\).

In case that AOS is applied to atmospheric observation, we have to consider two properties in addition to normal instrumental specifications of the spectrometer such as resolution, bandwidth, channel separation etc. Those are noise dynamic range and differential non-linearity of the analog to digital converter. These are important because a signal level of reference spectrum is different from observed spectrum in typical atmospheric observation. The details are discussed in the following sections.

2-2. Noise dynamic range (NDR)

The concept of 'Noise dynamic range (NDR)' is different from usual 'dynamic range' used in ordinary spectrometer, and is very important in the treatise of the signals embedded in the noise. The noise characteristics of RF signal that comes from IF amplification unit is basically determined by noise characteristics of the front end system of the radiometer. The radio signal is converted to optical one in the AOS, and it is detected by a CCD array. The read-out voltages, or the number of collected charges in each cell of the CCD array, should be proportional to the input RF power levels, but they are usually modified by several additional factors in reality. The variance of the original RF noise at CCD is expressed by the following modified radiometric equation;

\[
N_{RF}^2 = \frac{Q^2}{Bt}
\]

where \(Q\), \(B\), and \(t\) correspond to the number of collected charge at CCD, noise band width, and integration time for collecting charge, respectively. The contributors of modification of the noise characteristics can be photon shot noise, CCD dark noise, quantization noise of analog to digital converter, and detection circuit noise, namely;
\[ N_{\text{add}}^2 = N_{\text{photon}}^2 + N_{\text{CCD}}^2 + N_{\text{AD}}^2 + N_{\text{Detection-circuit}}^2 \]
\[ = \left( \sqrt{Q} \right)^2 + (q_0)^2 + \left( \frac{Q_{\text{sat}}}{\sqrt{2^{2n} \cdot 12}} \right)^2 + \left( q_{\text{eff}} \right)^2 \]

where, \( q_0 \), \( Q_{\text{sat}} \), \( n \), and \( q_{\text{eff}} \) are dark current noise, the amount of saturation charge, quantization bit of the A/D converter to be used and equivalent amount of charge of detection circuit noise, respectively.

The read out noise of the AOS is the sum of the RF noise and the additional ones;

\[ N_{\text{read-out}}^2 = N_{\text{RF}}^2 + N_{\text{add}}^2. \]

The modification of the noise characteristics means an increase of effective system noise temperature. In the case of AOS, the relative weight of the additional noise will increase as the RF power decreases. So if a criterion is settled so that the noise variance ratio \( N_{\text{read-out}}^2 / N_{\text{RF}}^2 \) to be less than 1.21, then we can define usable signal range of the spectrometer with less than 10 \% increase of effective system noise temperature. We call this ‘noise dynamic range’. As far as the observed spectra lie within the noise dynamic range, the increase of the effective system noise due to the spectrometer can be negligible.

Alternatively, we can calculate an increase of noise at a given signal level. Its coefficient is a function of the signal level, and expressed as \( f(D) \), where \( D = \frac{Q_{\text{sat}}}{Q} \cdot T_{\text{sys}}^{\text{eff}} = T_{\text{sys}}^{\text{org}} \cdot f(D) \).

\[ f(D) \] is expressed as the following;

\[ f(D) = \sqrt{1 + \frac{B \cdot t}{Q_{\text{sat}}} \cdot D + B \cdot t \left( \frac{q_0^2 + q_{\text{eff}}^2}{Q_{\text{sat}}^2} + \frac{1}{2^{2n} \cdot 12} \right) \cdot D^2} \] (1)

It is essential for obtaining a wide noise dynamic range to minimize coefficients of a series of \( D \) in equation (1). This result tells the following suggestions in designing AOS. Given the noise bandwidth,

- Integration time should be shortened to increase RF noise.
- Selection of the CCD having large saturation charge and low dark noise is important.
- State-of-the-art detection circuit is necessary to minimize \( q_{\text{eff}} \).
- The number of bit of the A/D converter must be large enough for quantization noise to be negligible.

2.3 Differential non-linearity (DNL)

Another concern with the AOS in obtaining the limb spectrum is 'differential non-linearity (DNL)' of the analog to digital converter, which was first claimed by R. Schieder of the University of Cologne. In characterizing linearity of A/D converter, there are two categories for describing its performance. One is integral non-linearity (INL), and this indicates the same characteristics as the non-linearity of amplifiers. On the contrary, the DNL is different concept from the former one. The DNL is irregularities in the "monotonic character" of the conversion from input analog voltages to digitized values. Noise due to this effect is non-statistical, because it is reproducible if we repeat measurements under the same conditions. It is troublesome that this effect is never visible as far as the signal and reference power input to the AOS are of the same power level, which is usually the case when a long-term integration test is performed in a laboratory. The Allan variance test also can never be an indicator of this effect. For atmospheric observations, however, the input power levels are largely separated between signal and reference. This makes it indispensable for us to pay an extra attention to this issue.

The effect of DNL to atmospheric spectrum heavily depends on the DNL characteristics of A/D converter, difference of the input power to the spectrometer between atmosphere and reference, and frequency characteristics of the input spectrum.
3. AOS OF JEM/SMILES

3.1 General specifications

AOS of SMILES consists of three parts, acousto-optical unit (AOU), RF amplifier unit (RFU) and control and video unit (CVU). The AOU includes two spectrometers each of which has 1200 MHz frequency coverage with 1500 spectral channels. A combination of two spectrometers by selecting appropriate IF switch network enables us to observe a limb spectrum of 2000 MHz bandwidth with 3000 spectral channels. Channel separation is typically 0.8 MHz, and the relation between channel number and corresponding frequency is not linear. Frequency calibration of the spectrometer will be accomplished by using a frequency reference with the absolute accuracy of about 10 kHz over the whole mission life. It is installed in the IFA (IF Amplifier unit) section, generating a series of carrier signals with an interval of 100 MHz. The output of this comb generator will be injected to the AOS once in every scan of the antenna (53 seconds). Peak positions of each picket are derived against channel number, and the relation between them and corresponding frequencies is analyzed by a polynomial fit. The residuals of the fit will be less than 30 kHz, which gives the error in frequency of the AOS spectra.

The spectrometer response upon input of a carrier signal can be obtained, the input spectrum of AOS is convoluted with this 'frequency response function'. The full width at half maximum of it will be 1.8 MHz, which is called 'resolution bandwidth' of the spectrometer. On the other hand, when we deal with noise characteristics of the AOS, we should use the 'noise bandwidth', which represents the width of such an equivalent boxcar filter that gives the same fluctuations on the output spectra. The noise bandwidth for the AOS on SMILES is expected to be 2.5 MHz. The unit exposure time of CCD is set to 4.9 ms and the collected charges are read-out at the rate of 750 kHz. Each output spectrum is obtained every 500 ms by accumulating the 96 unit spectra. The net integration time is therefore calculated to be 470.4 ms. This accumulation sequence is controlled by CVU, it covers also receiving tele-commands and sending data and telemetry.

Figure 2 shows the architecture of SMILES/AOS preliminary designed at Astrium, general specifications of the spectrometer are summarized in Table 1

Table 1 Specifications of SMILES/AOS (at PDR)

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of optical head</td>
<td>2</td>
</tr>
<tr>
<td>Input Frequency Range</td>
<td>1.55 - 2.75 GHz</td>
</tr>
<tr>
<td>-3dB Frequency resolution</td>
<td>1.8 MHz</td>
</tr>
<tr>
<td>CCD channel</td>
<td>1500 channel / 1.2GHz</td>
</tr>
<tr>
<td>Frequency Deviation from the best fitted curve</td>
<td>&lt; 30 kHz</td>
</tr>
<tr>
<td>Frequency Drift (medium term)</td>
<td>&lt; 170 kHz</td>
</tr>
<tr>
<td>Absolute Allan variance minimum time</td>
<td>&gt; 60 sec.</td>
</tr>
<tr>
<td>Noise dynamic range</td>
<td>1.1 (noise variance ratio) @ 7.5dB</td>
</tr>
<tr>
<td>Non linearity of power response</td>
<td>&lt; 3.1 % over 3dB dynamic range</td>
</tr>
<tr>
<td>Exposure time</td>
<td>4.9 ms</td>
</tr>
<tr>
<td>Accumulation time</td>
<td>470.4 ms</td>
</tr>
<tr>
<td>Data rate</td>
<td>110.7 kbps</td>
</tr>
</tbody>
</table>

Figure 2. The architecture of the AOS
3.2 Expected additional noise

The system noise temperature of JEM/SMILES will be 500 K thanks to adopting SIS mixer operated at 4K. This is one of the distinguished features of SMILES mission when compared to other atmospheric observation program from the space. Therefore it is important not to deteriorate this performance by AOS. To achieve this purpose, AOS should have a noise dynamic range as wide as possible. As described in the previous section, there are several guidelines for having a wide noise dynamic range, such as short integration time, selection of CCD having a highest saturation charge capacitance, and A/D converter with suitable resolution. In SMILES/AOS, parameters listed in TABLE 2 is used. With this condition, \( f(D) \) in equation (1) can be calculated, the coefficients \( f(D) \) is a function of the inverse of the normalized illumination level at CCD and shows 'effective increase' of system noise temperature as formulated in the equation. Figure 3 shows the plot of \( f(D) \). It can be found that at the illumination level of 9dB down from the saturation, the additional noise contribution is still less than 10%.

<table>
<thead>
<tr>
<th>Noise Bandwidth</th>
<th>( B )</th>
<th>2.5 MHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure time</td>
<td>( t )</td>
<td>4.9 ms</td>
</tr>
<tr>
<td>Saturation charge of CCD</td>
<td>( Q_{sat} )</td>
<td>1.3 Me^-</td>
</tr>
<tr>
<td>Read-out noise</td>
<td>( q_{eff} )</td>
<td>450 e^ - rms</td>
</tr>
<tr>
<td>A/D converter resolution</td>
<td>( n )</td>
<td>12</td>
</tr>
</tbody>
</table>

Table 2. Expected parameters relating to noise dynamic range of AOS

Figure 3  Plot of noise variance ratio.

3.2 Simulation of the DNL effect

In order to evaluate an effect of DNL, we first have to simulate the properties of the A/D converter to be used in SMILES/AOS as precise as possible because it heavily depends on the characteristics. The A/D converter which we plan to adopt is AD1671 made by analog devices, and the specifications for non-linearity are +/- 3 LSB and +/- 1 LSB for integral and differential characters, respectively. In making a model, we have referenced actual performance of the same type of the converter which were measured in another space program. According to them, DNL of measured pieces all lied within +/- 0.5 LSB at any experimental conditions, and a distinctive pattern has been observed in error curve of the non-linearity. We have regarded these features as typical behaviors of AD1671 and tried to simulate this trend precisely in the model as depicted in figure 4. The DNL of the used model is +/- 0.7 LSB which is less than manufacture's specifications but greater than our requirements (+/- 0.5 LSB).

Frequency characteristic of the observed spectrum is also a driver in evaluating the effect of DNL. We assumed the following normalized functions for it. For the 512 spectral channels,

\[
S(i) = (0.8 + 0.2 \sin \frac{2 \pi \cdot i}{340}) \cdot (1 - 0.1 \frac{i}{512}), \quad 0 \leq i \leq 512
\]
The equivalent temperature at full-scale of the AOS is set to 850 K. The calibration of the antenna temperature for the limb spectrum can be done by the following well-known equation;

\[ T_{\text{digital}} = \frac{D_{\text{digital}}^\text{limb}}{D_{\text{digital}}^\text{hot}} - \frac{D_{\text{digital}}^\text{reference}}{D_{\text{digital}}^\text{reference}} (T_{\text{hot}} - T_{\text{reference}}) \]

where \( D^\text{digital} \) means normalized digitized value of limb, reference or hot load observation. In the same way, we can calculate \( T^\text{analog} \) to evaluate the noise generated by the A/D converter. If we define \( \Delta T \) as;

\[ \Delta T = T^\text{digital} - T^\text{analog} \]

The contributor to \( \Delta T \) can be originated by both quantization and non-linearity. In the condition of the present simulation, however, the unit integration time is short enough (4.9ms) that the former can be negligible. We have carried out precise simulation with the modeled A/D converter, the 'one shot' temperature spectrum is calculated from limb data, reference data, and Hot load data with each observation time being 500 ms, 4 s, and 4 sec., respectively. This is actual configuration of JEM/SMILES observation.

![AD1671 SIMULATION](image1.png)

Figure 4 The A/D converter model used in DNL simulation.

INL : +/- 1.5 LSB, DNL : +/- 0.7LSB

![Fig. 5](image2.png)

Fig. 5 Plot of \( \Delta T \) against spectral channel for 1shot, after 2, 3, and 60 accumulations. The latter three spectra are shifted upward by 0.1, 0.2 and 0.3 K respectively. The difference of radiation temperature between limb and reference is 20 K and no gain variation over time is assumed.

Figure 5 shows \( \Delta T \) against spectral channels for various accumulation number of the spectrum. 60 accumulations corresponds to a one-day and 5 degree latitude zonal average the data at mid latitude region. Distinctive pattern remains unchanged over 60 accumulations of the spectrum which can be attributed to the cause of differential non-linearity. The pattern reflects frequency characteristics of the spectrum, and is not sensitive integral non-linearity. As can be seen in

![Fig. 6](image3.png)

Fig. 6 Plot of the rms of \( \Delta T, T^\text{digital}, \) and, \( T^\text{analog} \) against spectral accumulation number
figure 6, the both of the rms’ of $T^{\text{digital}}$ and $T^{\text{analog}}$ reduces as the inverse square of accumulation time, while the difference between them, $\Delta T$, becomes greater. At small number of accumulations, the radiometric noise dominates the spectral rms, however as the accumulation number increases, the noise due to DNL cannot be ignored and limits system sensitivity. This clearly indicates the DNL is an non-statistical effect.

![Figure 7 Plot of the rms of $\Delta T$ against the difference of the radiation temperature between limb spectrum and reference spectrum](image)

Though the DNL is troublesome in measuring the atmospheric spectra, it is found that a small variation of the system gain has a possibility to smooth out this effect efficiently. Figure 7 shows the effect of DNL against the difference in the input power levels between the two spectra. The lowest plot of the figure depicts an improvement of the sensitivity by including 'random' gain variation over 60 observational opportunities. This phenomenon will be rationalized by the shift of the 'operational point' of the A/D converter in digitizing a spectrum due to the gain variation. This plot tells us that if a gain variation occurs randomly (which is probably an ideal case), the DNL effect will be removed by accumulation. In the real observational conditions, the result will be between the two plots in the figure. The increase of rms in the plot toward the right side (large $T_{\text{limb}} - T_{\text{ref}}$) is due to INL of A/D converter. The DNL effect itself is cancelled even at this region.

### 4. EFFECTS ON THE RETRIEVAL ERROR

Among the causes that can contribute to the error in retrieving a height profile from the observed spectra, we investigate here the effect of the instrumental characteristics peculiar to the AOS. The potential items to be treated are, additional noise due to the spectrometer, and non-linearity of the A/D converter. As discussed in section 2, the additional noise of the spectrometer increases as $D$ increases, where $D$ is defined by the inverse ratio of collected charges against saturation of CCD well. If a frequency characteristic for an observed spectrum at CCD is large enough to exceed the defined noise dynamic range, increase of effective system noise can be 10% in some spectral region. The DNL of A/D converter generates undulation of spectral base line, whose pattern depends on the frequency characteristics of the observed spectrum.

![Figure 8 Plots of error ratio by changing measurement noise. Calculations were based on mid-latitude standard atmosphere modeled by Rutherford Appleton Laboratory.](image)
According to the present simulation the amplitude of the undulation corresponds to 10% increase of system noise. Covariance of retrieval error $S$ can be evaluated by using the following equation;

$$S = (K^T S^{-1}_e K + S_a)^{-1}$$

where, $K$ is a weighting function matrix and its elements can be calculated by SMILES forward model$^{12}$. $S_e$ and $S_a$ represents covariance matrix of measurement and a priori errors, respectively. The effect of system noise on the retrieval error has been simulated by varying it from 500 K to 800 K. In this situation a change in system noise affects $S_e$ only. Figure 8 shows an example of the simulation in which error ratios in retrieving a profile of the ClO molecule have been plotted. The further analysis should be done by taking a rigorous model of frequency characteristics of the spectrum, which will be clarified with the progress of SMILES development.

5. SUMMARY

With the consequence of the trade off in terms of spectrometer performance and resource consumption, AOS has been adopted as the radio spectrometer of SMILES. AOS has a capability of wideband, multi-species spectrometry, which meets our scientific mission objectives. However there are two major technical concerns except for normal instrumental specifications of the spectrometer in order to fully utilize SMILES spectroscopic performance, which are noise dynamic range and differential non-linearity of the A/D converter. Important instrumental specifications governing these two factors are discussed. SMILES/AOS has been designed so as to minimize these influences.

6. REFERENCES


11. R. Schieder, private communication.