Assessment of the MTG IR Sounding Mission Spectral Calibration Algorithm

Part 1: Instrument input analysis and candidate algorithm design

For the attention of: Rolf STUHLMANN (EUMETSAT)

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Assessment of the MTG IR Sounding Mission Spectral Calibration Algorithm

Part 1: Instrument input analysis and candidate algorithm design

### Summary

The present technical report describes the software system that has been implemented for the MTG/IRS spectral calibration algorithm assessment. All instrumental and geophysical input parameters are specified. The spectral calibration algorithm design and several design options are presented.

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**Assessment of the MTG IR Sounding Mission Spectral Calibration Algorithm**

**Part 1: Instrument input analysis and candidate algorithm design**

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0. Abstract

Spectral calibration of the MTG Infrared Sounder is not explicitly addressed in ongoing pre-phase A studies at industry level.

The objective of the present study is to consolidate the spectral calibration noise budget at system level and to initiate the trade-off with future instrument design activities.

The Spectral Calibration Sub-System of the IASI Numerical Performance Model has been adjusted to currently available MTG IR sounder baseline concepts for a dispersive and a Fourier Transform spectrometer.

Algorithms design options are analysed in terms of the selection of spectral calibration windows.

The spectral calibration algorithm performance is assessed in terms of radiometric errors and spectral shift errors.

Compliance between the current system allocation for the spectral calibration noise budget and the expected algorithm performance is stated. Requirements on focal plane co-alignment and instrument stability are derived from the spectral calibration budget allocation and the estimated spectral calibration algorithm performance.
1. Introduction

The Meteosat Third Generation (MTG) Infrared Sounding Mission is one of five initially identified observation missions of the MTG Programme. It is dedicated to the support of regional and global Numerical Weather Prediction by providing information on vertical profiles of wind (first priority), temperature and humidity compatible with user requirements projected in the 2015 timeframe. Secondary objectives address chemistry and air quality applications.

Due to the lack of a clear instrumental heritage, the instrument concept of the future MTG Infrared Sounder (IRS) is not yet chosen. The two possible concepts, a Fourier Transform Spectrometer (FTS) or a Dispersive Spectrometer (DS), are currently investigated in the frame of MTG pre-phase A studies at industry level conducted by ESA.

Observational requirements for all MTG missions are specified in the MTG Mission Requirements Document (MRD) [RD 1]. Concerning the IRS mission, these requirements refer to the quality of level 1b observational data (i.e., calibrated and geo-located, but unapodised measurements at the original spatial sampling). However, [RD 1] cannot be considered as a complete system specification that would allow to provide all necessary information for deriving unambiguously a full set of requirements at instrument level for the two candidate concepts. While most of the relevant aspects are investigated in the pre-phase A studies at industry level, the issue of spectral calibration is not.

In accordance with the conclusion of activities dedicated to the consolidation of IRS observational requirements prior to the start of the pre-phase A [RD 2], a system hypothesis on the noise related to spectral calibration at level 1b (inferior to 0.1 K NEdT@280K) has been introduced in the latest issue of [RD 1].

The radiometric resolution at level 1b as specified in [RD 1] is composed mainly of conventional radiometric noise (radiometric noise at instrument level, including the uncertainty of radiometric calibration) and spectral calibration noise.

Spectral calibration noise is defined as the uncertainty of spectrally calibrated radiances emanating from a spatially homogeneous Earth scene. It can be separated into two components. The first one represents the impact of instrument knowledge errors and instability, i.e., the capacity of the instrument model to predict the actual Instrument Spectral Response Function (ISRF) for a perfectly known instantaneous state of the instrument. The second one, the spectral calibration algorithm noise, represents the uncertainty related to instrument state estimation errors. The instrument state estimation consists mainly in the determination of a spectral shift between a measured spectrum and a reference spectrum related to a known instrument state. Thus spectral calibration algorithm noise depends on the radiometric resolution, the suitability of the calibration source (sharpness/amplitude of atmospheric absorption/emission line pattern and their stability with respect to atmospheric variability), and the accuracy of the forward radiative transfer model.

In the present study, we assess the spectral calibration algorithm noise to verify first the compliance with the MRD spectral calibration noise budget hypothesis. Secondly, the residual between overall budget and algorithm noise is allocated to the instrument components of spectral calibration noise. This initiates the system/instrument trade-off, in particular with regard to the requirements on instrument stability and instrument model accuracy quoted from [RD 1] here below and applicable in future IRS instrument design phases.
• **MRD_IRS.50**: The position of the ISRF$_{ij}$ centroid of a channel $j$ relative to a spatial sample $i$, shall not vary by more than $10^{-6}$ (TBC) over TBD seconds, equivalent to the calibration period.

• **MRD_IRS.60**: The shape index of the ISRF$_{ij}$ of a channel $j$ relative to a spatial sample $i$, shall not vary by more than 0.02 (TBC) over TBD seconds, equivalent to the calibration period.

These specifications are currently not exploitable at instrument level because the spectral calibration period is not defined. A quantitative consolidation of the above requirements is one of the objectives of the present study. In the same time, the related system specifications (acceptable knowledge errors of ISRF centroid and shape index) can be formulated for defined instrument concepts according to the spectral calibration noise allocation hypothesis.

A second system hypothesis in [RD 1] prescribes an in-flight spectral calibration procedure by means of an ISRF Estimation Model (ISRF-EM). In the operational phase, this model consists of

• an instrument model containing all parameters that influence the spectral response of the instrument,

• a spectral calibration algorithm that determines the discrepancy between measured and expected spectra,

• auxiliary data such as reference spectra for reference atmospheric conditions and, if required, a-priori knowledge on the atmospheric state.

It is emphasised that the main function of the ISRF-EM in the development phase is the control of the instrument specifications, in particular MRD_IRS.50 and MRD_IRS.60 because it constitutes the link between system (spectral calibration performance via a defined spectral calibration algorithm) and instrument (stability, radiometric and spectral resolution) specifications.

In more concrete terms, the objectives of the study are to identify the elements to be traded off between system and instrument level, to quantify the sensitivity of instrument parameters to the spectral calibration algorithm performance, and to provide a recommendation for candidate spectral calibration algorithms for the two possible instrument concepts.

The present part 1 of the study report describes the software system that has been implemented for the IRS spectral calibration algorithm assessment in section 2. All instrumental and geophysical input parameters are specified in sections 3 and 4, respectively. Spectral calibration algorithm design options in terms of correlation methods for spectral shift determination and in terms of spectral calibration windows are presented in section 5.

Part 2 [RD 3] establishes radiometric sensitivity to ISRF shift and shape knowledge errors for the two instrument concepts. Furthermore, performance estimations at low level of the spectral calibration sub-system, for a unique spatial sample in various spectral calibration windows, are obtained. The impact of radiometric noise and of atmospheric variability on the spectral shift determination is quantified and a consolidated list of spectral calibration windows is derived.

Part 3 [RD 4] is dedicated to full spectral calibration experiments to assess the spectral calibration algorithm noise quantitatively. The spectral calibration noise budget is consolidated and requirements on instrument knowledge and stability are derived.
1.1. Acronyms

AGIRS  Advanced Geostationary InfraRed Sounder
DISORT  Discrete-Ordinate-Method Radiative Transfer
DS  Dispersive Spectrometer
ESA  European Space Agency
EUMETSAT  European Organisation for the Exploitation of Meteorological Satellites
E/W  East-West
FIR  Finite Impulse Response
FT  Fourier Transform (correlation space)
FTS  Fourier Transform Spectrometer
HRRS  High Resolution Radiance Spectra
IASI  Infrared Atmospheric Sounding Interferometer
IFOR  Instantaneous Field of Regard
IFOV  Instantaneous Field of View
IPSF  Instantaneous Point Spread Function
IR  InfraRed
IRS  (MTG) InfraRed Sounder
ISRF  Instrument Spectral Response Function
ISRF-EM  ISRF Estimation Model
LOS  Line of Sight
MIPAS  Michelson Interferometer for Passive Atmospheric Sounding
MRD  Mission Requirements Document
MTG  Meteosat Third Generation
NEdT  Noise equivalent brightness temperature difference
N/S  North-South
OPD  Optical Path Difference
PSF  Point Spread Function
RD  Reference Document
rms  root mean square
RPD  Reference Path Difference
SAF  Self-Apodisation Function
SCS  Spectral Calibration Subsystem
SDB  Spectral Data Base
Shr  High-resolution spectrum
SNR  Signal-to-Noise Ratio
SOS  Spectral Oversampling
SP  Spectral (correlation space)
SSD  Spectral Shift Determination
SSI  Spectral Sampling Interval
SSP  Sub-Satellite Point
S1A/S1B  Level 1a/Level 1b spectra
TBC  To be confirmed
TBD  To be defined
WP  Work Package

Noveltis 2006
1.2. References


[RD 2] Infrared Atmospheric Sounding Mission (IASM) Requirements Justification.


2. Spectral calibration software system

This section describes the baseline assumptions on the MTG/IRS spectral calibration processing as well as the structure of the spectral calibration software system and its implementation in view of the spectral calibration algorithm assessment in upcoming study phases.

2.1. General definitions

2.1.1. Instrument states

The instrument state is the best knowledge of the set of instrument state parameters, which are used in the ISRF Estimation Model.

Nominal instrument states are represented by sets of instrument state parameters within their specified range.

The actual instrument state is defined by an instantaneous set of instrument state parameters. The objective of the spectral calibration algorithm is the retrieval of the actual instrument state (possibly followed by filtering of variations in time).

It may be efficient to determine the actual instrument state by interpolation in a look-up table. This table, referred to as Spectral Data Base (SDB), contains shift and shape parameters of the ISRF for a sub-set of nominal instrument states.

2.1.2. Spectrum levels

Prior to spectral calibration, the level 1a spectrum is associated with a theoretical frequency basis $\nu_{1b}$. The spectral calibration function $F_{sc}$ computes the calibrated frequency basis $\nu_{1a} = F_{sc}(\nu_{1b})$. The level 1a product consists of the level 1a spectrum and its calibrated frequency basis (i.e., $F_{sc}$).

The level 1b spectrum is the level 1a product resampled on the theoretical frequency basis. For long term analysis, the theoretical frequency basis will not move during the mission life time, i.e., level 1b centroid frequencies are fixed.

A reference spectrum is a level 1a or a level 1b spectrum corresponding to a perfectly defined instrument state and thus to a perfectly known ISRF shape and centroid frequency.

2.2. Baseline assumptions

The spectral calibration procedure consists in fitting the ISRF Estimation Model with the observations. The model can be fitted offline for long term parameters variations and online for short term parameters variations.

The objective is to determine the actual instrument state (stable within margins to be specified over a period referred to as spectral calibration period). This instrument state is estimated by determination of the spectral shift of a measured spectrum from a reference spectrum. The shift is linked to instrument state parameters retrieved within the ISRF Estimation Model, possibly by interpolation between nominal instrument states in the Spectral Data Base.
The operational spectral calibration software system will include those parts of the instrument model that link relevant instrument state parameters (e.g., focal plane distortion and position offset) to the spectral response functions of individual detectors. At present, in absence of explicit instrument models, the objective is to derive requirements in terms of ISRF knowledge and stability, verifiable during upcoming instrument design activities.

2.3. Spectral calibration algorithm design parameters

2.3.1. Correlation space

The spectral calibration is based on a correlation of stable absorption line pattern in selected spectral calibration windows between observed and theoretical reference spectra. Two correlation methods can be applied for the spectral shift determination of the measured spectrum. The first procedure is carried out in the radiance space by maximising the correlation between an observed and a reference spectrum. A second approach uses the correlation method in the Fourier space by analysing in carefully chosen spectral domains the phase of the Fourier transform of the measured spectrum compared to the phase of a nominal reference spectrum.

The approach for most of the IR sounding instruments is the correlation procedure in the radiance space. The correlation procedure in the Fourier space will be applied operationally in the IASI ground processing [RD 6]. Both approaches have been tested for AGIRS [RD 7], an IR sounder concept at moderate spectral resolution in the meantime considered for post-MSG-3 platforms and then abandoned due to the initiation of the MTG programme.

2.3.2. Spectral correlation domain

The spectral correlation domain is limited in size and position by various factors:

- Spectral signatures resolved by the instrument, governed by the instrument’s spectral resolution and the characteristics of atmospheric absorption line pattern (spectral distribution, strength).
- Stability of spectral signatures with respect to atmospheric variability.
- Variation of the spectral shift between the extremities of the spectral domain. The spectral shift determination is based on the assumption of a constant shift parameter over the entire spectral correlation domain. In practice, this constraint excludes spectral calibration domains including detectors of different arrays.
- Radiometric noise figures.

All these points have to be evaluated for the choice of the size and the position of the spectral correlation domain, also called spectral calibration window.
2.3.3. Scene filtering

Atmospheric variability is relevant to spectral calibration by the following aspects:

- In fully cloudy conditions, the spectral features of troposphere species disappear as a function of cloud top height. Therefore, spectral domains that are sensitive to stratospheric height levels only are first candidates for spectral calibration. In other spectral domains, it may be necessary to reject cloudy spatial samples for instrument state determination.

- Absorption line pattern become invisible in an isotherm atmosphere and become less sharp if the weighting functions peak in altitudes characterised by a small temperature gradient. If the line pattern exploited for spectral calibration appears in emission in certain atmospheric conditions and in absorption in others, the performance of the correlation procedure becomes dependent on the atmospheric state. This requires a-priori information on the atmospheric state and a set of reference spectra corresponding to these a-priori conditions.

- In particular cold scenes, associated with weak vertical temperature gradients and with weakened spectral signatures, may be subject of rejection from the spectral calibration procedure. This statement is amplified by the generally lower SNR at low brightness temperatures.

- The effect of scene heterogeneity, referred to as spectral calibration pseudo-noise or ISRF pseudo-noise, may be incompatible with the hypothesis of a homogeneous scene. Spatial samples characterised by strong radiometric gradients are inapt to be used for spectral shift determination if there is a significantly different spectral response of the various radiometric components present in the spatial sample. These cases need to be filtered by analysing the spatial variability of the scene content using integrated imager measurements. A quantitative analysis of the spectral calibration pseudo-noise is carried out in a parallel study [RD 5].

Obviously, the scene filtering criteria depend on the spectral correlation domain. In the present spectral calibration assessment study, scene rejection criteria are derived qualitatively. These may be used for estimating a realistic time accumulation scenario for the number of exploitable observations in the spectral calibration algorithm.

2.3.4. Number of spectral correlation domains

The number of spectral correlation domains required for instrument state determination depends on the instrument model. In general, a dispersive spectrometer (with a spectral dimension of the detector array) requires at least two domains to account for the spectral variation of the spectral calibration function (except if the array is rigid in the spectral dimension). A single domain is sufficient for a Fourier Transform spectrometer.

In case of several focal planes, the quality of the spectral calibration will depend on the capability to extrapolate the spectral calibration function estimated in a given array to the entire spectrum. In practice, the application of a global spectral calibration function requires a good knowledge of the alignment between different spectral bands or focal planes. If co-alignment is not ensured by instrument design, each spectral band has to be calibrated individually in a dedicated spectral calibration window.
2.3.5. Instrument parameters

Without knowledge of explicit instrument models, the spectral calibration algorithm has to be assessed on reasonable hypotheses on the instrument characteristics:

- **Spectral sampling, spectral resolution** and **spectral coverage** govern the resolved spectral signature of observed and reference spectra, the choice of spectral calibration windows and thus the accuracy of the shift estimation between the two spectra.
- **Radiometric resolution** affects the observed spectrum and influences the accuracy of the shift estimation with the reference spectrum.
- **Spectral band or focal plane separations** may introduce discontinuous spectral sampling and spectral resolution and put constraints on the choice of spectral calibration windows.
- The **ISRF model** provides the shape of the spectral response function as well as its spectral variation. It also provides ISRF shape variations over different spatial samples (if any).
- **Focal plane assembly and array dimensions** govern the range of ISRF variation within detector arrays and define, together with the ISRF model, the spectral calibration functions.

The above instrument parameters are inputs to the spectral calibration software system. They are discussed in section 3.

2.4. Spectral calibration subsystem (SCS)

This section describes the software architecture of the spectral calibration subsystem and of auxiliary sub-systems necessary for the spectral calibration algorithm assessment (spectra simulation and ISRF computation, level 1a simulation, direct level 1b simulation). The flowchart of the overall software system is shown in Figure 1.

Input data to the simulation process are spectra in high spectral resolution and instrument state parameters.

High-resolution spectra are generated for defined geophysical conditions: reference geophysical conditions for the generation of reference spectra, observed geophysical conditions for the simulation of actual level 1a spectra.

The ISRF model provides the spectral response function at levels 1a or 1b for a given instrument state. It is applied for:

- Generation of the SDB (red arrows, upper branch). The spectral data base consists of spectral shift and ISRF shape look-up tables for a selection of nominal instrument states.
- Computation of the reference level 1b spectra (red arrows, lower branch) for at least one nominal instrument state.
- Simulation of observed level 1a spectra for actual instrument state parameters (black arrows).
- Computation of perfectly calibrated level 1b spectra for actual instrument parameters (blue arrows).
Figure 1: Spectral calibration software system flowchart. The green box represents the spectral calibration subsystem (detailed in Figure 2), pale green boxes are auxiliary modules for spectra simulation (S1A: observed, S1Bref: reference, S1Btrue: perfectly calibrated). Yellow and steel blue boxes represent input and output data, respectively. The red branch (broken lines) is relevant to the generation of spectra and ISRF shift and shape parameters in reference conditions (instrumental and atmospheric). It is applied once for all and provides the static input to the spectral calibration subsystem. The black branch (straight lines) is applied to all measured spectra that are analysed in the spectral calibration process. It provides the dynamical input to the spectral calibration subsystem, i.e., observed spectra in various atmospheric conditions and instrument states. The blue branch describes the generation of truly calibrated spectra for validation purpose of the output of the spectral calibration subsystem; i.e., the calibrated spectrum S1B for the considered atmospheric conditions and instrument states.

The resulting ISRF are applied to high-resolution spectra in the convolution operator CNV to generate the calibrated reference spectra, simulated uncalibrated spectra in any geophysical and instrument conditions, and the corresponding, perfectly calibrated spectra, S1Bref, S1A, and S1Btrue, respectively. A noise operator is applied to the simulated level 1a spectra only.

The output of the spectral calibration sub-system is a calibrated spectrum S1B. It can be compared with the theoretical, perfectly calibrated spectrum S1Btrue. However, the practical interest for this comparison is limited, because the difference between the two spectra is dominated by radiometric noise, rather than by the spectral calibration algorithm noise.

SDB, calibrated reference spectra and uncalibrated spectra are the input to the spectral calibration sub-system (SCS), which constitutes the operational part of the software. The SCS is detailed in Figure 2.

Input spectra and the SDB are adapted to the selected spectral calibration windows.

The determination of the spectral shift between observed and reference spectrum is carried out alternatively in the spectrum space (dotted lines) or in the Fourier space (broken lines). In the spectrum space, the correlation between the two spectra is maximised. The reference spectrum is oversampled in order to minimize the interpolation errors in the correlation process. In the Fourier space, both spectra are oversampled in order to minimize the interpolation errors in the resampling process on a periodic basis. The spectral shift determination relates to the determination of the phase difference between the reference pseudo-interferogram and the observed interferogram.
Having determined the spectral shift of a set of level 1a spectra, the associated ISRF are estimated by the ISRF-EM. The actual instrument state is interpolated from the SDB by fitting the instrument parameters to the determined spectral shift, the actual ISRF parameters (shape/shift) are estimated for all spatial samples, and the spectral calibration function is estimated as function of the actual instrument state.

For level 1b spectra computation, the measured level 1a spectra, expressed on the calibrated wave number basis, are oversampled, then resampled (i.e., calibrated) on the regular spectral basis of level 1b.
2.4.1. Modular description

This section summarises the functionality of individual modules of the spectral calibration subsystem and of auxiliary modules.

SDB: Spectral Data Base computation

Computation of spectral shifts, ISRF shapes and spectral calibration functions for pre-defined instrument state parameters. The pre-defined instrument states are sets of parameters within their specified nominal variation. The spectral data base is computed separately for the two candidate instrument designs.

- SDB_FT: For FTS, instrument states are defined in terms of interferometer axis position.
- SDB_DS: For DS, a spectral data base is currently not used. Instrument state parameters are directly linked to spectral shift so that interpolation of the actual instrument state from the SDB is not required. Use of SDB becomes relevant when explicit instrument models are available.

SRF: Spectral Response Function (ISRF model, levels 1a or 1b)

Computation of ISRF for a defined instrument state. This module also evaluates the main ISRF characteristics: spectral shift, spectral calibration function, shape error index (comparison with a reference ISRF). This module is linked with an instrument model only for FTS design. For DS, the ISRF is read in directly, and spectral shifts are simulated as function of the instrument state. The input parameters are listed in § 2.4.2.

CNV: Computation of level 1a or level 1b spectra

- Spectral interpolation of ISRFs at predefined wave numbers to the considered wave numbers
- Convolution of high resolution spectrum with level 1a ISRFs (including spectral shift)
- Convolution of high resolution spectrum with level 1b ISRFs (neglecting spectral shift)

GNR: Gaussian Noise Generator

Addition of noise to convolved level 1a spectra. Random draw of a Gaussian distribution with specified standard deviation $1\sigma$ in each spectral sample.
SCS: Spectral Calibration Sub-system

- Estimation of the Spectral Shift between a level 1a spectrum and a reference spectrum (per spectral correlation window and per spatial sample)
  
  **SSD_FT**: In the Fourier Space  
  **SSD_SP**: In the Spectrum Space  

- Filtering of the individual spectral shift estimations (not applied in this study)
  
  Quality check by comparison with minimum and maximum values to be completed with scene filtering criteria
  
  **SSS_FT**: In the Fourier Space  
  **SSS_SP**: In the Spectrum Space  

- Estimation of the actual instrument state
  
  **FTS**: Computation of the interferometer axis position by interpolation between the pre-defined positions in the SDB. Minimisation of the mean square shift deviation between estimated and SDB predicted spectral shifts for all spatial samples and calibration windows.
  
  **IAX_FT**: for spectral shift determination in the Fourier Space  
  **IAX_SP**: for spectral shift determination in the Spectrum Space  

  **DS**: Computation of spectral offset and distortion by minimisation of the root mean square deviation between estimated and (spectral calibration function) predicted spectral shifts for all spatial samples and calibration windows (**RSF**).

- Temporal filtering of the instantaneous instrument state (not applied in this study)
  
  Polynomial temporal filtering of the instrument state parameters over a defined number of measurement steps

- Extraction of the Spectral Calibration Function for the entire spectrum
  
  **FTS**: Extraction of the spectral calibration function determined as function of a unique interferometer axis position estimation per focal plane derived from all available spectral calibration windows (**ISF**).
  
  **DS**: The spectral calibration function depends directly on the instrument state parameters.

- Spectrum Oversampling (**SOS**): this module is a combination of two parametrised non-linear operators. The first one operates in the Fourier space by application of different phases on the Fourier transform of the spectrum, the phases correspond to the different fractions of the spectral sampling. The second one is a cubic spline interpolator.

- Spectrum calibration and resampling (**S1B**)
  
  Computation of the calibrated wave number basis for the oversampled level 1a spectrum; Resampling to the theoretical wave number basis (by cubic spline interpolator).

**SCS_anal: Spectra calibration analysis**

Computation of spectral calibration errors

- Relative spectral shift errors
- Spectral radiance errors in NEdT (S1B – S1Btrue)
2.4.2. Parameterisations

The whole set of instrument parameters and processing software parameters are defined in a configuration file. This configuration file is at the input interface of all processing operators.

The software system is controlled by the following principal user parameterisations:

- Instrument parameters, ISRF models and the ISRF-EM Spectral Data Base (SDB) are parameterised by an instrument concept identifier, DS or FTS. Instrument inputs are at present:
  - for DS:
    - the level 1b ISRF (identical for all spatial samples),
    - the nominal level 1b centroid wavelengths/wave numbers,
    - a user-defined sub-selection of spatial samples (in coordinates relative to the spatial samples corresponding to the array borders),
    - the spectral offset at array borders in the spatial dimension,
    - the array distortion in the spectral dimension.
  - for FTS:
    - the PSF shape (assumed identical for all spatial samples),
    - the nominal PSF barycentre coordinates (parameterised by the optical magnification factor, the orbit height, and the spatial sample line and column number in the detector array) for a user-defined sub-selection of spatial samples,
    - the laser RPD wave length,
    - the laser RPD interferogram detector (PSF and field angle position in the focal plane),
    - the corner cube motion law (constant offset term, constant tilt term, parabolic term, higher frequency terms)
    - the interferometer axis position.

- A sub-selection of spatial samples of the detector array is parameterised by a user defined sequence of spatial samples with corresponding instrument coordinates.
- Each selected spatial sample is associated with a user defined geophysical scene that can be any of the available high-resolution spectra.
- A time sequence of measurements can be simulated by a loop over the spatial sample selection, possibly with different assignments to high-resolution spectra.
- The reference spectrum per spatial sample is user defined.
- Nominal level 1b convolution points are user parameterised. In particular, IRS mission bands can be considered separately, in any combination, or as a whole.
- Spectral calibration windows are defined in a list. Spectral shift estimations are carried out window by window, while the instrument state is determined once combining the information available from all spectral calibration windows.
- The correlation space is user defined.
- The sampling of instrument states considered in the SDB as well as the instrument state to be considered for level 1a spectra simulation is parameterised.
3. Instrument input analysis

At this stage of the MTG/IRS development process, there is no unique baseline for the two IRS instrument concepts. Nevertheless, the spectral calibration algorithm assessment, requires such baseline to define a simplified but realistic instrument model as starting point.

The baseline for this study is derived from first results of the ongoing MTG pre-phase A instrument studies (two studies are carried out independently of each other). Since the choice of the instrument concept, dispersion spectrometer (DS) or Fourier Transform Spectrometer (FTS) will be left open at least during pre-phase A, a baseline has to be defined for both concepts.

The following sub-sections provide an explicit description of the instrument baseline assumptions applicable to the IRS spectral calibration assessment analysis (section 3.1) and a description of concept dependent parameterisations for the practical application of the spectral calibration processing scheme (section 3.2).

3.1. Baseline concepts for spectral calibration assessment

The baseline for the two possible IRS concepts is described in [RD 8] and summarised in the following subsections.

Reported performances refer to a certain number of pre-processing steps that are intended to reduce the onboard data transfer rate and to increase the radiometric resolution. A summary of the spectral and spatial processing is provided in [RD 9]. Some of the processing is penalising for spectral calibration (e.g., the decrease of spectral resolution by spectral filtering may exclude the use of otherwise suitable calibration windows). Therefore, we adapt the performances reported in [RD 8] according to the following assumptions.

- Apodisation (FTS only): According to the MRD, no apodisation is applied to FTS spectra. The relevant spectral resolution is at level 1b (about 1.21 times better than the reported level 1c spectral resolution). On the other hand, radiometric noise is higher at level 1b (division by 0.63 after [RD 9]).

- Spectral filtering: The spectral filtering is intended to reduce the number of spectral samples according to the specifications and to increase the radiometric resolution and to render typical ISRF shapes comparable for the two concepts. The present study considers the spectral and radiometric performances after spectral filtering as baseline. However, the related loss in spectral resolution might be contradictory to user requirements. In particular for DS, it should be kept in mind that the investigated ISRF model does not exclusively depend on the instrument design, but also on the spectral filter characteristics.

- Spatial filtering is claimed to concentrate Integrated Energy of a spatial sample closer to its centre. Independently of the reservation that a global spatial filter without use of sub-pixel information renders a subsequent scene decomposition practically impossible, we assume that spectral calibration takes place prior to any spatial filtering. Thus, reported radiometric performances in [RD 8] are corrected by spatial ‘finite impulse response’ (FIR) correction factors reported in [RD 9] for both concepts.

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Thus the baseline concepts consider a spectrally filtered, unapodised (in case of FTS) and spatially unfiltered spectrum as input to the spectral calibration sub-system.

### 3.1.1. DS baseline

#### 3.1.1.1. Focal plane assembly

The Dispersive Spectrometer operates in 4 spectral bands (arrays S2 to S5, c.f., Table 1). Implementation of IRS-5 or IRS-6 is alternative. According to a decision during the ongoing pre-phase A instrument studies, IRS-0 (14.29 to 15 \(\mu\)m) is removed.

The E/W IFOV size (spectral dimension) is 3 km (IRS-5 to IRS-9) and 6 km (IRS-1 to IRS-4), respectively. This is obtained by two spectrometer slits of different width. The E/W motion smear is identical to the E/W IFOV size, implying an integration time (7.8 ms and 15.5 ms, respectively) identical to the sampling interval. The N/S IFOV size is 2.9 km and 5.7 km, respectively. The number of N/S array pixels is 64, reduced to 32 in bands IRS-1 to 4 by spatial averaging, corresponding to a N/S IFOR of 192 km. The entire Earth disk is scanned in 64 E/W strips within 30 minutes (repeat cycle).

#### 3.1.1.2. Spectral and radiometric characteristics

The spectral and radiometric performances are summarised in Table 1. A spectral gap of width 36 nm between IRS-1 and IRS-2 is not relevant in the study context. Radiometric performance depends on the spectral radiance itself, maximum and minimum noise is reported per mission band considering a typical radiance per spectral channel. Noise spectra are available as numerical tables.

<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>Wavelength range [(\mu)m]</td>
<td>12.99-14.3</td>
<td>10.2-12.99</td>
<td>9.34-10.2</td>
<td>8.26-9.34</td>
<td>6.25-8.26</td>
<td>5.00-6.25</td>
<td>4.44-5.00</td>
<td>4.17-4.44</td>
<td>4.00-4.17</td>
</tr>
<tr>
<td>Wavenumber range [(\text{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></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>req. spect. resolution [(\text{nm;cm}^{-1})]*</td>
<td>9.3</td>
<td>0.82</td>
<td>0.47</td>
<td>0.65</td>
<td>0.5</td>
<td>3.2</td>
<td>0.625</td>
<td>1.9</td>
<td>1.4</td>
</tr>
<tr>
<td>spect. resolution [(\text{nm;cm}^{-1})]*</td>
<td>12.5</td>
<td>12.5</td>
<td>7.1</td>
<td>7.1</td>
<td>7.1</td>
<td>4.8</td>
<td>2.9</td>
<td>2.1</td>
<td>1.1</td>
</tr>
<tr>
<td>SSI [(\mu)m]</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>
</tr>
<tr>
<td>spectral samples</td>
<td>199</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>
</tr>
<tr>
<td>equivalent SSI [(\text{cm}^{-1})]</td>
<td>0.37</td>
<td>0.52</td>
<td>0.405</td>
<td>0.505</td>
<td>0.525</td>
<td>0.512</td>
<td>0.535</td>
<td>0.96</td>
<td>1.69</td>
</tr>
<tr>
<td>1st and last nominal 1b centroid [(\text{cm}^{-1})]</td>
<td>700.04</td>
<td>770.12</td>
<td>980.505</td>
<td>1090.605</td>
<td>1209.475</td>
<td>1210.222</td>
<td>1599.334</td>
<td>1999.872</td>
<td>2399.04</td>
</tr>
<tr>
<td>req. rad. resolution NEdT@280K [(\text{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>0.2</td>
<td>0.3</td>
<td>as feasible</td>
</tr>
<tr>
<td>rad. res. NEdT@280K [(\text{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>
</tr>
<tr>
<td>(\kappa_{\text{IR}})</td>
<td>1.22</td>
<td>1.22</td>
<td>1.20</td>
<td>1.20</td>
<td>1.20</td>
<td>1.17</td>
<td>1.18</td>
<td>1.18</td>
<td>1.19</td>
</tr>
</tbody>
</table>

Table 1: Spectral and radiometric characteristics for the IRS/DS baseline. Radiometric performance as provided in [RD 8] is corrected by a factor \(1/\kappa_{\text{IR}}\) provided in [RD 9]. Legend: *=at band centre.

Nominal level 1b centroids (i.e., the convolution points of the level 1b spectral response function) are not explicitly defined in [RD 8]. For our investigation, we calculate an integer number of spectral samples as function of the spectral sampling and the mission band width as specified in wavelength in Table 1. Using this number of spectral samples per mission band, we resample the level 1b centroids to a constant spectral sampling grid in wave number and define level 1b centroids as a multiple of the spectral sampling interval. This virtual resampling is applied for practical reasons: All computations are carried out in terms of wave number (high-resolution spectra are available on a constant wave number spectral sampling interval) avoiding numerous
wavelength/wave number conversions in the convolution and spectral calibration modules. This simplification is consistent with the concept independent formulation of IRS spectral resolution requirements in terms of resolving power in [RD 1]. It can be reasonably assumed that spectra of a given sample number at constant wavelength or at constant wavenumber sampling interval conserve the information content over the typical width of IRS mission bands.

3.1.1.3. ISRF model

System Point Spread Functions (PSF) have been delivered by ESA as numerical tables at the edges and the centre of each mission band. Though not explicitly used in the present study, the PSF model is briefly discussed since governing the ISRF shapes.

Expressed in object space coordinates (i.e., lengths projected on Earth surface), the system PSF is obtained by convolution of the different contributors:

$$PSF(x, y) = PSF_{opt}(x, y) \otimes PSF_{IFOV}(x, y) \otimes PSF_{MS}(x, y) \otimes PSF_{LOS}(x, y)$$ (1.)

The optical PSF takes into account the diffraction for a circular aperture of 300mm, and optical aberrations assuming a geometric image quality equal to one quarter of the IFOV (rms). The IFOV PSF is a rectangular top-hat function. The motion PSF is a one-dimensional (E/W) top-hat function for the motion smear values defined above. The Line-of-Sight PSF is assumed as a circular top-hat considering a pointing stability of 3µrad rms during integration time.

Due to motion smear and LOS instability, the system PSF is the time integral of the instantaneous PSF (IPSF), defined via the IFOV center coordinates $(x_0, y_0)$ as:

$$IPSF(x, y) = PSF_{opt}(x, y) \otimes PSF_{IFOV}(x + x_0(t), y + y_0(t))$$ (2.)

Defining $IPSF_j(x)$ as the projection of the IPSF of a spectral detector $j$ on the spectral dimension (i.e., the E/W direction), the instrument spectral response function of spectral detector $j$ for a spatially uniform scene is given by

$$ISRF_j(\delta \lambda) = \prod \left( \frac{x}{\Delta X_S} \right) \otimes \left( IPSF_j(x) \right) \left( K_{\lambda j} \delta \lambda \right)$$ (3.)

with the notations

- $\otimes_x$: the convolution operator with respect to $x$,
- $\Delta X_S$: the slit size in the spectral dimension, projected in object space,
- $\delta \lambda$: the wavelength distance from the ISRF barycentre in spectral detector $j$,
- $\Pi(a/b)$: a top-hat function in $a$ of width $b$.

The relation between the spectral scale $\delta \lambda$ and the spatial scale in the spectral dimension $dx$ is defined by the coefficient $K_{\lambda j}$ that depends on the optical instrument parameters, the linear dispersion function, the spectral magnification and the orbit height. In absence of an explicit instrument model, it can be simply approximated by the ratio between the detector size in the spectral dimension, projected in object space, $\Delta X_D$, and the spectral sampling interval, SSI

$$K_{\lambda j} = \frac{dx}{d\lambda}(j) = \frac{\Delta X_D}{SSI_j}$$ (4.)
Equation (3) applies to an individual spectral detector $j$. In practice, spectral on-board binning has to be considered. The spectral response function of a linearly binned spectral channel $J$ transmitted to ground is a linear combination of adjacent spectral detector response functions. Neglecting any variation of the spectral response over adjacent detectors, we obtain

$$\text{ISRF}_J(d\lambda) = \frac{1}{N_B} \sum_{k=1}^{N_B} \text{ISRF}_j\left(d\lambda + \left(k - \frac{N_B}{2} + 1\right) \frac{\text{SSI}_j}{2}\right)$$

with $N_B$ the number of binned detectors and $\text{SSI}_j$ the spectral sampling interval at detector level in channel $J$. In the baseline concept, the number of binned detectors is 2 in bands IRS-1 to IRS-7, 3 in IRS-8 and 5 in IRS-9. The detector/slit size ratio is optimised for a binning of 2 spectral samples.

However, linear binning is not applied in the DS baseline concept [RD 8]. Instead, adjacent spectral samples are filtered numerically, at the expense of spectral resolution, according to filter coefficients fitting the spectral MTF to a Hamming window.

These filtered spectral response functions represent the ‘ISRF model’ for the DS spectral calibration algorithm assessment. They are available as numerical tables for the edges and the centre wavelength in each mission band, consistently with values of spectral sampling and spectral resolution reported in Table 1.

### 3.1.2. FTS baseline

#### 3.1.2.1. Focal plane assembly

After [RD 8], the Fourier Transform Spectrometer has four focal plane arrays (A1 to A4, c.f. Table 2) with 128 by 128 elements (A1, A2, after averaging over 2 by 2 elementary detector elements) or 256 by 256 elements (A3/3’, A4). Implementation of mission bands IRS-5 and IRS-6 is alternative. The scan mirror pupil diameter is 300 mm, the magnification factor of the telescope is 6. The IFOR is 1.19° by 1.19° (768 by 768 km SSP). The entire Earth disk is scanned in 16 E/W steps and 16 N/S steps within 30 minutes (repeat cycle). The IFOV size is 5.7 km and 2.9 km, respectively. Integration time is 6 s in bands IRS-1 to IRS-4 and 4.8 s in bands IRS-5/6 to IRS-9, respectively. Dwell periods are synchronised, the difference corresponds to a cut-off of the interferograms in arrays A3/3’ and A4.

#### 3.1.2.2. Spectral an radiometric characteristics

The spectral and radiometric characteristics are summarised in Table 2.

The Maximum OPD is related to the integration time and the spectral sampling and amounts to roughly ±1.22 cm in arrays A1 and A2, and to ±0.96 cm in arrays A3/3’ and A4. Spectral sampling and resolution are adapted to the MRD requirement by spectral filtering in mission bands IRS-2, 4, 8, and 9 through interferogram decimation. The spectral resolution is derived as 1.21 times the spectral sampling, which is the theoretical value for a perfect cardinal sine spectral response without any self-apodisation effect.

Nominal level 1b centroids are derived in analogy to DS by calculating an integer number of spectral samples as function of the spectral sampling and the mission band width as specified in wave number in Table 2. The centroids are defined as multiples of the specified spectral sampling interval.
Radiometric performance in [RD 8] refers to apodised spectra after spectral and spatial filtering. The radiometric resolution considered for spectral calibration assessment is corrected for the effects of apodisation and spatial filtering applying the correction factors provided in [RD 9]. Values refer to a typical radiance per spectral channel.

### Table 2: Spectral and radiometric characteristics for the IRS/FTS baseline. Radiometric performance as provided in [RD 8] is corrected by a factor 1/(k'FIR k'noise-apo) provided in [RD 9]. Legend: *excluding self-apodisation.

<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>A3</td>
<td>A3'</td>
<td>A4</td>
<td></td>
<td></td>
<td></td>
<td></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>Spect. resolution [cm⁻¹]</td>
<td>0.5</td>
<td>0.62</td>
<td>0.85</td>
<td>0.62</td>
<td>0.62</td>
<td>0.62</td>
<td>1.25</td>
<td>2.45</td>
<td></td>
</tr>
<tr>
<td>SSI [cm⁻¹]</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>
<td>2.03</td>
<td></td>
</tr>
<tr>
<td>Spectral samples</td>
<td>171</td>
<td>219</td>
<td>200</td>
<td>750</td>
<td>769</td>
<td>481</td>
<td>145</td>
<td>49</td>
<td></td>
</tr>
<tr>
<td>1st and last nominal 1b centroid [cm⁻¹]</td>
<td>700.28</td>
<td>980.31</td>
<td>1070.30</td>
<td>1210.04</td>
<td>1600.56</td>
<td>2000.44</td>
<td>2250.55</td>
<td>2401.49</td>
<td></td>
</tr>
<tr>
<td>Centroid [cm⁻¹]</td>
<td>769.98</td>
<td>979.68</td>
<td>1069.69</td>
<td>1209.60</td>
<td>1599.52</td>
<td>1999.92</td>
<td>2250.04</td>
<td>2398.87</td>
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</tr>
<tr>
<td>Required rad. resolution</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NEdT@280K [K]</td>
<td>0.2</td>
<td>0.24</td>
<td>0.2</td>
<td>0.2</td>
<td>0.62</td>
<td>0.62</td>
<td>0.62</td>
<td>0.62</td>
<td>0.62</td>
</tr>
<tr>
<td>Rad. res. NEdT@280K [K]</td>
<td>0.40-0.85</td>
<td>0.31-0.49</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>
<td></td>
</tr>
<tr>
<td>k'noise-apo</td>
<td>0.63</td>
<td>0.63</td>
<td>0.63</td>
<td>0.63</td>
<td>0.63</td>
<td>0.63</td>
<td>0.63</td>
<td>0.63</td>
<td>0.63</td>
</tr>
<tr>
<td>k'FIR</td>
<td>1.08</td>
<td>1.08</td>
<td>1.08</td>
<td>1.08</td>
<td>1.08</td>
<td>1.08</td>
<td>1.08</td>
<td>1.08</td>
<td>1.08</td>
</tr>
</tbody>
</table>

3.1.2.3. ISRF model

System PSF are provided by ESA as numerical tables at the edges and the centre of each mission band. The system PSF is obtained by convolution of the different contributors:

\[
PSF(x, y) = PSF_{opt}(x, y) \otimes PSF_{IFOV}(x, y) \otimes PSF_{LOS}(x, y) \tag{2}
\]

The optical PSF accounts for the diffraction for a circular aperture of 300mm, and for optical aberrations assuming a geometric image quality equal to one quarter of the IFOV (rms). The IFOV PSF is a rectangular top-hat function. The Line-of-Sight PSF is assumed as a circular top hat considering a pointing stability of 10µrad rms during integration time.

The ISRF of a spectral sample \( j \) is given by:

\[
ISRF_j(\delta \nu) = TF^{-1} \left[ SAF_j (ddm_0(m)) \right] \tag{6}
\]

the inverse Fourier Transform of the self-apodisation function \( SAF \) in channel \( j \) for the optical path difference \( ddm_0 \) of sample \( m \) of the ideal interferogram (at zero field angle, defined with respect to the interferometer axis, and zero angular extension). Defining \( ddm(m, x, y) = ddm_0(m) \cos(\alpha(x, y)) \) as the optical path difference for the same interferogram sample at a given field angle \( \alpha(x, y) \), the self-apodisation function is:

\[
SAF_j (ddm_0(m)) = \frac{I(ddm(m), \nu_0(j))}{I_0(ddm_0(m), \nu_0(j)))} \tag{7}
\]

the ratio between the measured and the ideal interferograms \( I \) and \( I_0 \), respectively, with:

\[
I_0(ddm_0(m), \nu_0(j)) = \exp(i \cdot 2 \pi \cdot \nu_0(j) \cdot ddm_0(m)) \tag{8}
\]

\[
I(ddm(m), \nu_0(j)) = \int \int \exp(i \cdot 2 \pi \cdot \nu_0(j) \cdot ddm_0(m, x, y) \cdot \cos(\alpha(x, y))) \cdot PSF(x, y) \, dx \, dy \tag{9}
\]
In case of IRS/FTS, the angular extension of spatial samples is small, so the SAF is dominated by the field angle generating a spectral shift $\Delta \nu$ while shape variations with field angle are small and all shapes are close to a cardinal sine.

The above formulation does not consider drifts of the reference laser frequency. It is assumed that for operational spectral calibration, the reference laser frequency stability is controlled offline and parameterised in the explicit instrument model.

Spectral response functions are not available from [RD 8] and have been generated by NOVELTIS every 20 to 40 cm$^{-1}$ depending on mission bands. The computation is consistent with the reported values of the spectral sampling interval SSI reported in Table 2 and parameterised internally via the maximum OPD (MOPD=0.5/SSI) and with the PSF model without spatial filter provided by ESA as input. Figure 3 illustrates representative nominal spectral response functions at zero field angle.

![MTG/IRS nominal spectral response 1b](image)

Figure 3: Nominal IRS/FTS level 1b spectral response functions at the lower wave number limit of selected mission bands. Spectral variation for bands with identical maximum OPD as well as field angle variations are insignificant at the scale of the figure axes.

It is recalled that the spectral calibration algorithm is assessed on unapodised spectra with the spectral and radiometric characteristics reported in Table 2, i.e., after interferogram decimation.

### 3.2. Practical application

The practical application of the SCS is detailed in this section in order justify parameter choices for the upcoming spectral calibration assessment investigations.

#### 3.2.1. Instrument state parameters and spectral calibration functions

Instrument state parameters that control the spectral response function estimation of any spectral and spatial sample differ considerably for the two instrument concepts.

##### 3.2.1.1. DS

A DS detector array has a spectral dimension (spectral samples $j$ aligned in the direction of motion smear, E/W) and a spatial dimension (spatial samples $i$, aligned perpendicular to the direction of motion smear, N/S).
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:

\[
\lambda_{i1a} - \lambda_{i1b} = \delta\lambda = A_i + (D-1) \lambda_{ilb}
\]  

(10.)

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., \(p=0\) and \(p=1\) 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:

\[
\lambda_{i1a} - \lambda_{i1b} = \delta\lambda = A_0 + p_i(A_1-A_0) + (D-1) \lambda_{ilb}
\]  

(11.)

In wave number (\(\nu\)), this yields:

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

(12.)

The spectral calibration function is given by

\[
F_{SC} = \nu_{ib}/\nu_{i1a} = \nu_{ib}/(\delta\nu_i + \nu_{ib}) = (A_0 + p_i(A_1-A_0))\nu_{ib} + D
\]  

(13.)

and the spectral calibration procedure has to determine the instrument state parameters \(A_0, A_1, D\).

3.2.1.2. FTS

The two dimensions of an FTS detector array are spatial. The spectral shift \(\delta\nu_i\) depends on the average field angle \(\alpha_i\) of a spatial sample \(i\)

\[
\alpha_i = \arccos \left( \iint \cos(\alpha(x, y)) \cdot PSF_i(x, y) \, dxdy \right)
\]  

(14.)

by:

\[
\delta\nu_i = \nu_{i1a} - \nu_{ib} = \nu_{ib} (\cos \alpha_i - 1)
\]  

(15.)

The spectral calibration function is given by

\[
F_{SC} = \nu_{ib}/\nu_{i1a} = \nu_{ib}/(\delta\nu_i + \nu_{ib}) = 1/\cos \alpha_i
\]  

(16.)

Spectral shift determinations translate into average field angle estimations for each considered spatial sample. The system is then fully characterised by the interferometer axis position, i.e., the focal plane coordinates where the field angle is zero. The interferometer axis position is the only instrument state parameter, allowing for the computation of the field angle (thus the spectral shift) for every detector in the array.

The above formulation is an approximation applicable to IRS/FTS. In general, the spectral shift depends in addition on the field angle variation within a spatial sample (see section 3.1.2.3). Due to the small angular dimension of spatial samples, field angle variations are negligible against the average field angle. If the average field angle itself is small (in a spatial sample near the interferometer axis), the absolute spectral shift is so small that the observed spectrum can be considered as calibrated.

Due to IASI heritage, our spectral calibration software system takes both effects into account, but a simplified formulation of the spectral calibration function after equation (16) should be investigated in the frame of future activities.
3.2.2. **Content of the spectral data base**

The content of the FTS Spectral Data Base is a collection of relative spectral shifts and the related spectral calibration functions for selected spatial samples and for predefined instrument states, i.e. a collection of interferometer axis positions. In the present study, we have arbitrarily chosen nine interferometer axis positions (3 by 3 samples of 1 mrad in N/S and E/W direction) around the nominal interferometer axis position in the centre of the detector array. This choice is not constraining the general applicability. In practice, it is required that SDB interferometer axis positions cover the (not yet known) nominal range of actual axis positions. The final choice depends on the specification of this nominal range.

In absence of an explicit instrument model, there is for instance no specific functionality of a Spectral Data Base for DS. The instrument state parameters defined in section 3.2.1 are not yet linked with instrument parameters that predict ISRF shift and shape parameters. The instrument state and the spectral calibration function can be directly retrieved from shift determinations in individual spatial samples and calibration windows through equations (12) and (13). It is expected though that upon availability of an explicit DS instrument model, the spectral calibration subsystem will use a Spectral Data Base in a similar way as outlined for FTS here above.

3.2.3. **Selection of spatial samples**

Operational spectral calibration will be applied to each measured spectrum in Earth observation mode from any detector element. On the other hand, it is unlikely that all available measurements (after scene filtering) will be exploited in the SCS for the determination of the instrument state. In the case of FTS, it is obvious that 128 by 128 (256 by 256 in bands 5 to 9) simultaneous spectral shift determinations provide redundant information on the interferometer axis position. Similarly for DS, the use of all 32 (64 in band 5 to 9) array positions in the spatial dimension is not required to derive a linear variation of the spectral offset along this dimension.

This suggests a sub-sampling of spatial samples to be considered in the SCS.

For FTS, the sub-selection needs to be adapted to the objective to determine the interferometer axis position. The sub-selection shall provide spectral shift determinations in the two spatial dimensions of the detector array. The minimum requirement for interferometer axis position estimation is a selection of three non-aligned detectors in the array.

For DS, instrument state determination requires a selection of at least two spatial samples (and of at least two calibration windows) for the estimation of the linear variation of the spectral offset in the spatial dimension (and the distortion in the spectral dimension).

Sub-selections of spatial samples are defined in detail in [RD 4, section 3.2.2], where the impact of various sub-selections on the instrument state estimation performance is investigated.
4. Geophysical inputs

The assessment of the MTG/IRS spectral calibration algorithm performance requires the availability of radiance spectra at high spectral resolution (as compared to the spectral resolution of the instrument), referred to as HRRS.

In a more advanced stage of the IRS development, the HRRS data base should allow for the representation of realistic scenes over a surface of the dimension covered by the IRS detector matrix (FTS) or a corresponding surface scanned by the IRS detector matrix (DS).

In the isolated context of the spectral calibration assessment investigation, it is too early to spend considerable effort on the time consuming simulation of HRRS data that may have no further use in future system assessment activities. Therefore, the available spectra from former investigations in the frame of [RD 2] are reused. These HRRS have been simulated between 600 cm\(^{-1}\) and 2565 cm\(^{-1}\) at a resolution of 0.01 cm\(^{-1}\) by coupling the radiative transfer codes 4A/OP and DISORT in order to accurately consider gaseous absorption at high spectral resolution and scattering in clouds. 44 clear-sky and 97 cloudy spectra are available for Meteosat viewing conditions, covering a large range of atmospheric conditions over the complete Meteosat disk. The simulations consider only variations of temperature, humidity and ozone profiles, they should not be overexploited when considering absorption line pattern of other trace gases. A detailed description of the data base, the simulation parameters and the atmospheric conditions is given in [RD 10].

4.1. Selection of representative radiance spectra

Use of the entire set of simulations puts too much weight on the investigation of atmospheric variability. In the MTG pre-phase A context, such detailed investigation is not justified, since not revealing elements for the IRS concept choice. However, the selection of HRRS data shall allow for an investigation of the principal impact of atmospheric variability:

- Impact of cloudiness on the spectral calibration performance
- Stability of the spectral calibration performance with various atmospheric regimes

The investigation should hint at the necessity for filtering cloud contaminated observations or not. It depends strongly on the choice of the spectral calibration windows and its sensitivity to cloud contamination. Second, the investigation of the spectral calibration performance in various atmospheric conditions will reveal indications for numerous system relevant trade-off decisions to be made in future:

- Is it possible to use a unique reference spectrum or is atmospheric prior knowledge for selection between different reference spectra required to obtain an acceptable performance?
- Does the use of several spectral calibration windows with different impact of atmospheric variability yield a stable algorithm performance?
- Which windows minimise the impact of atmospheric variability? Are related requirements in terms of spectral resolution met?
- Is the spectral calibration algorithm noise governed by the impact of radiometric resolution or by the impact of atmospheric variability?
In the above context, the selection of HRRS focuses on representing the following atmospheric regimes:

- moderately humid and temperate atmospheric conditions, used as global reference spectrum,
- hot and humid, hot and dry, cold and dry atmospheric conditions without clouds,
- high and opaque, high and semi-transparent, low and opaque clouds.

The selected high-resolution spectra at sampling 0.01 cm\(^{-1}\) for atmospheric conditions corresponding to the above criteria are characterised in Table 3.

The characterisation provides surface pressure \(p_{\text{surf}}\), surface temperature \(T_{\text{surf}}\), total water vapour content \(T_{\text{WC}}\), and a spectral surface emissivity classification \(I_{\text{emm}}\) (oce=ocean, des=desert, wsa=woody savannah). For cloudy components, the cloud layer is characterised by the cloud type \(C\) (Sc=stratocumulus, Ns=nimbostratus, Cb=cumulonimbus, Ci=cirrus), the total optical depth in the visible \(\tau\), cloud bottom and cloud top pressure \(p_b\) and \(p_t\), respectively and the cloud top temperature \(T_{\text{ctop}}\). Each clear-sky/cloud couple, is simulated at the reported, realistic satellite zenith angle \(\theta\) and is described in view of the general synoptic conditions.

<table>
<thead>
<tr>
<th>spectrum identifier</th>
<th>(p_{\text{surf}}) [hPa]</th>
<th>(T_{\text{surf}}) [K]</th>
<th>(T_{\text{WC}}) [kg/m(^2)]</th>
<th>(I_{\text{emm}})</th>
<th>(T_{\text{ctop}}) [K]</th>
<th>(\tau)</th>
<th>(p_b) [hPa]</th>
<th>(p_t) [hPa]</th>
<th>(\theta)</th>
<th>Synoptic conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>0511</td>
<td>1017.1</td>
<td>290.08</td>
<td>30.8</td>
<td>oce</td>
<td>10</td>
<td>950.9</td>
<td>900</td>
<td>NE trade wind regime, temperate and moderately humid</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0512</td>
<td>1017.1</td>
<td>290.08</td>
<td>31.2</td>
<td>oce</td>
<td>284.14</td>
<td>Sc</td>
<td>950</td>
<td></td>
<td>47°</td>
<td></td>
</tr>
<tr>
<td>0721</td>
<td>965.89</td>
<td>305.18</td>
<td>52.2</td>
<td>wsa</td>
<td>242.11</td>
<td>Cb</td>
<td>800</td>
<td>300</td>
<td>22°</td>
<td>Central Africa, ITCZ deep-convection, hot and humid</td>
</tr>
<tr>
<td>0722</td>
<td>963.88</td>
<td>304.89</td>
<td>65.6</td>
<td>wsa</td>
<td>243.24</td>
<td>Ns</td>
<td>700</td>
<td>500</td>
<td>61°</td>
<td>South Atlantic depression system, cold and dry</td>
</tr>
<tr>
<td>0931</td>
<td>979.54</td>
<td>271.53</td>
<td>6.78</td>
<td>oce</td>
<td>206.44</td>
<td>Ci</td>
<td>200</td>
<td>150</td>
<td>24°</td>
<td>West Sahara high-pressure belt, hot and dry</td>
</tr>
<tr>
<td>0932</td>
<td>980.82</td>
<td>271.97</td>
<td>7.81</td>
<td>oce</td>
<td>206.44</td>
<td>Ci</td>
<td>200</td>
<td>150</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3: Surface, atmospheric and cloud parameters for selected high-resolution radiance spectra.

The selected components are associated with a precise investigation purpose in Table 4.

<table>
<thead>
<tr>
<th>Investigation purpose</th>
<th>atmospheric state</th>
<th>spectrum identifier</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference spectrum</td>
<td>clear-sky, temperate, moderately humid</td>
<td>0511</td>
</tr>
<tr>
<td>Impact of atmospheric variability</td>
<td>clear-sky, hot, humid</td>
<td>0721 vs. 0511</td>
</tr>
<tr>
<td></td>
<td>clear-sky, hot, dry</td>
<td>1611 vs. 0511</td>
</tr>
<tr>
<td></td>
<td>clear-sky, cold, dry</td>
<td>0931 vs. 0511</td>
</tr>
<tr>
<td>Impact of cloudiness</td>
<td>high, opaque cloud</td>
<td>0722 vs. 0721</td>
</tr>
<tr>
<td></td>
<td>high, semi-transparent cloud</td>
<td>1614 vs. 1611</td>
</tr>
<tr>
<td></td>
<td>low, opaque cloud</td>
<td>0512 vs. 0511 and 0932 vs. 0931</td>
</tr>
</tbody>
</table>

Table 4: Link between HRRS selection and investigation purpose.

In the upcoming spectral calibration algorithm assessment, the calibrated spectrum 0511 will be considered as reference spectrum to be correlated with any uncalibrated spectrum for the spectral shift determination. Applying uncalibrated spectra in various atmospheric conditions will provide impact estimations of atmospheric variability on the spectral calibration algorithm performance.
Figure 4: Nominal IRS/DS level 1b spectra for geophysical conditions defined in Table 3.

For illustration of spectrum variability within the considered variation of atmospheric conditions, Figure 4 shows nominal 1b spectra for IRS/DS in the eight atmospheric conditions identified in Table 3. It can be noticed that all spectra appear smooth in bands IRS-8 and –9. This indicates not only a small potential for spectral calibration in these bands at the proposed spectral resolutions, but also limited information content with respect to vertical sounding.

4.2. Practical application

Independently of the instrument concept, IRS will provide a rate of several thousands spectra per second. In the frame of initial spectral calibration assessment activities that are dedicated to the consolidation of system requirements rather than to an explicit performance evaluation, it is necessary to define simplified simulations of the spectral calibration subsystem. This concerns both the geographical and the geophysical distribution scenario of spatial samples the spectral calibration algorithm is applied to.

The observations analysed by the operational SCS are associated to various geophysical conditions. An explicit simulation of the SCS for the above defined sub-selection of spatial samples would require the knowledge of the spatial distribution of geophysical conditions and the explicit simulation of high-resolution spectra for a huge number of geophysical conditions.
This explicit simulation is not desirable in the current state of the spectral calibration assessment. First, merging different geophysical conditions does not allow for a separation of the different contributions to the spectral calibration algorithm noise, in particular the impact of radiometric resolution from the impact of atmospheric variability. Second, as long as the duration of the spectral calibration is undefined, the geophysical variability to be considered cannot be reliably fixed. Atmospheric variability corresponds to the scene variation accumulated over the spectral calibration period. Global variability must be considered if the spectral calibration period is of the order of the IRS repeat cycle or beyond. This is not justified for a spectral calibration period small against the repeat cycle when IRS observation stem from only a small part of the visible Earth.

Therefore, in this study we will assume identical geophysical conditions for an instantaneous sub-selection of spatial samples. The impact of radiometric noise on the spectral calibration algorithm noise can be evaluated for a given geophysical state by comparison between performances for noisy and noise-free spectra. The impact of atmospheric variability is evaluated by application of the SCS to spectra representing various but spatially homogeneous geophysical conditions, facilitating the identification of those conditions that are unsuitable for spectral shift determination, thus spectral calibration processing.
5. Candidate spectral calibration algorithm design

Candidate spectral calibration algorithm design is distinguished in terms of the correlation space between observed (uncalibrated) spectra and reference (calibrated) spectra, and the selection of spectral calibration windows.

5.1. Correlation space

Two correlation methodologies are applied. The first one maximises the correlation coefficient between the measured and the reference spectra in one or more spectral calibration windows.

The second methodology is inspired by the IASI spectral calibration algorithm [RD 6]. The correlation coefficient is maximised by minimisation, in the dual Fourier space, of the phase difference between reference and measured interferograms (for DS, Fourier Transforms of the reference and measured spectra). The spectral correlation domain is required to represent periodic and stable absorption line pattern.

5.1.1. Spectral correlation space

The spectral shift is estimated in the spectrum space by the correlation coefficient computation between a measured spectrum and the oversampled calibrated reference spectrum shifted successively in different positions. The spectral shift corresponding to the maximum correlation coefficient is determined.

5.1.2. Fourier correlation space

A periodic absorption line structure is analysed via the components of its Fourier transform, since a translation of a function is represented by a phase shift of its Fourier transform, i.e., by a rotation of the complex pseudo-interferogram in the complex plane.

First, measured and reference spectra are Fourier transformed and over-sampled by stepwise phase modification with the same over-sampling factor. From IASI experience, a reasonable oversampling factor is 10.

The window size is determined by the number of selected spectral lines, typically between 10 and 30. From the base of the spectral transition positions, a new base is built in order to render the line pattern periodic (spectral lines are equidistant in sample number). The correlation maximization is performed in the Fourier space of the distorted spectral window (distorted in wave number, equidistant in sample number). Both spectra are interpolated on this periodic base.

This equidistance in sample number between absorption lines leads to energy peaks in the Fourier transform. These peaks represent harmonics of the periodic line pattern. Their position depends only on the period in sample number of this structure. The phase computed at these peaks represents the contribution of the periodic components out of phase in comparison with the chosen spectral structure. The phase of the measured spectrum and the phase of the reference spectrum are computed.
The difference between both phases at a chosen harmonic (with the greatest modulus) represents the spectral shift between the measured and reference spectrum. This spectral shift is used to calibrate the measured spectrum. The calibration is adjusted by re-computing the phase of the measured spectrum. The actual spectral shift is obtained when the difference between the measured phase and the reference phase tends to zero. This convergence is achieved through an iterative process. The process converges generally after a few iterations (≤ 10).

5.2. Analysis of spectral calibration windows

A first selection of spectral calibration windows for use in the MTG/IRS spectral calibration algorithm assessment is based on existing investigations, but modulated by IRS band separation characteristics and achieved IRS spectral resolution: In case of poor knowledge of the co-alignment between focal planes, there should be at least one spectral calibration window per array (for DS at least two). With the purpose of establishing an initial selection of spectral calibration windows, a visual analysis of typical IRS spectra is carried out with regard to the strength of spectral signatures and their stability with respect to atmospheric variability.

5.2.1. Selection

Relevant spectral calibration windows are identified as function of the specified IRS instrument concepts. This identification accounts in particular for the band separation parameters of the IRS concepts. Since band separations are identical for the two concepts, the selection of calibration windows is not concept dependent. In view of the early IRS development phase, the objective is to identify suitable calibration windows rather than to fine tune spectral limits for performance optimisation. It is not intended to investigate a large number of neighbouring calibration windows in terms of performance since former investigations of this subject can be exploited:

- The specification of the IASI spectral calibration algorithm [RD 6] provides performance estimates for four windows (identified by species generating the absorption line pattern and the central wave number of the window) in the spectral range covered by IRS: CO$_2$/736 cm$^{-1}$; N$_2$O/1263 cm$^{-1}$; CO/2090 cm$^{-1}$; CO$_2$/2361 cm$^{-1}$. Recently, performance estimations on refined windows adjacent to the above mentioned have been obtained [RD 11].

- The specification of the AGIRS spectral calibration algorithm [RD 7] provides performance estimates for three H$_2$O calibration windows in the spectral range 1840 to 2120 cm$^{-1}$.

- The specification of the MIPAS spectral calibration windows provides a selection independent of the IASI investigations. However, MIPAS spectral calibration windows appear hardly exploitable for IRS. This is due to the much higher spectral resolution of MIPAS and due to limb view induced substantially different spectral signatures in large parts of the spectrum.

First, we define candidate windows for the MTG/IRS spectral calibration in the Fourier space. A preliminary list is provided in Table 5. It eliminates those windows that are characterised by a line spacing that is obviously not resolved by both IRS concepts (except in bands IRS-8 and -9 where a strong degradation of spectral resolution is due to a non-mandatory on-board processing). This elimination concerns in particular N$_2$O absorption line pattern in bands IRS-4 and IRS-5 with a typical line spacing of 1.0 cm$^{-1}$ or smaller.
Windows F3, F8 and F12 have been investigated in [RD 6], F1, F2, F3, F6, F8, F9, F11, and F12 in [RD 11]. A first visual analysis of the high-resolution reference spectrum and the same spectrum convolved with a hypothetical spectral resolution of approximately 0.6 cm$^{-1}$ and a spectral sampling of 0.5 cm$^{-1}$ (simulations performed in [RD 2]) suggests elimination of F2, F7, F8, F9, F10 (these windows are strongly perturbed by other absorption line pattern), F4, F5, F13 (absorption line pattern are too weak). From the above preliminary list, windows are selected taking account of the following criteria:

- Both IRS instrument concepts have a common separation of bands and/or focal planes. In order to keep the possibility to relax requirements on focal plane co-alignment at instrument level it shall be investigated whether each band can be calibrated separately. The selection shall therefore contain at least one window (ideally two for DS) in the spectral domains of IRS-0/1/2, IRS-3/4, IRS-5/6, IRS-7/8/9. It can be noticed that the preliminary list does not contain any windows in bands IRS-3 to -6.

- Since band IRS-0 is not pursued anymore in the current pre-phase A studies, the selection shall preferably focus on IRS-1/2. This suggests selection of F3. F1 should be reconsidered if the spectral calibration performance in F3 is not satisfying.

- Since the implementation of IRS-5 and IRS-6 is alternative, spectral calibration windows shall be selected in both bands.

- Due to the relatively low user priority of IRS-8 and IRS-9, at least one calibration window should be selected in IRS-7. This suggests selection of F6. However, F11 and F12 are also investigated in anticipation of critical aspects regarding the expected performance in all three windows (weakness of the absorption line pattern in F6, limiting spectral resolution in F12, perturbed absorption line pattern in F11).

Based on the results of [RD 7] showing a higher spectral calibration performance by correlation in the spectrum space in windows characterised by high atmospheric variability, we do not look for defining windows containing regular absorption pattern at any cost. It is anticipated that spectral calibration in the Fourier space will not be possible in bands IRS-3/4, IRS-5 and IRS-6. The corresponding windows will only be applied for spectral shift determination in the spectrum space.
The resulting list of IRS spectral calibration windows investigated in this study is presented in Table 6. W02 to W05 (ex F3,6,11,12) will be investigated in the Fourier and in the spectrum space, W11 to W17 will only be considered for spectral calibration in the spectrum space. W11 to W17 have been selected by a simple visual analysis of typical spectral signatures. A typical window width of 50 cm\(^{-1}\) has been considered in view of keeping spectral shift variations small within a calibration window. Moreover, calibration windows must neither include a spectral band limit (spectral shift discontinuity due to imperfect focal plane co-alignment), nor a mission band limit (mission band dependent spectral onboard filtering).

<table>
<thead>
<tr>
<th>Window id</th>
<th>Wavenumber range (cm(^{-1}))</th>
<th>IRS Band</th>
<th>Species</th>
<th>Absorption line spacing (cm(^{-1}))</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>
<tbody>
<tr>
<td>W01F</td>
<td>673 - 695</td>
<td>IRS-0</td>
<td>CO(_2)</td>
<td>1.6</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>W02F</td>
<td>720 - 750  722 - 743</td>
<td>IRS-1</td>
<td>CO(_2)</td>
<td>1.5</td>
<td>0.5</td>
<td>0.50</td>
<td>0.67</td>
</tr>
<tr>
<td>W03F</td>
<td>2040 - 2070  2044 - 2066</td>
<td>IRS-7</td>
<td>CO(_2)</td>
<td>1.55</td>
<td>0.625</td>
<td>0.62</td>
<td>0.94</td>
</tr>
<tr>
<td>W04F</td>
<td>2300 - 2350  2303 - 2348</td>
<td>IRS-8</td>
<td>CO(_2)</td>
<td>1.8</td>
<td>1.25</td>
<td>1.24</td>
<td>1.67</td>
</tr>
<tr>
<td>W05F</td>
<td>2345 - 2375  2350 - 2370</td>
<td>IRS-8</td>
<td>CO(_2)</td>
<td>1.35</td>
<td>1.25</td>
<td>1.24</td>
<td>1.67</td>
</tr>
<tr>
<td>W11</td>
<td>1125 - 1195</td>
<td>IRS-4</td>
<td>-</td>
<td>-</td>
<td>0.85</td>
<td>0.85</td>
<td>0.92</td>
</tr>
<tr>
<td>W12</td>
<td>1145 - 1195</td>
<td>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</td>
<td>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</td>
<td>IRS-5</td>
<td>-</td>
<td>-</td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
<tr>
<td>W15</td>
<td>1650 - 1700</td>
<td>IRS-6</td>
<td>-</td>
<td>-</td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
<tr>
<td>W16</td>
<td>1800 - 1850</td>
<td>IRS-6</td>
<td>-</td>
<td>-</td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
<tr>
<td>W17</td>
<td>1880 - 1980</td>
<td>IRS-6</td>
<td>-</td>
<td>-</td>
<td>0.625</td>
<td>0.62</td>
<td>0.93</td>
</tr>
</tbody>
</table>

Table 6: Consolidated list of IRS candidate spectral calibration windows. Windows applied in the Fourier space are indicated by ‘F’ and are defined at slightly different spectral limits.

This consolidated list is a first specification of spectral calibration windows. A visual analysis for further consolidation is carried out by analysing the spectral dynamics of the reference spectrum. In Figure 5, the reference spectrum is shown in high spectral resolution as well as convolved with the nominal FTS level 1b spectral response in all chosen windows. DS spectra are not shown. Due to a similar or lower spectral resolution of the DS baseline in comparison to the FTS baseline, evidence of unsuitability of a calibration window for FTS let conclude the same for DS.

The suitability of each spectral calibration window is briefly commented:

**W01:** This window is out of the current IRS spectral coverage and will only be investigated if unsatisfactory spectral calibration performance for the baseline design is shown.

**W02:** The regular CO\(_2\) absorption line pattern is resolved with relatively high radiometric dynamics by three spectral samples per absorption line spacing. This window appears suitable in the two correlation spaces.

**W03:** The regular CO\(_2\) absorption line pattern is resolved by three spectral samples per absorption line spacing. Radiometric dynamics is reduced due to the sharpness of the absorption lines. Perturbation by H\(_2\)O absorption lines might render this window more suitable in the radiance correlation space.

**W04:** The CO\(_2\) absorption line pattern is hardly resolved.
**W05:** The CO₂ absorption line pattern is not resolved. It is recalled that W05 is used in the Fourier correlation space for the spectral calibration of IASI.

**W11/12:** CO₂ absorption pattern at small line spacing are not resolved. Strong H₂O absorption lines at larger spacing are relatively well resolved and may be exploitable in the radiance correlation space.

**W13, W16:** Dominated by H₂O absorption with an additional contribution from CH₄ at low wave numbers in W13, these windows have been chosen alternatively depending on the implementation of IRS-5 or IRS-6. Symmetric with respect to the H₂O absorption maximum at 1600 cm⁻¹, these windows show similar characteristics, i.e., irregular reference spectra with relatively high radiometric dynamics. W16 appears slightly smoother than W13, suggesting a preference for the implementation of IRS-5 from the point of view of spectral calibration.

**W14, W15:** Statements made for W13/W16 apply similarly, except that due to the proximity to the H₂O absorption maximum the radiometric dynamics is reduced.

**W17:** A similar window has been investigated in [RD 7] for an instrument at much lower spectral resolution. H₂O absorption lines generate irregular reference spectra with high radiometric dynamics. Weak CO₂ absorption lines at small line spacing are hardly resolved.
Figure 5: Overlay of the nominal IRS/FTS reference spectrum (black) with the corresponding high-resolution spectrum (grey) in spectral calibration windows W02-W05 and W11-W17.

It is concluded that all spectral calibration windows defined in Table 6, except W01 (for missing implementation of IRS-0), W04 and W05 (for insufficient spectral resolution) appear exploitable for spectral calibration of the current IRS baseline concepts.
5.2.2. Analysis of atmospheric stability

The impact of atmospheric variability is analysed qualitatively by estimating the variability of the exploited signature in the IRS level 1b spectra per calibration window with the atmospheric state. The selected geophysical conditions provide information on the impact of the variability of temperature and humidity profiles and of homogeneous clouds. Displayed on Figure 6, IRS/FTS nominal level 1b spectra (in atmospheric conditions identified in Table 3) are analysed following the investigation purpose summarised in Table 4. The objective is to identify those spectral calibration windows exhibiting obviously unstable line pattern due to atmospheric variability and to conclude on the necessity for cloud identification prior to the spectral calibration process. The quantitative impact of atmospheric variability will be obtained in future study phases, by explicit spectral calibration of IRS level 1a spectra in various atmospheric conditions with a level 1b reference spectrum corresponding to reference atmospheric conditions.

Figure 6 here below is spread over several pages.
IRS/FTS nominal 1b spectra: atmospheric/cloud variability

Window W05

Brightness temperature [K]

Wave number [cm⁻¹]

Window W11/W12

Brightness temperature [K]

Wave number [cm⁻¹]
IRS/FTS nominal 1b spectra: atmospheric/cloud variability

Window W13

Window W14

Noveltis 2006
IRS/FTS nominal 1b spectra: atmospheric/cloud variability

Window W15

1650 1655 1660 1665 1670 1675 1680 1685 1690 1695 1700

wave number [cm⁻¹]

brightness temperature [K]

Window W16

1800 1805 1810 1815 1820 1825 1830 1835 1840 1845 1850

wave number [cm⁻¹]

brightness temperature [K]
Figure 6: Overlay of nominal IRS/FTS spectra for geophysical conditions identified in Table 3 in spectral calibration windows W02-W05 and W11-W17.

In detail, we state window by window:

**W02:** The spectrum shape appears stable in all atmospheric conditions, even high opaque cloud conserve the spectral signature. If this signature proves radiometrically too weak, a simple brightness temperature threshold for filtering cold scenes out of the spectral calibration process might be considered. However, a definite conclusion requires the investigation of the impact of CO2 variations, which are not considered in the spectra simulations.

**W03:** The pure CO2 absorption region shows stable spectral signatures, strongly weakened in case of high opaque clouds and cold scenes. Furthermore, humidity variations have a visible perturbation potential (c.f. spectral shape of clear-sky spectra near H2O absorption lines).

**W04, W05:** Spectra are stable with respect to atmospheric conditions, the impact of clouds is tiny. Obviously, these windows are only useful if spectral resolution in IRS-8 is increased.

**W11/12:** Strong H2O absorption lines at large spacing are conserved, except at low brightness temperatures. In between these strong lines that may govern the correlation performance, weaker H2O absorption lines lead to considerable variations of the spectral shape in the hottest spectrum parts (c.f. hot and dry vs. hot and humid).

**W13, W16:** Spectral shapes are relatively well conserved, except for high opaque clouds that hide spectral features originating from the mid-troposphere.
**W14, W15:** The radiometrically weak spectral shapes are conserved except for the cold and dry cases (clear-sky and cloudy). Clouds have no strong impact due to the weighting function maximum near tropopause level in these windows. The decisive parameter for the spectral signature is then the lower stratospheric temperature gradient, which is much weaker in the case of the cold and dry atmosphere, associated to a mid-latitude depression system in winter.

**W17:** In a larger radiometric range, the same statements as for W13/W16 apply.

From the above considerations, some general hints at the necessity for scene filtering can be formulated. Scenes covered with opaque clouds are not exploitable for spectral calibration in those windows that are characterised by weighting functions pointing near or below cloud top height. In practice, this concerns high opaque clouds or mid- and low level clouds in dry and cold conditions in windows W03, W11/12, W13/16 and W17. The statement that hot scenes are more suitable for spectral calibration than cold scenes has to be interpreted with caution. First, inherent to the MTG/IRS scan cycle, hot scenes are regularly not observable over a few minutes. Second, cold scenes appear radiometrically less heterogeneous and thus introduce less pseudo-noise. Spectral calibration pseudo-noise due to different spectral response of the scene components is investigated in a parallel study and may be the dominating factor for a scene filtering prior to the spectral calibration process.

In conclusion for the upcoming quantitative IRS spectral calibration assessment, we will estimate shift determination performance for the defined spectral calibration windows (with little hope for success in W04 and W05) in all of the above analysed atmospheric conditions upon the selected global reference spectrum.
6. Conclusion and Outlook

The present part 1 of the MTG/IRS spectral calibration algorithm assessment report describes the algorithm baseline and the related software system. The algorithm baseline is linked to explicit instrument baseline assumptions. Geophysical application conditions are defined and algorithm design options discussed. In particular, a list of potential spectral calibration windows is established.


6.1. Part 2: Sensitivity analysis

The first task is to establish the relationship between ISRF shift and shape errors and radiometric spectrum errors. This is required to translate algorithm/instrument performance (knowledge errors and instability) in radiometric errors (to be specified in the spectral calibration noise budget).

The impact of radiometric noise on the spectral calibration noise is evaluated by estimating shift determination errors for a known atmospheric state, with and without radiometric noise. The impact of atmospheric variability on the spectral calibration noise is evaluated by estimating shift determination errors for various but known differences between atmospheric state and atmospheric reference state. Both components are translated into radiance errors and represent the spectral calibration algorithm error from a single spectral shift determination in a given spectral calibration window. Performance comparison between windows allows for a consolidation of the spectral calibration window selection. Additional windows or existing windows with improved spectral resolution are investigated in domains where separate array-by-array calibration is not ensured.

6.2. Part 3: Spectral calibration algorithm performance evaluation

Based on the results of the sensitivity analysis, a spectral calibration algorithm design is defined for the two instrument concepts, in particular in terms of the choice of spectral calibration windows.

The full spectral calibration algorithm, including instrument state determination and explicit spectral calibration of level 1a spectra (spectral resampling), will be applied to both instrument concepts.

The resulting spectral calibration algorithm noise governs the allocations for the instrument contributions to the spectral calibration noise budget. Upon the consolidated spectral calibration noise budget, requirements for ISRF knowledge and stability as well as for array co-alignment will be derived.