Assessment of the MTG IR Sounding Mission Spectral Calibration Algorithm

Part 3: Overall performance analysis

For the attention of: Rolf STUHLMANN (EUMETSAT)

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<td>Carsten STANDFSUSS,</td>
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<td>Carsten STANDFSUSS</td>
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Assessment of the MTG IR Sounding Mission Spectral Calibration Algorithm

Part 3: Overall performance analysis

Summary
In the frame of the MTG IR Sounding Mission Spectral Calibration Assessment study, the present third task report is dedicated to the overall spectral calibration performance analysis.

Section 2 briefly recalls the characteristics of the instrument baseline concepts (DS and FTS), of the spectral calibration windows, and of the considered geophysical conditions. The application conditions of full spectral calibration experiments for the two concepts in terms of extrapolation over the IRS spectral coverage and of spatio-temporal selection criteria are established in section 3. The overall spectral calibration performance is quantified for hypotheses of perfect inter-array co-alignment and of separate array calibration in section 4. Upon these performances, conclusions on spectral calibration design options and on requirements and error allocations related to spectral calibration are drawn in sections 5 and 6. Section 7 provides the overall study conclusions and perspectives.

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Author(s) Carsten STANDFUSS, Bernard TOURNIER
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#### Assessment of the MTG IR Sounding Mission Spectral Calibration Algorithm

**Part 3: Overall performance analysis**

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<td>I</td>
<td>4.1.2</td>
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<td>allocation justification for shape knowledge errors, transferred from part 2</td>
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* *I = Inserted  D = deleted  M = Modified*
Table of contents

1. INTRODUCTION ..................................................................................................................................... 7
   1.1. Acronyms .......................................................................................................................................... 8
   1.2. References ........................................................................................................................................ 8

2. INSTRUMENT, ALGORITHM AND GEOPHYSICAL PARAMETERS .................................................. 9
   2.1. Instrument baseline concepts ........................................................................................................ 9
   2.2. Consolidated list of spectral calibration windows ..................................................................... 10
   2.3. Geophysical conditions ................................................................................................................. 10

3. APPLICATION CONDITIONS FOR FULL SPECTRAL CALIBRATION EXPERIMENTS .................. 11
   3.1. Spectral calibration functions and instrument state parameters.............................................. 11
   3.2. Spatio-temporal selection criteria ................................................................................................ 12
       3.2.1. Scene filtering requirements ............................................................................................. 12
       3.2.2. Selection of detector array elements ................................................................................ 13
       3.2.3. Simulation of atmospheric variability ............................................................................. 14
       3.2.4. Spectral calibration period .............................................................................................. 14
       3.2.5. Radiometric noise ............................................................................................................. 15

4. QUANTIFIED SPECTRAL CALIBRATION PERFORMANCE ............................................................. 16
   4.1. DS baseline ..................................................................................................................................... 16
       4.1.1. Impact of spatial sample selection ..................................................................................... 17
       4.1.2. Performance for different spectral calibration windows ................................................... 19
   4.2. FTS baseline ................................................................................................................................... 28
       4.2.1. Impact of spatial sample selection ..................................................................................... 28
       4.2.2. Performance for different spectral calibration windows ................................................... 30
   4.3. Overall algorithm performance summary .................................................................................... 38
   4.4. Limitations and open issues ......................................................................................................... 39
       4.4.1. Spatial scene distribution ..................................................................................................... 39
       4.4.2. Time filtering ........................................................................................................................ 39
       4.4.3. Numerical algorithm noise ................................................................................................. 39
       4.4.4. Concept choice .................................................................................................................... 40

5. CONCLUSION ON SPECTRAL CALIBRATION ALGORITHM DESIGN ............................................ 41
   5.1. Both concepts ................................................................................................................................ 41
   5.2. DS baseline ..................................................................................................................................... 42
   5.3. FTS baseline ................................................................................................................................... 42

6. CONSOLIDATION OF REQUIREMENTS ............................................................................................ 43
   6.1. Spectral calibration noise budget ............................................................................................... 43
   6.2. Recommendation of requirements related to spectral calibration ........................................... 45

7. STUDY CONCLUSIONS AND PERSPECTIVES ............................................................................... 47
1. Introduction

Part 1 of the study on the ‘Assessment of the MTG IR Sounding Mission Spectral Calibration Algorithm’ [RD 1] describes the software system implementation for the IRS spectral calibration algorithm assessment as well as the instrumental and geophysical input parameters.

In part 2 [RD 2], the relation between shift and shape knowledge errors of the Instrument Spectral Response Function (ISRF) and radiometric errors is established. This relation will eventually link the radiometric specification of the spectral calibration noise budget to its components depending on algorithm and instrument performance. Moreover, part 2 provides performance estimations at low level of the spectral calibration sub-system, i.e., in terms of algorithm noise generated by ISRF shift determination errors for individual spectra in various spectral calibration windows. In particular, the impact of radiometric noise and of atmospheric variability on the spectral shift determination is investigated. A consolidated list of spectral calibration windows is derived.

The present report (part 3) is dedicated to full spectral calibration experiments. The first objective is to explicitly quantify the spectral calibration algorithm noise by estimating instrument state parameters from individual shift determinations. These instrument state parameters prescribe the ISRF in all spatial samples for each spectral channel. This requires the application of various spatio-temporal selection scenarios of individual measurements in different atmospheric conditions, and of various configurations of consolidated spectral calibration windows. The latter includes in particular an optimised window choice in case of good focal plane co-alignment and the case of an individual spectral calibration per focal plane. Then, based on the spectral calibration algorithm noise quantification, the overall spectral calibration noise budget is consolidated and allocations are recommended for instrument dependent contributions (focal plane co-alignment, ISRF centroid stability, ISRF shape knowledge).

Section 2 briefly recalls the characteristics of the instrument baseline concepts (dispersive spectrometer DS and Fourier Transform spectrometer FTS), of the spectral calibration windows, and of the considered geophysical conditions. The application conditions of full spectral calibration experiments for the two concepts in terms of extrapolation over the IRS spectral coverage and of spatio-temporal selection criteria are established in section 3. The overall spectral calibration performance is quantified for hypotheses of perfect inter-array co-alignment and of separate array calibration in section 4. Upon these performances, conclusions on spectral calibration design options and on requirements and error allocations related to spectral calibration are drawn in sections 5 and 6. Section 7 provides the overall study conclusions and perspectives.
1.1. Acronyms

Cb  cumulonimbus
Ci  cirrus
DS  Dispersive Spectrometer
ESA European Space Agency
EUMETSAT European Organisation for the Exploitation of Meteorological Satellites
E/W East-West
FIR Finite Impulse Response
FTS Fourier Transform Spectrometer
IASI Infrared Atmospheric Sounding Interferometer
IR InfraRed
IRS (MTG) InfraRed Sounder
ISRF Instrument Spectral Response Function
ISRF-EM ISRF Estimation Model
MRD Mission Requirements Document
MTG Meteosat Third Generation
NEdT Noise equivalent brightness temperature difference
N/S North-South
NWP Numerical Weather Prediction
RD Reference Document
rms root mean square
SCS Spectral Calibration Subsystem
SDB Spectral Data Base
SDE Shift Determination Error
SEI Shape Error Index
SSI Spectral Sampling Interval
TBD To be defined
WP Work Package

1.2. References


2. Instrument, algorithm and geophysical parameters

This section recalls the instrument baseline parameters for the two possible concepts, the principal characteristics of pre-selected spectral calibration windows as well as of the considered atmospheric conditions. A detailed description is given in [RD 1].

2.1. Instrument baseline concepts

Instrument baseline concepts are based on [RD 3].

Spectral and radiometric characteristics of the DS and FTS instrument baseline are summarised in Table 1 and Table 2, respectively.

It is recalled that the implementation of mission bands 5 and 6 is alternative.

<table>
<thead>
<tr>
<th>Mission Band</th>
<th>IRS-1</th>
<th>IRS-2</th>
<th>IRS-3</th>
<th>IRS-4</th>
<th>IRS-5</th>
<th>IRS-6</th>
<th>IRS-7</th>
<th>IRS-8</th>
<th>IRS-9</th>
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<tbody>
<tr>
<td>Wavenumber range [cm⁻¹]</td>
<td>700-770</td>
<td>770-980</td>
<td>980-1070</td>
<td>1070-1210</td>
<td>1210-1600</td>
<td>1600-2000</td>
<td>2000-2250</td>
<td>2250-2400</td>
<td>2400-2500</td>
</tr>
<tr>
<td>Array band index</td>
<td>S2</td>
<td>S3</td>
<td>S4</td>
<td>S4</td>
<td>S5</td>
<td>S5</td>
<td>S5</td>
<td>S5</td>
<td>S5</td>
</tr>
<tr>
<td>req. spect. resolution [nm/cm⁻¹]*</td>
<td>9.3</td>
<td>8.2</td>
<td>6.5</td>
<td>5.2</td>
<td>3.2</td>
<td>2.3</td>
<td>1.4</td>
<td>1.25</td>
<td>1.25</td>
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<tr>
<td>spect. resolution [nm/cm⁻¹]*</td>
<td>0.5</td>
<td>0.625</td>
<td>0.85</td>
<td>0.625</td>
<td>0.625</td>
<td>0.625</td>
<td>0.625</td>
<td>0.625</td>
<td>0.625</td>
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<tr>
<td>SSI [nm]</td>
<td>6.9</td>
<td>6.9</td>
<td>3.9</td>
<td>3.9</td>
<td>2.7</td>
<td>1.6</td>
<td>1.2</td>
<td>1.73</td>
<td>2.9</td>
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<tr>
<td>spectral samples</td>
<td>189</td>
<td>404</td>
<td>221</td>
<td>277</td>
<td>745</td>
<td>781</td>
<td>467</td>
<td>156</td>
<td>59</td>
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<tr>
<td>equivalent SSI [cm⁻¹]</td>
<td>0.37</td>
<td>0.52</td>
<td>0.505</td>
<td>0.505</td>
<td>0.523</td>
<td>0.512</td>
<td>0.535</td>
<td>0.96</td>
<td>1.69</td>
</tr>
<tr>
<td>req. rad. resolution NEdT@280K [K]</td>
<td>0.2</td>
<td>0.24</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.3</td>
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<td>as feasible</td>
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<tr>
<td>rad. res. NEdT@280K [K]</td>
<td>0.25-0.45</td>
<td>0.08-0.25</td>
<td>0.05-0.09</td>
<td>0.04-0.07</td>
<td>0.09-0.17</td>
<td>0.10-0.25</td>
<td>0.12-0.22</td>
<td>0.12-0.18</td>
<td>0.16-0.36</td>
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</table>

Table 1: Spectral and radiometric characteristics for the IRS/DS baseline. *=at band centre.

<table>
<thead>
<tr>
<th>Mission Band</th>
<th>IRS-1</th>
<th>IRS-2</th>
<th>IRS-3</th>
<th>IRS-4</th>
<th>IRS-5</th>
<th>IRS-6</th>
<th>IRS-7</th>
<th>IRS-8</th>
<th>IRS-9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavenumber range [cm⁻¹]</td>
<td>700-770</td>
<td>770-980</td>
<td>980-1070</td>
<td>1070-1210</td>
<td>1210-1600</td>
<td>1600-2000</td>
<td>2000-2250</td>
<td>2250-2400</td>
<td>2400-2500</td>
</tr>
<tr>
<td>Array band index</td>
<td>A1</td>
<td>A2</td>
<td>A2</td>
<td>A3</td>
<td>A3</td>
<td>A3</td>
<td>A3</td>
<td>A4</td>
<td>A4</td>
</tr>
<tr>
<td>integration time [s]</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>4.8</td>
<td>4.8</td>
<td>4.8</td>
<td>4.8</td>
<td>4.8</td>
</tr>
<tr>
<td>req. spect. res. [cm⁻¹]*</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.625</td>
<td>0.625</td>
<td>0.625</td>
<td>1.25</td>
</tr>
<tr>
<td>spect. resolution [cm⁻¹]*</td>
<td>0.50</td>
<td>0.50</td>
<td>0.505</td>
<td>0.505</td>
<td>0.523</td>
<td>0.512</td>
<td>0.535</td>
<td>0.96</td>
<td>1.69</td>
</tr>
<tr>
<td>SSI [cm⁻¹]</td>
<td>0.41</td>
<td>0.41</td>
<td>0.41</td>
<td>0.41</td>
<td>0.70</td>
<td>0.52</td>
<td>0.52</td>
<td>0.52</td>
<td>1.03</td>
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<tr>
<td>spectral samples</td>
<td>171</td>
<td>403</td>
<td>219</td>
<td>200</td>
<td>750</td>
<td>769</td>
<td>481</td>
<td>145</td>
<td>49</td>
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<tr>
<td>req. rad. resolution NEdT@280K [K]</td>
<td>0.2</td>
<td>0.24</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.3</td>
<td>as feasible</td>
<td>as feasible</td>
</tr>
<tr>
<td>rad. res. NEdT@280K [K]</td>
<td>0.40-0.85</td>
<td>0.31-0.49</td>
<td>0.22-0.45</td>
<td>0.19-0.46</td>
<td>0.28-1.43</td>
<td>0.29-1.43</td>
<td>0.34-0.60</td>
<td>0.44-0.75</td>
<td>0.56-1.69</td>
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Table 2: Spectral and radiometric characteristics for the IRS/FTS baseline. *=excluding self-apodisation.
2.2. Consolidated list of spectral calibration windows

Table 3 recalls the list of spectral calibration windows pre-selected in [RD 1] and consolidated in [RD 2].

<table>
<thead>
<tr>
<th>Window id</th>
<th>Wavenumber range (cm⁻¹)</th>
<th>IRS Band</th>
<th>used for DS only</th>
<th>Spectral resolution required (cm⁻¹)</th>
<th>Spectral resolution IRS/FTS(cm⁻¹)</th>
<th>Spectral resolution IRS/DS(cm⁻¹)</th>
</tr>
</thead>
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<tr>
<td>W02</td>
<td>720 - 750 IRS-1</td>
<td></td>
<td></td>
<td>0.5</td>
<td>0.50</td>
<td>0.67</td>
</tr>
<tr>
<td>W21</td>
<td>790 - 860 IRS-2</td>
<td>X</td>
<td></td>
<td>0.625</td>
<td>0.62</td>
<td>0.94</td>
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<tr>
<td>W11</td>
<td>1125 - 1195 IRS-4</td>
<td></td>
<td></td>
<td>0.85</td>
<td>0.85</td>
<td>0.92</td>
</tr>
<tr>
<td>W13</td>
<td>1350 - 1400 IRS-5</td>
<td></td>
<td></td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
<tr>
<td>W14</td>
<td>1500 - 1550 IRS-5</td>
<td>X</td>
<td></td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
<tr>
<td>W15</td>
<td>1650 - 1700 IRS-6</td>
<td>X</td>
<td></td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
<tr>
<td>W16</td>
<td>1800 - 1850 IRS-6</td>
<td></td>
<td></td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
<tr>
<td>W03</td>
<td>2040 - 2070 IRS-7</td>
<td></td>
<td></td>
<td>0.625</td>
<td>0.62</td>
<td>0.94</td>
</tr>
</tbody>
</table>

Table 3: List of IRS candidate spectral calibration windows.

For **FTS**, one window per array is chosen (W02, W11, W13/16, W03). This allows

- either a single-window approach (**all-array calibration**) by extrapolation of the spectral calibration function over the entire spectrum under the condition that co-alignment between detector arrays is better than 5 \(10^{-7}\) in terms of relative shift knowledge error, corresponding to a noise allocation of 0.025K NEdT@280K,
- or a quadruple-window approach (**array-by-array calibration**) by calibrating each array independently if the above co-alignment requirement is not met.

For **DS**, at least two windows are required in order to determine the spectral distortion. An individual spectral calibration of arrays S3 (IRS-3/4) and S5 (IRS-7/8/9) appears hardly possible. We investigate

- a two-window approach (**all-array calibration**) in W02, W03 that requires an inter-array co-alignment better than 1 \(10^{-6}\) in terms of the relative shift knowledge error, corresponding to a noise allocation of 0.025K NEdT@280K,
- a quadruple-window approach (**two-by-two array calibration**), calibrating arrays S2/S3 (W02+W11) and S4'/S5 (W16+W03), requiring the above co-alignment between combined arrays,
- the individual spectral calibration of arrays S2 (W02+W21), S4 (W13+W14) and S4' (W15+W16) (**partial array-by-array calibration**).

Co-alignment requirements are quantitatively justified in [RD 2, section 3.4.3]

2.3. Geophysical conditions

Spectral calibration of MTG/IRS spectra is considered for four representative atmospheric regimes (hot and humid, hot and dry, temperate and moderately humid, cold and dry). Each regime is represented by a clear-sky and a cloudy spectrum. The atmospheric and surface conditions are characterised in more detail in [RD 2, §2.3]. [RD 2] analysis of the impact of atmospheric variability on the spectral shift determination encouraged the use of a unique, globally applicable reference spectrum, corresponding to reference atmospheric conditions. The atmospheric reference case is defined as the temperate, moderately humid atmospheric state without clouds.
3. Application conditions for full spectral calibration experiments

3.1. Spectral calibration functions and instrument state parameters

From [RD 1, section 3.2.1], we recall the spectral shift dependency on the instrument state for the two instrument concepts. For DS in each spatial sample $i$ (associated to a detector line in the spectral dimension), we assume the shift (in wavelength) $\delta \lambda$ as the sum of a spectral offset $A$ and a distortion $D$ of the detector array in the spectral dimension. To account for the rigidity of the detector array, we assume a linear variation of the spectral offset in the spatial (N/S) dimension. Therefore, we define $A_0$ and $A_1$ as the spectral offset in the lower (southern) and upper (northern) swath edges of the detector array, respectively, and the position $p$ of a spatial sample $i$ in relative N/S swath coordinates, i.e., $p_i=0$ and $p_i=1$ for the spatial samples at the southern and northern swath edges. The description of the spectral shift over the entire DS detector array is then given by:

$$\lambda_{i1a} - \lambda_{i1b} = \delta \lambda_i = A_0 + p_i (A_1 - A_0) + (D-1) \hat{\lambda}_{ib}$$

or in wave number ($\nu$):

$$\delta \nu_i = \nu_{ib} (1/( (A_0 + p_i (A_1 - A_0) ) \nu_{ib} + D) - 1)$$

The spectral calibration function is given by:

$$F_{SC} = \nu_{ib}/\nu_{ia} = \nu_{ib}/(\delta \nu_i + \nu_{ib}) = (A_0 + p_i (A_1 - A_0) ) \nu_{ib} + D$$

The instrument state is described by the three parameters $A_0$, $A_1$, $D$, to be estimated by the spectral calibration procedure. The nominal instrument state is given by $D=1$, $A_0=A_1=0$.

With

$$A_i = A_0 + p_i (A_1 - A_0)$$

the minimum requirement for the solution of the system

$$D = \frac{\nu_2}{\nu_2 - \nu_1} \frac{\nu_1}{\nu_1 + \delta \nu_{li}} - \frac{\nu_1}{\nu_2 - \nu_1} \frac{\nu_2}{\nu_2 + \delta \nu_{li}}$$

is the determination of the distortion factor $D$ through at least two shift estimations $\delta \nu_1$ and $\delta \nu_2$ at wave numbers $\nu_1$ and $\nu_2$, and of spectral offsets $A_i$ in at least two relative swath positions. $A_0$, $A_1$, and $D$ are determined by a multi-linear regression (equation 1) and minimisation of the root mean square difference between estimated and approximated wavelength shifts.

It is emphasised that the above spectral calibration function considers a very simple instrument model (e.g., constant linear dispersion, ISRF model independent of the spatial sample). In practice, the spectral calibration function will be more complex and needs to be adapted to the detailed instrument model all along the upcoming development phases. On the other hand, the spectral calibration function may be simplified if offset variations over the spatial dimension or if distortion in the spectral dimension is negligible by design.
The current assumption on the spectral calibration function is not limiting the validity of the results presented in this report as long as:

- the spectral shift is a known analytical function of instrument parameters,
- the impact of instrument state variations on the ISRF shape is negligible.

For **FTS**, the spectral shift $\delta \nu_i$ depends on the average field angle $\alpha_i$ of a spatial sample $i$ in good approximation by:

$$\delta \nu_i = \nu_{i1a} - \nu_{i1b} = \nu_{i1b} (\cos \alpha_i - 1)$$

(7.)

The spectral calibration function is given by:

$$F_{SC} = \frac{\nu_{i1b}}{\nu_{i1a}} = \frac{\nu_{i1b}}{(\delta \nu_i + \nu_{i1b})} = \frac{1}{\cos \alpha_i}$$

(8.)

Spectral shift determinations translate into average field angle estimations for each spatial sample. The system is then fully characterised by a single instrument state parameter, the interferometer axis position, i.e., the focal plane coordinates where the field angle is zero. Its estimation requires a simultaneous spectral shift determination for at least three non-aligned spatial samples in at least one spectral calibration window.

### 3.2. Spatio-temporal selection criteria

#### 3.2.1. Scene filtering requirements

The analysis of the spectral shift determination errors of individual measurements [RD 2] yields critical performances for cold scenes, either due to polar atmospheric regimes where small vertical temperature gradients lead to attenuated spectral signatures, or due to high opaque clouds hiding spectral signatures from below the cloud top. In addition, any cold scene is associated with a relatively low signal-to-noise ratio.

Moreover, [RD 5] suggests a filtering of scenes characterised by a cloud border appearance near the spatial sample centre due to a critical amount of spectral calibration pseudo-noise (induced by scene heterogeneity) in the following conditions: (a) the cloudy and clear-sky component have a strong radiometric contrast, (b) in case of FTS, the spatial sample is associated with a high field angle and the cloud border is oriented perpendicular to the field angle gradient, (c) in case of DS, the cloud border is oriented perpendicular to the spectral dimension, i.e., it has a meridional component.

Scene filtering is part of the spectral calibration pre-processing and thus requires external or internal scene identification. A qualitative identification of scene filtering requirements is desirable by now, since potentially affecting the instrument design. The identification of cold scenes might be obtained by simple threshold tests in atmospheric window regions applied either on predefined IRS spectral clusters or on co-registered spatial clusters of the IRS built-in imager. The identification of cloud border conditions requires co-registered measurements at the sub-scale of IRS spatial samples from the built-in imager in the thermal window region.

Far beyond the study scope, a detailed analysis of the scene filtering requirements on the spectral calibration performance requires a realistic description of the spatial variation of atmospheric conditions and the simulation of the corresponding high-resolution spectra.
3.2.2. Selection of detector array elements

Due to the large number of detector elements per array, it appears neither beneficial, nor feasible to exploit each spatial sample for the determination of instrument parameters. Therefore, a sub-selection of spatial samples for instantaneous instrument state determination is carried out such that first indications of the impact of different sub-selections on the instrument state estimation accuracy are obtained.

3.2.2.1. DS

A spatial sample $i$ corresponds to an E/W detector line in the spectral dimension. We select four spatial samples with relative swath coordinates $p_1=0$, $p_2=0.33$, $p_3=0.67$ and $p_4=1$. This allows to investigate the impact of various selections on the instrument state estimation performance.

![Illustration of the DS detector array (in focal plane coordinates) in nominal (black) and actual (green) instrument states. Four spatial samples (detector lines) $i=1,2,3,4$ with $p_1=0$, $p_2=0.33$, $p_3=0.67$ and $p_4=1$ are selected for full spectral calibration examples. Sub-selection of $i=1,4$ and $i=2,3$ is also considered. The selection in the spectral dimension is governed by the choice of spectral calibration windows (c.f. section 2.2).](image)

3.2.2.2. FTS

A spatial sample $i$ corresponds to a detector element in the array. We select nine spatial samples in the diagonals of the detector array. This allows in particular to investigate the impact of various selections on the instrument state estimation performance as function of the nominal distance of the selected detectors from the interferometer axis. We select four detectors at two third ($i=1-4$) and four others ($i=5-8$) at one third of the maximum field angle (87.5 mrad). In addition, we consider a detector at zero nominal field angle ($i=9$).
3.2.3. Simulation of atmospheric variability

In this early phase of the MTG/IRS spectral calibration algorithm development, we abstain from a detailed analysis of spatial atmospheric variations. The spectral calibration experiments are applied to a homogeneous atmosphere over the entire spatial sample selection in the eight conditions recalled in section 2.3.

3.2.4. Spectral calibration period

While a time filter function of successive instrument state estimations is prepared for implementation in the used software, it is not applied in the current study, where we provide quantified spectral calibration noise estimations for an instantaneous determination of the instrument state. The impact of time filtering on the spectral calibration performance is discussed qualitatively as study conclusion.

This is conform with the development logic of the MTG/IRS spectral calibration algorithm: In a first step (this study), we quantify the instrument stability requirements. In a second step, an investigation in which time frame these requirements are feasible is requested, before a trade-off between requirement and feasibility leads to the specification of the spectral calibration period.
3.2.5. Radiometric noise

Radiometric noise is randomly generated according to the spectral noise figures of the two concept baselines (see section 2.1 and Figure 3).

![MTG/IRS radiometric noise](image)

Figure 3: Radiometric noise (1σ) as function of wave number for IRS DS and FTS concepts. With respect to the baseline [RD 3], performances are rescaled by elimination of the spatial FIR filtering effect (both concepts) and the apodisation effect (FTS only). The reported performance applies to level 1a/1b for both concepts.

It is important to note that radiometric noise is added in a random way separately for each selected spatial sample and the corresponding level 1a spectrum. While a single noise draw can be favourable or unfavourable for an individual spectral shift determination, the probability for a favourable or unfavourable noise configuration in view of the instrument state parameter determination over several spatial samples is reduced.
4. Quantified spectral calibration performance

We investigate in this section the overall spectral calibration algorithm performance at the instantaneous scale, i.e., spectral calibration of all spatial samples independently for each dwell period. The results will hint at the necessity or not to accumulate and temporally filter observations over longer (spectral calibration) periods in order to reduce the impact of radiometric noise on the spectral calibration accuracy.

4.1. DS baseline

As discussed in section 2.2, at least two windows are required in order to determine the spectral distortion. We investigate the all-array calibration (W02/IRS-1 + W03/IRS-7) that represents the most favourable case for the system but might be unfeasible. It requires a good inter-array co-alignment and equivalent spectral distortion in all arrays. The alternative two-by-two array configuration calibrates bands at low and at high spatial sampling independently of each other, but still combines windows from two different arrays (W02/IRS-1 + W11/IRS4 and W16/IRS-6 + W03/IRS-7). Finally, the single-array approach calibrates three arrays independently of each other (W02/IRS-1+W21/IRS-2), (W13+W14/IRS-5) and (W15+W16/IRS-6). If this configuration reveals advantageous performances, solutions for the remaining arrays IRS-3/4 and IRS-7/8/9 should be re-investigated.

In practice, the spectral calibration procedure consists of an individual spectral shift determination in each calibration window and each selected spatial sample for the selections i=1,2,3,4; i=1,4; i=2,3 (see section 3.2.2.1), respectively referred to as ‘full’, ‘outer’ and ‘inner’, hereafter.

The instrument state parameters $D, A_0, A_1$ in equation (1) are determined by a least-square linear regression over four (in spatial sample selection ‘inner’ or ‘outer’) or eight (‘full’) individual shift determinations.

The performance is evaluated for eight instrument states, listed in Table 4.

<table>
<thead>
<tr>
<th>DS instrument state index</th>
<th>$A_0$ [nm]</th>
<th>$A_1$ [nm]</th>
<th>$D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (reference)</td>
<td>0.000</td>
<td>0.000</td>
<td>1.0000</td>
</tr>
<tr>
<td>2</td>
<td>0.400</td>
<td>0.399</td>
<td>0.9999</td>
</tr>
<tr>
<td>3</td>
<td>0.400</td>
<td>0.399</td>
<td>1.0000</td>
</tr>
<tr>
<td>4</td>
<td>0.000</td>
<td>0.000</td>
<td>0.9999</td>
</tr>
<tr>
<td>5</td>
<td>-0.400</td>
<td>-0.399</td>
<td>0.9999</td>
</tr>
<tr>
<td>6</td>
<td>-0.400</td>
<td>-0.399</td>
<td>1.0001</td>
</tr>
<tr>
<td>7</td>
<td>0.000</td>
<td>0.000</td>
<td>1.0001</td>
</tr>
<tr>
<td>8</td>
<td>0.400</td>
<td>0.399</td>
<td>1.0001</td>
</tr>
</tbody>
</table>

Table 4: DS instrument states investigated for spectral calibration performance assessment. State 1 is the reference state corresponding to the reference spectrum in the shift determination processing.
The corresponding relative shift is shown for the spatial sample \( i=1 \) in Figure 4. It is independent of wave number only if the spectral offset \( A_0 \) is zero (straight lines).

\[
\text{relative shift for eight DS instrument states (spatial sample } i=1)\]

![Figure 4: Relative spectral shift as function of wave number in spatial sample \( i=1 \) \((p_r=0)\) for eight instrument states defined in Table 4.](image)

The instrument states have been chosen such that the maximum relative shift is limited to \( \pm 2 \times 10^{-4} \).

### 4.1.1. Impact of spatial sample selection

The impact of the number and the position of the spatial sample selection on the accuracy of the regression is investigated for the all-array spectral calibration (using windows W02/IRS-1 and W03/IRS-7) upon the spatial sample selections defined in section 3.2.2.1.

Figure 5 presents the rms regression error of \( \delta \lambda_i \) in equation (1) in calibration windows W02+W03 as function of atmosphere and instrument state. Expectedly, the accuracy of the regression for cold scenes 0722 (high opaque Cb) and 0933 (sub-polar atmosphere with mid-level cloud) is significantly lower than for warmer scenes. We focus the discussion on the latter. The regression error for the selections ‘outer’ and ‘inner’ appears quite noisy with the instrument state. The noise is not correlated with the instrument state for both sample sub-selections, but dominated by the radiometric noise. This is why the regression error for the full sample selection is often close to the average of the regression errors of the two sample sub-selections. The random impact of radiometric noise is reduced, but a selection of four spatial samples instead of two provides in average no advantage in view of the regression accuracy. This is documented by the average regression rms error over the eight instrument states, presented separately for the six remaining atmospheres in Table 5. The best performance is associated to either the ‘inner’ or the ‘outer’ two-sample selection. Nonetheless, we consider the ‘full’ four-sample selection in the upcoming performance analysis in order to dampen the random impact of the small number of considered instrument states on the overall performance analysis. In terms of the operational algorithm design, however, a two-sample selection filtered in time over several integration periods might be a more suitable choice.
Figure 5: Regression error (rms) for the determination of the instrument state $A_0$, $A_1$, and $D$ in calibration windows W02/IRS-1+W03/IRS-7 as function of atmosphere (first abscissa index, c.f. [RD 2, Table 4]) and instrument state (second abscissa index, from 1 to 8 for each atmosphere) for three spatial sample selections.

<table>
<thead>
<tr>
<th>Atmosphere</th>
<th>spatial sample selection</th>
<th>W02/IRS-1+W03/IRS-7</th>
</tr>
</thead>
<tbody>
<tr>
<td>0511 – temperate /moderately humid – clear-sky</td>
<td>full</td>
<td>17.9</td>
</tr>
<tr>
<td>0512 – temperate /moderately humid – low stratus</td>
<td>outer</td>
<td>11.6</td>
</tr>
<tr>
<td>0721 – hot/humid – clear-sky</td>
<td>inner</td>
<td>13.0</td>
</tr>
<tr>
<td>1611 – hot/dry – clear-sky</td>
<td>full</td>
<td>11.5</td>
</tr>
<tr>
<td>1614 – hot/dry – thin cirrus</td>
<td>outer</td>
<td>14.1</td>
</tr>
<tr>
<td>0931 – cold/dry – clear-sky</td>
<td>inner</td>
<td>29.9</td>
</tr>
</tbody>
</table>

Table 5: Regression rms error averaged over eight instrument states in $[10^{-12} \text{ m}]$ for six atmospheric conditions and three spatial sample selections in calibration windows W02/IRS-1+W03/IRS-7. Best performance per atmosphere is highlighted.
Moreover, the fact that the outer sample selection does not provide systematically better results than the inner sample selection indicates that the sample-dependent determination of a spectral offset between $A_0$ and $A_1$ is not driving the regression, at least over the investigated instrument states. A spectral offset common to all spatial samples would yield similar results. The necessity to consider a spectral offset variable with the spatial sample should be consolidated upon the explicit instrument design.

### 4.1.2. Performance for different spectral calibration windows

In the full spatial sample selection, spectral calibration experiments are carried out separately in six combinations of spectral calibration windows for eight atmospheric conditions and eight instrument states. Opposite to an FTS concept, the performance in terms of relative spectral shift errors depends on the wavelength and has to be analysed separately by spectral band.

This section summarises the obtained 4 (spatial samples) by 6 (window combinations) by 8 (atmospheres) by 8 (instrument states) by 9 (bands) relative shift error determinations in view of an overall performance assessment.

Figure 6 is intended to illustrate the different dimensions of the relative spectral shift error determinations and to develop a strategy to analyse them. The performance variation with the spectral calibration window selection is not represented, all results refer to the all-array calibration configuration W02/IRS-1+W03/IRS-7.

Performance variation with the atmosphere is important. At first glance, a weak performance for cold scenes with respect to warmer scenes is noticeable. For a given atmosphere, the performance does not strongly depend on the spatial sample, at least for those atmospheres yielding relatively good performances. This result indicates the desired homogeneity of the spectral calibration performance over all spatial samples.

The performance variation with the instrument state is not negligible, but can be referred to a random impact of radiometric noise. Negative performance accidents cannot be systematically referred to a specific instrument state.

A strong performance variation over spectral bands becomes obvious for certain atmospheres (e.g., 0721 and 0931). Hence, the spectral calibration leads to relative shift determination errors ($\text{SDE}_r$) that must be analysed at the scale of spectral bands. The band dependence of the performance variation indicates a monotonous, more or less linear variation with wave number. In numerous cases, relative $\text{SDE}$ in IRS-1 and IRS-9 are of opposite sign. However, the sign appears as randomly induced by the atmospheric conditions, it has no physical meaning.

We conclude from Figure 6 that the rms relative spectral shift errors over spatial samples and instrument states represent the overall spectral calibration algorithm performance

- for a specific choice of spectral calibration windows,
- for a given geophysical scene distribution,
- within a spectral band.

By consequence, we analyse here below the rms relative $\text{SDE}$ for eight atmospheric conditions in nine bands for the six window combinations.
Figure 6: Relative spectral shift determination error SDE, after spectral calibration in calibration windows W02/IRS-1+W03/IRS-7 as function of the selected spatial sample (pixel, first abscissa index from 1 to 4), the instrument state (second abscissa index, from 1 to 8 for each pixel) and the type of atmosphere (symbols) in bands IRS-1, -5 and –9 (from top to bottom).
Figure 7 shows the rms relative shift errors for an instantaneous all-array calibration (in windows W02/IRS-1 and W03/IRS-7) under the condition of good inter-array co-alignment.

![Diagram showing relative shift errors for different atmospheric conditions](image)

**Figure 7:** DS all-array spectral calibration. Relative shift error (rms over four spatial samples and eight instrument states) per mission band for eight atmospheric conditions in spectral calibration window configuration W02/IRS-1 + W03/IRS-7.

Relative rms shift errors are spectrally constant for certain atmospheres. For the other atmospheres there is a more or less clear tendency to error minimisation in IRS-4/IRS-5 (i.e., midway between the two calibration windows) while maximum errors occur outside the range covered by the windows in IRS-8 and IRS-9. The ratio between maximum and minimum errors does not exceed 4.

In terms of performance variation with the atmosphere type, the coldest scenes (0722, 0932) perform worst (about $10^{-5}$) as expected. It is interesting to notice that the best performance (about $10^{-6}$) is obtained with the reference atmosphere (0511) and the radiatively similar case of the reference atmosphere with low clouds (0512). It is about two times better than for the hot and dry atmosphere type (without and with cirrus, 1611 and 1612, respectively) and better (except in IRS-5) by a variable factor up to 3 than for the hot and humid atmosphere type (0721). A tendency to higher performance for the reference atmosphere has not been clearly observed for the individual shift determination in individual calibration windows [RD 2, section 5.1]. This let us conclude that a performance gain for the reference atmosphere is due to a spectrally consistent SDE in the two calibration windows, while SDE for scenes deviating from the reference state, though of the same magnitude, may be less consistent over the two calibration windows (e.g., by their sign).

Figure 8 and Figure 9 provide the rms relative shift errors in case of an independent calibration of arrays S2/S3 (in W02/IRS-1 and W11/IRS-4) and of arrays S4'/S5 in (W16/IRS-6 and W03/IRS-7). This configuration represents the two-by-two array calibration. Results are shown over the full spectral range, but apply in first place to bands 1-4 (Figure 8) and 6-9 (Figure 9). For the other bands, results indicate the in general decreasing, theoretical performance if results are extrapolated beyond the spectral range covered by the calibration windows, assuming perfectly co-aligned arrays.
For all but cold scenes, calibration of bands 1 to 4 in W02 and W11 provides slightly better results between $5 \times 10^{-7}$ and $25 \times 10^{-7}$ as for the all-array calibration. The tendency towards an improved performance for the reference scene is weakened in comparison to Figure 7.
Calibration of bands 6 to 9 in W16 and W03 slightly improves the results for the all-array calibration in bands 6 and 7 only. The performance decrease in IRS-8 and IRS-9 is uncritical due to the low radiometric sensitivity to spectral shift errors in these bands.

Accordingly to the previous figures, Figure 10, Figure 11 and Figure 12 address the possibility for independent array-by-array calibration of arrays S2 in W02/IRS-1 and W21/IRS-2, S4 in W13 and W14/IRS-5, and S4’ in W15 and W16/IRS-6, respectively. Again, results are shown over the full spectral range, but apply in first place to the bands where the calibration windows are situated. Extrapolation to other arrays, even if perfectly co-aligned, yields poor performance.

Array S2 calibration (Figure 10, IRS-1 and –2) is comparable in performance with the preceding configurations in band IRS-1 only. The relatively low performance of W21/IRS-2 as individual spectral calibration window explains a systematic increase of the rms relative shift error in IRS-2 by more than a factor 2.

Individual array S4(IRS-5) calibration (Figure 11) generates relative shift errors of the order of $4 \times 10^{-6}$ for warmer scenes. For the reference scene a much better performance ($1 \times 10^{-6}$) is observed.

Individual array S4’(IRS-6) calibration (Figure 12) performs at an accuracy of $1 \times 10^{-6}$ to $2 \times 10^{-6}$ for all but cold scenes.

The array-by-array calibration performs generally at a lower level than the preceding configurations. Nevertheless, the compliance with the specification must be evaluated upon radiometric errors. So array-by-array spectral calibration should not be excluded as algorithm design option for the only reason of a performance loss with respect to the (possibly unfeasible) all-array and two-by-two array configurations.

**Figure 10:** As Figure 7 for individual array S2 calibration in windows W02/IRS-1 + W21/IRS-2.
The link of relative spectral shift errors, discussed here above, with radiometric errors is established using the relation between radiometric noise (rms over channels per mission band) and relative spectral shift, and its variation with the atmosphere type. These relations are derived in [RD 2, Table 6 and Figure 8].
For the all-array spectral calibration, Figure 7 translates directly into radiometric errors by multiplication of relative spectral shift errors with the radiometric sensitivity coefficients. The resulting radiometric noise per mission bands is shown in Figure 13 for the four investigated clear-sky atmospheres. For clarity, the results for the cloudy scenes 0512 (low opaque clouds, similar to 0511) and 1612 (thin cirrus, similar to 1611) are not shown.

Figure 13: DS all-array spectral calibration, perfect array co-alignment

From Figure 13 it is concluded that the spectral calibration noise due to spectral shift errors is for the investigated scenes in all bands within the allocated 0.10K NEdT@280K. This statement applies to an instantaneous instrument state determination over a single dwell period of 15.5 ms (7.8 ms in bands 5 to 9). In case of a stable instrument, the performance can be significantly improved by accumulation of measurements over longer periods and sub-sequent time filtering.

Secondly, the performance is best for the reference atmosphere, indicating that atmospheric prior knowledge is beneficial for the spectral calibration algorithm performance. However, using a unique, global reference spectrum yields still a largely acceptable performance for all but the coldest scenes.

The only reservation for the applicability of Figure 13 is the possibly unfeasible requirement on inter-array co-alignment, more precisely the incapacity to predict a spectral shift in bands IRS-3 to IRS-6 from the only spectral shift determination in IRS-1 and IRS-7.

In this context, Figure 14 presents the radiometric noise in the configuration of the two-by-two-array spectral calibration, i.e., independently in bands with low (IRS-1 to IRS-4) and with high (IRS-5 to IRS-9) spatial resolution. In this configuration, a perfect co-alignment is only required between arrays within these band groups.
Figure 14: DS two-by-two-array spectral calibration in W02/IRS-1 + W11/IRS-4 and W16/IRS-6 + W03/IRS-7 in case of perfect co-alignment of arrays S2/S3 and S4'/S5. Radiometric spectral calibration noise in cK NEdT@280K (rms per mission band) for instantaneous determination of the spectral calibration function over one dwell period without time filtering. Also shown (as isolated data points) is the radiometric spectral calibration noise for separate array-by-array calibration of S2 (in W02/IRS-1 and W21/IRS-2), S4 (in W13 and W14/IRS-5) and S4’ (in W15 and W16/IRS-6).

The general comments given for Figure 13 apply again. In particular, the spectral calibration in conditions of the reference atmosphere is associated with the best performance. It is then interesting to compare the performances of all-array and two-by-two array calibration (excluding IRS-5, which is not addressed by the spectral calibration in windows W16/IRS-6 and W03/IRS-7). The performances are similar in magnitude with slight variations in both directions depending on spectral band and atmosphere type.

The array-by-array spectral calibration algorithm noise, also shown in Figure 14, is increased by a factor 4 in IRS-2 with respect to the all-array and two-by-two array configurations, while an equivalent performance for all three configurations is noticed for IRS-1 and IRS-6. A performance loss with respect to the all-array calibration is observed for IRS-5. This reduction is variable with the atmosphere type. Nevertheless, all noise estimations for the separate array-by-array configurations are reasonably low with respect to the overall spectral calibration noise allocation.

In summary, the spectral calibration performance for DS over a single dwell period, using a unique, global reference spectrum is within the specification of the 0.10K NEdT@280K in all investigated cases except for the coldest scenes. Therefore, an investigation of the potential for performance increase by accumulation of measurements over periods much longer than the dwell period (reduced impact of radiometric noise), is not of first priority at this stage of the spectral calibration algorithm assessment.

As potentially critical aspects, we mention the high relevance of IRS-1 as provider of a suitable calibration window in all investigated configurations. The above statements are less optimistic if IRS-1 should be abandoned during the further mission development phases.
Furthermore, a separate calibration of array S3 (IRS-3 and –4) is difficult to obtain. An instrument concept optimised from the spectral calibration point of view would require a mandatory implementation of IRS-1 with good co-alignment of arrays covering IRS-1 on the one hand and IRS-3/4 on the other hand.

For mission bands at high spatial resolution, a separate calibration of array S5 (IRS-7, -8, -9) has not been investigated. Considering IRS-8 and IRS-9 as candidate bands for elimination, and implementation of IRS-6 and IRS-7 on a common array would resolve potential alignment problems in this spectral domain.

With respect to the high relevance of IRS-1 as spectral calibration window provider, feasibility issues in terms of radiometric resolution rise the question if the considered spectral calibration window W02 in IRS-1 (720 – 750 cm\(^{-1}\)) is still useful in case of degraded radiometric resolution. In this context, EUMETSAT provided a relaxed specification of radiometric resolution referred to as ‘bad noise’ configuration. It defines three values (NEdT@280K) in band IRS-1: 1K below 715 cm\(^{-1}\), 0.6K above 730 cm\(^{-1}\), and 0.8K in between. Radiometric resolution in all other bands is 0.4K.

The spectral calibration algorithm is applied to the array spectral calibration of low-resolution bands IRS-1 to –4 in windows W02/IRS-1 and W11/IRS-4. Results are compared to those obtained with DS baseline noise (Figure 8, Figure 14, results for IRS-1 to IRS-4). Table 6 reports the error ratio between the ‘bad noise’ and DS baseline noise configurations.

<table>
<thead>
<tr>
<th>Atmosphere</th>
<th>IRS Mission band</th>
</tr>
</thead>
<tbody>
<tr>
<td>0511 – temperate /moderately humid – clear-sky</td>
<td>2.1 2.2 2.7 3.2</td>
</tr>
<tr>
<td>0512 – temperate /moderately humid – low stratus</td>
<td>1.9 2.5 3.9 4.9</td>
</tr>
<tr>
<td>0721 – hot/humid – clear-sky</td>
<td>1.3 1.3 1.3 1.5</td>
</tr>
<tr>
<td>1611 – hot/dry – clear-sky</td>
<td>1.4 1.6 3.7 2.9</td>
</tr>
<tr>
<td>1612 – hot/dry – thin cirrus</td>
<td>1.6 2.3 3.6 3.2</td>
</tr>
<tr>
<td>0931 – cold/dry – clear-sky</td>
<td>1.4 1.2 1.1 1.2</td>
</tr>
</tbody>
</table>

Table 6: Rms error ratio for DS spectral calibration in W02/IRS-1 and W11/IRS-4 in bands 1 to 4 for six atmospheres: Bad noise over DS baseline noise.

We state an increase of the rms relative shift error by factors between 1.1 and 4.9, depending on atmosphere type and the mission band. The noise degradation has a stronger impact for reference and close-to-reference scenes 0511 and 0512 where the impact of atmospheric noise on the shift error is zero or low. For the other scenes, noise degradation due to the loss in radiometric resolution is smaller.

It is further noticed that shift error degradation in IRS-1 is limited to a factor 2, which corresponds roughly to the radiometric resolution ratio of ‘bad noise’ and DS baseline noise. Higher factors are observed in IRS-4 where bad noise is equal to about six times the DS baseline noise.

With the performance loss in the ‘bad noise’ configuration as reported in Table 6, the spectral calibration algorithm noise over a single dwell period is still below 0.05K for all atmosphere types in all bands. Therefore, even in case of an unfavourable radiometric resolution, IRS-1 has an important impact on the spectral calibration performance of bands IRS-1 to IRS-4.
4.2. FTS baseline

As mentioned in section 2.2, the IRS/FTS spectral calibration is applied in five mono-window configurations (W02/IRS-1, W11/IRS-4, W13/IRS-5, W16/IRS-6, W03/IRS-7) corresponding to a separate calibration of each focal plane (A1, A2, A3, A3’, A4, respectively). In case of sufficient inter-array co-alignment, the results obtained for a given array can be extrapolated over other arrays.

In practice, the theoretical spectral shift for each selected spatial sample (after Figure 2) is stored in the spectral data base (SDB) for nine interferometer axis positions in focal plane coordinates at –1, 0, +1 mrad in both dimensions with respect to the nominal interferometer axis position. The actual interferometer axis position is interpolated in the SDB by least-square minimisation of individual shift determinations for the selected spatial samples within the pre-calculated theoretical shifts.

For the simulation of FTS level 1a spectra we consider four interferometer axis positions on the upper right half-diagonal of the array:

<table>
<thead>
<tr>
<th>axis position</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>x/y [µrad]</td>
<td>0/0</td>
<td>10/10</td>
<td>100/100</td>
<td>400/400</td>
</tr>
</tbody>
</table>

Table 7: IRS/FTS interferometer axis positions [µrad] in focal plane coordinates considered for full spectral calibration experiments.

The underlying hypothesis related to the practical algorithm is that instantaneous axis positions are limited such that no border position in the SDB grid is closest to the actual axis positions, i.e., that axis position variations are constrained to the range ±0.5 mrad in both dimensions. Otherwise, the axis position determination is flagged as failure. This quantitative assumption is not constraining for the spectral calibration algorithm itself, but it has impact on the initialisation parameters of the spectral shift determination procedure, in particular on the spectral range where a correlation maximization between measured and reference spectrum is attempted. In this context, it is important that a nominal range of interferometer axis positions is quantified during the instrument design phase.

4.2.1. Impact of spatial sample selection

The impact of the number and the position of selected spatial samples for interferometer axis position determination is investigated in two spectral calibration windows (W02/IRS-1 and W03/IRS-7) for three sub-selections of spatial samples defined by Figure 2:

a) all nine spatial samples (i=1-9)
b) the four outer spatial samples (i=1-4)
c) the four inner spatial samples (i=5-8)
Figure 15: Interferometer axis position determination error as function of atmosphere (first abscissa index, c.f. [RD 2, Table 4]) and axis position (second abscissa index, from 1 to 4 for each atmosphere, see Table 7) for three spatial sample selections in calibration window W02/IRS-1.

Figure 16: As Figure 15, but in calibration window W03/IRS-7.
Figure 15 and Figure 16 present the axis determination errors in calibration windows W02 and W03, respectively. Values out of range indicate failure of the position determination process and occur exclusively for cold scenes (“0722 high opaque Cb” and “0933 sub-polar atmosphere with mid-level cloud”). For the other atmospheres, there is no obvious relation between performance and axis position. The impact of the spatial sample selection can then be evaluated by the average error over the four axis positions as provided in Table 8.

<table>
<thead>
<tr>
<th>Atmosphere</th>
<th>Window W02/IRS-1</th>
<th>Window W03/IRS-7</th>
</tr>
</thead>
<tbody>
<tr>
<td>i = 1-9</td>
<td>i = 1-4</td>
<td>i = 1-4</td>
</tr>
<tr>
<td>i = 5-8</td>
<td>i = 1-9</td>
<td>i = 1-4</td>
</tr>
<tr>
<td>i = 5-8</td>
<td>i = 1-4</td>
<td>i = 1-4</td>
</tr>
<tr>
<td>0511 – temperate /moderately humid – clear-sky</td>
<td>36.5</td>
<td>19.0</td>
</tr>
<tr>
<td>0512 – temperate /moderately humid – low stratus</td>
<td>15.6</td>
<td>18.0</td>
</tr>
<tr>
<td>0721 – hot/humid – clear-sky</td>
<td>20.2</td>
<td>11.4</td>
</tr>
<tr>
<td>1611 – hot/dry – clear-sky</td>
<td>18.5</td>
<td>11.8</td>
</tr>
<tr>
<td>1614 – hot/dry – thin cirrus</td>
<td>14.7</td>
<td>10.4</td>
</tr>
<tr>
<td>0931 – cold/dry – clear-sky</td>
<td>52.9</td>
<td>40.3</td>
</tr>
</tbody>
</table>

Table 8: Interferometer axis position determination error in [µrad] averaged over four axis positions in six atmospheric conditions and three spatial sample selections in calibration windows W02/IRS-1 and W03/IRS-7. Best performance per window and atmosphere is highlighted.

Except for three atmospheres in window W02, the selection of nine spatial samples shows the best performance. However, the sub-selection of four pixels at two third of the maximum field angle performs almost equivalently. A strong performance decrease is observed for the sub-selection of the four spatial samples at one third of the maximum field angle. This is explained by the fact that the spectral shift of a spatial sample $i$ is proportional to the nominal average field angle $\alpha_{0i}$. Is $\Delta \alpha_i$ the difference between actual and nominal field angle, the relative spectral shift deviation from nominal, $\Delta (\delta \nu/\nu)_{0i}$, is given by

$$
\Delta \left( \frac{\delta \nu}{\nu} \right)_{0i} = \cos(\alpha_{0i} + \Delta \alpha_i) - \cos \alpha_{0i} = \cos \alpha_{0i} \cdot (\cos \Delta \alpha_i - 1) - \sin \alpha_{0i} \cdot \sin \Delta \alpha_i \approx -\alpha_{0i} \cdot \Delta \alpha_i
$$

(9.)

as long as self-apodisation is negligible ($\alpha_{0i}$ not too close to zero) and $\Delta \alpha_i$ small. Shift determinations at smaller field angles are then less significant for the axis position determination.

For validation purposes we apply the full pixel selection (9 spatial samples) to the spectral calibration experiments although it is anticipated that an operational spectral calibration algorithm can exploit the information from four spatial samples at preferably high field angles without a significant performance loss.

4.2.2. Performance for different spectral calibration windows

Spectral calibration experiments are carried out separately in five spectral calibration windows for eight atmospheric conditions and four actual interferometer axis positions as described above.

The estimated axis positions are shown in Figure 17 distinguishing the actual axis position by colours and the calibration window by symbols (performance variation with atmospheric conditions is not explicitly shown on this figure).
Figure 17: Estimated interferometer axis positions for four true axis positions (colours), five spectral calibration window (symbols) and eight atmospheric conditions (not further distinguished here).

It can be noticed that the typical estimation accuracy of the axis position is of the order of 50 µrad, independently of the actual axis position itself. The corresponding axis position estimation errors are shown in Figure 18 as function of the true axis position, the atmosphere and the calibration window. Failure of the position determination procedure concerns exclusively the cold scenes 0722 and 0933. For the other atmospheres, the position estimation error does not systematically depend on the axis position itself. Again, the performance is analysed on errors averaged over the four axis positions. These are provided in Table 9.

Interestingly, since opposite to the performance characteristics of the DS spectral calibration, the FTS spectral calibration has no tendency to a performance increase when atmospheric conditions correspond to the reference atmosphere (0511). In most of the calibration windows, the axis position determination errors are smaller for the hotter scenes (0721, 1611, 1612) than for the reference scene (0511).
Figure 18: Interferometer axis position determination error as function of atmosphere (first abscissa index, c.f. [RD 2, Table 4]) and axis position (second abscissa index, from 1 to 4 for each atmosphere, see Table 7) for five spectral calibration windows.

<table>
<thead>
<tr>
<th>Atmosphere</th>
<th>Spectral calibration window</th>
<th>W02</th>
<th>W11</th>
<th>W13</th>
<th>W16</th>
<th>W03</th>
</tr>
</thead>
<tbody>
<tr>
<td>0511 – temperate /moderately humid – clear-sky</td>
<td>IRS-1</td>
<td>36.5</td>
<td>44.1</td>
<td>37.5</td>
<td>77.9</td>
<td>19.0</td>
</tr>
<tr>
<td>0512 – temperate /moderately humid – low stratus</td>
<td>IRS-1</td>
<td>15.6</td>
<td>40.8</td>
<td>49.7</td>
<td>45.4</td>
<td>18.0</td>
</tr>
<tr>
<td>0721 – hot/humid – clear-sky</td>
<td>IRS-4</td>
<td>20.2</td>
<td>17.4</td>
<td>45.5</td>
<td>50.2</td>
<td>11.4</td>
</tr>
<tr>
<td>1611 – hot/dry – clear-sky</td>
<td>IRS-5</td>
<td>18.5</td>
<td>36.1</td>
<td>21.9</td>
<td>31.2</td>
<td>11.8</td>
</tr>
<tr>
<td>1614 – hot/dry – thin cirrus</td>
<td>IRS-6</td>
<td>14.7</td>
<td>38.6</td>
<td>30.3</td>
<td>40.8</td>
<td>10.4</td>
</tr>
<tr>
<td>0931 – cold/dry – clear-sky</td>
<td>IRS-7</td>
<td>52.9</td>
<td>67.0</td>
<td>50.0</td>
<td>126.9</td>
<td>40.3</td>
</tr>
<tr>
<td>0722 – hot/humid – high opaque Cb</td>
<td>-</td>
<td>70.2</td>
<td>246.1</td>
<td>50.5</td>
<td>-</td>
<td>134.8</td>
</tr>
<tr>
<td>0933 – cold/dry – moderately high opaque</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>183.4</td>
<td>158.1</td>
</tr>
</tbody>
</table>

Table 9: Interferometer axis position determination error in [µrad] averaged over four axis positions for five spectral calibration windows.

 Except for one atmosphere, calibration window W03/IRS-7 yields the highest performance and is confirmed as the window with the best extrapolation potential of the spectral calibration function in case of a good inter-array co-alignment. Second best performance is observed in W02/IRS-1, the performances in the other windows are variable with the type of the atmosphere. The coldest scenes, corresponding to atmospheres 0722 and 0933 are definitely excluded from the further analysis due to low performance or even failure of the axis position determination.
The typical interferometer axis determination errors of Table 9 are translated into relative spectral shift errors through equation (11). It is recalled that spectral shift errors decrease to a negligible value close to the interferometer axis (i.e., near to the centre of the detector arrays) and are maximised near the array corners at maximum nominal field angle (87.5 µrad). The performance assessment should focus on maximum errors because spectral calibration requirements apply to any spatial sample. Any other assessment would lead to an undesired systematic spatial heterogeneity of the quality of observations.

Figure 19 presents the maximum relative shift error (i.e., at maximum field angle) for the five investigated calibration windows and the six remaining atmospheres. It is assumed that the vector between the true and the estimated axis position is oriented parallel to a diagonal of the detector array. Results refer then to a corner detector in this diagonal.

Except for the coldest, sub-polar atmosphere (0931), relative shift errors are limited to below 2 \(10^{-6}\) in W03, 3 \(10^{-6}\) in W02 and about 4 \(10^{-6}\) in W11 and W13. The performance decrease in W16 with respect to W13 is most likely due to higher radiometric noise (c.f. Figure 3).

Figure 19: Maximum relative shift error corresponding to average axis position determination error.

![Figure 19](image)

Figure 20 to Figure 23 translate relative spectral shift errors into radiometric errors using the noise-shift relationship derived in [RD 2, Table 6] and its variation with the atmospheric type [RD 2, Figure 8]. Each figure represents the performance for a clear-sky atmosphere type (hot/humid, hot/dry, temperate/moderately humid, cold/dry, respectively), the remaining cloudy atmospheres are associated with a performance similar to their clear-sky counter-parts (not shown). Each figure presents the rms spectral calibration noise per mission band, corresponding to the maximum relative shift errors of Figure 19.

Noveltis 2006
Figure 20: Maximum FTS all-array spectral calibration noise (rms per mission band) corresponding to relative
shift errors shown in Figure 19 for five spectral calibration windows. Crosses emphasise the performance in case

Figure 21: As Figure 20, for atmosphere type: hot/dry.
Figure 22: As Figure 20, for atmosphere type: temperate/moderately humid.

Figure 23: As Figure 20, for atmosphere type: cold/dry.
Six curves are shown. The five straight curves represent an all-array spectral calibration (determination of the interferometer axis position in one of the five windows, extrapolated over the entire spectral domain) in case of perfect inter-array co-alignment. The sixth curve (broken line) emphasises the performance in the window associated to the array of the respective mission bands, i.e., W02 in IRS-1 and −2, W11 in IRS-3 and −4, W13 in IRS-5, W16 in IRS-6, and W03 in IRS-7, -8, and −9. It represents the performance of a separate array-by-array calibration without stringent requirements on inter-array co-alignment.

Key results are:

- For all atmosphere types, the all-array calibration in W03/IRS-7 yields the best performance. In this configuration, maximum noise occurs in IRS-7, but is limited to 0.05K NEdT@280K, except for the cold and dry atmosphere (0.07 K).
- The separate array-by-array spectral calibration yields performances better than 0.1 K in all bands for all atmosphere types. IRS-7 is not anymore the only driving band in terms of radiometric noise, similar noise levels are observed in IRS-1, -3, -5, and −6.
- Strikingly, the radiometric noise is relatively independent of the atmosphere type. Increasing precision the interferometer axis position estimation for hotter scenes is approximately balanced by decreasing radiometric errors at a given spectral shift (due to decreasing spectrum derivatives) for colder scenes.

The two latter observations are emphasised in Figure 24 and Figure 25, illustrating the maximum rms spectral calibration noise per mission band for the four atmosphere types in case of all-array calibration in W03/IRS-7 and of separate array-by-array calibration, respectively.

In summary, as for DS, the spectral calibration algorithm performance for FTS over a single dwell period, using a unique, global reference spectrum, is within the specification of the 0.10K NEdT@280K in all investigated cases except for the coldest scenes.

Thus, the potential for performance increase by accumulation of measurements over periods much longer than the dwell period is not an issue of first priority. It is likely to be smaller than for DS, because the FTS dwell period is longer by a factor 400. It should be evaluated upon an explicit instrument design and a quantified instrument stability estimation (in terms of ISRF knowledge).

Potentially critical aspects identified for DS do not apply to the FTS concept because a simultaneous exploitation of at least two calibration windows is not required. In particular, the two extreme configurations of the spectral calibration algorithm design, all-array and array-by-array calibration, have been assessed as valid options to be chosen as function of the instrument performance. Moreover, the implementation of IRS-1 as provider of a mandatory calibration window is not required.
Figure 24: Expected spectral calibration noise (instantaneous axis position determination without time filtering) for all-array spectral calibration in window W03 in case of perfect co-alignment between detector arrays. Maximum noise for a corner detector in worst-case axis position error orientation.

Figure 25: Expected spectral calibration noise (instantaneous axis position determination without time filtering) for separate array-by-array spectral calibration in windows W02, W11, W13, W16, W03. Maximum noise for a corner detector in worst-case axis position error orientation.
4.3. **Overall algorithm performance summary**

This section summarises the assessment of spectral calibration algorithm noise due to spectral shift determination errors for the two instrument concepts derived in sections 4.1 and 4.2 on the basis of Figure 13, Figure 14, Figure 24 and Figure 25. The variation with the atmosphere is not considered anymore, all estimations refer to an average performance over the four investigated clear-sky scenes, using a global reference spectrum.

All estimations represent the radiometric error related to a temporally unfiltered determination of the spectral calibration function over one dwell period (15.5 ms and 6s for DS and FTS, respectively). In particular for DS, and in trade-off with instrument stability characteristics, a performance increase is expected by accumulation and filtering of spectral calibration functions over longer time periods. Finally, it is recalled that FTS algorithm performance estimates refer to the worst case, i.e. a detector element at maximum field angle (87.5 mrad for the FTS baseline concept, algorithm noise decreasing linearly with decreasing field angle).

<table>
<thead>
<tr>
<th>mission band</th>
<th>IRS-1</th>
<th>IRS-2</th>
<th>IRS-3</th>
<th>IRS-4</th>
<th>IRS-5</th>
<th>IRS-6</th>
<th>IRS-7</th>
<th>IRS-8</th>
<th>IRS-9</th>
</tr>
</thead>
<tbody>
<tr>
<td>DS all-array: W02/IRS-1+W03/IRS-7</td>
<td>0.03</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.02</td>
<td>0.01</td>
<td>0.05</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>DS 2-by-2-arrays: W02/IRS-1+W11/IRS-4</td>
<td>0.03</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.07*</td>
<td>0.01</td>
<td>0.04</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td></td>
<td>W16/IRS-6+W03/IRS-7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FTS all-array: W03/IRS-7</td>
<td>0.04</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>0.03</td>
<td>0.02</td>
<td>0.05</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td>FTS array-by-array: W02/IRS-1</td>
<td>0.05</td>
<td>0.02</td>
<td></td>
<td>0.04</td>
<td>0.03</td>
<td>0.06</td>
<td></td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td></td>
<td>W11/IRS-4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>W13/IRS-5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>W16/IRS-6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>W03/IRS-7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 10: Spectral calibration algorithm noise [K] in NEdT@280K for temporally unfiltered spectral calibration functions determined over one dwell period for DS all-array and 2-by-2-array calibration and for FTS all-array and array-by-array calibration configurations. FTS estimations are for corner detectors of the array (worst case). *Performance decrease due to unsuitable selection of calibration windows.

Table 10 provides the expected spectral calibration algorithm noise per mission band in realistic configurations of spectral calibration windows. A performance within 0.05K NEdT@280K can be expected in all mission bands. An explicit assessment of the spectral calibration noise budget requires the knowledge of inter-array co-alignment and instrument stability and should be consolidated on explicit instrument design hypotheses.

As overall conclusion of Table 10, we state that with respect to algorithmic spectral shift determination errors, the spectral calibration for both IRS instrument concepts is feasible without major problems within the current spectral calibration noise allocation of 0.1K NEdT@280K. A revision of this statement may be required for DS in case of weak inter-array co-alignment (necessity for array-by-array calibration) or in case of elimination of IRS-1 (providing a suitable calibration window).
4.4. Limitations and open issues

The performance assessment of full spectral calibration experiments in this section is based on the evaluation of radiometric errors due to spectral shift knowledge errors for a unique determination of the instrument state.

4.4.1. Spatial scene distribution

Instrument state determinations are derived for explicit scene distributions and randomly drawn noise figures for each measured spectrum according to the baseline performance. In particular, no spatial variation of the scene over the selected spatial samples has been investigated. In the current state of the spectral calibration algorithm assessment, this is justified by the fact that the spectral calibration period (depending on instrument stability) is unknown. Thus, the natural variation of scene types observed during this period cannot be prescribed in a realistic way.

It is emphasised that the Spectral Calibration Subsystem (SCS) developed in this study is capable to process any geophysical scene distribution in future investigations, the limiting factor is the availability of high-resolution radiance spectra for all considered geophysical scenes.

4.4.2. Time filtering

Time filtering of spectral calibration functions over longer periods is prepared in the SCS development by generation of a historical product storing time series of instrument state estimations. It should be implemented in future investigations in accordance with explicit instrument stability hypotheses. In the current SCS, the historical product is overwritten for each SCS application, the time filtering process is thus neutralised.

4.4.3. Numerical algorithm noise

A clear separation of the spectral calibration algorithm noise from radiometric noise is difficult to obtain. A direct comparison between a calibrated spectrum and the theoretical reference spectrum tends to reproduce the radiometric instrument noise figure (in general large against spectral calibration noise). However, if the spectral calibration procedure introduces systematic errors, these must be detected and constrained.

In order to evaluate sources of algorithmic noise other than those associated to the intrinsic shift determination (already investigated in [RD 2]), spectral calibration experiments have to be applied to noiseless measurements. A demonstration is given below at the example of FTS where we consider a spectrum without radiometric noise after convolution with the theoretical calibrated ISRF and the same spectrum as output of the spectral calibration processing.

Figure 26 shows in red the difference between these two spectra and exhibits a Gibbs effect introduced by the spectral over-sampling algorithm. The amplitude of this effect depends on a variety of initialisation parameters:

- Spectral width of the calibration window and its position relative to the spectral band limits
- Spectral sampling and spectral resolution of the measured spectra
- Windowing length in both interferogram and spectrum space
- Oversampling factor in both interferogram and spectrum space
In an operational application context, windowing and oversampling parameters need to be optimised in order to minimise the observed Gibbs effect. This issue has to be investigated in more detail upon explicit instrument design during future spectral calibration algorithm development activities.

Secondly, we consider two spectra in identical atmospheric conditions as output of the spectral calibration processing, but for interferometer axis positions different by the typical axis position determination error (40 µrad). The black curve in Figure 26 represents the difference between these two calibrated noiseless spectra.

Since both spectra are processed identically the major part of the Gibbs effect is eliminated, not exceeding 0.01K NEdT@280K. It is concluded that the observed Gibbs effect for the current initialisation of the windowing and oversampling parameters is acceptable in the frame of the present MTG/IRS spectral calibration assessment. A comparison between calibrated spectra is affected by algorithm noise that is negligible in the spectral calibration noise budget.

4.4.4. Concept choice

Performance differences for the two concepts have to be interpreted with caution. This is due to incompliance of the two baseline concepts with [RD 4] at different levels. While the FTS baseline is in compliance with the radiometric resolution requirements (see Figure 3), the DS baseline fails in meeting the spectral resolution requirements (see Table 1).
5. Conclusion on spectral calibration algorithm design

5.1. Both concepts

The performance estimation of a spectral calibration algorithm for the IRS DS and FTS baseline concepts indicates compliance with the spectral calibration noise allocation for a single instrument state determination over one dwell period. The following recommendations for future spectral calibration design activities can be expressed for both concepts:

- The spectral calibration period is at least equal to the dwell period. It is to be optimised in accordance with the feasible stability of the ISRF, the limiting factor for its duration. Individual spectral calibration for each dwell period is costly at system level and not optimised with regard to the impact of radiometric noise. Spectral shift and instrument state determination should be applied to a spatio-temporal selection of measurements over the spectral calibration period. The spatial selection criteria depend strongly on the length of the spectral calibration period and the number of reference spectra.

- Scene filtering is required for cold scenes (due to high opaque clouds or due to low surface temperature). These scenes are likely to be identified by simple brightness temperature threshold tests in spectral domains of high atmospheric transmittance, applicable to spectrally uncalibrated sounder data (level 1a).

- As shown in [RD 5], scene filtering is also required for measurements with heterogeneous scene content, in particular in case of strong radiometric gradients. The identification of these scenes requires observations at high spatial resolution and would be ideally provided by an IRS built-in imager.

- Inherent to the scan characteristics, IRS observations will consist of mid- and high-latitude observations over two periods of several minutes within each repeat cycle. It is important to note that spectral calibration of scenes in sub-polar regions has been shown successful for a clear-sky ocean scene with surface temperature 271 K. This hints at the feasibility of spectral calibration independently of the spectral calibration period. If short against the repeat cycle, spectral calibration functions are determined on scene types similar to the observed scenes they are applied to. In case of spectral calibration periods of the order of the repeat cycle or longer, spectral calibration functions are determined preferentially on suitable scenes in tropical and sub-tropical regions, and then applied globally. It is concluded that the IRS spectral calibration algorithm puts no quantitative requirement on the spectral calibration period.

Recommendations applying specifically to each of the two concepts are summarised here below.
5.2. DS baseline

- **Spectral shift determination is feasible** with sufficient accuracy on a global reference spectrum. However, use of atmospheric a-priori information (i.e., use of several reference spectra chosen as function of the prior information) improves the spectral calibration performance.

- Since separate array-by-array calibration for the current DS baseline concept is not an optimised option in terms of performance, extrapolation of the spectral calibration function within mission bands IRS-1 to IRS-4 on the one hand and IRS-5 and IRS-9 on the other hand should be ensured. This can be obtained either by implementation of these bands in a common focal plane or by a stable co-alignment of different focal planes carrying these bands.

- The preferred spectral calibration window configuration is:
  - in terms of performance an independent calibration of bands IRS-1 to IRS-4 in W02/IRS-1 and W11/IRS-4 and of bands IRS-5 to IRS-9 in (W13/IRS-5 or ) W16/IRS-6 and W03/IRS-7.
  - in terms of system resources an all-array calibration in W02/IRS-1 and W03/IRS-7.

- In any investigated spectral calibration algorithm option, W02/IRS-1 and W03/IRS-7 have an important impact on the overall performance.

5.3. FTS baseline

- **Spectral shift determination is feasible** with sufficient accuracy on a global reference spectrum. Use of several reference spectra chosen as function of available prior information on the scene content does not significantly improve the spectral calibration performance.

- **Spectral calibration is feasible over all arrays** (in case of sufficient inter-array co-alignment stability) as well as separately for each array. The preferred spectral calibration window configuration is:
  - W03/IRS-7 for an all-array calibration approach. Spectral shift determination in the Fourier space may be reconsidered in this configuration in order to reduce ground segment requirements at the expense of a small performance loss.
  - W02/IRS-1, W11/IRS-4, W13/IRS-5, W16/IRS-6, W03/IRS-7 for an array-by-array calibration.

- Spatial scene selection should be based on at least four pre-defined areas of the detector arrays at moderate or high field angles in an approximate square distribution around the theoretical interferometer axis position. Within these areas, the warmest scenes should be selected dynamically for spectral shift determination.
6. Consolidation of requirements

6.1. Spectral calibration noise budget

As a high-level study output, a review and a declination of the spectral calibration noise allocation 0.1K NEdT@280K [RD 4] is carried out in this section. The radiometric sensitivity to spectral shift and ISRF shape errors, expressed in terms of relative spectral shift $SDE_r$ and shape error index $SEI$, respectively, is adopted from the analysis in [RD 2, section 3.4]. It is recalled that IRS-7 is the mission band of highest sensitivity to spectral shift errors, IRS-1 the band the most sensitive to ISRF shape errors. Requirements are driven by these bands, relaxations are acceptable in other bands. The sensitivities are concept dependent due to the distinct typical line shapes of the spectral response functions.

The overall budget is declined in a component of algorithmic spectral calibration uncertainty due to spectral shift determination algorithm errors (as quantified in section 4), of ISRF shape knowledge errors, of inter-array misalignment, and of instrument instability during the spectral calibration period.

Table 11 presents a quantitative declination of the spectral calibration noise budget together with the corresponding specifications in terms of shift and shape knowledge errors. A justification for individual allocations is given here below.

<table>
<thead>
<tr>
<th>Overall budget DS</th>
<th>NEdT@280K [K] at level 1b</th>
<th>corresponding specification</th>
<th>remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Algorithmic shift determination</td>
<td>0.05</td>
<td>-</td>
<td>estimation, single dwell period</td>
</tr>
<tr>
<td>Shape error (symmetric)</td>
<td>0.05</td>
<td>SEI = 0.012</td>
<td></td>
</tr>
<tr>
<td>Shape error (asymmetric)</td>
<td>0</td>
<td>-</td>
<td>assumption</td>
</tr>
<tr>
<td>Shift due to array mis-alignment</td>
<td>0.025</td>
<td>see text</td>
<td>two-by-two array approach</td>
</tr>
<tr>
<td>Shift variation during spectral calibration period</td>
<td>0.066</td>
<td>$SDE_r = 2.6 \times 10^{-6}$</td>
<td>residual of other comp.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Overall budget FTS</th>
<th>NEdT@280K [K] at level 1b</th>
<th>corresponding specification</th>
<th>remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Algorithmic shift determination</td>
<td>0.05</td>
<td>-</td>
<td>estimation, single dwell period</td>
</tr>
<tr>
<td>Shape error (symmetric)</td>
<td>0.05</td>
<td>SEI = 0.036</td>
<td></td>
</tr>
<tr>
<td>Shape error (asymmetric)</td>
<td>0.025</td>
<td>TBD</td>
<td></td>
</tr>
<tr>
<td>Shift due to array mis-alignment</td>
<td>0</td>
<td>-</td>
<td>separate calibration of each focal plane</td>
</tr>
<tr>
<td>Shift variation during spectral calibration period</td>
<td>0.066</td>
<td>$SDE_r = 1.3 \times 10^{-6}$</td>
<td>residual of other comp.</td>
</tr>
</tbody>
</table>

Table 11: Consolidated MTG/IRS spectral calibration noise budget for DS and FTS baseline concepts.

After Table 10, we allocate 0.05 K to the algorithmic shift determination noise. This allocation refers to the unfavourable assumption of separate spectral calibration for each dwell period and thus includes a not yet quantifiable margin in view of possible time filtering of spectral calibration functions over longer periods.
0.05 K are allocated to **shape knowledge errors due to symmetric line shape variations** (e.g., self-apodisation, corner cube motion deviations for FTS, any kind of variation for DS). Corresponding SEI requirements apply as knowledge and as stability requirements, i.e. the ISRF must be predictable and stable over the spectral calibration period within this specification. The present study provides no justification for the quantitative allocation itself. The currently applied instrument baseline assumptions do not yet allow for an explicit and reliable simulation of instrument state variations and their impact on the ISRF shape. The strategy is to specify a shape error index for symmetric shape variations such that related radiometric noise is a small contributor in comparison to the contribution from spectral shift variations during the spectral calibration period. A future trade-off between the two contributions can be envisaged. It is anticipated that ISRF shape knowledge errors are small by design in case of a DS concept. In case of FTS, the impact of field angle knowledge errors on the ISRF shape is expected to be negligible.

**Asymmetric shape knowledge errors**, e.g., ‘ghosts’ in the case of FTS, are more severely restricted since potentially affected with a bias. They are strongly dependent on micro-vibration frequencies. Results obtained in [RD 2] indicate that SEI is not a suitable parameter to control ghost in the spectral response. A specification on forbidden frequencies appears more reliable. For the current concept these frequencies would be lower than about 20 Hz. Dedicated investigations on a known spectrum of vibration frequencies are required to consolidate this specification. Assuming that this error type is inherent to the FTS concept, zero is allocated for this component in the DS spectral calibration noise budget.

**Spectral shift knowledge errors due to inter-array mis-alignment** apply only if the spectral calibration function is extrapolated from one array to another. For the FTS concept, separate array-by-array calibration is validated as a design option compliant with an 0.05K allocation for algorithmic shift determination noise. Therefore it is set to zero. For the DS concept, the allocation is severe (0.025K) in order to ensure consistency of spectral shift determinations in different windows commonly used for the instrument state determination. As discussed in section 4.3, the most suitable spectral calibration algorithm option is a separate calibration of bands IRS-1 to IRS-4 and IRS-5 to IRS-9. Involved calibration windows are situated in IRS-1 and –4 and in IRS-6 (or –5) and –7, respectively. Recalling the radiometric sensitivity to relative spectral shifts from [RD 2, Table 6] for IRS-4, -5, -6 (0.10K/10^-5, 0.14K/10^-5; 0.08K/10^-5, respectively), it is required that

a) for a known ISRF centroid frequency in IRS-1, the ISRF centroid frequency in IRS-4 is predictable to within a relative shift error of 2.5 10^-6,

b) for a known ISRF centroid frequency in IRS-7, the ISRF centroid frequency in IRS-5 (IRS-6) is predictable to within a relative shift error of 1.8 10^-6 (3 10^-6).

The remaining component due to **spectral shift variations during the spectral calibration period** is calculated as the residual of individual allocations with respect to the spectral calibration budget allocation. It is assumed that the mentioned contributions add independently of each other to the spectral calibration noise budget. This hypothesis appears reasonable at the current state of the spectral calibration assessment, but should be consolidated in future on explicit instrument design.

It can be stated that the above allocation of spectral calibration noise components is compliant with the overall budget allocation. The major part of the budget can be allocated to instrument instability contributions. It is emphasised that the above spectral calibration noise allocation should be understood as a basis for further adjustments during the instrument design process. Reallocations within the budget are expected, depending on the actual instrument performance with respect to the allocations.

Noveltis 2006
6.2. Recommendation of requirements related to spectral calibration

In this section we comment and formulate recommended modifications of MTG/IRS definitions and specifications [RD 4] relative to spectral calibration.

- Definition of the spectral calibration period

The spectral calibration period is the time span providing observations that can be consistently used for an independent estimation of the instrument state dependent instrument spectral response function in all spatial samples i and all spectral channels j. Its theoretical minimum duration is equivalent to one dwell period. The maximum duration is limited by instrument instability.

- Conclusion on the length of the spectral calibration period

The spectral calibration period can be designed according to feasible instrument stability and to timeliness requirements at system level. There are no specific requirements with respect to the spectral calibration algorithm design.

- MRD_IRS.40 (ISRF centroid frequency knowledge)

This requirement is deleted in [RD 4]. The investigations in this study, in particular in view of the initialisation of the shift determination algorithm, reveal the necessity to characterise the expected range of the spectral shift between measured and reference spectra. A quantitative specification can be justified with respect to spectral shift determination in the Fourier space (windows W02F/IRS-1 and W03F/IRS-7). The shift determination in the Fourier space is ambiguous by a multiple of the line spacing (1.5 and 1.55 cm⁻¹, respectively) of the exploited regular absorption pattern. In terms of relative shift, W02F/IRS-1 is driving the requirement to a value of 2 10⁻⁴. The following specification is recommended:

The maximum relative shift of the ISRF centroid of each sample i in each channel j with respect to the nominal centroid shall be characterised. As a goal, it shall be within 2 10⁻⁴.

The co-alignment requirement derived in section 6.1 applies only to the DS concept:

Additionally for the DS concept, it is required that

- for a known ISRF centroid frequency in IRS-1, the ISRF centroid frequency in IRS-4 is predictable to within a relative shift error of 2.5 10⁻⁶,
- for a known ISRF centroid frequency in IRS-7, the ISRF centroid frequency in IRS-5 (resp. IRS-6) is predictable to within a relative shift error of 1.8 10⁻⁶ (resp. 3 10⁻⁶).
**MRD_IRS.50 (Stability of the ISRF centroid frequency)**

After section 6.1, the following specification is recommended:

*The position of the ISRF centroid of each spatial sample i in each spectral channel j shall not vary by more than*

- $2.6 \times 10^{-6}$ relative (DS)
- $1.3 \times 10^{-6}$ relative (FTS)

*during the spectral calibration period.*

**MRD_IRS.60 (ISRF shape error index)**

Opposite to the current formulation in [RD 4], the requirement on the ISRF shape error index characterises in first place the error on the ISRF knowledge, i.e. the capability of the instrument model to predict the ISRF shape for a given instrument state determination (per spectral calibration period). Possible variations of the ISRF shape are to be constrained consistently with the knowledge requirement. In practice, the most relevant issue for time variation of the ISRF are micro-vibrations in case of an FTS concept. These cannot be constrained reliably by a maximum shape error index without a knowledge of amplitudes and the frequency spectrum of micro-vibrations. In a first step, it is recommended to require their characterisation:

*For any spatial sample i and each spectral channel j the ISRF shape error index shall be lower than*

- 0.012 (DS)
- 0.036 (FTS)

*The specification applies to actual and modelled ISRF estimations averaged over the spectral calibration period.*

*Time variation of the instantaneous actual ISRF with respect to the modelled ISRF (averaged over the spectral calibration period) shall be characterised in terms of Shape Error Index and not exceed the above specification.*

*Additionally for FTS, it is required to characterise the impact of micro-vibrations on the ISRF shape and on its variation during the spectral calibration period.*
7. Study conclusions and perspectives

The major output of this study consists in a first quantification of requirements related to spectral calibration, derived upon realistic MTG/IRS baseline concepts.

The next step is to assess the feasibility of these requirements at instrument level. This investigation requires the development of detailed instrument models and yields performance estimations in terms of instrument instability and ISRF knowledge. This assessment might suggest an adjustment of the allocations for the spectral calibration noise budget and its individual contributions and leads eventually to a first specification of the spectral calibration period.

After this assessment at instrument level, the MTG/IRS spectral calibration subsystem (SCS) developed in the frame of the present study is ready for reuse. On a short-term perspective (before the instrument qualification phase), it constitutes a valuable model dedicated to the control and the validation of instrument specifications with respect to spectral calibration and to the consolidation of the detailed spectral calibration algorithm design.

In this context, the necessary extensions concern:

- the implementation of updated instrument models in SCS,
- the refinement of the formulation of the spectral calibration function according to the updated instrument models,
- the explicit implementation of measurement accumulation in time, consistently with the spectral calibration period,
- the generation of a larger amount of high-resolution spectra, representative for a realistic spatio-temporal variation of observed scenes during the spectral calibration period,
- the implementation of a scene filtering algorithm, based on either spectrally integrated sounder observation, or simultaneous built-in imager observations at high spatial sampling, or external data (e.g., MTG Imaging mission observations, NWP model or climatological prior information).

The above extensions enable a refined spectral calibration performance assessment for explicit instrument design options on the one hand, and a fine-tuning of spectral calibration algorithm design and initialisation parameters (e.g., calibration window selection, choice of the correlation space, initialisation parameters for spectral oversampling, shift determination) on the other hand.

The interest for such optimisation in the current state of the instrument and system design phase, i.e. in absence of explicit instrument design and system requirements, appears limited.

The principal intention of this first assessment of the MTG/IRS spectral calibration algorithm is to provide up to now missing system specifications and basic algorithm design options that initiate a trade-off process between system requirements and instrument specifications during the upcoming MTG/IRS development phases.