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A simulation-based error budget of the TES method for the design of the spectral configuration of the micro-bolometer based MISTIGRI thermal infrared sensor

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Abstract—In preparation of the micro-bolometer based Micro Satellite for Thermal Infrared GRound surface Imaging (MISTIGRI) mission, we study the error budget of the Temperature-Emissivity Separation (TES) method using several spectral configurations that differ in channel numbers, locations, and widths. The error budget quantifies the contribution of (1) the TES underlying assumption about emissivity spectral contrast, (2) the errors on atmospheric corrections, and (3) the instrumental noise. When dealing with atmospheric corrections, we consider errors on atmospheric temperature, water vapor content, and concentrations of CO₂ and O₃. To that end, we design an end-to-end simulator of MISTIGRI measurements in order to simulate the radiative and biophysical quantities involved in the data processing. We conduct numerous simulations over a wide range of realistic setups that include cavity effect, i.e., radiance trapping within vegetation canopy. In the case of micro-bolometer based sensing, the current study highlights that atmospheric and instrumental noises have similar impacts on the TES retrievals, with resulting errors twice as large as those due to the TES intrinsic assumption about spectral contrast, where the latter contributes to the TES error budget within the [0.005 - 0.009] interval for emissivity, and within the [0.3 K - 0.4 K] interval for LST. Also, we show that retrieval performance of surface temperature is very similar across all considered MISTIGRI spectral configurations, with RMSE variation within 0.2 K.

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Eventually, our study permits to select a 4-channels spectral configuration as the most suited for the MISTIGRI instrument, notably because it enables a moderately better capture of the emissivity contrast than a 3-channels one.

Index Terms—Thermal infrared remote sensing, Satellite mission design, Temperature / emissivity separation, Vegetation canopy - scaled cavity effects, Micro-bolometers detectors, Atmospheric corrections, TES error budget

I. INTRODUCTION

THERMAL InfraRed (TIR) remote sensing is a powerful tool for Earth system monitoring, since it provides proxies of Earth surface emissivity spectrum / radiometric temperature that are widely used in several thematic studies. Involved processes are related to radiation budget [1]–[5], land surface energy balance and evapotranspiration [6]–[15], soil moisture and vegetation water status [16]–[18], crop micro-meteorological conditions [19], urban heat island and urban atmospheric flows [20]–[22], volcanic ashes with sulfate and sulfur dioxide deposits [23], [24], lava flow monitoring and modeling [25], [26], mineral mapping [27], [28], cryospheric inventory and worldwide glacier balance [29], [30], as well as numerical weather prediction and ocean forecasting modeling [31], [32]. Various satellite TIR missions have been dedicated to the estimation of land surface temperature (LST) during the last three decades, either with high spatial resolution sensors such as Landsat [33], [34] and ASTER [7], [35], [36], or with high temporal resolution sensors such as AVHRR [37], [38], MSG [39], [40], MODIS [41], [42], or SLSTR onboard Sentinel 3 [31], [43]. Although disaggregation approaches have been explored to overcome the lack of TIR data with both high spatial and temporal resolutions [44], [45], several studies have campaigned for satellite missions providing such TIR data, including IRSUTE [46], SPECTRA [47], ECOSTRESS [48], or LSTM [49].

The Micro Satellite for Thermal Infrared GRound surface Imaging (MISTIGRI) preparatory mission was initiated and conducted by CNES (French space agency) in collaboration with Spain, between 2010 and 2015 [50]. Follow-on from IRSUTE and SPECTRA, it was the precursor of the Thermal InfraRed Imaging Satellite for High-resolution Natural resource Assessment (TRISHNA) mission, to be launched in

2025 [51]. The primary objective of the MISTIGRI mission was the monitoring of land surface energy and water budgets. The spatial resolution was set to 50 m, and the revisiting rate was set to one day, with an overpass within the [12:00-13:00] solar time interval. The one-day revisit induced a constant off-nadir viewing with a view zenith angle lower than 40° . Finally, the MISTIGRI instrument was designed with micro-bolometer sensors, which led to set large spectral channels for reducing instrumental noise, whose expected values were between 0.2 and 0.5 K at 290 K. The baseline instrument spectral configuration included 4 channels labelled TIR3, TIR4, TIR1, and TIR2, respectively centered at $8.6 \mu\text{m}$ ($0.32 \mu\text{m}$ width), $9.1 \mu\text{m}$ ($0.32 \mu\text{m}$ width), $10.3 \mu\text{m}$ ($1.02 \mu\text{m}$ width), and $11.5 \mu\text{m}$ ($1.02 \mu\text{m}$ width).

Retrieving surface emissivity and temperature from TIR remote sensor measurements is an ill-posed problem, with N_b equations from channel measurements and $N_b + 1$ unknowns that include N_b channel emissivities and one radiometric temperature. Among the existing solutions that consist in adding an $N_b + 1$ equation to the system [52]–[54], we chose the Temperature Emissivity Separation method (TES, [35], [55]). This choice is motivated by the TES capability to retrieve surface emissivity and temperature from a unique multispectral snapshot at the satellite overpass time, thus making possible the monitoring of temporal changes of surface temperature on the basis of a one-day revisiting rate. The TES method relies on the assumption that any natural surface emissivity spectrum includes a value close to unity within the TIR spectral range, which induces the possibility to derive the emissivity minimum value from emissivity contrast by using an empirical relationship [56], [57]. The TES method has been extensively used and studied in the past three decades, notably in order to enhance its stability and performance, with regards to observation conditions driven by sensor capabilities, atmospheric conditions and land surface spectral properties [1], [3], [36], [55]–[75].

When designing any satellite mission, an important step is the definition of the mission characteristics in accordance to the approaches that are used for data processing and thematic uses. As overviewed by [50] for the MISTIGRI mission, some instances are the revisiting rate / overpass time in the light of evapotranspiration diurnal course, or the viewing direction in the light of radiative transfer processes. In the context of monitoring land surface temperature, the definition of the spectral configuration of the MISTIGRI sensor has to be investigated with regards to sensor technologies (i.e., micro-bolometers detectors) and used methods (e.g., TES retrieval of emissivity / temperature with prior atmospheric corrections). More particularly, the appropriate locations and widths for the MISTIGRI spectral channels should balance between three constraints: capturing spectral contrasts of the observed emissivity spectra, minimizing atmospheric perturbations, and minimizing instrumental noise.

The current study aims to conduct an error budget for the TES method when used over MISTIGRI imagery of vegetated land surfaces (mission primary objective), in order to find an appropriate sensor spectral configuration among predefined configurations, on the basis of balancing between the three

forementioned constraints. To that end, an end-to-end simulator is implemented, which is dedicated to: (1) the simulation of TIR multispectral measurements, and (2) use of the TES method for LST retrieval after prerequisite atmospheric corrections. The simulator relies on simulated land surface emissivity spectra that account for radiance trapping within vegetation canopy, since [57] showed that the subsequent cavity effect induces an upper shift of emissivity for both the TES empirical relationship and the subsequent retrievals. We first detail the process flow of both the TES method and the end-to-end simulator in § II and § III, respectively. Next, we present the simulator implementation in § IV, and the simulation strategy when addressing the MISTIGRI mission in § V. We finally present and discuss our results in § VI, and we conclude with current limitations and further perspectives in § VII.

II. TES PRESENTATION

A. TES principle and overview

Rather than associating the maximum emissivity with a nominal value [76], the TES approach assumes that the emissivity spectrum of a natural surface in the TIR spectral domain includes a maximum value bounded within the [0.98-1] interval. Subsequently, any change in the emissivity spectrum minimum value is related to a change in the spectral contrast across the emissivity spectrum [57]. Thus, by empirically relating the minimum emissivity to the spectral dynamics observed across the N_b channels [68], TES overcomes the indetermination by removing the $(N_b + 1)^{th}$ unknown of the ill-posed problem for LST retrieval (see § I). To that end, channel emissivities and radiometric temperature are retrieved via an iterative process that includes four steps described below.

B. TES processing flow

The first step estimates radiometric surface temperature T_R^{sur} as the maximum temperature over the N_b channels j :

$$T_R^{sur} = \max(T_j) \quad (1)$$

where radiometric temperature T_j for channel j is deduced via the inverse Planck's law L_{BB}^{-1} applied to the corresponding surface-emitted radiance L_j^{em} , itself derived from measured surface outgoing radiance $L_j^{sur\uparrow}$ after atmospheric corrections, and from atmospheric downwelling irradiance $E_j^{atm\downarrow}$:

$$L_j^{em} = L_j^{sur\uparrow} - (1 - \varepsilon_j) \frac{E_j^{atm\downarrow}}{\pi} \quad (2)$$

$$T_j = L_{BB}^{-1} \left(\frac{L_j^{em}}{\varepsilon_j}, \lambda_j \right) \quad (3)$$

$$L_{BB}^{-1}(L_j, \lambda_j) = c_2 \left[\lambda_j \ln \left(\frac{c_1}{\pi \lambda_j^5 L_j} + 1 \right) \right]^{-1} \quad (4)$$

with c_1 and c_2 the first and second radiation constants, equal to $3.74151 \cdot 10^{-16} \text{ W.m}^{-2}$ and 0.0143879 m.K , respectively. ε_j and λ_j are channel emissivity and central wavelength, respectively.

The second step is the calculation of relative emissivities as the ratios of channel emissivities ε_j to the mean emissivity over the N_b channels:

$$\beta_j = \frac{\varepsilon_j}{\langle \varepsilon_j \rangle} = \frac{L_j^{em} / L_{BB}(T_R^{sur}, \lambda_j)}{\langle L_j^{em} / L_{BB}(T_R^{sur}, \lambda_j) \rangle} \quad (5)$$

where L_{BB} is the Planck's law:

$$L_{BB}(T_R^{sur}, \lambda_j) = c_1 \left[\lambda_j^5 \pi \left[\exp \left(\frac{c_2}{\lambda_j T_R^{sur}} \right) - 1 \right] \right]^{-1} \quad (6)$$

The third step consists of calculating the minimum value of the emissivity spectrum as an empirical relationship of the Maximum Minimum Difference (MMD \equiv spectral contrast) of the relative emissivities β_j :

$$MMD = \beta_{max} - \beta_{min} = \frac{\max(\varepsilon_j) - \min(\varepsilon_j)}{\langle \varepsilon_j \rangle} \quad (7)$$

$$\varepsilon_{min} = A + B \times MMD^C \quad (8)$$

where A , B , and C are coefficients that depend on the spectral configuration of the instrument, and which are estimated from non-linear regression over a database of emissivity spectra (see details in [57]).

In the fourth and last step, the channel emissivities over the N_b channels are derived from the minimum channel emissivity value as:

$$\varepsilon_j = \frac{\varepsilon_{min}}{\beta_{min}} \beta_j \quad (9)$$

The TES iterative process is initialized by setting to unity the emissivity values ε_j in Equation 2 for each channel j (radiometric temperature is set to brightness temperature). From this initialization, the iterative procedure follows Equation 1 to 9. For our study, we set a maximum of ten iterations, but the process systematically converges in fewer than six iterations. Once convergence is reached, TES retrievals of both channel emissivity TES- ε_j over the N_b channels and radiometric temperature surface TES- T_R^{sur} are obtained from the last iteration on Equation 9 and 1, respectively.

III. SiMi DESCRIPTION

A. SiMi overview

The specification of the optimal MISTIGRI spectral configuration is performed using simulated data. The simulator for MISTIGRI measurements (SiMi) is designed, on a single pixel basis, 1/ to simulate radiative transfer processes involved in TIR data measurements along with related quantities, and 2/ to analyse the performance of the retrieval procedure for the variables of interest, including atmospheric corrections and recovering of land surface emissivity / temperature with the TES method. The simulations cover the TIR spectral range ([7.5 - 13.5] μm) with a 10^{-3} μm resolution. SiMi includes five connected modules illustrated in Figure 1 and described below (quantities mentioned in Figure 1 are defined in Table I).

- 1) The synthetic scene module (Module 1) describes the scene at the land surface level, by considering an equivalent homogeneous body with the same radiative characteristics, namely emissivity spectrum and radiometric

temperature, than the actual composite of plant canopy and underlying soil [77].

- 2) The atmosphere module (Module 2) is dedicated to the simulation of atmospheric effects on the measured signal. On the basis of predefined atmospheric conditions, it simulates the atmospheric radiative transfer and the resulting signal at the sensor input (top of atmosphere - TOA), and it quantifies the atmospheric radiative quantities to be used for atmospheric corrections.
- 3) The instrument module (Module 3a) computes the quantities measured by the instrument (channel radiances / brightness temperatures) in accordance to spectral response function and instrumental noise for each channel.
- 4) The calibration module (Module 3b) deals with the calibration of the TES empirical relationship $\varepsilon_{min} = f(MMD)$ (Equation 8). This relationship depends upon the channel locations and widths, and has to be calibrated for each spectral configuration [57].
- 5) The inversion module (Module 4) performs the inversion of the simulated measurements. It first applies atmospheric corrections, and then makes use of the TES method to separate target emissivity and temperature.

B. The land surface module (Module 1)

The land surface module generates emissivity spectra for a given scene consisting of vegetation canopy and underlying soil, using the Scattering by Arbitrarily Inclined Leaves-Thermique (SAIL-Thermique) radiative transfer model [78], [79]. It describes land surface as a turbid medium, with a stack of homogeneous vegetation layers above a soil substrate. Vegetation canopy is characterized by canopy structure (i.e., leaf area index LAI and leaf inclination distribution function ALA) and leaf optical properties (reflectance and transmittance spectra). Underlying soil surface is characterized by optical properties (soil reflectance spectra). Radiative transfer is simulated by accounting for successive scattering within the canopy, and between the canopy and the soil. SAIL-Thermique considers the Kirchhoff's law at the thermodynamical equilibrium, where directional surface emissivity ε_λ is calculated from the directional-hemispherical reflectance ρ_λ : $\varepsilon_\lambda = 1 - \rho_\lambda$. SAIL-Thermique is used to generate two datasets.

- The first dataset, called DB1, is used to compute the spectral surface leaving radiance $L_\lambda^{sur\uparrow}$, by combining any emissivity spectrum ε_λ with prescribed values of surface radiometric temperature T_R^{sur} . Each pair $\{\varepsilon_\lambda$ spectrum, T_R^{sur} value $\}$ corresponds to a land surface scene. This pair is provided to Module 2, and further serves as a reference for validation exercises. The first exercise consists in validating the TES semi-empirical relationship, once calibrated. The second exercise consists in validating TES retrievals of channel emissivity and radiometric temperature (Figure 1).
- The second dataset, called DB2, is used to calibrate the TES semi-empirical relationship (Module 3b).

C. The atmosphere module (Module 2)

For any pair $\{\varepsilon_\lambda$ spectrum, T_R^{sur} value $\}$, the atmosphere module computes several spectral quantities: atmo-

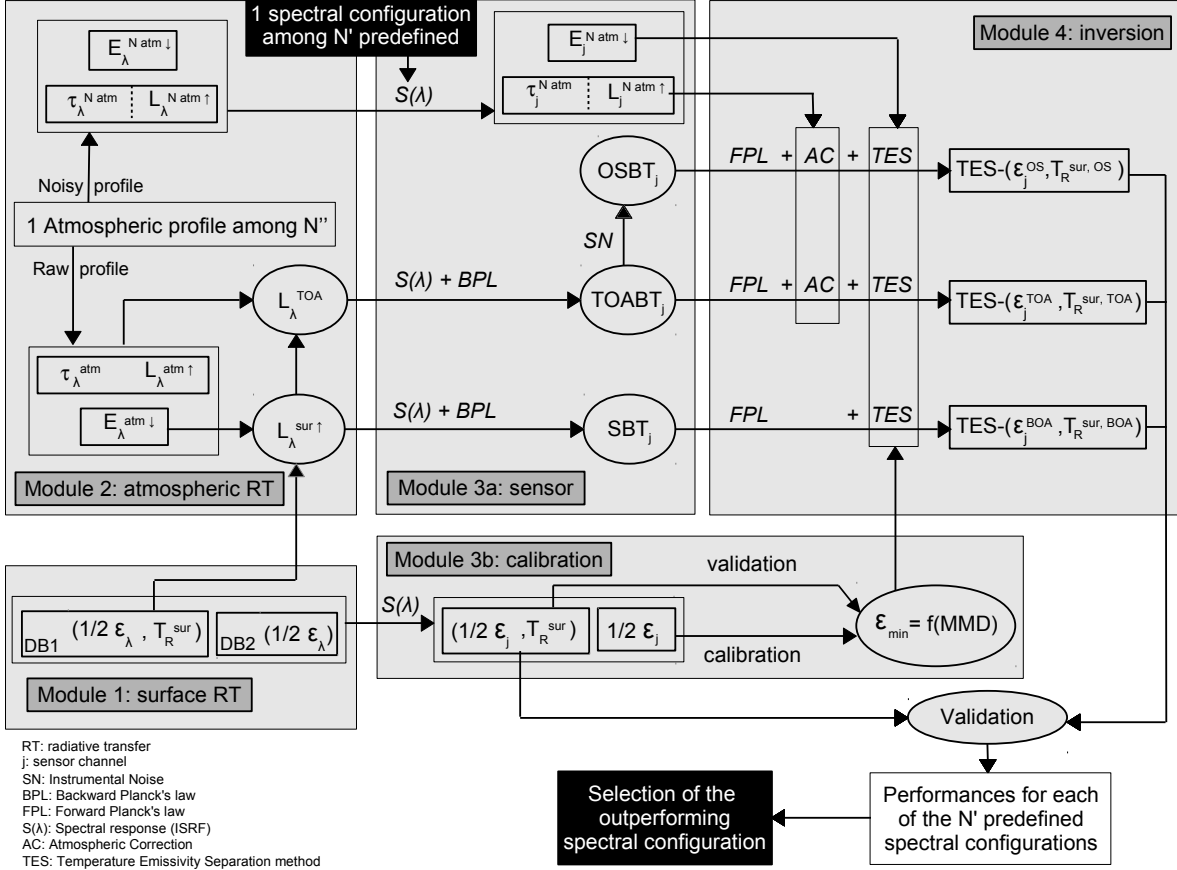


Fig. 1. Overview of the approach used to identify an optimal spectral configuration in the TIR range for the MISTIGRI instrument. Quantities mentioned in the Figure are defined in Table I.

spheric downwelling irradiance $E_{\lambda}^{atm\downarrow}$, surface-leaving radiance $L_{\lambda}^{sur\uparrow}$ (Equation 10 and 11), atmospheric transmittance τ_{λ}^{atm} , atmospheric upwelling radiance at the sensor level $L_{\lambda}^{atm\uparrow}$, and TOA radiance at the sensor entrance L_{λ}^{TOA} (Equation 12).

$$L_{\lambda}^{sur\uparrow} = L_{\lambda}^{em} + (1 - \varepsilon_{\lambda}) \frac{E_{\lambda}^{atm\downarrow}}{\pi} \quad (10)$$

$$L_{\lambda}^{em} = \varepsilon_{\lambda} L_{BB}(T_R^{sur}, \lambda) \quad (11)$$

$$L_{\lambda}^{TOA} = \tau_{\lambda}^{atm} L_{\lambda}^{sur\uparrow} + L_{\lambda}^{atm\uparrow} \quad (12)$$

The calculations of $E_{\lambda}^{atm\downarrow}$, τ_{λ}^{atm} , and $L_{\lambda}^{atm\uparrow}$ involve the simulation of atmospheric radiative transfer based on atmospheric profiles of pressure, temperature, humidity, as well as of concentrations in carbon dioxide [CO₂] and ozone [O₃] [80], [81]. The radiative transfer is simulated using the MATISSE-v2 code [82], [83]. MATISSE is chosen for its consistent atmospheric profile database, given that it is very similar to its counterparts such as MODTRAN for radiative transfer simulation. After these calculations, each atmospheric profile is characterized by a triplet $\{E_{\lambda}^{atm\downarrow}, \tau_{\lambda}^{atm}, L_{\lambda}^{atm\uparrow}\}$, to be combined with each pair $\{\varepsilon_{\lambda}$ spectrum, T_R^{sur} value $\}$.

The atmosphere module also computes the atmospheric radiative quantities, namely $E_{\lambda}^{N\,atm\downarrow}$, $\tau_{\lambda}^{N\,atm}$, and $L_{\lambda}^{N\,atm\uparrow}$, to be used for atmospheric corrections in Module 4 after convolution with the instrumental spectral response function

(ISRf) in Module 3a (Figure 1). To that end, and in order to account for errors on atmospheric corrections due to partial knowledge on atmospheric status, atmospheric profiles are noised on temperature $T_{atm}(z)$ and humidity $hr(z)$, as well as on concentrations of carbon dioxide [CO₂](z) and ozone [O₃](z), where z is the altitude above sea level. Each variable profile $Var(z)$ is noised using a Gaussian white noise:

$$Var(z) = Var(z) + \mathcal{N}(0; \alpha \cdot Var(z) + \beta) \quad (13)$$

$$Var(z) \in \{T_{atm}(z), hr(z), [CO_2](z), [O_3](z)\} \quad (14)$$

where α and β are set up as following:

- in accordance with [84], we set a standard deviation of 0.8 K for $T_{atm}(z)$ ($\alpha = 0$, $\beta = 0.8$), which corresponds to a maximum error of 2 K;
- in accordance with [85] and [84], we set a standard deviation of $0.1 \times hr(z)$ for $hr(z)$ ($\alpha = 0.1$, $\beta = 0$), which corresponds to a maximum relative error of 25%;
- in accordance with [81], we set a standard deviation of $0.15 \times [CO_2](z)$ for $[CO_2](z)$ ($\alpha = 0.15$, $\beta = 0$), which corresponds to a maximum relative error of 40%;
- In accordance with [85], we set a standard deviation of $0.2 \times [O_3](z)$ on $[O_3](z)$ ($\alpha = 0.2$, $\beta = 0$), which corresponds to a maximum relative error of 50%.

TABLE I
SIGNIFICATION OF THE RADIATIVE QUANTITIES THAT ARE MENTIONED IN FIGURE 1.

Parameters	Description
ε_λ	Spectral land surface emissivity
ε_j	Channel land surface emissivity
ε_{min}	Minimum value of ε_j across N_b channels
MMD	Maximum-Minimum Difference (Equation 7)
T_R^{sur}	Land surface radiometric temperature
$E_\lambda^{atm\downarrow}$	Spectral atmospheric downwelling irradiance
$E_\lambda^{N,atm\downarrow}$	Noised spectral atmospheric downwelling irradiance (1)
$E_j^{atm\downarrow}$	Channel atmospheric downwelling irradiance
$E_j^{N,atm\downarrow}$	Noised channel atmospheric downwelling irradiance (1)
τ_λ^{atm}	Spectral atmospheric transmittance
$\tau_\lambda^{N,atm}$	Noised spectral atmospheric transmittance (1)
τ_j^{atm}	Channel atmospheric transmittance
$\tau_j^{N,atm}$	Noised channel atmospheric transmittance (1)
$L_\lambda^{atm\uparrow}$	Spectral atmospheric upwelling radiance
$L_\lambda^{N,atm\uparrow}$	Noised spectral atmospheric upwelling radiance (1)
$L_j^{atm\uparrow}$	Channel atmospheric upwelling radiance
$L_j^{N,atm\uparrow}$	Noised channel atmospheric upwelling radiance (1)
$L_\lambda^{sur\uparrow}$	Spectral surface leaving radiance
$L_j^{sur\uparrow}$	Channel surface leaving radiance
$L_\lambda^{TOA\uparrow}$	Spectral top of atmosphere radiance
$L_j^{TOA\uparrow}$	Channel top of atmosphere radiance
SBT_j	Surface brightness temperature
$TOABT_j$	Top-of-atmosphere brightness temperature
$OSBT_j$	Out-of-sensor brightness temperature
$TES - (\varepsilon_j^{BOA}, T_R^{sur,BOA})$	TES retrievals of emissivity / temperature from SBT_j
$TES - (\varepsilon_j^{TOA}, T_R^{sur,TOA})$	TES retrievals of emissivity / temperature from $TOABT_j$
$TES - (\varepsilon_j^{OS}, T_R^{sur,OS})$	TES retrievals of emissivity / temperature from $OSBT_j$
(1) from noised atmospheric profile to account for uncertainties on atmospheric status	

D. The instrument module (Module 3a)

The instrument module accounts for the sensitivity of each spectral channel, and for the associated Noise Equivalent Difference Temperature (NEDT) that depends upon channel width.

To account for sensitivity of channel j , any spectrum (e.g., emissivity, radiance, transmittance) Q_λ is convolved with the dedicated ISRF that spreads over the $[\lambda_{min,j} - \lambda_{max,j}]$ interval, thus providing the waveband equivalent value Q_j :

$$Q_j = \frac{\int_{\lambda_{min,j}}^{\lambda_{max,j}} Q_\lambda S_j(\lambda) d\lambda}{\int_{\lambda_{min,j}}^{\lambda_{max,j}} S_j(\lambda) d\lambda} \quad (15)$$

Accounting for instrumental noise on measured temperature consists of adding, for any channel j , a Gaussian white noise with a standard deviation equal to the corresponding NEDT $_j$:

$$OSBT_j = BT_j + \mathcal{N}(0, NEDT_j) \quad (16)$$

where BT_j is the brightness temperature at the sensor level, and $OSBT_j$ is the output sensor brightness temperature with instrumental noise. $NEDT_j$ is provided by the sensor manufacturer as function of both measured brightness temperature and channel width (full width at half maximum - FWHM).

In the context of satellite mission design, it is valuable to characterize the error budget at different levels. To that end, Module 3a provides estimates of measured brightness temperatures over the N_b channels j for three different cases of BT_j (Figure 1):

- 1) SBT_j corresponds to brightness temperatures at the surface level, it is derived from radiance spectrum $L_\lambda^{sur\uparrow}$;
- 2) $TOABT_j$ corresponds to brightness temperatures at the satellite level above the atmosphere, it is derived from radiance spectrum L_λ^{TOA} ;
- 3) $OSBT_j$ is derived from $TOABT_j$ by applying the Gaussian white noise formulation (Equation 16).

Note that both SBT_j and $TOABT_j$ are derived from corresponding radiances after convolution with the dedicated ISRF and application of the inverse Planck's Law L_{BB}^{-1} (Equation 4).

E. The calibration module (Module 3b)

The calibration module aims to calibrate the TES empirical relationship $\varepsilon_{min} = f(MMD)$ that derives minimum emissivity from the spectral contrast captured by multispectral TIR measurements over N_b channels. To that end, emissivity minimum and maximum values, as well as MMD (Equation 7), are derived for each emissivity spectrum from DB2 database, after convolution with ISRF $S(\lambda)$ (Equation 15).

The calibration is performed by computing the empirical coefficients A , B and C of the $\varepsilon_{min} = f(MMD)$ relationship

(Equation 8) using the "Optim" R function [86]. The latter minimizes the calibration residual error expressed as the root mean square error $RMSE_{cal}^{\varepsilon_{min}}$ [87]:

$$RMSE_{cal}^{\varepsilon_{min}} = \sqrt{\frac{\sum (\varepsilon_{min}^{obs-cal} - \varepsilon_{min}^{est})^2}{n2}} \quad (17)$$

where $\varepsilon_{min}^{obs-cal}$ and ε_{min}^{est} are respectively the ε_{min} reference values from the DB2 subset of emissivity spectra and the ε_{min} estimates from Equation 8 with the calibrated coefficients, and $n2$ is the number of emissivity spectra within the DB2 subset:

The validation of the calibrated empirical relationship is conducted using the DB1 subset of emissivity spectra, by computing $RMSE_{val}^{\varepsilon_{min}}$ as:

$$RMSE_{val}^{\varepsilon_{min}} = \sqrt{\frac{\sum (\varepsilon_{min}^{obs-val} - \varepsilon_{min}^{est})^2}{n1}} \quad (18)$$

where $\varepsilon_{min}^{obs-val}$ are the ε_{min} reference values from DB1 subset of emissivity spectra, and $n1$ is the number of emissivity spectra within the DB1 subset.

F. The inversion module (Module 4)

The inversion module aims to retrieve land surface emissivity and radiometric temperature from the MISTIGRI simulated measurements. It first corrects sensor data from atmospheric perturbations, and second applies the TES method to retrieve emissivity ε_j over the N_b channels j along with the associated radiometric surface temperature T_R^{sur} (see Figure 1).

Upon entry in the inversion module, brightness temperatures from Module 3a are converted into channel radiances by using the Planck's law L_{BB} (Equation 6). Atmospheric corrections are then performed using the noised atmospheric radiative quantities that are computed from noised atmospheric profiles in Module 2 and next ISRF-convolved in Module 3a, namely the noised channel atmospheric transmittance $\tau_j^{N atm}$ and the noised upwelling radiance at the sensor level $L_j^{N atm \uparrow}$:

$$L_j^{sur \uparrow} = \frac{L_j^{OS} - L_j^{N atm \uparrow}}{\tau_j^{N atm}} \quad (19)$$

where L_j^{OS} and $L_j^{sur \uparrow}$ are the radiances over channel j at the sensor level (before atmospheric corrections) and at the surface level (after atmospheric corrections), respectively.

Afterwards, the TES method is applied on the channel radiances at the surface level $L_j^{sur \uparrow}$, by using the ISRF-convolved values of noised atmospheric downwelling irradiance $E_j^{N atm \downarrow}$ (see Figure 1 and Equation 2). As explained in the previous section, it is valuable to characterize the error budget at different levels, in the context of satellite mission design. To that end, SiMi permits to apply the inversion procedure at three levels (Figure 1):

- 1) applying the TES method on sensor measurements of surface brightness temperature at the surface level, so-called SBT_j, to quantify errors resulting from TES assumptions only;

- 2) applying atmospheric corrections and the TES method on TOA brightness temperature at the sensor level, so-called TOABT_j, to quantify errors resulting from both atmospheric perturbations and TES assumptions;
- 3) applying atmospheric corrections and the TES method on output sensor (OS) brightness temperature, so-called OSBT_j, to quantify errors resulting from instrumental noise, atmospheric perturbations and TES assumptions.

Thus, TES retrieves the pairs $\{\text{TES-}\varepsilon_j^{BOA}, \text{TES-}T_R^{sur,BOA}\}$ from SBT_j (BOA stands for bottom of atmosphere), $\{\text{TES-}\varepsilon_j^{TOA}, \text{TES-}T_R^{sur,TOA}\}$ from TOABT_j (TOA stands for top of atmosphere), and $\{\text{TES-}\varepsilon_j^{OS}, \text{TES-}T_R^{sur,OS}\}$ from OSBT_j (OS stands for out of sensor), where each pair corresponds to each of the three aforementioned cases, respectively.

G. Performance analysis

For each spectral configuration characterized by a set of N_b channels with the corresponding ISRF $S_j(\lambda)$, the TES retrievals of surface emissivities and temperatures are compared with their initial counterparts at the simulator entrance (see Figure 1). For emissivity, these counterparts are the ISRF-convolved values of the emissivity spectra ε_λ within the DB1 subset. The comparison is based on the quantification of RMSE values between the initial counterparts (ε_j, T_R^{sur}) and their corresponding values for the three types of product considered ($\text{TES-}\varepsilon_j^k, \text{TES-}T_R^{sur,k}$) _{$k \in \{BOA, TOA, OS\}$} :

$$RMSE_{\varepsilon_j^k}^{TES} = \sqrt{\frac{\sum (\text{TES-}\varepsilon_j^k - \varepsilon_j)^2}{N_{ret}}} \quad (20)$$

$$RMSE_{T_R^{sur,k}}^{TES} = \sqrt{\frac{\sum (\text{TES-}T_R^{sur,k} - T_R^{sur})^2}{N_{ret}}} \quad (21)$$

where N_{ret} is the number of retrievals considered in each case.

IV. SiMi IMPLEMENTATION

Once the SiMi simulator is designed, the next step is implementation. This consists of providing ancillary information in order to document land surface and atmospheric conditions.

A. Database for land surface emissivity

We select for the current study the emissivity dataset computed with Module 1 in the framework of a previous study that evaluated the impact of vegetation cavity effect on the performance of the TES method [57]. The resulting dataset includes simulated emissivity spectra for a panel of soil / vegetation canopy combinations, which provides a representative dataset for satellite mission design. By considering a large range of inputs related to vegetation canopy architecture and vegetation / soil optical properties (LAI, ALA, spectra of leaf reflectance and transmittance, spectra of soil reflectance), the dataset includes 63,700 spectra of emissivity of vegetated surface over the [7.5-13.5] μm spectral range.

Since large similarities appears between several simulated spectra of emissivity, and in order to reduce computation time, the database is reduced by selecting emissivity spectra using

the Spectral Angle Mapper (SAM) method [88]. The resulting subset includes 271 emissivity spectra represented in Figure 2. Eventually, and as described in § III-B, a random equal split of the dataset is conducted (Figure 1). The first part, namely DB1, includes 135 spectra and is used for the simulations and for validation exercise. The second part, namely DB2, includes 136 spectra and is used to calibrate the MMD empirical relationship of the TES method.

We verify the robustness of the split between DB1 and DB2, by quantifying the variability of the calibrated coefficients for the TES empirical relationship when repeating the procedure 100 times on a random basis. The observed variability, about 1–2% relative, confirms the robustness of the split.

B. Atmospheric profile dataset

For documenting the atmospheric status, we used the MATISSE-v2 atmospheric profile database that includes three libraries called Air Force Geophysics Laboratory (AFGL)-lib, CLIMATO-lib and Thermodynamic Initial Guess Retrieval (TIGR)3-lib.

- AFGL-lib includes six profiles that are known as tropical, mid-latitude summer, mid-latitude winter, sub-arctic summer, sub-arctic winter and 1976 US Standard [89].
- CLIMATO-lib includes 144 profiles from a climatology database that provides an averaged thermodynamic profile for each latitude [90].
- TIGR3-lib includes 2311 atmospheric profiles. It is a climatological library of representative atmospheric situations selected by statistical methods from 80,000 radiosonde-based profiles [91].

Each of the 2461 atmospheric profiles of the database includes vertical profiles of atmospheric pressure $P_{atm}(z)$, temperature $T_{atm}(z)$, humidity $hr(z)$, as well as of concentration in carbon dioxide $[CO_2](z)$ and ozone $[O_3](z)$.

Given the large size of the MATISSE-v2 atmospheric profile database, and in order to minimize the computation load, a first step consists of reducing the number of atmospheric profiles to construct a representative dataset without redundancy. This process is conducted by considering main drivers of atmospheric radiative transfer in the TIR domain, namely atmospheric water vapor content (AWVC), which drives atmospheric transmittance and emission, and equivalent atmospheric temperature T_{atm}^{eq} , which drives atmospheric emission. Both values are computed by following Equation 22 and 23.

$$AWVC = \int_0^{z_{max}} \rho_v(z) dz \quad (22)$$

$$T_{eq}^{atm} = \frac{\int_0^{z_{max}} T_{atm}(z) \rho_v(z) dz}{AWVC} \quad (23)$$

where z_{max} is the highest altitude of the atmospheric profile and $\rho_v(z)$ is the water vapor density. Hence, the reduction method consists of selecting a set of profiles that verify two comparison criteria: (1) differences between two AWVC values are larger than 0.15 g.cm⁻², and (2) differences between two T_{eq}^{atm} values are larger than 2 K. This reduction method leads to the selection of a subset of 248 atmospheric profiles among the 2461 initial profiles, hereafter referred to as SEL1

subset. Figure 3 illustrates the distribution of the original dataset (top panels) and of the SEL1 subset (bottom panels) in the spaces $\{T_{atm}^{eq}, AWVC\}$, $\{[CO_2], AWVC\}$, and $\{[O_3], AWVC\}$. We note that the envelopes of the scatterplots are preserved, while their densities are reduced.

When conducting the inversion procedure to retrieve surface emissivity and radiometric temperature from the simulated MISTIGRI measurements (§ III-C), we account for uncertainties on atmospheric corrections by noising atmospheric profiles. When dealing with uncertainties on atmospheric temperature and humidity, we use the SEL1 subset of atmospheric profiles. For uncertainties on atmospheric concentrations of carbon dioxide $[CO_2]$ and ozone $[O_3]$, we use portions of the SEL1 subset, always with the objective of reducing the computation load. A portion of SEL1, namely SEL2, is generated by selecting SEL1 profiles that verify two comparison criteria: (1) differences between two AWVC values are larger than 1 g.cm⁻², and (2) differences between two vertically integrated values of $[CO_2(z)]$ are larger than 10 ppmv. Similarly, a portion of SEL1, namely SEL3, is generated by selecting SEL1 profiles that verify two comparison criteria: (1) differences between two AWVC values are larger than 0.5 g.cm⁻², and (2) differences between two vertically integrated values of $[O_3(z)]$ are larger than 0.15 ppmv. The resulting SEL2 and SEL3 selections contain 16 and 41 atmospheric profiles. We observe that SEL2 and SEL3 datasets are representative of the $[CO_2]$ and $[O_3]$ dynamics depicted by the SEL1 subset. Indeed, the envelopes of the scatterplots are preserved, while their densities are reduced (figure not shown).

C. Computation of radiative quantities and of variables of interest

First, each of the 135 emissivity spectra of DB1 (see § IV-A) is associated to ten values of radiometric temperature T_R^{sur} . These temperatures are determined by a random selection within the [270 - 340] K interval, by setting up a constraint to provide realistic cases: for large canopy coverage (LAI larger than 4), the T_R^{sur} value is lower than 315 K.

Second, each pair {emissivity spectra ε_λ , radiometric temperature T_R^{sur} } is combined with each atmospheric profile within the SEL1 subset, when the following condition is verified: $T_R^{sur} \in [T_{atm}(1)-10; T_{atm}(1)+30]$, where $T_{atm}(1)$ is the temperature of the lowest atmospheric level. For this, we combine each pair $\{\varepsilon_\lambda, T_R^{sur}\}$ with the triplet {atmospheric transmission τ_λ^{atm} , atmospheric downwelling irradiance $E_\lambda^{atm\downarrow}$, atmospheric upwelling radiance $L_\lambda^{atm\uparrow}$ } of any atmospheric profile, by using Equations (10)-(12) to compute surface-leaving $L_\lambda^{sur\uparrow}$ and top-of-atmosphere L_λ^{TOA} radiances (Figure 1). This process results in a number of simulated MISTIGRI measurements = 52 916 sets of SBT_j , $TOABT_j$ and of $OSBT_j$ (Figure 1).

Third, atmospheric profiles from subsets SEL1, SEL2 and SEL3 are noised on $T_{atm}(z)$ and $hr(z)$ only, on $[CO_2](z)$ only and on $[O_3](z)$ only, respectively, by following the procedure detailed in § III-C, to next calculate the corresponding radiative atmospheric quantities, namely $\tau_\lambda^{N\,atm}$, $L_\lambda^{N\,atm\uparrow}$ and $E_\lambda^{N\,atm\downarrow}$. Then, the latter are used to perform atmospheric

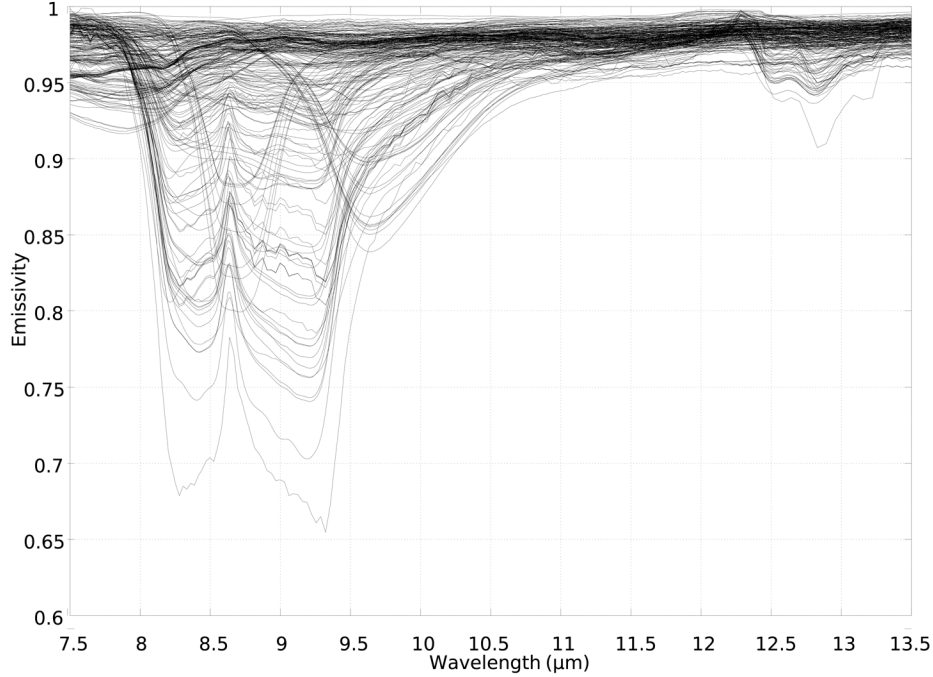


Fig. 2. The 271 SAIL-generated emissivity spectra of vegetation canopy over soils.

corrections in Module 4 (Equation 19) after convolution with channel filters (ISRF $S(\lambda)$, Equation 15). Atmospheric corrections are performed on simulated data at the sensor level (prior to instrumental noise, $TOABT_j$), and on simulated data of output sensor brightness temperature (after instrumental noises, $OSBT_j$).

For both $OSBT_j$ and $TOABT_j$, atmospheric corrections using the SEL1, SEL2 and SEL3 subsets respectively result in $N_{ret} = 52\,916$, $3\,126$ and $8\,531$ sets of corrected MISTIGRI measurements. Finally, the TES method is applied on all sets of atmospherically corrected MISTIGRI measurements. When dealing with SBT_j , we apply TES on sensor measurements at the surface level by including errors on atmospheric downwelling radiance, which is consistent with former studies based on field measurements [71], [92]–[94].

V. SETUP OF THE SIMI SIMULATOR FOR MISTIGRI

A. Instrumental configuration

As mentioned in introduction, the solution chosen for the MISTIGRI was micro-bolometer sensors. This solution imposes to consider wide spectral channels of at least $0.5\ \mu\text{m}$ full width at half maximum (FWHM), in order to minimize radiometric noise (NEDT, see Equation 16). For comparison, in the case of the ASTER sensor, which used first-generation MCT detectors, the minimum FWHM is $0.25\ \mu\text{m}$ [95]. The ISRF set for the reference configuration is provided by the sensor manufacturer (top panel of Figure 4). This configuration includes four channels: TIR1 over $[9.8 - 10.8]\ \mu\text{m}$, TIR2 over $[11 - 12]\ \mu\text{m}$, TIR3 over $[8.15 - 9.1]\ \mu\text{m}$, and TIR4 over $[8.6 - 9.55]\ \mu\text{m}$. According to the sensor manufacturer, uncertainty on both central wavelengths λ_j and FWHMs is $0.15\ \mu\text{m}$. For

the current study, this reference configuration is disregarded since the TIR1 channel significantly overlaps the strong ozone absorption region around $9.6\ \mu\text{m}$.

From the reference configuration, other configurations are generated by varying the number of channels, their positions, and their FWHM, with the following constraints.

- The number of spectral channels N_b is fewer than five as regard to mission requirements, and greater than two in order to capture the spectral variability of natural surfaces, for the sake of consistency with the use of the TES method.
- The spectral channels are as wide as possible to minimise instrumental noise, and as narrow as possible to capture emissivity variations, especially between 8 and $10\ \mu\text{m}$.
- The spectral channels are located on atmospheric windows, i.e., spectral intervals where atmospheric transmittance is large.

From these considerations, six spectral configurations are proposed for the MISTIGRI mission (see Figure 4): two sets of two configurations with $N_b = 4$ channels (MIS-1, MIS-2) on the one hand, and (MIS-3, MIS-4) on the other hand; as well as one set of two configurations with $N_b = 3$ channels (MIS-5, MIS-6). These six configurations are selected for the reasons discussed below.

- The set of configurations (MIS-5, MIS-6) differs from the sets (MIS-1, MIS-2) and (MIS-3, MIS-4) by the number of spectral channels N_b . These differences permit to study the impact of channel number over the $[8 - 10]\ \mu\text{m}$ spectral interval that is typified by large emissivity variations (see Figure 2).
- The sets (MIS-1, MIS-2) and (MIS-3, MIS-4) differ in the

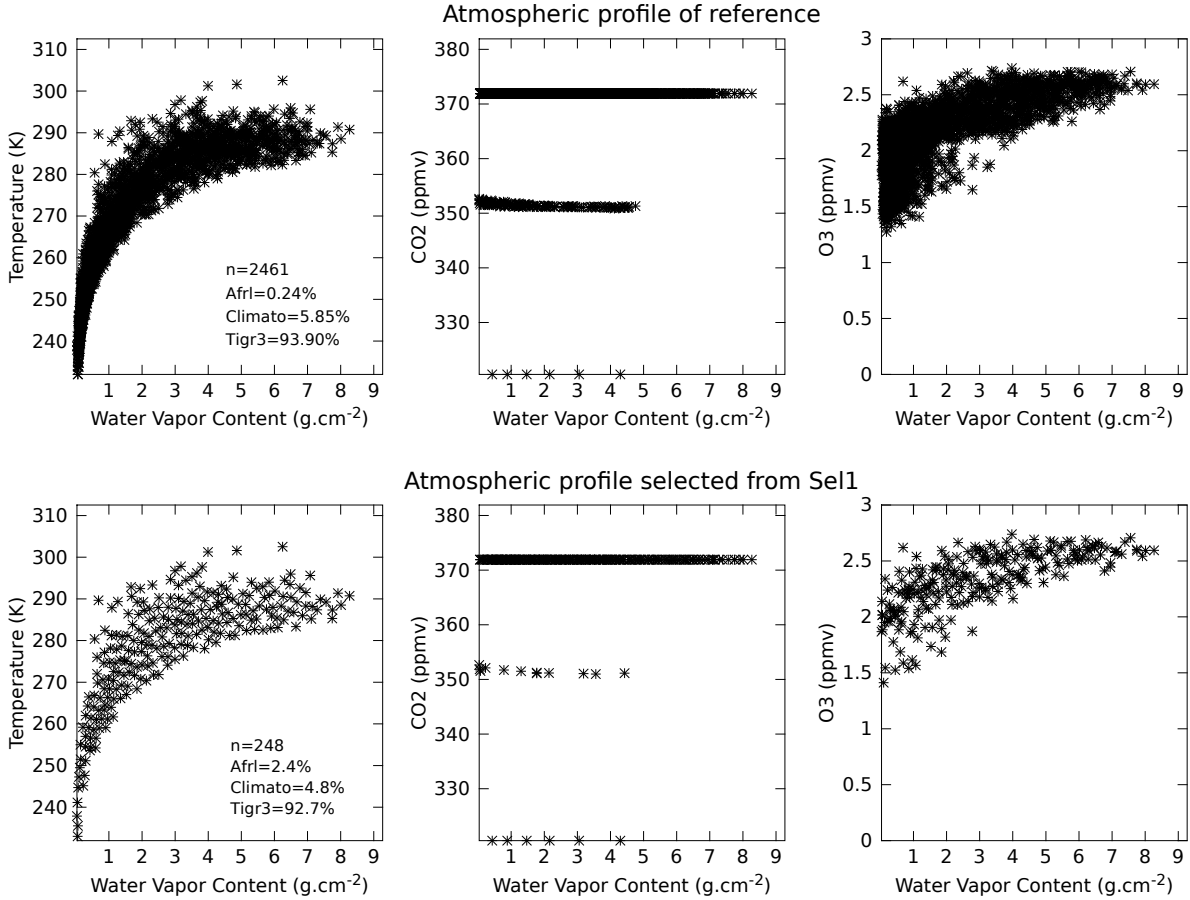


Fig. 3. Representation of the MATISSE-v2 and SEL1 subset of atmospheric profiles in the $\{T_{atm}^{eq}, AWVC\}$, $\{[CO_2], AWVC\}$ and $\{[O_3], AWVC\}$ spaces. $AWVC$ and T_{atm}^{eq} are computed using Equations 22 and 23, respectively. $[CO_2]$ and $[O_3]$ are integrated values across the vertical profiles.

Fig. 4.

location of the two channels over the $[8 - 10] \mu m$ range. Similarly, the MIS-5 and MIS-6 configurations differ in the location of the single channel over the $[8 - 10] \mu m$ range. Again, these differences permit to study the impact of channel localisation within the $[8 - 10] \mu m$ spectral interval that is characterized by large emissivity variations (see Figure 2).

- The MIS-1 and MIS-2 configurations differ in channel widths for TIR1 and TIR2, as do MIS-3 and MIS-4 configurations for TIR3 and TIR4. These differences permit to evaluate the impact of channel FWHM.

Each spectral channel j has a Gaussian shape with a central wavelength λ_j and a $FWHM_j$ (Table II).

From the abacuses provided by the manufacturer, the $NEDT_j$ values are finally computed for all channels included in each of the six MISTIGRI spectral configurations to be evaluated (see Figure 5). Any abacus expresses $NEDT_j$ as function of both measured brightness temperature and channel width (full width at half maximum - FWHM). Using microbolometer detectors, $NEDT_j$ is significantly larger when chan-

nel width decreases. Furthermore, $NEDT_j$ decreases when the measured brightness temperature is larger, whereas channel central wavelength as negligible impact.

B. MMD calibration and validation

The empirical relationship $\varepsilon_{min} = f(MMD)$ is calibrated by using the DB2 subset of emissivity spectra that contains 135 samples, and it is validated by using the 136 emissivity spectra included into the DB1 subset. Emissivity spectra are ISRF-convolved by using the MISTIGRI spectral configurations defined in § V-A. Initial values of empirical coefficients are set according to previous studies [55]: $A = 0.994$, $B = -0.687$, and $C = 0.737$. Note that we obtained the same calibration results regardless of initial guess.

VI. RESULTS AND DISCUSSION

We report and discuss the results we obtain when calibrating the TES empirical relationship, and when validating the TES retrievals of emissivity and radiometric temperature. For TES retrievals, we report results by considering first uncertainties

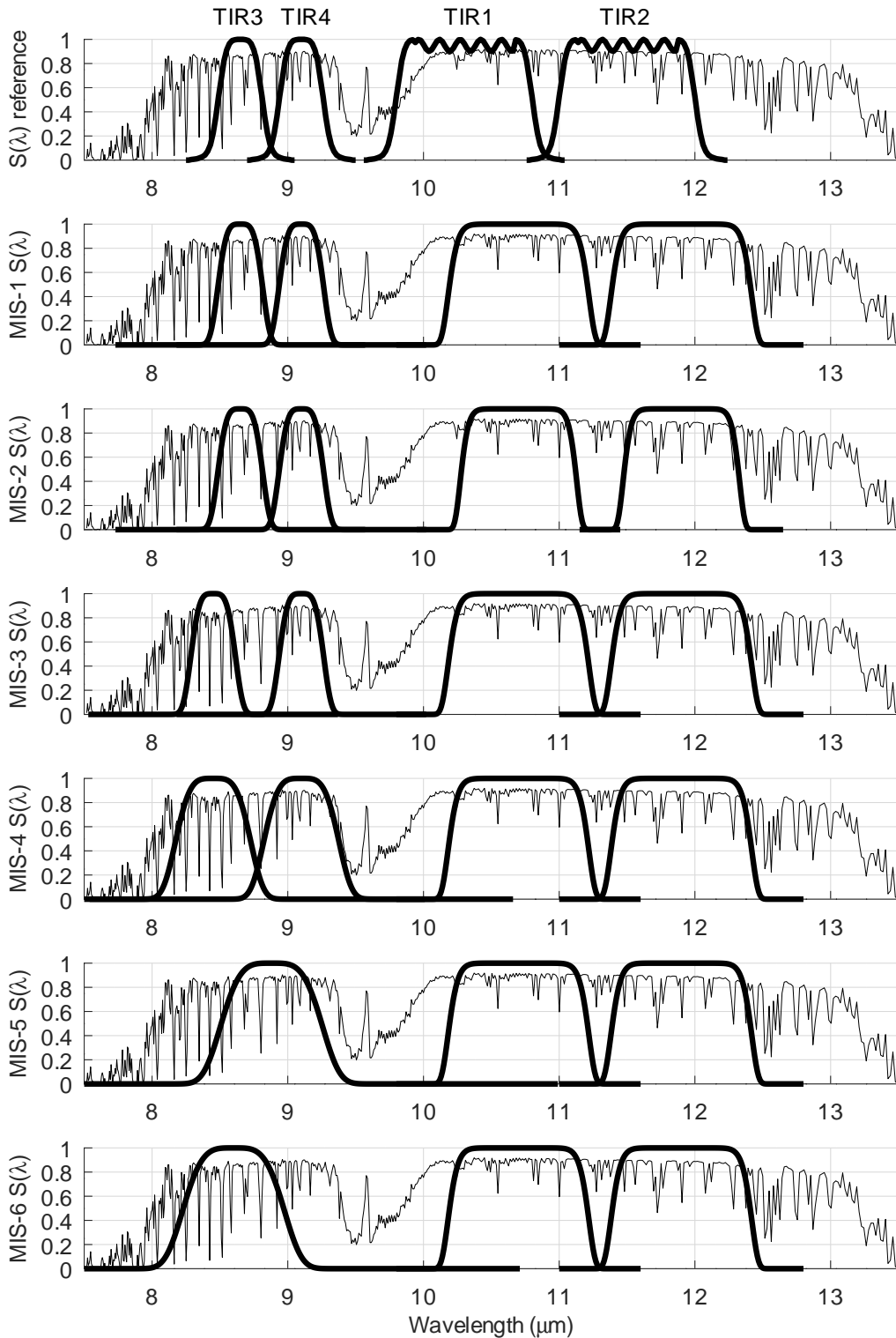


Fig. 4. The various MISTIGRI spectral configurations considered in the current study, typified by their instrumental spectral response function (ISRF), along with a typical example of atmospheric transmittance. Central wavelengths and FWHMs are given into Table II.

TABLE II
SUMMARY OF THE SIX MISTIGRI SPECTRAL COMPOSITIONS WE CONSIDER IN THE CURRENT STUDY. CHANNELS ARE ORDERED ACCORDING TO INCREASING WAVELENGTHS.

Channel	TIR3		TIR4		TIR1		TIR2	
	λ_3	FWHM ₃	λ_4	FWHM ₄	λ_1	FWHM ₁	λ_2	FWHM ₂
MIS-1	8.65	0.32	9.1	0.32	10.7	1.02	11.9	1.02
MIS-2	8.65	0.32	9.1	0.32	10.7	0.84	11.9	0.84
MIS-3	8.45	0.32	9.1	0.32	10.7	1.02	11.9	1.02
MIS-4	8.45	0.54	9.1	0.54	10.7	1.02	11.9	1.02
MIS-5	8.88	0.74	-	-	10.7	1.02	11.9	1.02
MIS-6	8.60	0.74	-	-	10.7	1.02	11.9	1.02

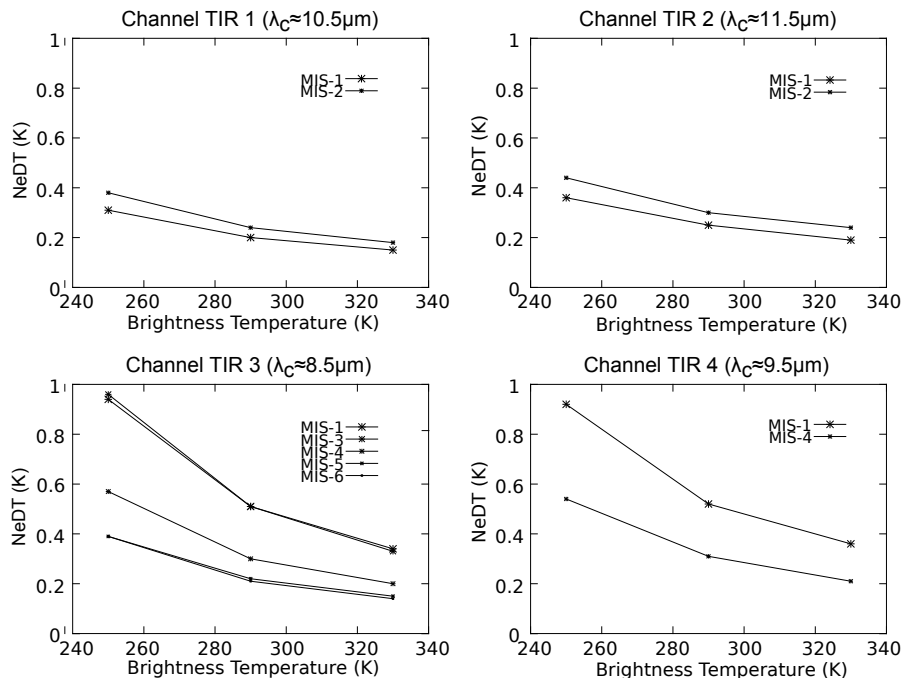


Fig. 5. NeDT values as a function of brightness temperature and channel width (FWHM), for all channels in each of the six MISTIGRI spectral configurations to be evaluated. A unique illustration is given when a channel is identical across several spectral configurations (see Table II for channel equality across configurations).

on atmospheric profiles of temperature and humidity, and second uncertainties on carbon dioxide and ozone concentrations. In both cases, we compare TES retrievals derived from brightness temperature at the surface level ($\text{TES-}\varepsilon_j^{BOA}$, $\text{TES-}T_R^{sur,BOA}$), from brightness temperature at the sensor level ($\text{TES-}\varepsilon_j^{TOA}$, $\text{TES-}T_R^{sur,TOA}$), and from out-of-sensor brightness temperature ($\text{TES-}\varepsilon_j^{OS}$, $\text{TES-}T_R^{sur,OS}$). The results are discussed in the light of spectral configuration, including channel number, widths, and locations, in order to highlight any influence of these factors in the context of the MISTIGRI mission.

A. Calibrating the TES empirical relationship.

Figure 6 displays the MMD calibration results obtained for each of the six MISTIGRI configurations, along with the corresponding values for the A, B, and C coefficients (Equation 8) and the associated residual errors $RMSE_{cal}^{\varepsilon_{min}}$ (Equation 17).

In all cases, the calibration results are good, with $RMSE_{cal}^{\varepsilon_{min}}$ values lower than 0.007. The MIS-3 and MIS-4 configurations have the lowest calibration residual errors, which is ascribed to the combination of channel locations (Subplots 4 and 5 in Figure 4) and emissivity spectral dynamics (Figure 2), where location of TIR3 below $8.5 \mu\text{m}$ allows a better capture of the spectral contrasts. The 3-channels configurations MIS-5 and MIS-6 have the largest calibration residual errors, since they capture less spectral variability of emissivity with only one channel over the $[8 - 9.5] \mu\text{m}$ spectral range. The A, B, C coefficients are different from one configuration to another, but they are similar when channel numbers are equal, i.e., spectral configurations MIS-1 to MIS-4 with 4 channels versus spectral configurations MIS-5 and MIS-6 with 3 channels.

The validation results are very similar to the calibration results, both in error magnitude and error variations from one spectral configuration to another (figure not shown). Indeed,

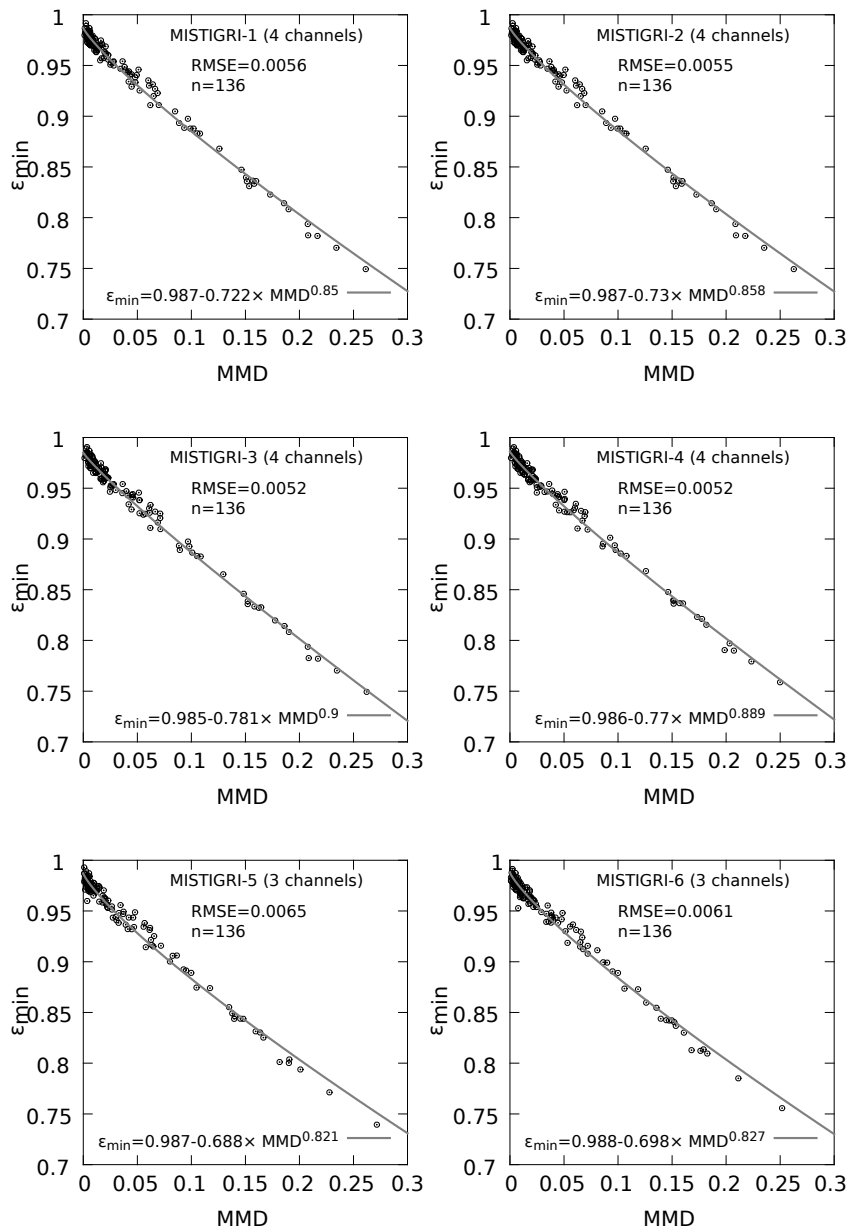


Fig. 6. Results of the $\varepsilon_{min} = f(MMD)$ calibration for each of the six MISTIGRI spectral configurations.

Fig. 7.

the $RMSE_{val}^{\varepsilon_{min}}$ values are consistent with those obtained for calibration and remain as well below 0.007 for all MISTIGRI spectral configurations. However, the similitude between RMSE values for calibration and validation must be considered with caution. Indeed, the calibration and validation datasets are not fully independent since they are extracted from a unique dataset that was simulated by the same model. Overall, the calibration errors we report here are similar to those reported in previous studies [1], [56], [57], [62], [63], [66], [68], [74].

B. Retrieval accuracies with errors on atmospheric corrections related to temperature and humidity.

Table III displays the validation results obtained with the TES method when using the SEL1 subset of atmospheric profiles noised on temperature and humidity. We consider each of the three types of retrievals to be considered (Figure 1): retrievals from brightness temperatures SBT_j at the surface level ($TES-\varepsilon_j^{BOA}$, $TES-T_R^{sur,BOA}$), retrievals from brightness temperatures $TOABT_j$ at the top of atmosphere ($TES-\varepsilon_j^{TOA}$, $TES-T_R^{sur,TOA}$), and retrievals from output sensor brightness

temperature $OSBT_j$ at the top of atmosphere with instrumental noise ($TES-\varepsilon_j^{OS}$, $TES-T_R^{sur,OS}$).

For the BOA retrievals ($TES-\varepsilon_j^{BOA}$, $TES-T_R^{sur,BOA}$), the RMSE values on channel emissivities $RMSE_{\varepsilon_j^{BOA}}^{TES}$ and radiometric temperature $RMSE_{T_R^{sur,BOA}}^{TES}$ across all MISTIGRI configurations range between 0.005 and 0.009, and between 0.30 and 0.45 K, respectively. These RMSE values correspond to the errors due to the TES underlying assumptions (i.e., empirical relationship), as well as to the errors on the quantification of atmospheric downwelling radiance (§ IV-C). Regardless of spectral configuration, the relative variations in emissivity RMSE values across spectral channels range up to 20%, and larger RMSE values are observed at lower wavelengths. This can be explained by two factors in this range of wavelength. The first factor is related to sharp changes in emissivity between 8 and 9.5 μm , which are more difficult to capture as compared to flatter spectra portions between 10 and 12.5 μm (Figure 2). The second factor is related to error propagation in the right term of Equation 2, for which errors in emissivity combine with magnitude of atmospheric downwelling irradiance that increases at lower wavelengths [57]. Given a large part of MMD values are below 0.03 over our dataset of simulated emissivity spectra (Figure 6), this can also be explained by the grey body problem of the TES method that occurs over land surfaces with low spectral contrasts [36], [57], [70], [96]. When dealing with spectral configuration, the inclusion of one more channel over the [8 - 9.5] μm spectral interval induces slightly lower RMSE values on channel emissivities and radiometric temperature (i.e., MIS-1 to MIS-4 versus MIS-5 and MIS-6). This is associated with a better capture of spectral variability across the aforementioned spectral interval with large emissivity variations (Figure 2). When considering the four-channels configurations, a larger gap between the TIR3 and TIR4 channels over the [8 - 9.5] μm spectral interval induces lower RMSE values (MIS-3 and MIS-4 versus MIS-1 and MIS-2), which is also explained by a better capture of spectral variability. Finally, decreasing channel widths over both spectral intervals (i.e., [8 - 9.5] μm and [10 - 12.5] μm) does not impact the captured spectral variability, since the RMSE values are similar (MIS-1 versus MIS-2 and MIS-3 versus MIS-4). Beyond the changes in RMSE values explained above, it is worth noting that differences in RMSE values remain low from one spectral configuration to another, up to 0.0023 and 0.13 K on channel emissivity and radiometric temperature, respectively.

For the TOA retrievals ($TES-\varepsilon_j^{TOA}$, $TES-T_R^{sur,TOA}$), the RMSE values on channel emissivities $RMSE_{\varepsilon_j^{TOA}}^{TES}$ and radiometric temperature $RMSE_{T_R^{sur,TOA}}^{TES}$ across all MISTIGRI configurations range between 0.008 and 0.0140, and between 0.70 and 0.80 K, respectively. These RMSE values are due to the combination of uncertainties related to the TES implementation (see previous paragraph) and uncertainties on atmospheric corrections. Regardless of spectral configuration, the relative variations in emissivity RMSE values across spectral channels range up to 85%, and larger RMSE values are observed at extreme wavelengths, namely 8.6 μm and

11.9 μm . This is ascribed to lower atmospheric transmittances at these wavelengths (Figure 4), which enhance errors on atmospheric corrections [36], [80], [97]. When dealing with spectral configuration, the inclusion of one more channel over the [8 - 9.5] μm spectral interval induces slightly lower RMSE values on channel emissivities and radiometric temperature (i.e., MIS-1 to MIS-4 versus MIS-5 and MIS-6), which, as in the BOA case, can be explained by a better capture of spectral variability. When considering the four-channels configurations, a larger gap between the TIR3 and TIR4 channels over the [8 - 9.5] μm spectral interval does not induce any change in RMSE values (MIS-3 and MIS-4 versus MIS-1 and MIS-2). This is converse to what is reported for the BOA retrievals, and it is therefore ascribed to uncertainties on atmospheric corrections. Finally, decreasing channel widths does not induce significant changes on RMSE values (MIS-1 versus MIS-2 and MIS-3 versus MIS-4). Overall, the differences in RMSE values remain low from one spectral configuration to another, up to 0.002 and 0.1 K on channel emissivity and radiometric temperature, respectively.

For the OS retrievals ($TES-\varepsilon_j^{OS}$, $TES-T_R^{sur,OS}$), the RMSE values on channel emissivities $RMSE_{\varepsilon_j^{OS}}^{TES}$ and radiometric temperature $RMSE_{T_R^{sur,OS}}^{TES}$ across all MISTIGRI configurations range between 0.0160 and 0.037, and between 0.8 and 0.9 K, respectively. These larger RMSE values result from the combination of uncertainties related to the TES implementation, of uncertainties on atmospheric corrections, and of uncertainties induced by instrumental noise. Regardless of spectral configuration, the relative variations in emissivity RMSE values across spectral channels range up to 85%, and larger RMSE values are observed at extreme wavelengths, namely 8.6 μm and 11.9 μm . This is ascribed to the combined effects of uncertainties induced by instrumental noise and uncertainties on atmospheric corrections at wavelengths with lower atmospheric transmittances. Moreover, the RMSE values for emissivity are larger than in the TOA case, with increases up to a factor 3 for some channels, which highlights the impact of instrumental noise when dealing with micro-bolometer detectors. In terms of spectral configuration, the largest (respectively lowest) RMSE values are observed for configurations with lowest (respectively largest) channel widths, namely MIS-2 (respectively MIS-5 and MIS-6), which is ascribed to the impact of channel width on instrumental noise (Figure 5). Overall, the differences in RMSE values remain low from one spectral configuration to another, up to 0.0185 and 0.1 K on channel emissivity and radiometric temperature, respectively. Figure 7 displays examples of scatterplots when considering the TES retrievals from output sensor brightness temperature $OSBT_j$ after atmospheric corrections, for the three-channels spectral configuration MIS-5. It is shown that retrievals and reference values are in agreement for channel emissivity at 8.88 μm and radiometric temperature, whereas a moderate (respectively large) discrepancy is observed for channel emissivity at 10.7 μm and 11.9 μm . Such discrepancies are not observed when validating TES retrievals from measurements of brightness temperature at the surface level [57], and they underline the impact of inaccurate atmospheric corrections on

TABLE III

ERRORS ON RETRIEVALS OF EMISSIVITY AND RADIOMETRIC TEMPERATURE FROM THE TES METHOD ALONG WITH ATMOSPHERIC CORRECTIONS FROM PROFILES NOISED ON TEMPERATURE AND HUMIDITY. WE REPORT RMSE VALUES FOR (1) THE PAIR $\{\text{TES}-\varepsilon_j^{BOA}, \text{TES}-T_R^{sur,BOA}\}$ THAT CORRESPONDS TO APPLYING THE TES METHOD ON SENSOR MEASUREMENTS OF SURFACE BRIGHTNESS TEMPERATURE AT THE SURFACE LEVEL, (2) FOR THE PAIR $\{\text{TES}-\varepsilon_j^{TOA}, \text{TES}-T_R^{sur,TOA}\}$ THAT CORRESPONDS TO APPLYING ATMOSPHERIC CORRECTIONS AND THE TES METHOD ON TOA BRIGHTNESS TEMPERATURE AT THE SENSOR LEVEL, AND (3) THE PAIR $\{\text{TES}-\varepsilon_j^{OS}, \text{TES}-T_R^{sur,OS}\}$ THAT CORRESPONDS TO APPLYING ATMOSPHERIC CORRECTIONS AND THE TES METHOD ON OUTPUT SENSOR (OS) BRIGHTNESS TEMPERATURE (FIGURE 1). CHANNEL EMISSIVITIES ARE ORDERED ACCORDING TO INCREASING WAVELENGTHS.

BOA	$RMSE_{\varepsilon_3^{BOA}}^{TES}$	$RMSE_{\varepsilon_4^{BOA}}^{TES}$	$RMSE_{\varepsilon_1^{BOA}}^{TES}$	$RMSE_{\varepsilon_2^{BOA}}^{TES}$	$RMSE_{T_R^{sur,BOA}}^{TES}$
MIS-1	0.0077	0.0067	0.0061	0.0063	0.35
MIS-2	0.0074	0.0065	0.0059	0.0061	0.34
MIS-3	0.0071	0.0059	0.0054	0.0054	0.30
MIS-4	0.0074	0.0059	0.0053	0.0054	0.30
MIS-5	0.0084	-	0.0074	0.0077	0.43
MIS-6	0.0086	-	0.0068	0.0070	0.40
TOA	$RMSE_{\varepsilon_3^{TOA}}^{TES}$	$RMSE_{\varepsilon_4^{TOA}}^{TES}$	$RMSE_{\varepsilon_1^{TOA}}^{TES}$	$RMSE_{\varepsilon_2^{TOA}}^{TES}$	$RMSE_{T_R^{sur,TOA}}^{TES}$
MIS-1	0.0112	0.0098	0.0082	0.0131	0.70
MIS-2	0.0104	0.0093	0.0076	0.0141	0.68
MIS-3	0.0124	0.0095	0.0076	0.0124	0.68
MIS-4	0.0125	0.0100	0.0075	0.0121	0.69
MIS-5	0.0118	-	0.0095	0.0135	0.78
MIS-6	0.0122	-	0.0089	0.0128	0.76
OS	$RMSE_{\varepsilon_3^{OS}}^{TES}$	$RMSE_{\varepsilon_4^{OS}}^{TES}$	$RMSE_{\varepsilon_1^{OS}}^{TES}$	$RMSE_{\varepsilon_2^{OS}}^{TES}$	$RMSE_{T_R^{sur,OS}}^{TES}$
MIS-1	0.0299	0.0246	0.0203	0.0289	0.89
MIS-2	0.0311	0.0251	0.0211	0.0321	0.91
MIS-3	0.0376	0.0247	0.0203	0.0298	0.89
MIS-4	0.0277	0.0194	0.0165	0.0258	0.79
MIS-5	0.0191	-	0.0161	0.0232	0.85
MIS-6	0.0212	-	0.0159	0.0230	0.83

the performance of the TES method.

The aforementioned results for the BOA, TOA, and OS retrievals, permit to address the TES error budget at different levels, and to compare the combined effects of uncertainties that accumulate at each step, namely TES implementation, atmospheric corrections, and instrumental noise related to the use of bolometer-based sensors.

- First, the impacts of sharp emissivity changes at lower wavelengths (i.e., larger RMSE values for lower wavelengths, benefit of larger gap between channels within the [8 - 9.5] μm spectral interval, benefit of a second channel over the [8 - 9.5] μm spectral interval) tend to vanish when accumulating errors induced by atmospheric corrections and uncertainties related to instrumental noise.
- Second, the impact of errors on atmospheric correction is large, since it almost doubles the RMSE values on channel emissivities and radiometric temperature, with largest impacts for channels located close to the atmospheric window boundaries (8 μm and 12.5 μm).
- Third, consideration for additional instrumental noise significantly increases the errors on channel emissivity, but the resulting impact on radiometric temperature is limited. However, the benefit of adding a second channel over the [8 - 9.5] μm spectral interval is very limited when alternatively considering a unique channel with a large width. This underlines the balance between capturing spectral contrast and minimizing instrumental noise for bolometer-based sensors with large instrumental noise.

The MIS-5 configuration seems to be the most robust to the coupling of errors on atmospheric corrections and instrumental

noise, since it corresponds to the lowest error increase on radiometric temperature (from 0.43 K to 0.85 K). In absolute terms, i.e., by adding the intrinsic uncertainty of TES, the most accurate configuration is MIS-4, since it provides the lowest error on radiometric temperature (0.79 K). Overall, the RMSE values that encompass all uncertainties range between 0.83 K and 0.91 K across all MISTIGRI spectral configurations. This shows that the spectral configuration is not a critical issue for surface temperature retrieval in our study case with bolometer-based detectors. We note we deal here with accuracy on radiometric temperature, in accordance to the primary objectives of the MISTIGRI mission on land surface energy and water budgets. Nevertheless, we note that there is no systematic agreement between RMSE values on channel emissivities and on radiometric temperature, especially when the number of channel varies (i.e., from three to four channels). This is ascribed to the high non linearity of the TES equation system (Equations 1 to 9), where any retrieval of radiometric temperature results from an iterative process that involves an incremental estimation of minimum emissivity across N_b channels. Eventually, the TES performance we observe here is moderately larger than those reported in former studies also based on modeling approaches, with RMSE values ranging between 0.6 and 1 K [48], [59], [63], [74], [75].

C. Retrieval accuracies with errors on atmospheric corrections related to carbon dioxide and ozone concentration.

Table IV and V display the validation results obtained with the TES method when using the SEL2 and SEL3 subset of atmospheric profiles noised on $[\text{CO}_2]$ and $[\text{O}_3]$. We consider each of the three types of retrievals to be considered (Figure 1):

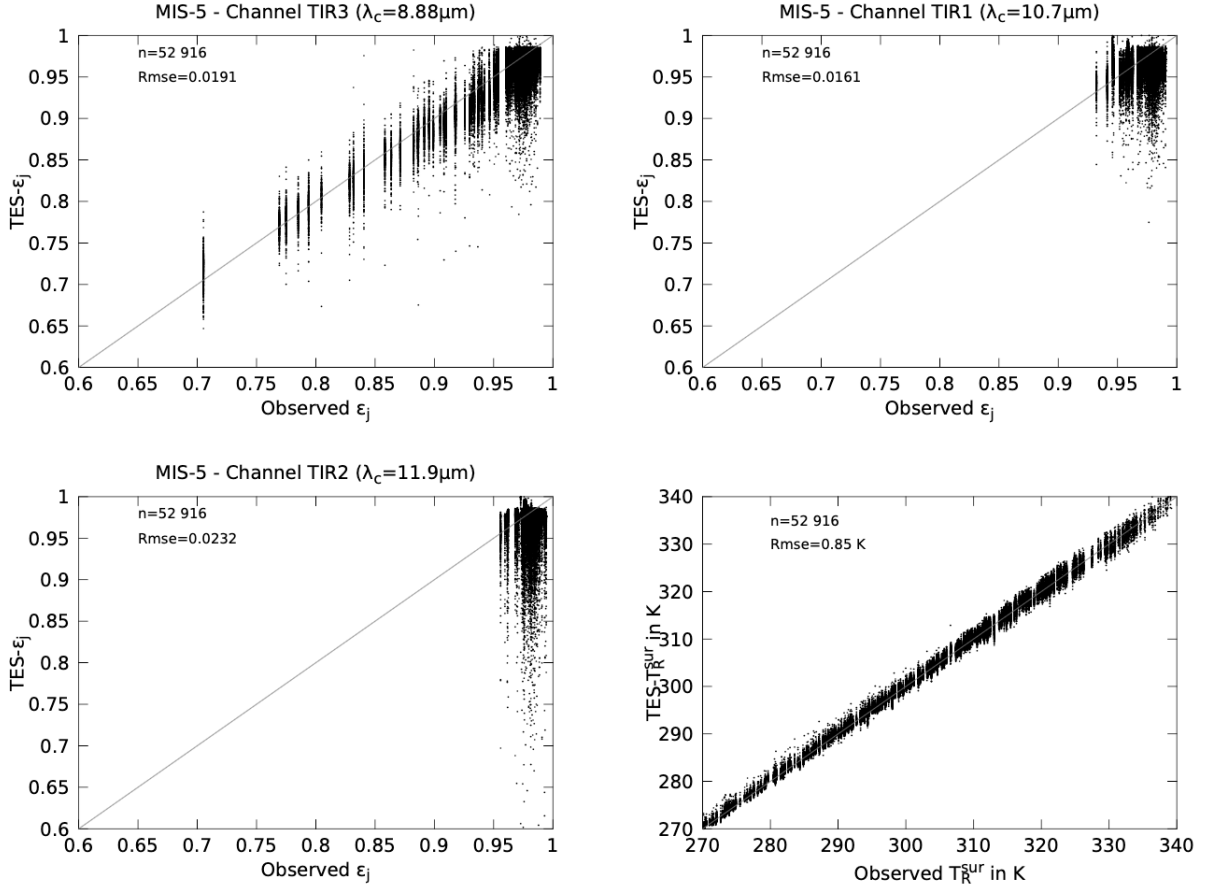


Fig. 7. Comparison of TES retrievals against reference values when considering (1) the MIS-5 spectral configuration with 3 channels (Figure 4), (2) atmospheric corrections from atmospheric profiles noised on temperature and humidity, and (3) the TES retrievals of channel emissivities and radiometric temperature from output sensor brightness temperatures $OSBT_j$ ($TES-\varepsilon_j^{OS}$, $TES-T_R^{sur,OS}$).

retrievals from brightness temperatures SBT_j at the surface level ($TES-\varepsilon_j^{BOA}$, $TES-T_R^{sur,BOA}$), retrievals from brightness temperatures $TOABT_j$ at the top of atmosphere ($TES-\varepsilon_j^{TOA}$, $TES-T_R^{sur,TOA}$), and retrievals from output sensor brightness temperature $OSBT_j$ at the top of atmosphere with instrumental noise ($TES-\varepsilon_j^{OS}$, $TES-T_R^{sur,OS}$). Since the TES retrievals from brightness temperatures SBT_j at the surface level were previously analysed in § VI-B, we do not discuss them here, and they are included in Table IV and V to serve as references when analysing (1) the TOA retrievals that involve errors on atmospheric corrections related to $[CO_2]$ and $[O_3]$, and (2) the OS retrievals that additionally involve uncertainties related to instrumental noise. We note the results for BOA retrievals are not identical in Table III, Table IV and V, since they correspond to different numbers of retrievals (52 916 with the SEL1 subset, 3 126 with the SEL2 subset, and 8 531 with the SEL3 subset, see § IV-C), as well as to different values for noised atmospheric downwelling irradiance.

For the TOA retrievals ($TES-\varepsilon_j^{TOA}$, $TES-T_R^{sur,TOA}$), the RMSE values on channel emissivities $RMSE_{\varepsilon_j^{TOA}}^{TES}$ and radiometric temperature $RMSE_{T_R^{sur,TOA}}^{TES}$ across all MISTIGRI configurations range between 0.060 and 0.013, and between 0.30 and 0.45 K, respectively, for both SEL2 and SEL3 subsets

of atmospheric profiles noised on $[CO_2]$ and $[O_3]$. Across both subsets, errors on TOA retrievals are very similar to those observed on BOA retrievals, which indicates that errors on atmospheric corrections related to $[CO_2]$ and $[O_3]$ have a very small impact on the TES retrievals.

For the OS retrievals ($TES-\varepsilon_j^{OS}$, $TES-T_R^{sur,OS}$), the RMSE values on channel emissivities $RMSE_{\varepsilon_j^{OS}}^{TES}$ and radiometric temperature $RMSE_{T_R^{sur,OS}}^{TES}$ across all MISTIGRI configurations range between 0.02 and 0.05, and between 0.8 and 1 K, respectively, for both SEL2 and SEL3 subsets. Thus, additional consideration of instrumental noise has a significant impact on the RMSE values, since these values reach the same magnitude than those reported for TOA retrievals with the SEL1 subset (Table III). This indicate that the impact on TES retrievals of uncertainties due to instrumental noise is similar to that of errors on atmospheric corrections related to atmospheric temperature and humidity. Then, the similar RMSE values observed for TOA and OS retrievals in Table III are explained by compensation effects between atmospheric and instrumental perturbations, the latter being characterized by Gaussian processes (Equations 13 and 14).

Eventually, and similarly to the result obtained with the SEL1 subset, the spectral configuration that seems robust to coupling between $[CO_2]$ / $[O_3]$ concentration errors and

TABLE IV

ERRORS ON RETRIEVALS OF EMISSIVITY AND RADIOMETRIC TEMPERATURE FROM THE TES METHOD ALONG WITH ATMOSPHERIC CORRECTIONS FROM PROFILES NOISED ON $[\text{CO}_2]$. WE REPORT RMSE VALUES FOR (1) THE PAIR $\{\text{TES}-\varepsilon_j^{BOA}, \text{TES}-T_R^{sur,BOA}\}$ THAT CORRESPONDS TO APPLYING THE TES METHOD ON SENSOR MEASUREMENTS OF SURFACE BRIGHTNESS TEMPERATURE AT THE SURFACE LEVEL, (2) FOR THE PAIR $\{\text{TES}-\varepsilon_j^{TOA}, \text{TES}-T_R^{sur,TOA}\}$ THAT CORRESPONDS TO APPLYING ATMOSPHERIC CORRECTIONS AND THE TES METHOD ON TOA BRIGHTNESS TEMPERATURE AT THE SENSOR LEVEL, AND (3) THE PAIR $\{\text{TES}-\varepsilon_j^{OS}, \text{TES}-T_R^{sur,OS}\}$ THAT CORRESPONDS TO APPLYING ATMOSPHERIC CORRECTIONS AND THE TES METHOD ON OUTPUT SENSOR (OS) BRIGHTNESS TEMPERATURE (FIGURE 1). CHANNEL EMISSIVITIES ARE ORDERED ACCORDING TO INCREASING WAVELENGTHS.

BOA	$RMSE_{\varepsilon_3^{BOA}}^{TES}$	$RMSE_{\varepsilon_4^{BOA}}^{TES}$	$RMSE_{\varepsilon_1^{BOA}}^{TES}$	$RMSE_{\varepsilon_2^{BOA}}^{TES}$	$RMSE_{T_R^{sur,BOA}}^{TES}$
MIS-1	0.0075	0.0066	0.0061	0.0063	0.34
MIS-2	0.0073	0.0064	0.0058	0.0061	0.33
MIS-3	0.007	0.0058	0.0054	0.0054	0.29
MIS-4	0.0073	0.0058	0.0053	0.0054	0.29
MIS-5	0.0082	-	0.0073	0.0076	0.41
MIS-6	0.0085	-	0.0067	0.007	0.38
TOA	$RMSE_{\varepsilon_3^{TOA}}^{TES}$	$RMSE_{\varepsilon_4^{TOA}}^{TES}$	$RMSE_{\varepsilon_1^{TOA}}^{TES}$	$RMSE_{\varepsilon_2^{TOA}}^{TES}$	$RMSE_{T_R^{sur2}}^{TES}$
MIS-1	0.0102	0.008	0.0069	0.0061	0.35
MIS-2	0.0086	0.0067	0.0058	0.0059	0.32
MIS-3	0.0124	0.0077	0.0065	0.0055	0.32
MIS-4	0.0129	0.0086	0.0065	0.0056	0.32
MIS-5	0.0107	-	0.0084	0.0079	0.44
MIS-6	0.0117	-	0.0078	0.0074	0.41
OS	$RMSE_{\varepsilon_3^{OS}}^{TES}$	$RMSE_{\varepsilon_4^{OS}}^{TES}$	$RMSE_{\varepsilon_1^{OS}}^{TES}$	$RMSE_{\varepsilon_2^{OS}}^{TES}$	$RMSE_{T_R^{sur,OS}}^{TES}$
MIS-1	0.0356	0.029	0.0249	0.0324	0.93
MIS-2	0.0389	0.0324	0.0275	0.0385	0.99
MIS-3	0.047	0.0305	0.0272	0.0383	0.97
MIS-4	0.0336	0.0239	0.021	0.0332	0.76
MIS-5	0.0245	-	0.0217	0.0249	0.8
MIS-6	0.0276	-	0.0213	0.0269	0.79

TABLE V

ERRORS ON RETRIEVALS OF EMISSIVITY AND RADIOMETRIC TEMPERATURE FROM THE TES METHOD ALONG WITH ATMOSPHERIC CORRECTIONS FROM PROFILES NOISED ON $[\text{O}_3]$. WE REPORT RMSE VALUES FOR (1) THE PAIR $\{\text{TES}-\varepsilon_j^{BOA}, \text{TES}-T_R^{sur,BOA}\}$ THAT CORRESPONDS TO APPLYING THE TES METHOD ON SENSOR MEASUREMENTS OF SURFACE BRIGHTNESS TEMPERATURE AT THE SURFACE LEVEL, (2) FOR THE PAIR $\{\text{TES}-\varepsilon_j^{TOA}, \text{TES}-T_R^{sur,TOA}\}$ THAT CORRESPONDS TO APPLYING ATMOSPHERIC CORRECTIONS AND THE TES METHOD ON TOA BRIGHTNESS TEMPERATURE AT THE SENSOR LEVEL, AND (3) THE PAIR $\{\text{TES}-\varepsilon_j^{OS}, \text{TES}-T_R^{sur,OS}\}$ THAT CORRESPONDS TO APPLYING ATMOSPHERIC CORRECTIONS AND THE TES METHOD ON OUTPUT SENSOR (OS) BRIGHTNESS TEMPERATURE (FIGURE 1). CHANNEL EMISSIVITIES ARE ORDERED ACCORDING TO INCREASING WAVELENGTHS.

BOA	$RMSE_{\varepsilon_3^{BOA}}^{TES}$	$RMSE_{\varepsilon_4^{BOA}}^{TES}$	$RMSE_{\varepsilon_1^{BOA}}^{TES}$	$RMSE_{\varepsilon_2^{BOA}}^{TES}$	$RMSE_{T_R^{sur1}}^{TES}$
MIS-1	0.0075	0.0067	0.0061	0.0063	0.35
MIS-2	0.0073	0.0065	0.0059	0.0061	0.34
MIS-3	0.007	0.0058	0.0054	0.0054	0.3
MIS-4	0.0073	0.0059	0.0053	0.0054	0.3
MIS-5	0.0083	-	0.0074	0.0076	0.42
MIS-6	0.0085	-	0.0068	0.007	0.39
TOA	$RMSE_{\varepsilon_3^{TOA}}^{TES}$	$RMSE_{\varepsilon_4^{TOA}}^{TES}$	$RMSE_{\varepsilon_1^{TOA}}^{TES}$	$RMSE_{\varepsilon_2^{TOA}}^{TES}$	$RMSE_{T_R^{sur,TOA}}^{TES}$
MIS-1	0.0102	0.0081	0.0068	0.0062	0.36
MIS-2	0.0087	0.0069	0.0059	0.0059	0.33
MIS-3	0.0118	0.0078	0.0064	0.0055	0.32
MIS-4	0.012	0.009	0.0064	0.0056	0.33
MIS-5	0.0109	-	0.0084	0.0079	0.45
MIS-6	0.0113	-	0.0077	0.0073	0.42
OS	$RMSE_{\varepsilon_3^{OS}}^{TES}$	$RMSE_{\varepsilon_4^{OS}}^{TES}$	$RMSE_{\varepsilon_1^{OS}}^{TES}$	$RMSE_{\varepsilon_2^{OS}}^{TES}$	$RMSE_{T_R^{sur,OS}}^{TES}$
MIS-1	0.0367	0.0304	0.025	0.0303	0.89
MIS-2	0.0384	0.0312	0.0267	0.0386	0.94
MIS-3	0.05	0.0332	0.0413	0.0592	0.9
MIS-4	0.0378	0.026	0.0229	0.0307	0.79
MIS-5	0.0243	-	0.0206	0.0262	0.79
MIS-6	0.0288	-	0.0217	0.0255	0.79

instrumental noise is MIS-5. In absolute terms, the most accurate configuration is still MIS-4, although the differences with the other configurations also remain small (Tables IV and V).

D. Sensitivity of the MISTIGRI / TES retrievals to uncertainties on channel location and bandwidths.

Our results also provide information about the sensitivity of the TES retrievals to uncertainties on MISTIGRI channel locations and widths, which is an important issue for sensor design and subsequent accuracy on emissivity / temperature retrievals. On the one hand, uncertainty on both channel locations and widths is $0.15 \mu\text{m}$, according to the information provided by the detector manufacturer (§ V-A). On the other hand, the variability on channel location and widths across the six MISTIGRI spectral configurations is slightly larger than the aforementioned uncertainty, i.e., around $0.2 \mu\text{m}$, as indicated in Figure 4 and Table II. Therefore, it is possible to evaluate the impact of this uncertainty, by quantifying the variability we observe on TES retrieval accuracy across the six MISTIGRI spectral configurations.

On the basis of the TES retrieval accuracy across the six configurations, for each of the three cases (BOA, TOA, OS) reported by Table III, IV and V, we note a variability on TES retrieval accuracy that ranges between 0.05 K and 0.15

K. This underlines the low impact of changes in channel locations and bandwidths, and therefore the low impact of uncertainty on channel locations and bandwidths. Eventually, we note that changes between the six spectral configurations (i.e., channel locations and bandwidth) are similar to the uncertainty on channel locations and bandwidths. Indeed, the variability across spectral configurations is constrained by both channel overlaps and atmospheric windows, notably because of large bandwidths. This highlights that using bolometer-based detectors induces a trade-off between instrumental noise and bandwidth. Such constraint should be overcome by using last generation of MCT cooled detectors.

VII. CONCLUDING REMARKS

The current study aims to propose an appropriate spectral configuration for the micro-bolometer based TIR sensor of the MISTIGRI mission.

The strategy is typified by the following points. First, we address the various errors related to each step of the retrieval procedure: the TES underlying assumptions about emissivity spectral contrast, the errors on atmospheric corrections related to knowledge about atmospheric status when the satellite overpasses, and the instrumental noise related to filter response functions for micro-bolometer based detectors. Second, when dealing with uncertainties on atmospheric status, we consider atmospheric profiles of temperature and humidity, as well as of carbon dioxide and ozone concentrations. Third, the error budget analysis is based on numerical model simulations, by including last generation of land surface emissivity spectra that account for the cavity effect. Fourth, we evaluate six predefined spectral configurations for the MISTIGRI TIR

sensor, where the spectral configurations differ in terms of channel number, locations, and widths.

On the basis of the error budget analysis, the main outcomes of the current study are the following. First, errors on atmospheric corrections related to knowledge on temperature and humidity profiles have similar impact on TES retrievals than uncertainties related to instrumental noise. The equivalence in contribution to the error budget is ascribed to the large instrumental errors due to the use of micro-bolometer detectors. The resulting errors on TES retrievals are twice as large as those due to the TES underlying assumption about emissivity spectral contrast. Second, retrieval accuracies are very similar across all MISTIGRI spectral configurations, where differences are within 0.2 K on radiometric temperature. This shows that the spectral configuration to be chosen is not a critical issue in our study case that addresses the use of micro-bolometer based sensing with significant instrumental noises or large channel widths. Third, retrieval accuracies on radiometric temperature are moderately larger than those reported in former studies based on numerical model simulations, for MCT cooled detectors such as ASTER or ECOSTRESS sensors.

Main limitations of the current study, to be overcome with on-going works, are the following. First, we consider a micro-bolometer based sensor, and results may vary if considering last generation of MCT cooled detectors that permit to reduce both channel widths and instrumental noises. In this case, the challenge is to increase the accuracy of atmospheric corrections. Second, we consider a set of predefined spectral configurations to be evaluated by analysing the simulations based error budget. However, results are expected to be more robust if using an optimisation procedure that combines the simultaneous sliding of several channels, since it is possible to identify a global minimum on retrieval errors.

From a practical point of view, eventually, the study succeeds in defining the most suited spectral configuration for the MISTIGRI sensor, i.e., the spectral configuration that provides retrievals of land surface radiometric temperature with lower errors.

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