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Thermal structure and aerosols in Mars' atmosphere from TIRVIM/ACS onboard the ExoMars Trace Gas Orbiter : validation of the retrieval algorithm

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Key Points:

- We exploit TIRVIM spectra to determine Martian atmospheric, surface temperature, as well as integrated opacity of dust and water ice clouds.
- Different sources of biases are investigated with the help of simulated observations at different local times, latitudes and seasons.
- Atmospheric temperatures retrieved from TIRVIM in April-May 2018 are in excellent agreement with co-located MCS observations.

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Abstract

The Atmospheric Chemistry Suite (ACS) onboard the ExoMars Trace Gas Orbiter (TGO) monitors the Martian atmosphere through different spectral intervals in the infrared light. We present a retrieval algorithm tailored to the analysis of spectra acquired in nadir geometry by TIRVIM, the thermal infrared channel of ACS. Our algorithm simultaneously retrieves vertical profile of atmospheric temperature up to 50 km, surface temperature, and integrated optical depth of dust and water ice clouds. The specificity of the TIRVIM dataset lies in its capacity to resolve the diurnal cycle over a 54 sol period. However, it is uncertain to what extent can the desired atmospheric quantities be accurately estimated at different times of day. Here we first present an Observing System Simulation Experiment (OSSE). We produce synthetic observations at various latitudes, seasons and local times and run our retrieval algorithm on these synthetic data, to evaluate its robustness. Different sources of biases are documented, in particular regarding aerosol retrievals. Atmospheric temperature retrievals are found robust even when dust and/or water ice cloud opacities are not well estimated in our OSSE. We then apply our algorithm to TIRVIM observations in April-May, 2018 and perform a cross-validation of retrieved atmospheric temperature and dust integrated opacity by comparisons with thousands of co-located Mars Climate Sounder (MCS) retrievals. Most differences between TIRVIM and MCS atmospheric temperatures can be attributed to differences in vertical sensitivity. Daytime dust opacities agree well with each other, while biases are found in nighttime dust opacity retrieved from TIRVIM at this season.

Plain Language Summary

The Martian surface and atmosphere undergo strong variations in temperature and amount of aerosols (dust or water ice cloud particles). Our knowledge on their variations at diurnal scale is however limited, due to lack of appropriate observations. We present a method to analyze thermal emission spectra of Mars' surface and atmosphere recorded by TIRVIM, a spectrometer onboard the ExoMars Trace Gas Orbiter. We have developed a program to derive surface and atmospheric temperatures from these spectra, along with an estimation of the amount of aerosols. The specificity of the TIRVIM dataset is its capacity to resolve the diurnal cycle over a 54 sol period. However, atmospheric quantities cannot be accurately estimated at all times of day. One of the goals of our paper is to assess the robustness of our algorithm with the help of simulated observations. The

54 retrieval of aerosol opacity is assessed to be challenging at some times of day, but atmo-
55 spheric temperature is well determined. We have then applied our algorithm to tens of
56 thousands of TIRVIM observations obtained in April-May 2018 and showed that our de-
57 rived atmospheric temperatures compare very well with independent measurements ob-
58 tained from the Mars Climate Sounder, reinforcing our confidence in our method.

59 1 Introduction

60 The ESA-Roscosmos ExoMars Trace Gas Orbiter (TGO) was launched on March
61 14th, 2016 and was successfully inserted into Mars' orbit in November, 2016. After sev-
62 eral orbit manoeuvres including a 12-month aerobraking phase it reached its final, 400-
63 km altitude and near-circular orbit on April 13th, 2018. Onboard TGO, the Atmospheric
64 Chemistry Suite (ACS) comprises three spectrometers, each tailored for specific scien-
65 tific goals (Korablev et al., 2018). We focus here on the thermal infrared spectrometer,
66 named TIRVIM (Thermal InfraRed channel in honor of professor Vassilii Ivanovich Mo-
67 roz), which was operational from April, 2018 until December, 2019, hence almost a mar-
68 tian year (between mid- martian years 34 and 35). Through nadir-viewing soundings,
69 its main goal is to monitor the atmospheric temperature, surface temperature and in-
70 tegrated aerosol content – dust and water ice clouds – at a great variety of local times.
71 Indeed, TGO's orbit is designed in such a way that nadir observations sample the full
72 diurnal cycle in 54 sols, at all latitudes between 74°N and 74°S. Hence, it is able to cap-
73 ture both seasonal and diurnal variations of these climatological variables and comple-
74 ments other still-operating thermal infrared sounders, such as the Mars Climate Sounder
75 (MCS) onboard NASA's Mars Reconnaissance Orbiter, the Planetary Fourier Spectrom-
76 eter (PFS) onboard ESA's Mars Express and the Thermal Emission Imaging System (THEMIS)
77 onboard Mars Odyssey.

78 MCS is a radiometer operating in limb-viewing geometry, allowing the retrieval of
79 vertical profiles of atmospheric temperature from 5 to 80 km as well as dust and water
80 ice vertical profiles, with a vertical resolution of typically 5 km (Kleinböhl et al., 2009).
81 Being on a Sun-synchronous polar orbit, MCS mostly acquires data at local times 3:00
82 and 15:00 (± 1.5 hours when cross-track observations are performed). PFS is a thermal
83 infrared spectrometer operating in nadir-viewing geometry providing temperature pro-
84 files in the range 5–50 km with a vertical resolution of 10 km (Grassi et al., 2005) along
85 with surface temperature and the integrated content of dust and water ice clouds. The

86 same quantities can be retrieved from TIRVIM observations. The Mars Express orbiter
87 is such that PFS observations sample various local times but with a longer revisit time
88 compared to TIRVIM (150 sols for PFS versus 54 sols for TIRVIM), and a sparser spa-
89 tial coverage due to the elliptical orbit of Mars Express. Finally, the THEMIS instru-
90 ment comprises several cameras that image Mars in the visible and thermal infrared. It
91 is sensitive to atmospheric temperature in a broad altitude range centered on 50 Pa, and
92 allows for the retrieval of integrated dust and water ice opacity (Smith, 2009). It is on
93 a Sun-synchronous orbit, but the local time coverage has varied over the past 20 years;
94 it sampled local times 7AM–7PM during Martian Year 34. Another important instru-
95 ment to add to this list was the Thermal Emission Spectrometer (TES) mounted on the
96 Mars Global Surveyor that operated between 1997 and 2006. It was a spectrometer rather
97 similar to PFS with a coarser spectral resolution of either 5 or 10 cm^{-1} , sensitive to the
98 temperature in the range 5–35 km, dust and water ice cloud opacities in nadir mode (Conrath
99 et al., 2000; Smith et al., 2000). It performed measurements at local times near 2 AM
100 and 2 PM and also operated systematically in limb geometry, allowing the retrieval of
101 atmospheric temperature up to 65 km.

102 Deriving those atmospheric quantities is of high interest to study the Martian cli-
103 mate at various spatial and temporal scales, from diurnal variations to inter-annual vari-
104 ations. These measurements have helped to broadly characterize the vertical and merid-
105 ional structure of atmospheric temperature, dust loading and water ice clouds (e.g., Smith
106 et al., 2001; McCleese et al., 2010; Giuranna et al., 2021), which in turn bring insights
107 onto Mars atmospheric dynamics. In particular, the TES and MCS retrieval products
108 have been used in several data assimilation studies (e.g., Steele et al., 2014; Navarro et
109 al., 2014; Greybush et al., 2019). More recently, these thermal infrared measurements
110 have brought new insights on the diurnal variability of dust and water ice clouds (Kleinböhl
111 et al., 2020; Smith, 2019a; Wolkenberg & Giuranna, 2021; Giuranna et al., 2021). How-
112 ever, developing a retrieval algorithm that performs well at all conditions (dust load, lo-
113 cal time, etc) is a challenge. Particular care has to be taken regarding the reliability of
114 aerosol retrievals from nadir sounders when the contrast between the surface tempera-
115 ture and atmospheric layer where the aerosols lie is low, as already raised by several pre-
116 vious studies (Pankine et al., 2013; Smith, 2019a, 2019b; Wolkenberg & Giuranna, 2021).

117 The objective of this paper is to document a retrieval algorithm developed at Lab-
118 oratoire de Météorologie Dynamique (LMD) for the analysis of TIRVIM observations,

119 to discuss some challenges identified and validate our retrievals against independent ob-
120 servations from MCS. We first detail characteristics of TIRVIM observations in section 2.
121 We describe our algorithm in section 3 and apply it to synthetic measurements gener-
122 ated for a great variety of scenes (latitudes, local time, surface temperature, aerosol con-
123 tent, topography) in section 4. Challenges arise due to the degeneracy in the inverse prob-
124 lem, especially regarding the combined retrieval of surface temperature, dust and wa-
125 ter ice optical depth. This algorithm is then applied to the first 45 sols of TIRVIM ob-
126 servations from mid-March to end of April 2018, as described in section 5. The retrieved
127 temperature profiles are compared to co-located MCS observations near 3 AM and 3 PM
128 to perform a cross-validation of our retrievals and evaluate potential biases. A first as-
129 sessment of the quality of dust retrievals is also included. Detailed discussion regarding
130 the diurnal temperature variations derived from TIRVIM observations is deferred to an-
131 other paper. We conclude on the performance of TIRVIM and on our algorithm in sec-
132 tion 6.

133 2 ACS/TIRVIM nadir measurements

134 2.1 Instrument characteristics

135 TIRVIM is a double-pendulum Fourier-transform spectrometer sensitive in the spec-
136 tral range 1.7 to 17 μm (600 – 5200 cm^{-1}). It operates routinely in nadir-viewing ge-
137 ometry and can also operate in solar occultation mode; the former type is the focus of
138 this paper. In nadir geometry, spectra are only exploitable between 620 and 1300 cm^{-1} ,
139 as thermal emission from the surface and atmosphere quickly drops beyond 1000 cm^{-1} .
140 In this geometry, the apodized spectral resolution is 1.2 cm^{-1} and the integration time
141 for a single interferogram is 0.4 seconds. The individual projected field of view on Mars
142 from TGO’s circular orbit for a single observation is 14 km cross-track \times 16 km along-
143 track, accounting for the small (4 km/s) smearing due to the spacecraft’s motion dur-
144 ing acquisition. Further details on TIRVIM technical characteristics can be found in Korablev
145 et al. (2018).

146 2.2 Calibration and instrumental issues

147 Generation of calibrated spectra from raw interferograms is done at the Space Re-
148 search Institute (IKI) in Moscow, Russia. Absolute radiometric calibration was facili-

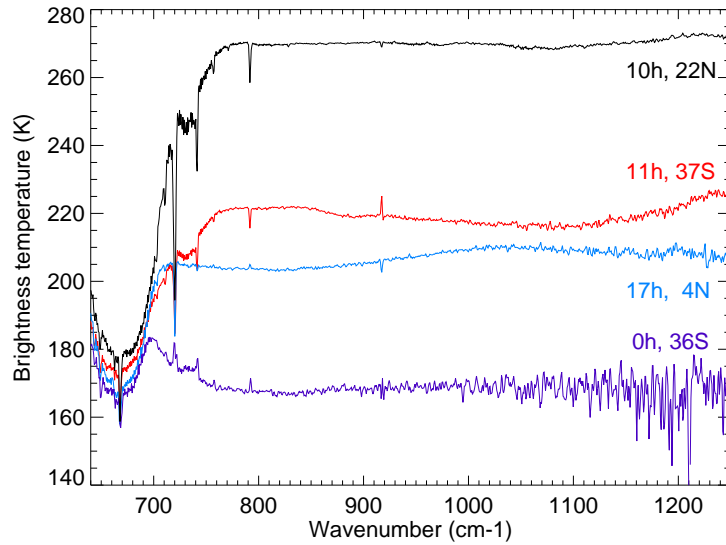


Figure 1. Examples of TIRVIM spectra acquired in March 2018 at four latitudes and local times, with different surface temperatures. They were acquired in the onboard averaging mode, where 8 interferograms were averaged by the instrument software onboard TIRVIM. Absorption by dust centered at 1090 cm^{-1} is particularly visible in the spectrum at 37°S , 11h (in red), while absorption by water ice clouds centered at 820 cm^{-1} is visible in the spectrum acquired at 4°N , 17h (in blue). An electric spike, which is an artifact, can be seen near 920 cm^{-1} .

149 tated by routine periodical measurements of the internal calibration black body and of
 150 the cold space. TIRVIM turned out to be an IR Fourier transform spectrometer with a
 151 source-dependent phase function. Radiometric calibration of such an instrument was con-
 152 sidered by Revercomb et al. (1988).

153 Ahead of the beginning of TIRVIM science operations, the chosen strategy to re-
 154 lay the data was to perform an on-board averaging of 8 consecutive interferograms in
 155 order to increase the signal-to-noise ratio (SNR). This was justified by the fact that the
 156 individual interferograms are recorded at very close locations on Mars, hence surface and
 157 atmospheric variables should not vary much amongst 8 sequential acquisitions. This on-
 158 board averaging mode was used for the first five months of the mission (except for the
 159 very first six days, where individual interferograms were relayed). However, the onboard
 160 interferogram averaging appeared to be sometimes incorrect. Interferograms must be aligned
 161 in the path difference space before averaging. The onboard TIRVIM software aligned in-
 162 terferograms before averaging according to their maxima. Since the source was chang-

163 ing, and the instrument had a source dependent phase, maxima of the interferograms
 164 did not always correspond to the same path difference. In such cases, the average inter-
 165 ferogram and therefore calibrated spectral radiance was incorrect. Those cases were flagged
 166 as poor-quality data and were excluded from our analysis. They could represent up to
 167 20% of all measurements. Fortunately, the other $\sim 80\%$ are of good quality and are ex-
 168 ploited in this paper. The corresponding field of view of the averaged interferograms is
 169 approximately 25×105 km. To limit data loss, this mode was later abandoned in favor
 170 of recording and relaying each individual interferograms. The drawback was the reduced
 171 signal-to-noise ratio (down to 3 times) and a higher data rate from the spacecraft. Among
 172 the other known issues in the calibrated spectra is an electrical spike near 920 cm^{-1} (that
 173 is excluded from our analysis).

174 Examples of TIRVIM spectra acquired in March 2018 at different local times and
 175 latitudes are shown in units of brightness temperature in Figure 1. Apart from the near
 176 blackbody surface emission, these spectra are dominated by the atmospheric CO_2 ab-
 177 sorption band centered at 667 cm^{-1} (sometimes visible in emission, when the atmosphere
 178 is warmer than the surface), a broad water ice feature centered at 820 cm^{-1} and a broad
 179 dust feature centered at 1090 cm^{-1} . We emphasize here that the left wing of the broad
 180 CO_2 absorption band is almost not captured by TIRVIM (unlike PFS). Apart from a
 181 few particular cases (mentioned later), this does not hamper the atmospheric temper-
 182 ature retrievals.

183 The Noise Equivalent Radiance (NER) of a calibrated spectrum obtained without
 184 interferogram averaging is of the order of $0.4 \times 10^{-7} \text{ W cm}^{-2} \text{sr}^{-1} / \text{cm}^{-1}$ for most of the
 185 spectral range, and increases near the edge of our spectral domain: it reaches $1.2 \times 10^{-7} \text{ W cm}^{-2} \text{sr}^{-1} / \text{cm}^{-1}$
 186 at 660 cm^{-1} and $0.8 \times 10^{-7} \text{ W cm}^{-2} \text{sr}^{-1} / \text{cm}^{-1}$ at 1300 cm^{-1} . These values are compa-
 187 rable to the NER of PFS spectra at 600 cm^{-1} but are up to 10 times lower than PFS
 188 NER at 1300 cm^{-1} (Giuranna et al., 2005). The resulting signal-to-noise ratio strongly
 189 depends on the Martian surface (or atmospheric) temperature and wavenumber. Fig-
 190 ure 2 illustrates these SNR variations: for a warm surface (eg. 280K) the SNR is in the
 191 range 30–200, depending on wavenumber, while for a colder surface (eg. 190K), the SNR
 192 is typically ten times lower. An exception is for wavenumbers $650\text{--}700 \text{ cm}^{-1}$, where sur-
 193 face emission does not contribute to the measured thermal emission from space and for
 194 which the SNR depends on atmospheric temperature, which varies less dramatically than
 195 the surface temperature. In this wavenumber range, the SNR is of the order of 30–100.

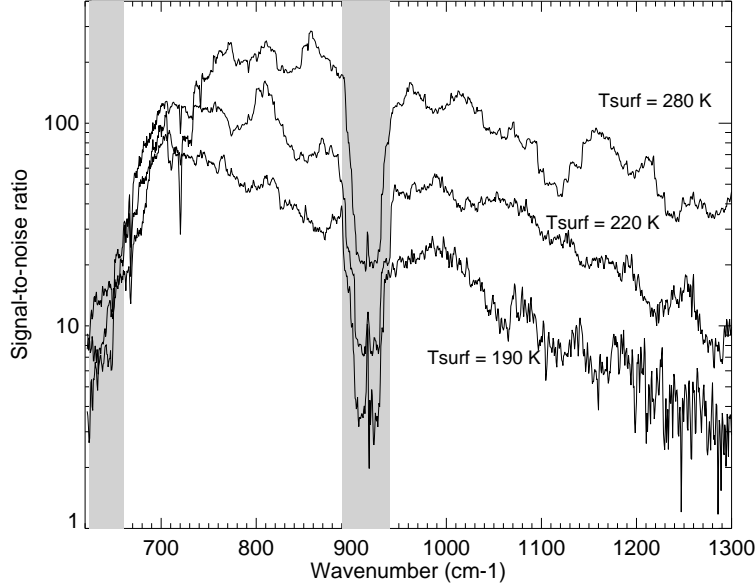


Figure 2. Signal-to-noise ratio for three individual spectra (no onboard averaging) acquired in October 2018, for which the retrieved surface temperature was 190K, 220K and 280K, as labeled. Note that the SNR is similar for the three spectra in the range $660\text{--}700\text{ cm}^{-1}$, as in this spectral range, the outgoing thermal radiation depends on the atmospheric temperature and not on surface temperature. The two grey shaded areas have large noise levels (low SNR) while not being essential to our analysis and are thus excluded. One corresponds to the left edge of the spectrum ($620\text{--}660\text{ cm}^{-1}$), the other one to an electric spike centered at 920 cm^{-1} .

196 If we consider spectra resulting from the onboard averaging of 8 interferograms, the afore-
 197 mentioned SNR values are multiplied by ~ 3 .

198 In this paper, we will include analysis of spectra acquired in both modes, predom-
 199 inantly the averaging mode. We will see that good performances are achieved with this
 200 mode. The calibration version we use is referred to as version 4, where orbit-average black
 201 body and space interferograms are used for calibration.

202 **2.3 Spatiotemporal coverage of TIRVIM nadir measurements**

203 The ExoMars Trace Gas Orbiter is set on a near-circular orbit at 400-km altitude
 204 with an inclination of 74° (implying that nadir observations cannot be made at latitudes
 205 poleward of 74°). TGO executes 12 orbits per (Earth) day, hence sampling 24 different

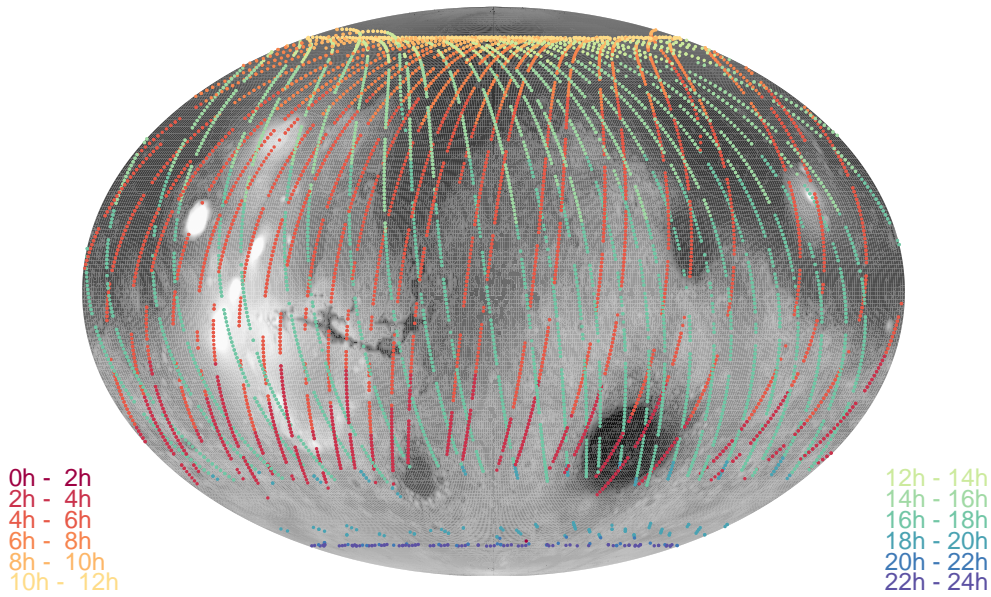


Figure 3. Coverage of TIRVIM nadir observations acquired on the 26th, 27th and 28th of March 2018, showing here only data that passed a set of initial quality filters. Different colors refer to the local time, as labeled. TGO’s orbit is such that the local time of TIRVIM observations shifts by ~ 13 minutes earlier every sol.

206 longitudes per day at a given latitude. An example of the coverage obtained after three
 207 days (36 orbits of TGO) is shown in Figure 3. At low latitudes, on this short time pe-
 208 riod, mostly two local times are sampled. However, TGO is not in a Sun-synchronous
 209 configuration: rather, the local time coverage slightly drifts earlier each day in such a
 210 way that after 54 sols (corresponding to 25° – 35° of Ls, depending on season), the diur-
 211 nal cycle has been evenly sampled in local times over the whole planet – providing that
 212 TIRVIM is operating continuously. The revisit time for a given (latitude, longitude, lo-
 213 cal time) targeted point on Mars is actually 108 sols ; however, if we consider an area
 214 of $\sim 5^\circ \times 5^\circ$, a 54-sol observation period provides coverage at all local times and is rele-
 215 vant for studying diurnal variations (with the caveat that $\sim 30^\circ$ of solar longitude has passed).

216 A Stirling cryo-cooler ensured the stability of the detector operating temperature
 217 at 65–75K. Several overheating events occurred in the first months of the mission, which
 218 required the cooler to be switched off for several weeks, which meant the absence of mean-
 219 ingful data. TIRVIM started its routine nadir observations on March 13, 2018 but en-

220 countered an issue with the stability controller of the double pendulum movement on
 221 April 28, 2018, which caused dramatic loss of the data quality. It resumed its quality ob-
 222 servations on May 26, 2018 until an overheating event occurred on July 15, 2018. Af-
 223 ter that, overheating events became more frequent. To overcome these issues, from Septem-
 224 ber, 2018 onwards, an automatic switch off of the cryo-cooler was programmed if its tem-
 225 perature exceeded 14°C. Another limitation stemmed from the lifetime of the Stirling
 226 cryo-cooler, which was estimated to last 10 000 hours (it actually operated 8,000 hours
 227 before failing in December, 2019). If TIRVIM had been switched ON all the time, then
 228 the cooler would have stopped functioning after 10 months. In order to mitigate this ef-
 229 fect, a duty cycle of ~50% was undertaken in October, 2018 at which time TIRVIM ac-
 230 quired data roughly 2 days out of 7, except for one 9-day long acquisition every month.
 231 This observing strategy largely prevented overheating events from occurring, and allowed
 232 TIRVIM to acquire data over almost a full martian year. In this paper, we will report
 233 in section 5 on the analysis of the first 45 days of TIRVIM data during March-April, 2018.

234 3 Retrieval algorithm

235 TIRVIM spectra contain information on the surface temperature, on the vertical
 236 profile of atmospheric temperature between a few kilometers above the surface and ~50 km
 237 (or 2–3 Pa) and on the column integrated opacity of dust and water ice clouds. We aim
 238 at retrieving simultaneously these quantities by exploiting TIRVIM spectra between 660
 239 and 1300 cm^{-1} . Our algorithm comprises a forward radiative transfer model used to gen-
 240 erate synthetic observations, coupled with a constrained linear inverse model, described
 241 below.

242 3.1 Radiative transfer model

243 Our forward radiative transfer model computes the spectral radiance I_ν of the out-
 244 going thermal emission of Mars' surface and atmosphere, neglecting scattering contri-
 245 butions, in the plane-parallel approximation :

$$I_\nu(\tau = 0, \mu) = \epsilon_\nu B_\nu(T_{\text{surf}}) e^{-\tau_{\text{total}}/\mu} + \frac{1}{\mu} \int_0^{\tau_{\text{total}}} B_\nu(T(\tau')) e^{-\tau'/\mu} d\tau' \quad (1)$$

246 with $\mu = 1/\cos(\theta)$ the airmass at an emission angle θ ; ϵ_ν the surface emissivity; B_ν
 247 the Planck function, τ' the partial integrated optical depth from the top of the atmo-

248 sphere to a given pressure level, T_{surf} the surface temperature and T the atmospheric
 249 temperature at a given pressure level. Our model atmosphere is discretized into 45 ver-
 250 tical sigma-levels, with the first level just above the surface. Hence, rather than using
 251 a fixed pressure grid, our pressure grid is tuned to local surface pressure to adapt to the
 252 topography. Radiances from TIRVIM and those calculated from equation 1 are converted
 253 in brightness temperatures $T_{B,\nu}$. Unless stated otherwise, in the following, we work in
 254 brightness temperature units and not radiances.

255 We use a line-by-line approach, where spectra are first computed at a high spec-
 256 tral resolution of 0.01 cm^{-1} , and are then convolved at the resolution of the instrument.
 257 TIRVIM spectra are apodized with a Hamming function and we use the appropriate in-
 258 strument function for this convolution. Note that the sampling is 0.645 cm^{-1} and the
 259 corresponding spectral resolution (full width at half maximum) is of 1.2 cm^{-1} . We take
 260 into account opacity from atmospheric CO_2 gas, dust and water ice clouds. Line-by-line,
 261 CO_2 absorption coefficients are tabulated offline for a set of 45 reference pressures equally
 262 spaced in natural logarithm space (from 1260 Pa to 5×10^{-3} Pa) and 12 temperatures.
 263 These sets of 12 reference temperature values themselves depend on pressure and are sam-
 264 pled to encompass climatological conditions over a full martian year, including global
 265 dust storm conditions with warmer temperatures. For instance, near the surface ($p > 300$
 266 Pa), reference temperature values range from 150K to 260K, every 10K while at 10 Pa,
 267 these levels comprise ten levels sampled from 100 to 190K (every 10K) plus two extra
 268 levels at 210K and 230K. These computations use the HITRAN 2016 spectroscopic database
 269 (Gordon et al., 2017). We tested another set of CO_2 coefficients generated from the GEISA
 270 2015 linelist (Jacquinet-Husson et al., 2016) and found that it yielded similar spectra,
 271 as far as the CO_2 $15 \mu\text{m}$ band is concerned. The temperature dependence of the line width
 272 due to pressure broadening is not taken from the HITRAN database (as it corresponds
 273 to air broadening) but instead is adapted for a CO_2 atmosphere. It is computed for each
 274 transition, as a function of the rotational quantum number J , based on values tabulated
 275 by Lamouroux et al. (2012). Furthermore, pressure broadening is not represented by a
 276 standard Lorentz function. Rather, we adopt an asymmetric sub-Lorentzian profile, which
 277 empirically takes into account the effects of collisional line mixing and the finite dura-
 278 tion of collisions. These line shapes are represented by a Lorentz function multiplied by
 279 a factor χ that depends on the distance from the line center and was derived from ex-
 280 perimental work relevant for the $4.3\text{-}\mu\text{m}$ CO_2 band (Perrin & Hartmann, 1989). We as-

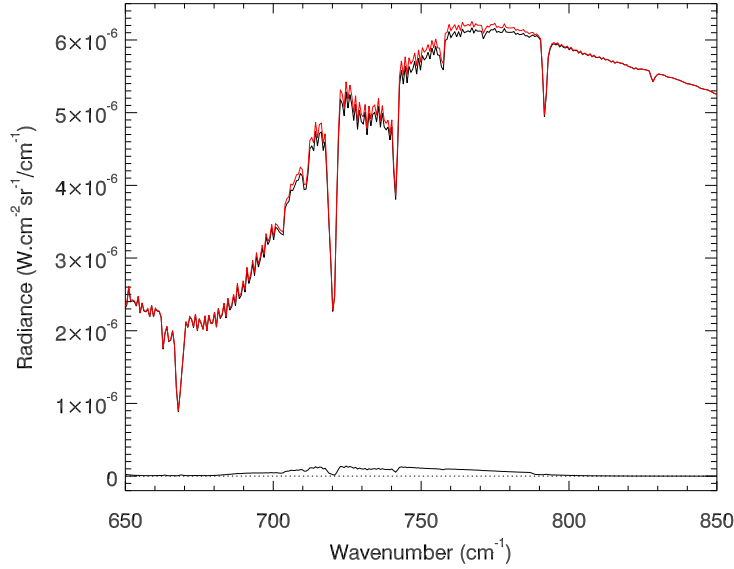


Figure 4. Synthetic TIRVIM spectra focusing here on the CO₂ band, assuming (in black) a Lorentz line profile or (in red) a sub-Lorentzian line profile to empirically take into account the effects of collisional line mixing and the finite duration of collisions, based on experimental work by Perrin and Hartmann (1989). The difference between the two spectra is plotted at the bottom.

281 sume that these χ factors can also be used for the 15- μm CO₂ band. The final line shape
 282 is obtained by a convolution of the sub-Lorentzian profile with a Gaussian profile (that
 283 represents Doppler broadening of the lines). An example of synthetic TIRVIM spectra
 284 is shown in Figure 4, which compares spectra computed with a Lorentz function or the
 285 sub-Lorentzian line profile. In this example, the radiance is increased by 1–2 % (hence,
 286 1 to 2- σ above the noise level) in the range 700–780 cm^{-1} when a sub-Lorentzian line
 287 profile is adopted. This effect is noticeable, but its influence is small regarding atmospheric
 288 temperature retrievals (typically $\sim 1\text{--}2$ K).

289 Extinction coefficients Q_{ext} for water ice particles are computed offline using Mie
 290 theory, assuming a log-normal size distribution, an effective radius r_{eff} of 1.45 μm , a vari-
 291 ance of 0.1 and optical constants from Warren (1984). Particle sizes of typically 1 to 3.5 μm
 292 are most frequently observed, as determined from CRISM observations (Guzewich & Smith,
 293 2019) or from MGS TES (Clancy et al., 2003). Assuming a single particle size for wa-
 294 ter ice clouds in our radiative transfer model should not affect our retrievals of the cloud

295 integrated optical depth because it is sensitive to the ratio $Q_{\text{ext}}/r_{\text{eff}}$. Indeed, the latter
296 quantity varies by less than 10% for particles sizes in the range 1–3.5 μm . Hence, the
297 uncertainty on total cloud opacity related to a wrong assumption of particle sizes should
298 be on the order of 10%.

299 Regarding dust particles, their extinction coefficients are computed from a T-matrix
300 code using an effective radius r_{eff} of 1.5 μm , a variance of 0.3 and optical constants de-
301 rived from CRISM observations by Wolff et al. (2009), which also used a T-matrix code
302 in the analysis. Particle effective sizes of 1–2 μm with a variance of the size distribution
303 of 0.2–0.4 are the most frequently observed (see review by Kahre et al. (2017) and re-
304 cent results from solar occultations recorded by ACS and analysed by Luginin et al. (2020)).
305 Changing the dust particle radius to 1 μm or 2 μm affects the ratio $Q_{\text{ext}}/r_{\text{eff}}$ by less than
306 10%, hence the uncertainty on total dust opacity linked to assuming a constant dust par-
307 ticle radius of 1.5 μm remains small as well ($< 10\%$).

308 Dust is assumed to be well-mixed (ie., with a constant mass mixing ratio) in the
309 first two scale heights above the surface, then its mixing ratio decreases linearly with height
310 (log-pressure, to be precise). The vertical profile of ice mixing ratio is parameterized by
311 a Gaussian profile centred at a condensation level that can either be set arbitrarily, or
312 is computed by combining knowledge on the temperature profile (being retrieved simul-
313 taneously) and the water vapor column, taken from the Thermal Emission Spectrom-
314 eter (TES) climatology (Smith, 2004). More information on the choice for *a priori* pa-
315 rameters for dust and water ice clouds is given in section 3.2.4. As we neglect scatter-
316 ing effects, our retrieved quantities are "effective" dust and water ice absorption. The
317 error induced by neglecting scattering was previously estimated by Smith (2004). The
318 authors ran tests including or not scattering effects and concluded that the actual ex-
319 tinction optical depth was approximately 1.3 and 1.5 times as large as the "effective" ab-
320 sorption optical depth for dust and water ice, respectively. Their work was based on the
321 same dust and ice features as ours, i.e. at 1075 and 825 cm^{-1} , and similar particle sizes.
322 Similar factors between absorption and extinction values were found by Wolff and Clancy
323 (2003).

324 Additional ancillary data are needed to compute synthetic spectra. For each TIRVIM
325 measurement, surface pressure is extracted at the corresponding season, local time and
326 location from the Mars Climate Database (MCD) version 5.3 (Millour et al., 2018) us-

327 ing the surface pressure predictor described in Forget et al. (2007). The latter exploit
328 high resolution MOLA (32 pixels/degree) topography. The CO₂ mixing ratio vertical pro-
329 file is also extracted from the MCD. Spectral surface emissivity for each observation is
330 interpolated from TES spectral emissivity map (Bandfield & Smith, 2003). As informa-
331 tion within the CO₂ band is missing, we adopt a simple linear interpolation of surface
332 emissivity in this spectral range. An error in surface emissivity in this region should not
333 impact our results, as the contribution from the surface to the outgoing thermal emis-
334 sion is negligible in this spectral range of strong CO₂ absorption.

335 3.2 Retrieval algorithm

336 The overall goal is to find a set of parameters (vertical profile of temperature, sur-
337 face temperature, integrated opacity of aerosols) that produces a synthetic spectrum (us-
338 ing the aforementioned forward radiative transfer model) in close agreement with a TIRVIM
339 spectrum, within noise levels. As we are facing an ill-posed and underconstrained inverse
340 problem, there exists a strong degeneracy of this set of parameters, including potentially
341 non-physical solutions that could still match the observed spectra. In order to regular-
342 ize the inverse problem, we choose the widely-used framework of optimal estimation re-
343 trieval, described in Rodgers (2000). In this framework, the cost function to be minimized
344 includes not only the evaluation of goodness-of-fit to the data (χ^2), but also an additional
345 regularization term that should contain our best *a priori* physical knowledge on the de-
346 sired quantities. To be more accurate, we use the same choice of cost function as Conrath
347 et al. (2000) that is slightly different from that described in Rodgers (2000) (see next sub-
348 section). The choice of the *a priori* values together with their covariance matrix is not
349 trivial, though, requiring a certain level of trial-and-error process.

350 We detail below the retrieval scheme for atmospheric temperature on the one hand,
351 surface temperature and aerosols on the other hand, and will lastly describe how they
352 are combined with a detailed description of the different steps of our algorithm.

353 3.2.1 Atmospheric temperature retrieval scheme

354 Regarding the retrieval of temperature vertical profiles, we adopt the same approach
355 as Conrath et al. (2000) for the analysis of the TES/MGS data, also successfully applied

356 to PFS/Mars Express data by Fouchet et al. (2007). A first guess temperature profile
 357 T_a is iteratively modified following this equation:

$$\mathbf{T}_{n+1} = \mathbf{T}_a + \mathbf{W}(\Delta\mathbf{T}_b + \mathbf{K}(\mathbf{T}_n - \mathbf{T}_a)) \quad (2)$$

$$\mathbf{W} = \mathbf{S}_a \mathbf{K}^T (\mathbf{K} \mathbf{S}_a \mathbf{K}^T + \frac{1}{\alpha} \mathbf{S}_e)^{-1} \quad (3)$$

358 where \mathbf{T}_n is the temperature profile at iteration n , $\Delta\mathbf{T}_b$ the difference between the
 359 synthetic spectrum (in brightness temperature) computed with temperature \mathbf{T}_n and the
 360 TIRVIM one, \mathbf{K} is the functional derivative matrix, with elements K_{ij} defined as the deriva-
 361 tive of the brightness temperature at wavenumber i over the temperature at a pressure
 362 level j ($K_{ij} = \frac{dT_i}{dT_j}$), \mathbf{S}_a the covariance matrix for the *a priori* temperature profile, and
 363 \mathbf{S}_e the error covariance matrix, whose diagonal elements contain the squared wavenumber-
 364 dependent NER of TIRVIM spectra. Finally, α is a parameter used to assign more or
 365 less weight to the observations with respect to our *a priori* knowledge. Based on sev-
 366 eral tests on retrievals on both synthetic and actual TIRVIM data, we find that a value
 367 of $\alpha = \beta \times \frac{\text{trace}(\mathbf{S}_e)}{\text{trace}(\mathbf{K} \mathbf{S}_a \mathbf{K}^T)}$, with a nominal value of 3 for β , yields satisfactory results.

368 3.2.2 Information content for the temperature

369 Only a portion of a TIRVIM spectrum is exploited in equations 2 and 3, as infor-
 370 mation on the atmospheric temperature comes from the CO₂ band in the range 660–780 cm⁻¹
 371 (recall that we exclude data in the range 620–660 cm⁻¹ due to low signal-to-noise ra-
 372 tio). Actually, within this spectral range, there exists a strong redundancy in the infor-
 373 mation content, where contribution functions at different wavenumbers peak at the same
 374 pressure level. While some level of redundancy is desirable (because of noise in the data),
 375 all individual spectral measurements within this range are not needed to achieve a sat-
 376 isfactory temperature profile retrieval. Hence, in order to reduce computation time, we
 377 select 50 out of the 177 wavenumbers in TIRVIM spectra in the range 660–780 cm⁻¹.
 378 This reduces the matrix size of \mathbf{K} , \mathbf{S}_e and $\Delta\mathbf{T}_b$ in equations 2 and 3. We keep all 14
 379 points between 665.3 cm⁻¹ and 673.7 cm⁻¹, then one every three points until 714.3 cm⁻¹,
 380 then one every five points up to 780 cm⁻¹. We emphasize that we have tested retrievals
 381 in different configurations (50 or 177 points in the CO₂ band) and confirm that retrieved
 382 temperature profiles are almost identical.

383 We present an example of the information content sampled by these 50 wavenum-
384 bers, as a function of pressure, in Figure 5 (examples at other latitudes and local times
385 will be given in section 4, focused on synthetic retrievals). The exact pressure levels at
386 which the functional derivatives peak and their relative amplitudes depend on the tem-
387 perature profile itself and on the aerosol load ; however, general trends can be drawn.
388 The radiance or brightness temperature at wavenumbers 670–780 cm^{-1} is mostly sen-
389 sitive to the atmospheric temperature at altitudes 4–35 km (20–400 Pa for a surface pres-
390 sure of 610 Pa). Despite having selected about a third of the spectral information in the
391 CO_2 band, we note that redundancy in functional derivatives peaking at similar levels
392 is still large. On the other hand, information on the temperature at altitudes 35–55 km
393 (2–20 Pa) exclusively comes from the two spectral points at the core of the CO_2 band,
394 at wavenumbers 667.7 and 668.4 cm^{-1} . We also notice that these two functional deriva-
395 tives have broader full width at half maximum (being about 15 km) compared to the con-
396 tribution functions peaking at 4–35 km, which have half-widths of ~ 10 km. This gives
397 a qualitative estimate of the vertical resolution of the retrieved profile, which varies be-
398 tween 1 scale height (in the lower troposphere) and 1.5 scale heights (in the middle tro-
399 posphere).

400 *3.2.3 Building the first guess temperature profile*

401 In a Bayesian approach, one possibility would be to compute both the *a priori* tem-
402 perature profile and its covariance matrix \mathbf{S}_a from a climatology of temperature profiles,
403 such as provided by the Mars Climate Database. The first guess can also be different from
404 the *a priori* temperature profile. This is the methodology employed for instance by Grassi
405 et al. (2005) for PFS data analysis. However, this method has its limits when atmospheric
406 conditions depart significantly from the "climate" scenario of the MCD (in the event of
407 a global dust event, for instance , see Wolkenberg et al., 2018). We choose instead the
408 same approach as Conrath et al. (2000): for each observation, we build the first guess
409 from TIRVIM spectra themselves. Furthermore, this first guess is chosen as our *a pri-*
410 *ori* profile. Hence, we are not here in a purely Bayesian formalism, as our *a priori* pro-
411 files already contain information from the spectra. The method of Conrath et al. (2000)
412 to build this first guess consists of computing a set of brightness temperatures from the
413 radiance at several wavenumbers within the CO_2 band (in our case, we use the set of 50
414 wavenumbers described above), corrected for atmospheric transmission and surface con-

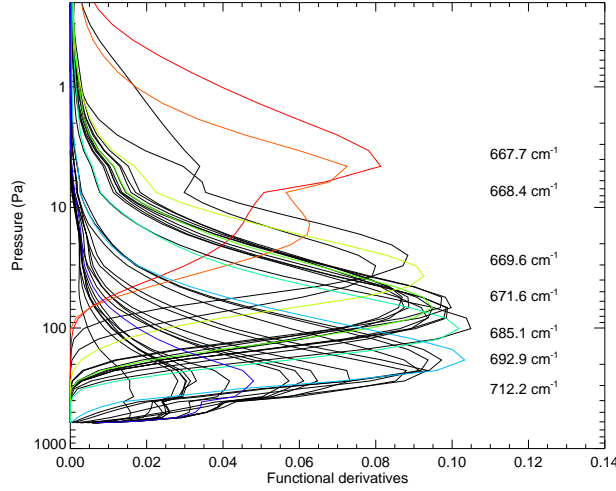


Figure 5. Functional derivatives of the temperature as a function of pressure, for fifty different wavenumbers in the range $665\text{--}780\text{ cm}^{-1}$. Seven out of fifty wavenumbers are highlighted in color and labeled. In general, TIRVIM spectra probe from lower to higher pressure regions starting from the core of the CO_2 band (at 667.7 cm^{-1}) to its wing. This example was generated for atmospheric conditions extracted from the Mars Climate Database for Martian Year 25, $L_s=180^\circ$, latitude 15°N and local time 9 AM.

415 tribution. This set of brightness temperatures is then attributed to different atmospheric
 416 pressure levels based on the contribution functions (see equations 13 and 14 of Conrath
 417 et al., 2000) to build a first rough temperature profile, typically constrained between 10
 418 and 40 km. This profile is then extrapolated upwards and downwards, using a method
 419 that differs from Conrath et al. (2000). For the upper part, we force the profile to smoothly
 420 go back to a climatology based on four martian years (MY29–MY33) of diurnal aver-
 421 ages of MCS temperature profiles, binned every 5° of L_s and 5° of latitude, zonally av-
 422 eraged. Regarding the extrapolation downwards, after several trials, we choose to im-
 423 pose the slope of the temperature profile in the first scale height based on an empirical
 424 relationship (determined from simulated synthetic spectra) between the temperature ver-
 425 tical gradient in the first scale height and the difference in brightness temperature be-
 426 tween 690 and 702 cm^{-1} . Finally, the entire profile is smoothed vertically by convolu-
 427 tion with a Gaussian function with a 0.75 scale height half width. Regarding the covari-
 428 ance matrix \mathbf{S}_a , it is defined like in Conrath et al. (2000) as to filter non-realistic ver-
 429 tical oscillations:

$$S_{\text{a}_{ij}} = \exp \left[-\frac{\log(p(i)/p(j))^2}{2c^2} \right] \quad (4)$$

with c a correlation length chosen nominally as 0.75 scale heights. Like β , this parameter c is read in an input file.

3.2.4 Surface temperature and aerosol retrieval scheme

We now focus on the range 780–1300 cm^{-1} of the spectra. The general idea is to iteratively update first guess values of the surface temperature T_{surf} and of the dust and water ice vertical mixing ratio profiles q_{d} and q_{i} by exploiting the calculated functional derivatives of the brightness temperature to these parameters (noted K_{Ts} , K_{qd} and K_{qi}). We emphasize that nadir spectra are generally not (or very weakly) sensitive to the vertical distribution of dust and water ice clouds, hence, we only retrieve a scaling factor to *a priori* profiles of their mixing ratio. The functional derivatives K_{qd} and K_{qi} we use actually relate to the change in brightness temperature associated with a *relative* change in q_{d} and q_{i} , rather than a change in absolute values of q_{d} and q_{i} . Minimization of a cost function leads to the following iterative increment in T_{surf} , q_{d} and q_{i} in the case of the simultaneous retrieval of all three quantities:

$$T_{\text{surf}(n+1)} = T_{\text{surf}(n)} + \sigma_{\text{Ts}} K_{\text{Ts}}^T Y \Delta I \quad (5a)$$

$$q_{\text{d}(n+1)} = q_{\text{d}(n)} (1 + \sigma_{\text{qd}} K_{\text{qd}}^T Y \Delta I) \quad (5b)$$

$$q_{\text{i}(n+1)} = q_{\text{i}(n)} (1 + \sigma_{\text{qi}} K_{\text{qi}}^T Y \Delta I) \quad (5c)$$

$$Y = \left(\sigma_{\text{Ts}} K_{\text{Ts}} K_{\text{Ts}}^T + \sigma_{\text{d}} K_{\text{qd}} K_{\text{qd}}^T + \sigma_{\text{i}} K_{\text{qi}} K_{\text{qi}}^T + \frac{1}{\gamma} S_e \right)^{-1} \quad (6)$$

where ΔI is the difference between the synthetic spectrum – computed with surface temperature $T_{\text{surf}(n)}$, aerosol mixing ratio profiles $q_{\text{d}(n)}$ and $q_{\text{i}(n)}$ – and the TIRVIM spectrum in the range 780–1300 cm^{-1} ; σ_{Ts} , σ_{d} and σ_{i} are the *a priori* covariance on surface temperature (set to 8K), dust and water ice cloud opacity (both set to a factor of three); and γ is a parameter used to assign more or less weight to the observations with respect to our *a priori* knowledge (determined similarly as α in equation 3). As for the atmospheric temperature retrieval, we do not use all spectral points in the retrieval of

451 these quantities, especially since dust and water ice exhibit smooth spectral features. A
452 set of 78 out of 805 spectral points in the range 785–1295 cm^{-1} was carefully selected
453 to optimize the information content and gain calculation time. This selection was based
454 on a study of the Jacobians for surface temperature, dust and water ice opacities (deriva-
455 tives of brightness temperature over these scalar quantities), computed for synthetic data.
456 We retain more points near the peaking values of these Jacobians (one point every ~ 3
457 cm^{-1}). Away from these regions of maximum information content, our sampling is sparser
458 (one point every $\sim 10 \text{ cm}^{-1}$).

459 We emphasize that dust and water ice cloud opacities cannot be retrieved at all
460 local times. This issue was already discussed e.g. by Smith (2019a) from the analysis of
461 THEMIS broadband thermal infrared images, and also by Wolkenberg et al. (2018) from
462 PFS/Mars Express spectra. The challenge in retrieving aerosol opacities from these nadir-
463 viewing instruments is that sensitivity to dust and/or water ice (given here by K_{qd} and
464 K_{qi}) tends to be zero in the event when most of the dust (or water ice) mass load lies
465 at altitudes where atmospheric temperature is close to surface temperature. In that case,
466 no absorption nor emission band will be visible in the spectra, irrespective of the aerosol
467 load, and we will not be able to determine the aerosols' opacity. This situation is mostly
468 encountered near 7–8 AM and 7–8 PM, as we will see in section 5.3. Of course, in the
469 event when there are no aerosol absorption or emission bands seen in TIRVIM data, but
470 at the same time the surface – atmosphere temperature contrast is high, even a small
471 amount of dust (or water ice) should have produced an absorption or emission feature,
472 hence we would confidently conclude that the atmosphere is clear.

473 We have also added the option to not retrieve a given variable among surface tem-
474 perature, dust and water ice opacity in case a TIRVIM spectrum is too noisy and does
475 not exhibit a clear dust or ice spectral feature. Indeed, we noticed that in such situa-
476 tions, our retrieval algorithm sometimes fitted the data (or rather, fitted the noise) with
477 a combination of values of surface temperature, dust or ice opacities that were unreal-
478 istic. Retrieving only a subset of parameters in this situation help regularize the inverse
479 problem. In more detail, we start by computing the standard deviation of TIRVIM bright-
480 ness temperature in the range 1210–1290 cm^{-1} as a proxy for the noise level (hereafter
481 called noise_{1250}). Indeed, beyond 1200 cm^{-1} , we find that the NER provided by the in-
482 strument team often underestimate the actual noise level so that we chose to estimate
483 it from the data itself in this rather flat (in brightness temperature) spectral region. We

484 then compute the contrast in TIRVIM average brightness temperature between the range
 485 1060–1130 cm^{-1} and the range 1225–1290 cm^{-1} (hereafter called $\text{contrast}_{\text{dust}}$) and the
 486 one between 810–860 cm^{-1} and 1225–1290 cm^{-1} (hereafter called $\text{contrast}_{\text{ice}}$). Differ-
 487 ent configurations are considered:

- 488 • If spectra are noisy (arbitrary threshold set to $\text{noise}_{1250} > 6\text{K}$) and $\text{contrast}_{\text{dust}}$ and
 489 $\text{contrast}_{\text{ice}}$ are smaller than noise_{1250} : we retrieve surface temperature only;
- 490 • If spectra are noisy and $\text{contrast}_{\text{dust}} < \text{noise}_{1250}$ and $\text{contrast}_{\text{ice}} > \text{noise}_{1250}$: we
 491 simultaneously retrieve surface temperature and water ice opacity;
- 492 • If spectra are noisy and $\text{contrast}_{\text{dust}} > \text{noise}_{1250}$ and $\text{contrast}_{\text{ice}} < \text{noise}_{1250}$: we
 493 simultaneously retrieve surface temperature and dust opacity;
- 494 • Else, we simultaneously retrieve surface temperature, dust and water ice opacity.

495 The retrieval of only one or two parameters among surface temperature, dust and wa-
 496 ter ice opacity follows the same form as equations 5a–6.

497 In order to evaluate the level of confidence we have on dust and water ice cloud re-
 498 trievals, we adopt a similar approach as Smith (2019a) and define the $1\text{-}\sigma$ relative error
 499 on dust opacity dust_{err} as the ratio between the $1\text{-}\sigma$ noise level (in brightness temper-
 500 ature; computed from the instrument NER estimates) at 1100 cm^{-1} and the functional
 501 derivative K_{qd} , computed at 1100 cm^{-1} as well. When this ratio equals one, this means
 502 that a 100% change in dust opacity results in a change in brightness temperature sim-
 503 ilar to the $1\text{-}\sigma$ noise level. In other words, the $1\text{-}\sigma$ error on dust opacity would be 100%
 504 in this case. We arbitrarily define a dust quality flag that considers only dust retrievals
 505 with dust_{err} values lower than one. Similarly, for ice, we define ice_{err} as the ratio between
 506 the noise level and K_{qi} , both estimated at 820 cm^{-1} . Examples of typical errors on dust
 507 and water ice cloud opacities will be detailed in section 4.

508 *3.2.5 Choice of a priori values for aerosols and setting of the cloud con-* 509 *densation level*

510 Another challenge is related to the fact that even though the functional derivatives
 511 used in the retrieval in equation 5a–5c are updated at each iteration, they are themselves
 512 first computed based on prior information on the vertical distribution of dust and wa-
 513 ter ice clouds that can be erroneous and hamper our retrievals. For instance, if we *a pri-*

514 *ori* assume that a cloud lies at an altitude where atmospheric temperature is warmer than
 515 the surface temperature, the functional derivative K_{q_i} will be positive in sign (the cloud
 516 is assumed to be seen in emission). However, if the cloud is actually at an altitude where
 517 atmospheric temperature is colder than the surface (i.e. the cloud is seen in absorption
 518 in TIRVIM data), the retrieval scheme will fail to reproduce the observed absorption band
 519 as we only retrieve a scaling factor to an initial mixing ratio profile. This actually im-
 520 plies that there are situations where we can say that TIRVIM spectra contain some level
 521 of information on the cloud altitude. This piece of information has to be exploited, if pos-
 522 sible. More generally speaking, the choice of *a priori* values for the vertical distribution
 523 of q_d and q_i can strongly influence our results while in the case of atmospheric temper-
 524 ature retrieval, this choice is less critical.

525 While dust is rather ubiquitous, water ice clouds can be discrete and exhibit a greater
 526 spatio-temporal variability than dust, which makes their choice of *a priori* properties not
 527 trivial. It would be tempting to run several retrievals for each observation, starting from
 528 different *a priori* values for dust and ice opacities, assuming different cloud condensa-
 529 tion levels, and then select *a posteriori* the solution (or solutions) that best match the
 530 considered TIRVIM spectrum. However, this would be too costly in computation time.
 531 We thus choose an intermediate path: in a first stage of our algorithm, we explore var-
 532 ious combinations of dust opacities ($\tau_{\text{dust}}=0.1, 0.3, 0.6$), ice opacities ($\tau_{\text{ice}}=0.1, 0.3, 0.7,$
 533 1.5 and 4) and cloud altitudes (three different values, among which the condensation level
 534 derived from TES water vapor climatology). We exclude combinations that are not re-
 535 alistic, e.g. large values of τ_{ice} at high altitudes. For each combination, we compute a
 536 first guess synthetic spectrum in the range $800\text{--}1290\text{ cm}^{-1}$. To compute these spectra,
 537 the surface temperature is evaluated directly from the brightness temperature of TIRVIM
 538 spectra in the range $1240\text{--}1290\text{ cm}^{-1}$, a portion of the spectrum that is rather transpar-
 539 ent. We pick up the combination of parameters that best match the considered TIRVIM
 540 spectrum at this stage as *a priori* values, and then start a retrieval. This way, we make
 541 sure to start our retrievals with prior values that match basic features of TIRVIM data
 542 (dust or ice seen in emission or absorption ; hints for a clear or a high dust load in the
 543 atmosphere, for instance) and hence, with sensible values of K_{q_d} and K_{q_i} .

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3.3 Algorithm steps

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The different steps of our algorithm, including those dealing with the special cases mentioned above, and the link between the retrieval of aerosol opacities, surface and atmospheric temperature, are summarized in this section.

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First, a pre-processing step discards observations with known issues and extract ancillary data (surface pressure and CO₂ profile from the MCD, surface emissivity and climatological water vapor from TES, temperatures from MCS climatology, etc). One NetCDF file per TGO orbit is created, which contains TIRVIM spectra with the aforementioned ancillary information. Typically, one file contains hundreds to thousands of spectra. After this pre-processing step, the retrieval algorithm works as follows :

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1. Read in the NetCDF file and a list of optional parameters in a text-format input file, begin loop on all observations within this file.
2. Assuming a small dust and water ice opacity (0.03), build first guess temperature profile from the spectrum and compute the condensation level $p_{\text{cond TES}}$ of water ice clouds, based on this first guess profile and TES water vapor climatology.
3. Compute noise_{1250} , $\text{contrast}_{\text{dust}}$ and $\text{contrast}_{\text{ice}}$.
4. If both absolute values of $\text{contrast}_{\text{dust}}$ and $\text{contrast}_{\text{ice}}$ are smaller than noise_{1250} , go to step 8 (the spectrum is considered \sim flat and there is no need to explore a range of first guess values), else continue.
5. Build a family of possible and realistic combinations of τ_{dust} , τ_{ice} , p_{cond} (among which the condensation level $p_{\text{cond TES}}$ determined above, but also encompassing potential lower and/or upper cloud, depending on the first value $p_{\text{cond TES}}$).
6. For each of the above combinations: build the corresponding first guess temperature profile from TIRVIM spectrum in the range 660–740 cm^{-1} ; estimate surface temperature from TIRVIM spectrum in the range 1240–1290 cm^{-1} ; compute a first synthetic spectrum; compare with the TIRVIM spectrum and store the corresponding χ^2 .
7. Select the combination of first guess values for $(\tau_{\text{dust}}, \tau_{\text{ice}}, p_{\text{cond}})$ corresponding to the minimum χ^2 ; keep the corresponding surface and atmospheric temperatures as first guesses as well.
8. Compute a first synthetic spectrum with the first guess values, this time along with the computation of the functional derivatives for all quantities. Initialize χ^2 .

- 576 9. Start a retrieval loop. Different configurations are considered.
- 577 • If spectra are noisy and $\text{contrast}_{\text{dust}}$ and $\text{contrast}_{\text{ice}}$ are smaller than noise_{1250} :
578 make one step of surface temperature retrieval only;
 - 579 • If spectra are noisy and $\text{contrast}_{\text{dust}} < \text{noise}_{1250}$ and $\text{contrast}_{\text{ice}} > \text{noise}_{1250}$:
580 make one step of simultaneous surface temperature and water ice opacity re-
581 trieval;
 - 582 • If spectra are noisy and $\text{contrast}_{\text{dust}} > \text{noise}_{1250}$ and $\text{contrast}_{\text{ice}} < \text{noise}_{1250}$:
583 make one step of simultaneous surface temperature and dust opacity retrieval;
 - 584 • Else: make one step of simultaneous surface temperature, dust and water ice
585 opacity retrieval following eq. 5a–5c.
- 586 10. Re-compute a synthetic spectrum with updated quantities (surface temperature
587 and / or τ_{dust} and / or τ_{ice}), calculate the functional derivatives for atmospheric
588 temperature.
- 589 11. Make one step of atmospheric temperature retrieval following eq. 2.
- 590 12. Re-compute a synthetic spectrum with updated atmospheric temperature, then
591 update χ^2 : if the change in χ^2 compared to the previous value is less than 2%, or
592 if the number of iteration is > 9 , then: end the retrieval loop, write outputs and
593 go on with the next observation; else go back to step 9.

594 A solution is reached most of the time in 4 or 5 iterations. Even though only a frac-
595 tion of the TIRVIM spectrum is exploited in equations 2, 5a–5c and in χ^2 calculations,
596 we do compute a synthetic spectrum on the full spectral range of TIRVIM after conver-
597 gence, that we keep for quality checks.

598 Our algorithm is not Bayesian, in particular as the so called *a priori* temperature
599 profile already contains information from the data themselves. We note that it is also
600 the case for the reference algorithm used for MGS/TES data, developed by Conrath et
601 al. (2000). Rapid convergence is achieved mostly because we start the retrievals from first
602 guess values already close to the "true" atmospheric state; however, in the next section,
603 we will also show examples starting from different *a priori* profiles to demonstrate that
604 our code still performs well in these conditions.

4 Synthetic retrievals and error analysis

4.1 Synthetic observations and approach

The precise tuning of the retrieval algorithm described previously results from several phases of trials and development, depending on how well the algorithm performs against synthetic measurements. To build these synthetic observations, we extract surface pressure, surface and atmospheric temperature as well as aerosol mixing ratio profiles from the Mars Climate Database for the scenario corresponding to Martian Year 25. We choose this year as it features a global dust event at Ls 190–240° (Smith et al., 2002). We extract these data at longitude 0° for various conditions: at five seasons (Ls= 0, 90, 180, 210 and 270°), 8 local times (every three hours) and 11 latitudes (from 75S to 75N, every 15°), hence 440 spectra in total. We then generate synthetic TIRVIM spectra with our forward model, then add noise (with realistic spectral dependency of the noise), and run our retrieval algorithm. This exercise is often referred to in the literature as an Observing System Simulation Experiment (OSSE).

Generally speaking, this exercise allows to test the sensitivity to, for instance, assuming a different vertical profile of dust and water ice clouds in the retrieval set-up compared to the forward model used to generate the synthetic data, and its impact on the retrieved quantities. It is also useful to identify flaws in our retrieval pipeline, fine-tune the sampling in wavenumber and refine our error analysis. We do not test the sensitivity of the retrieved quantities to an error in surface pressure, surface emissivity, spectroscopic database or aerosol particle sizes: these parameters are the same in the forward model and retrieval pipeline. Hence, the only forward model error that we consider comes from the different vertical mixing ratio profiles assumed for dust and water ice. Despite this quite favorable setting, we will see that many challenges arose solely due to the intrinsic degeneracy of the inverse problem and/or noise in the spectra.

4.2 Robustness of the synthetic retrievals: aerosols

Overall, synthetic retrievals perform quite as expected: cases with a warm surface temperature (hence high SNR) yield the most robust results for all retrieved parameters. For such cases, the integrated opacities of dust and water ice clouds are well estimated even if the assumed simplified vertical distributions of aerosols differs from the "actual" one (taken from the MCD), thanks to the large surface-atmosphere tempera-

636 ture contrast. A typical example of such a favorable case, with a surface temperature
637 of 285K, is presented in Figure 6.

638 For surface temperatures lower than 230K, the fraction of retrievals that fail to cor-
639 rectly retrieve dust and water ice opacity increases. These unsatisfactory cases fall in two
640 categories: either the quality criterion for dust or ice retrieval (defined in section 3.2.4)
641 is not met, or this criterion is met (in the sense that we consider there is enough sen-
642 sitivity to ice or dust in the spectra to trust the results) but the retrieved integrated ice
643 or dust opacity differs significantly from the "true" (MCD) one nonetheless. This occurs
644 (but not systematically) when the assumed dust mixing ratio at altitudes where the tem-
645 perature is similar to surface temperature differs significantly from that of the MCD (in
646 other words, TIRVIM spectra are blind to dust loading at some pressure levels but as
647 we integrate the whole dust column opacity, an error in this blind zone impacts the in-
648 tegrated optical depth) ; and/or when there is a high level of degeneracy between sur-
649 face temperature and dust and/or ice, in particular when spectra exhibit shallow dust
650 and/or ice features.

651 About 60% of the retrievals pass our quality filter for dust. We present a summary
652 of all these good quality-flagged retrieved dust opacities in Figure 7. Most of the scenes
653 that pass this quality filter also exhibit large ($>20\text{K}$) surface-lower atmosphere temper-
654 ature contrast, which is consistent as this situation corresponds to a greater sensitivity
655 to dust. Our algorithm performs well even in dusty conditions, ie. with an integrated
656 optical depth greater than one. However, this is probably too optimistic, as we neglect
657 multiple scattering by dust in both the forward model used to generate the synthetic spec-
658 tra and the retrieval pipeline. The Pearson correlation coefficient between MCD and re-
659 trieved dust opacity is 0.94. The standard deviation of the difference between retrieved
660 and "true" dust opacity is 0.12, which is larger than the mean absolute $1-\sigma$ error in dust
661 estimated from the ratio between noise level and K_d , which yields a value of 0.08. This
662 suggests that our formal error is underestimated, but this is not surprising, given differ-
663 ent sources of potential biases. We find that 12% of the dust retrievals that do pass the
664 dust quality filter suffer from a significant bias (compared to the "true" dust opacity),
665 ie. two times larger than our $1-\sigma$ error estimate. Some outliers are indeed visible in Fig-
666 ure 7, and we also identify several groups of cases where dust is systematically over or
667 underestimated in the retrievals. The physical reason behind these outliers will be fur-
668 ther discussed below for a few representative cases.

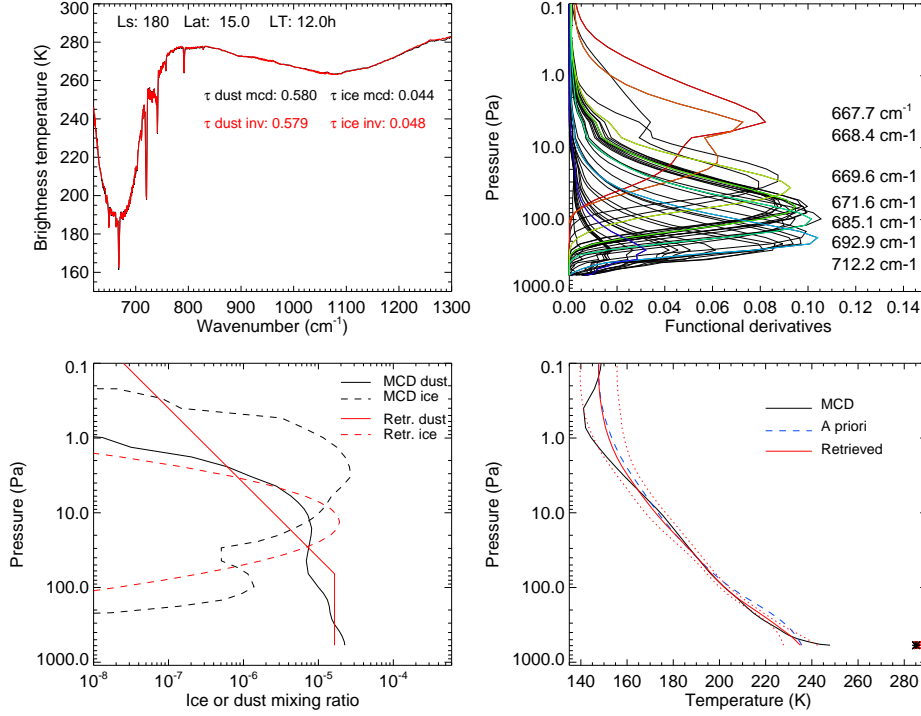


Figure 6. Summary of a synthetic retrieval for a MCD scenario extracted at $L_s=180^\circ$, latitude 15°N , local time 12 AM (noon). Top, left: Synthetic TIRVIM spectrum (black) along with the best fit (red). Retrieved and MCD dust and water ice cloud integrated opacities are indicated. Top, right: functional derivatives of the temperature as a function of pressure, for 50 different wavenumbers within the CO_2 band. Several wavenumbers are highlighted in different colors and labeled. Bottom, left: Mixing ratio vertical profiles for dust and water ice as taken from the MCD (used to generate the synthetic spectrum, in black) and as derived from the retrieval process (in red ; note that only a scaling factor to a generic *a priori* profile is retrieved). Bottom, right: Temperature vertical profile from the MCD (used to generate the synthetic spectrum, in black), *a priori* profile built from the synthetic spectrum (dashed blue line), and retrieved profile (red), with error bars in red dotted lines. The black and red stars stand for the MCD and retrieved surface temperature, respectively.

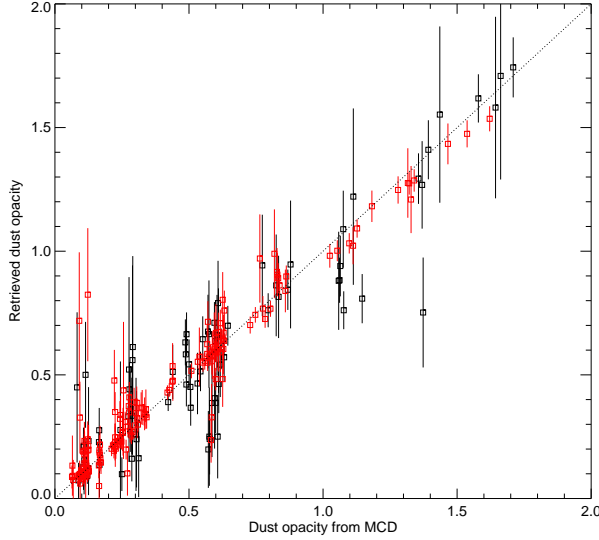


Figure 7. Retrieved versus input (MCD) integrated dust opacity in our OSSE. Only cases that passed the dust quality flag are shown. In red are cases for which the temperature contrast between surface and lower atmosphere (at 4 km) is greater than 20K. The dashed line highlights a one-to-one correspondence.

669 Retrieved and MCD dust opacities are shown for different seasons, latitudes and
 670 local times in Figure 8. A close-up of the $L_s=270^\circ$ case is shown in Figure A1. Daytime
 671 retrievals (red squares with error bars in Figures 8 and A1) are in general more robust,
 672 with smaller associated retrieval errors. This is mostly explained by a large surface-atmosphere
 673 temperature contrast and warmer temperatures (hence higher S/N ratio). Systematic
 674 overestimation of dust is visible in particular at $L_s=90^\circ$ at low latitudes (15S–30°N) for
 675 nighttime retrievals, where an integrated dust opacity of ~ 0.2 is retrieved at night, in-
 676 stead of ~ 0.1 in the MCD. Daytime retrievals on the other hand are robust at this sea-
 677 son and latitudes. These different behaviors create a spurious daily cycle of dust in the
 678 retrievals, not present in the MCD. Two examples of overestimated dust are shown in
 679 Figures A2 and A3. In the first case (latitude 15N, midnight), an optically thick cloud
 680 centered at ~ 100 Pa prevents the correct retrieval of atmospheric temperature in the lower
 681 atmosphere (see the functional derivatives of temperature in Figure A2). The retrieved
 682 surface-atmosphere temperature contrast is underestimated, and as a result, the dust load
 683 is overestimated by our algorithm. Indeed, there is a degeneracy in the solution of the
 684 inverse problem between dust opacity and temperature contrast, and we see here an ex-

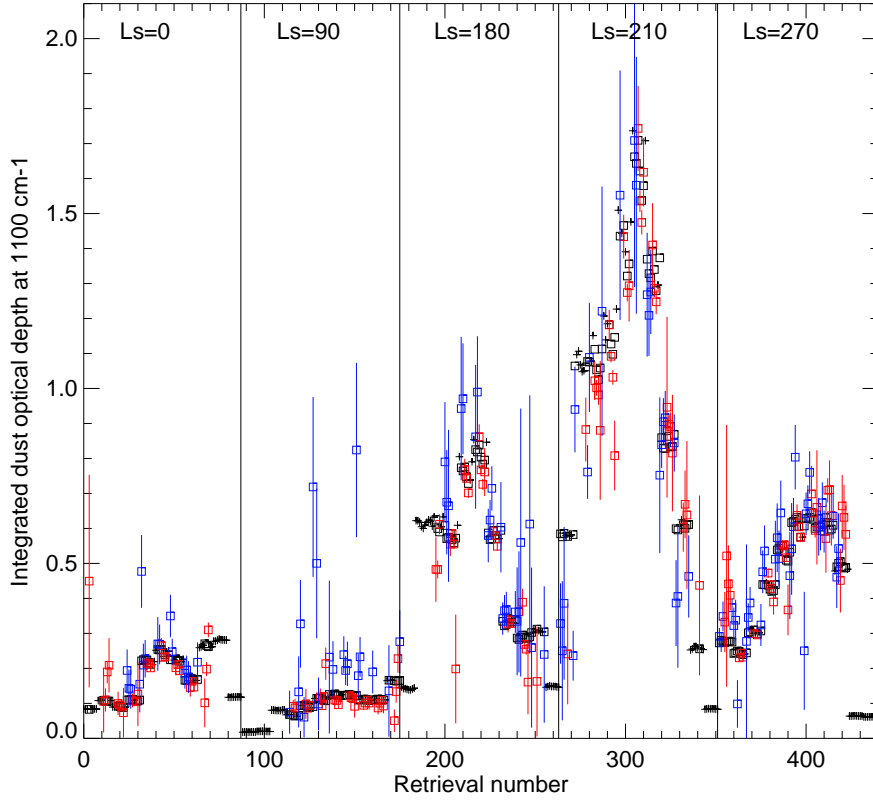


Figure 8. Evaluation of the robustness of dust retrievals sorted by season. Data points are grouped by values of Ls. Within each group, data are sorted by latitude from 75S to 75N, more clearly seen in Figure A1. Black crosses represent integrated dust opacities from the MCD, used to generate synthetic spectra in the OSSE. Blue squares are retrieved dust opacity that passed the dust quality flag for local times 0AM, 3AM, 6AM and 9PM, red squares for local times 9AM, 12AM, 3PM and 6PM. Vertical bars show the $\pm 1\text{-}\sigma$ error as defined in section 3.2.4. When no colored square is associated to a black cross, it means that the retrieval did not pass the dust quality flag, hence they were not plotted.

ample of a compensation of two errors. In the second example in Figure A3 (latitude 30N, 3AM), the atmospheric temperature is well estimated. Here, the issue seems to be the *a priori* dust vertical distribution, assumed well-mixed in the first two scale heights while it quickly decreases with height in the MCD profile. Because atmospheric temperature at 50–200 Pa is close to the surface temperature, we are not sensitive to the dust in this altitude range, but it will be anyhow added up in the calculation of integrated optical depth. Hence, while the amount of dust in the lower part of the atmosphere seems well estimated, the retrieved total integrated dust opacity is mechanically overestimated.

We detail another case study of challenging dust retrieval, this time during the global dust event of MY25 ($L_s=210^\circ$) and shown in Figure A4. Here, in spite of the high dust opacity (1.37) in the MCD scenario, the synthetic spectrum exhibits a very shallow dust emission feature. This is due to the modest surface-atmosphere temperature contrast in the first scale height, combined to the presence of dust at high (and colder) altitudes in the MCD profile at pressures lower than 60 Pa: the shallow dust feature results from a combination of dust thermal emission at various temperatures. Here, the underestimation of retrieved dust opacity by a factor of two by our algorithm is partly due to the wrong assumption on dust vertical distribution above 60 Pa, and partly due to the fact that the large dust opacity increases the degeneracy between surface temperature and dust retrieval. As a consequence, here, a slightly warmer surface temperature and less dust in the lower atmosphere yields a similar brightness temperature as the MCD scenario, that has a slightly colder surface and higher dust loading but over a greater column, with different emission temperatures. These three examples illustrate well some of the subtle challenges encountered (that we will have to keep in mind when interpreting actual TIRVIM data). In spite of this, we recall that overall, nearly 90% of the dust retrievals that pass our quality flag are found satisfactory.

Regarding cloud retrievals, about 62% of the retrievals pass our water ice quality filter. However, 32% of these cases are significantly biased compared to the MCD values: this fraction is almost three times greater than that for dust retrievals. Furthermore, we obtain a correlation of 0.74 between MCD and retrieved ice integrated optical depth. This confirms the overall worse performance of ice retrievals compared to dust retrievals. We first investigate whether our assumed cloud altitude is realistic or not. Figure 9 shows the MCD cloud "altitude" (pressure level of maximum ice mixing ratio) versus the cloud altitude set during the retrieval. Overall, the correspondence between the two is rather

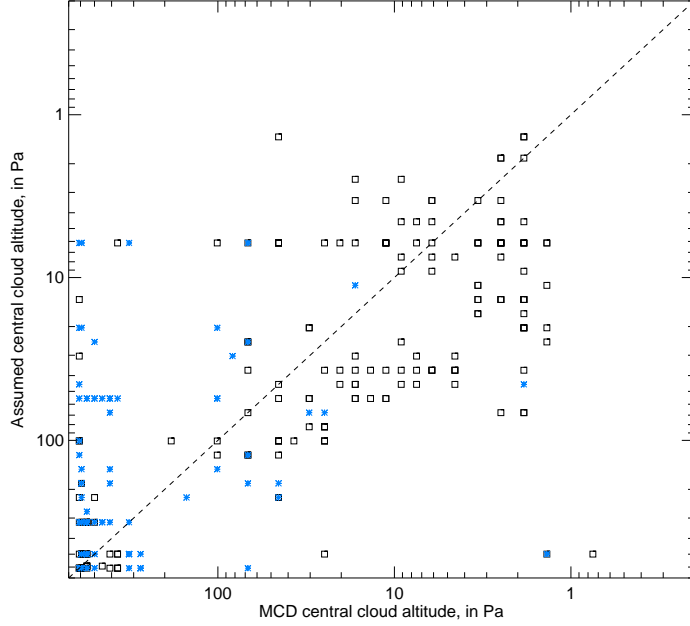


Figure 9. Cloud altitude as set up in the retrieval algorithm (see section 3.3) versus MCD central cloud altitude, in Pa. These values have been normalized to 610 Pa. Only cases that pass our ice quality flag are included. Blue stars highlight cases where ice opacity retrievals were significantly biased with respect to MCD values, despite having been flagged as robust ice retrievals.

718 good, except for low altitude clouds (in the MCD) whose altitude is not well captured.
 719 Actually, most of the biased cloud retrievals correspond to low altitude clouds in the MCD
 720 (see Figure 9), with large opacities (>3) in the MCD scenario. In these situations, the
 721 retrieval of surface temperature and/or lower atmospheric temperature is challenging,
 722 which in turn impacts the cloud opacity retrieval.

723 We also note that even a moderate error in the assumed cloud altitude can signif-
 724 icantly impact the retrieved optical depth. An example of a wrong determination of wa-
 725 ter ice cloud opacity linked to an error in the assumed water ice vertical mixing ratio pro-
 726 file is shown in Figure A5. Here, the MCD profile features a vertically extended cloud,
 727 from 3 to 300 Pa, with an integrated opacity of 0.325, while the retrieval assumes a thin-
 728 ner cloud centered at 10 Pa and yields a much lower ice opacity (0.136). Still, the fit to
 729 the synthetic spectrum is satisfactory. This illustrates well a degeneracy frequently ob-
 730 served, typically in the surface temperature range 180–220K, between the ice opacity and
 731 the surface-atmosphere (where the cloud resides) temperature contrast. An optically thicker

732 cloud located at an atmospheric temperature closer to the surface temperature yields a
733 similar spectral signature as a less opaque cloud located at significantly colder (or warmer,
734 if seen in emission) atmospheric temperature, compared to the surface. The chosen ex-
735 ample in Figure A5 is actually more subtle, as part of the vertically extended cloud is
736 located in a region of similar atmospheric temperature as the surface, making it invis-
737 ible to retrievals.

738 Hence, as for dust retrievals, several examples of over- or underestimation of cloud
739 opacity can be found while still presenting a good fit to the spectra, either linked to a
740 wrong assumption on the ice vertical distribution and/or a degeneracy with surface tem-
741 perature determination and/or wrong determination of atmospheric temperature near
742 the surface, or a subtle combination of these effects. A few difficult cases of combined
743 degeneracy between surface temperature and both dust and ice opacity are also found.

744 The degeneracy between surface temperature and aerosol retrievals is further il-
745 lustrated in Figure 10, which displays the error in surface temperature (the a posteri-
746 ori difference between retrieved and MCD surface temperature), only for cases that pass
747 the dust or ice quality flags. Cases for which dust or water ice opacities are significantly
748 biased with respect to the MCD values (defined by a difference with the MCD opacity
749 greater than two times our estimated $1\text{-}\sigma$ error) predominantly exhibit a greater error
750 in surface temperature as well. This illustrates the degeneracy between these quantities
751 in the inverse problem: these errors compensate and a combination of erroneous values
752 of surface temperature, dust and/or ice opacity can yield good fits to the synthetic TIRVIM
753 spectra nonetheless. On the positive side, as mentioned at the beginning of this section,
754 we note that for warm surface temperatures, the retrieval of all quantities remains ro-
755 bust.

756 **4.3 Robustness of the synthetic retrievals: atmospheric temperature**

757 Retrievals of atmospheric temperature profiles are found reliable in a vast major-
758 ity of cases, even when dust, water ice or surface temperature retrievals are not robust.
759 An exception is for observations featuring low altitude opaque clouds. In this case, we
760 can lose sensitivity to atmospheric temperature in the first scale height, as was shown
761 in Figure A2 during the aphelion cloud belt, or in Figure A6 for a high latitude winter
762 case. In such a situation, the retrievals are more impacted by a wrong *a priori* near-surface

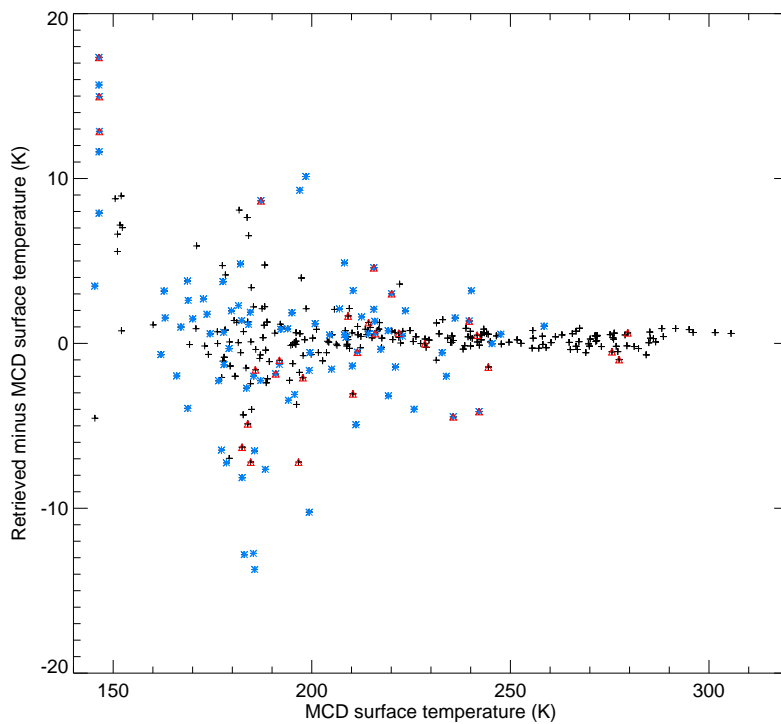


Figure 10. Error in surface temperature (defined as the difference between retrieved and "true" MCD surface temperature) as a function of the MCD surface temperature. We only show data points that pass either or both aerosol quality flags. We highlight as red triangles the dust retrievals that were significantly biased compared to MCD dust opacity, and as blue stars the cases where ice retrievals were significantly biased (greater than two times the $1\text{-}\sigma$ error).

763 temperature, which implies a wrong ice emission temperature and in turn, impacts the
764 retrieved ice optical depth. The case in Figure A6 illustrates another challenge for nadir
765 observations that constitutes the presence of a very steep temperature gradient in the
766 lower atmosphere: here, the temperature increases from 163K to 211K between 490 Pa
767 and 230 Pa, which represents a +48K increase over 7 km. Given the coarse vertical sen-
768 sitivity of TIRVIM retrievals, such a steep gradient cannot be captured properly. We note,
769 however, that this issue is localized and that the retrieved atmospheric temperature be-
770 haves well above 10 km as it does depart from the *a priori* profile and satisfactorily re-
771 produces the local temperature maximum seen in the MCD profile at 100–200 Pa, where
772 information content is high enough.

773 Apart from the caveat described above, we find that the atmospheric temperature
774 retrievals perform well. The difference between the retrieved temperature profiles and
775 that from the MCD, MY25 (used to generate the synthetic observations), along with the
776 mean and 1- σ standard deviation of this difference, are shown in Figure 11. Most of the
777 differences can be explained by the rather coarse vertical resolution of TIRVIM, as will
778 be demonstrated in the following section. In the region of maximum sensitivity (5–35 km),
779 the mean of the difference is close to zero and the 1- σ standard deviation generally lower
780 than 3K. In the 35–55 km (2–20 Pa) region, the vertical resolution is coarser. As a re-
781 sult, the retrieved temperature averaged over 35–55 km may be correct, although the slope
782 may not (as is the case for $L_s=180^\circ$ in our OSSE). This can result in rather large errors
783 at a given pressure level in the range 35–55 km while the fit to the data is correct: this
784 behavior is consistent with the information content of the data and illustrates the de-
785 generacy due to the coarse vertical resolution. Above the altitude of maximum sensitiv-
786 ity (peaking near 2–3 Pa, or 50 km), the temperature profile smoothly returns to the *a*
787 *priori* profile, and results should not be interpreted. This will have to be kept in mind
788 when actual TIRVIM retrievals are discussed. We report a similar issue in the first at-
789 mospheric scale height, in particular when very steep temperature gradient (in the MCD)
790 are not caught by our retrieval, as mentioned previously and illustrated in Figure A6.
791 This is frequently associated to elevated water ice content near the surface and mostly
792 occurs at $L_s=270^\circ$ in the winter high latitudes. Finally, we note that the atmospheric
793 temperature retrieved for global dust storm conditions is very satisfactory and is very
794 similar to the $L_s=180^\circ$ case.

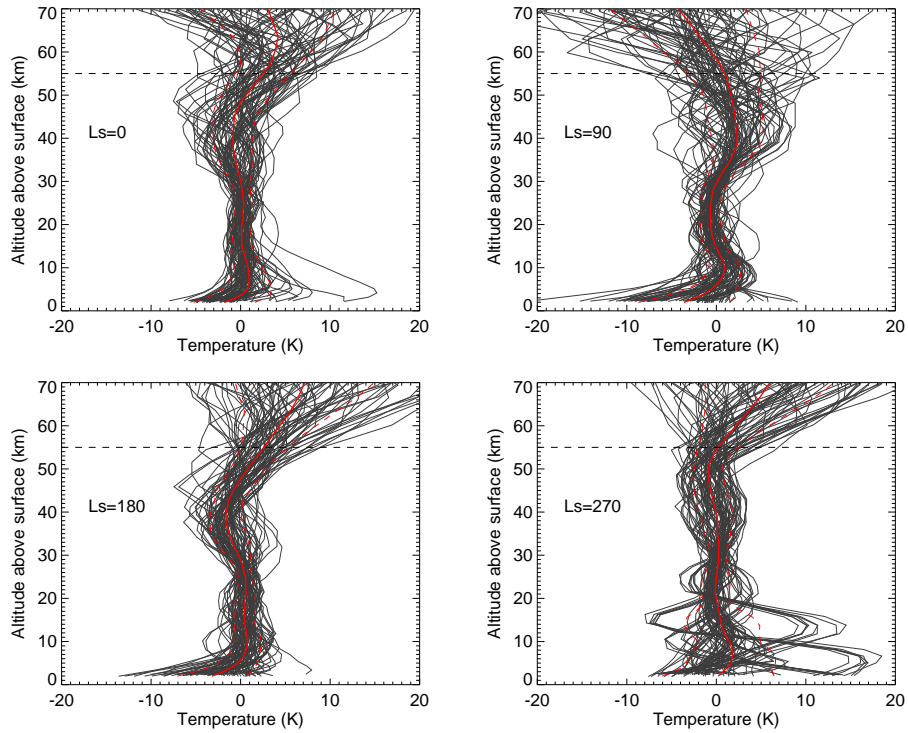


Figure 11. Vertical profiles of the difference between retrieved and MCD temperature profiles, sorted by seasons, as labeled. In each panel, the red solid line is the mean of the difference, and dashed red lines are $1\text{-}\sigma$ standard deviation added and subtracted from the mean. The case $Ls=210^\circ$ is not shown but is almost identical to the case $Ls=180^\circ$. Most of the error results from the rather coarse vertical resolution of TIRVIM (see Figure 13 for comparison).

795 It might seem that our algorithm for atmospheric temperature retrieval performs
796 well mostly because our *a priori* temperatures profiles are well chosen, but it's not fully
797 the case. To demonstrate the limited influence of the *a priori* on our results, we have
798 also run the 440 test cases of our OSSE with *a priori* profiles $\pm 10\text{K}$ warmer or colder
799 than our nominal profiles. Examples are shown in supplementary Figure A7. The retrieved
800 profiles converge towards a very similar solution between a few kilometers above the sur-
801 face and $\sim 3\text{ Pa}$, independently of the choice of the *a priori* profiles. Above 3 Pa , the pro-
802 files starts to diverge and go back to their own *a priori* profile, consistently with the in-
803 formation content of the data. The quality of the fit in the CO_2 band is overall a bit bet-
804 ter when using our nominal *a priori* profile, which is mostly due to slightly better fits
805 of the core of the CO_2 band. This illustrates well the difficulty for our retrieval algorithm
806 to depart far enough from the prior at $1\text{--}3\text{ Pa}$ (where information content is low) solely
807 to fit $1\text{--}2$ spectral points near 667 cm^{-1} , and justifies our choice of *a priori* profile to mit-
808 igate this challenge. Another advantage is a slightly faster convergence of the retrievals
809 (~ 4 iterations for our nominal profile instead of ~ 5 iterations for the other two profiles).
810 As we will rarely interpret observations above the $2\text{--}3\text{ Pa}$ level though, we show here that
811 our results are largely independent of the choice of the *a priori* profile.

812 Finally, we can also briefly compare the performance of our OSSE with that of Grassi
813 et al. (2005) done for synthetic PFS/Mars Express retrievals. As expected, the authors
814 highlighted a difficulty of their retrievals to capture strong vertical thermal gradients in
815 the lowest levels of the atmosphere. Based on 288 representative simulated spectra (ex-
816 tracted from the MCD at different seasons, local times and latitude), they found that
817 their algorithm performed very well between 5 and 25 km , with systematic errors near
818 zero and random error of the order of $2\text{--}3\text{K}$. However, their retrieval exhibited a system-
819 atic error in the retrieved temperature above 30 km that reached 4K at 50 km , while the
820 random error increased from 5 to 8K between 30 and 50 km . Random errors are thus
821 very comparable to ours, while we do not report any systematic errors up to 40 km . Grassi
822 et al. (2005) also emphasized that for altitudes $40\text{--}50\text{ km}$, the contribution of the *a pri-*
823 *ori* profile became more important than the weight of the data in constraining the so-
824 lution. This is consistent with our analysis and is not surprising, as PFS and TIRVIM
825 have similar spectral resolution and hence similar information content.

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4.4 Effect of averaging kernels on temperature profiles

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We can go one step further in the comparison of retrieved versus "true" profile by emulating the combined effects of TIRVIM coarse vertical resolution and the influence of the *a priori* profile on the MCD profile. Indeed, in theory, TIRVIM retrievals provide our best estimate $\hat{\mathbf{T}}$ of the true atmospheric state \mathbf{T}_{true} , with the caveat that these retrieved profiles represent a smoothed version of the true state and partly contain *a priori* information, in particular in altitude regions where information content is low. This is formally expressed by:

$$\hat{\mathbf{T}} = \mathbf{T}_{\mathbf{a}} + \mathbf{A}_{\mathbf{k}}(\mathbf{T}_{\text{true}} - \mathbf{T}_{\mathbf{a}}) \quad (7)$$

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with the averaging kernel matrix $\mathbf{A}_{\mathbf{k}}$ defined by $\mathbf{A}_{\mathbf{k}} = \mathbf{W}\mathbf{K}$. This matrix is proportional to the weighting kernels and reflects the fraction of information coming from the *a priori* and from the data. Examples of rows of $\mathbf{A}_{\mathbf{k}}$ are presented in figure 12. The FWHM of a row gives an estimate of the vertical resolution of our retrievals and illustrates well how it is significantly larger (coarser) at higher altitudes. Note that for this example, rows of $\mathbf{A}_{\mathbf{k}}$ at pressures higher than ~ 4 Pa exhibit a sensitivity peaking at the corresponding pressure level, but that for lower pressures, the peak sensitivity occurs below that level (at higher pressures). In this example, our peak sensitivity does not reach higher than the 3 Pa level. More details on the use of averaging kernels can be found in Rodgers (2000).

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By applying equation 7 to the "true" MCD profiles, we can thus run the MCD profiles through the retrieval filter, which degrades their vertical resolution and introduces a fraction of the *a priori* temperature profile. If the retrieval algorithm works without flaw, the retrieved temperature profiles obtained in this OSSE should be almost identical (within the formal retrieval error) to the best estimates $\hat{\mathbf{T}}$ obtained with equation 7. The updated comparison between our retrievals and $\hat{\mathbf{T}}$ profiles is shown in Figure 13. As expected, for most cases, the difference is smaller than 2K at all altitudes, since both profiles now go back to the same *a priori*. This signifies that 2K is a realistic estimate of the formal error linked to noise in the data and the non-linearity of the radiative transfer equation. However, there are a few cases where the difference between profiles significantly exceeds error bars. This happens in particular at $L_s=270^\circ$, for the challenging scenes with a thick low altitude cloud in the MCD. Here, the unexpected difference

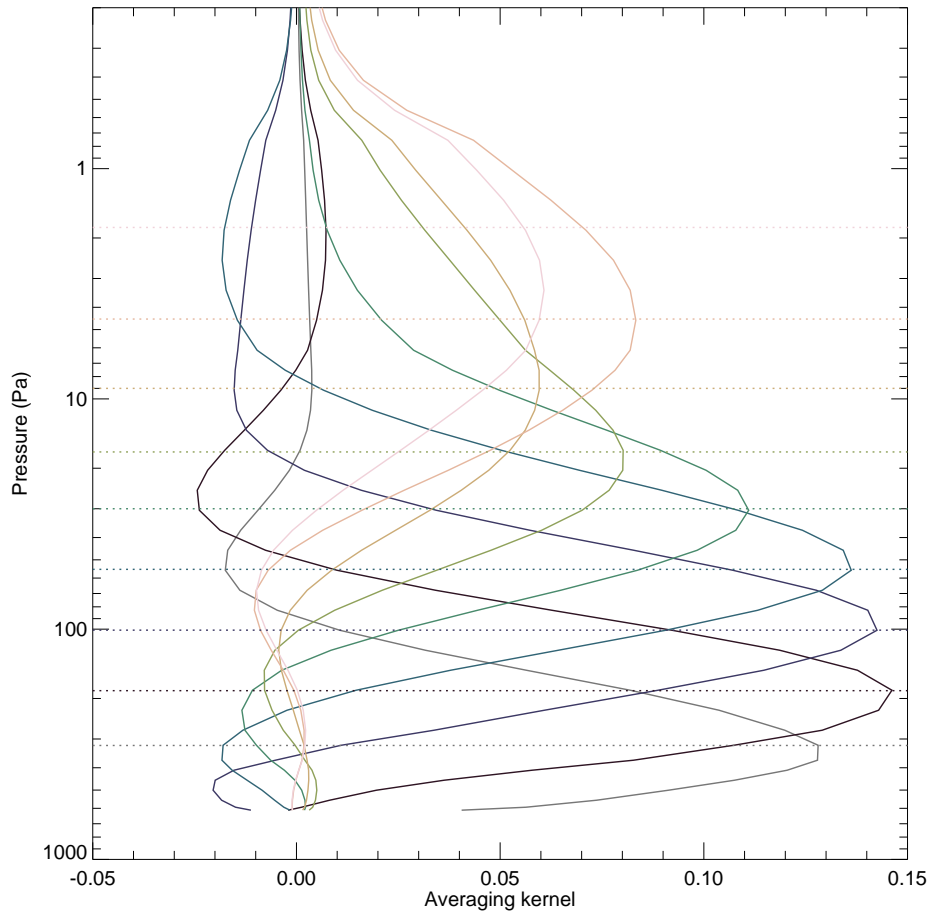


Figure 12. Example of nine rows of the averaging kernel matrix (solid lines), for nine pressure levels, materialized in dotted lines. This example was generated for atmospheric conditions extracted from the MCD for MY25, $L_s=180^\circ$, latitude 15°N and local time 9 AM (same as Figure 5).

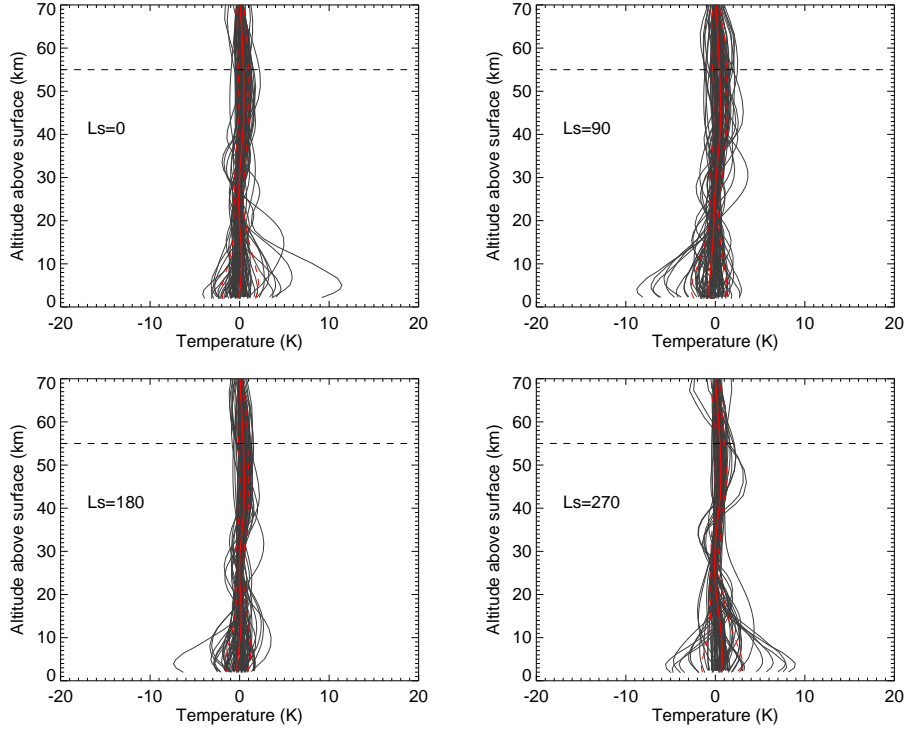


Figure 13. Same as Figure 11 but showing the difference between retrieved and "smoothed" MCD temperature profiles ($\hat{\mathbf{T}}$).

856 between the retrieval and $\hat{\mathbf{T}}$ stems from the wrong evaluation of the averaging kernel ma-
 857 trix \mathbf{A}_k . Indeed, our retrievals often fail to capture the actual high cloud optical depth,
 858 which impacts the calculated functional derivatives \mathbf{K} and hence, \mathbf{A}_k as well. In the ex-
 859 ample shown in Figure A6, the functional derivatives (wrongly) indicate that the sen-
 860 sitivity to the low atmospheric temperature should be rather good, which explains why
 861 $\hat{\mathbf{T}}$ is close to the MCD profile. However, the retrieved temperature is hampered here by
 862 a wrong estimate of water ice cloud opacity and the functional derivatives should not
 863 be as high in the first scale height. We emphasize though that these situations are not
 864 frequent, and that overall, the retrieval algorithm behaves as expected. To summarize,
 865 except for a few particular cases, based on this OSSE, our confidence in the retrieved
 866 temperature profiles is quite high.

867 5 Application to ACS/TIRVIM spectra and validation of the retrievals

868 We have applied our retrieval algorithm to the full TIRVIM dataset. The retrieved
 869 quantities, along with fits to the data, are distributed on the IPSL data center (Guerlet,

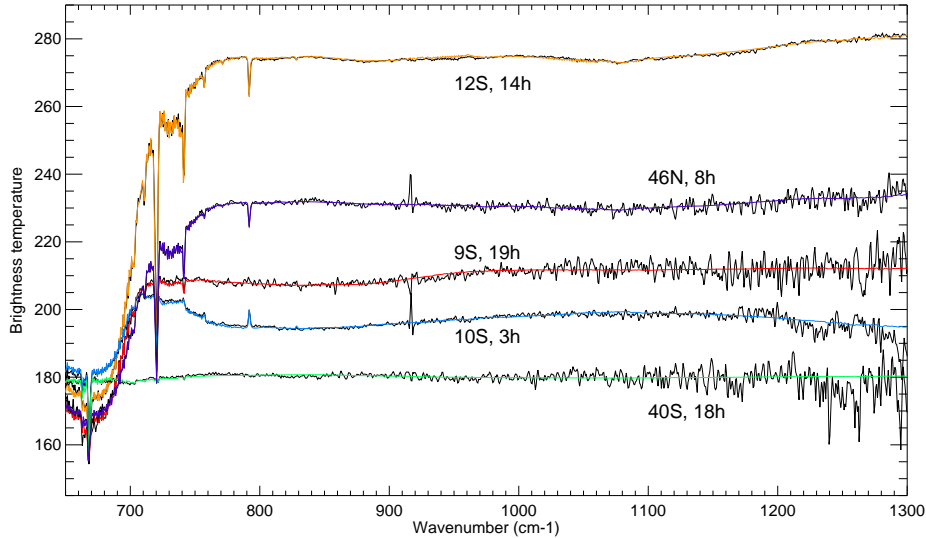


Figure 14. Examples of TIRVIM spectra (in black) and best fits (in color). These five spectra were all acquired close to $L_s=150^\circ$ of Martian Year 34 and near $40^\circ W$. Latitudes and true solar local times are labeled; these cases were chosen to sample different surface and atmospheric temperatures.

2021). We illustrate examples of five TIRVIM spectra and their corresponding best fits
 870 at different latitudes and local times in Figure 14. In the following, we cross validate the
 871 atmospheric temperature profiles retrieved from TIRVIM against Mars Climate Sounder
 872 (MCS) profiles and continue with an evaluation of the retrieved dust integrated optical
 873 depth. We focus in this paper on the first few weeks of TIRVIM scientific operations.
 874 Validation of water ice cloud opacity retrieval is deferred to future work for two reasons.
 875 Firstly, there were very few clouds at the season and latitude coverage corresponding to
 876 the first weeks of TIRVIM data (at $L_s \sim 150^\circ$). Secondly, the OSSE has shown that our
 877 cloud retrievals suffered from rather larger uncertainties and biases. We thus plan to im-
 878 prove our ice retrieval algorithm in the future before further validation and scientific ex-
 879 ploitation (see discussion in section 6).
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881 5.1 Description of TIRVIM and MCS datasets and co-location method

882 We focus on the validation of TIRVIM retrievals acquired during the first 45 sols
 883 of TGO science phase, ie. between March 13 and April 28, 2018. This corresponds to
 884 Martian Year 34 near the northern autumn equinox, from $L_s=142^\circ$ until $L_s=167^\circ$. This

885 dataset comprises both individual spectra (acquired during the first 6 days) and spec-
886 tra resulting from the onboard averaging of 8 consecutive interferograms. Only 3% of
887 the retrievals did not pass the post-processing quality filters (mostly related to the qual-
888 ity of the fits, based on χ^2), which is highly satisfactory. This is actually even more fa-
889 vorable than our exercise on synthetic retrievals (where overall, 9% didn't pass our set
890 of quality filters) and could be explained by the low number of challenging scenes (ie.
891 elevated aerosol load and/or cold surface) at this season and for the latitudinal cover-
892 age considered here.

893 We choose to validate our results against Mars Climate Sounder (MCS) observa-
894 tions. The MCS is a passive radiometer that records the thermal emission of the mar-
895 tian atmosphere in limb viewing geometry, in several thermal infrared channels, includ-
896 ing three channels covering the 15- μm CO₂ band. The MCS team provides retrieved ver-
897 tical profiles of the temperature with a vertical resolution of 5 km, from an altitude of
898 typically ~ 10 – 15 km (as low as 5 km in the event of a clear atmosphere) up to 80–90 km
899 altitude, or from typically ~ 300 to 0.02 Pa. Due to the Sun-synchronous orbit of MRO,
900 these profiles are only available near local times 3 AM and 3 PM, with a rather dense
901 coverage in latitude and longitude. The MCS retrieval algorithm includes a single-scattering
902 approximation to account for scattering effects (Kleinböhl et al., 2011) and accounts for
903 temperature and aerosol load variations along the line of sight (Kleinböhl et al., 2017).
904 Temperatures derived from MCS have been used in many scientific studies (e.g., Lee et
905 al., 2009; Kleinböhl et al., 2013). Because MCS samples a greater altitude range, achieves
906 a higher vertical resolution, and its data are known for their high reliability, we choose
907 to validate our TIRVIM temperature retrievals against MCS ones acquired at close lo-
908 cations, dates and local time.

909 For this exercise we select, for each TIRVIM observation, all MCS data acquired
910 within 6° of longitude, 3° in latitude, and half an hour in local time of the considered
911 TIRVIM profile (although we allow the date of observation to differ by \pm one sol between
912 the two data sets). These co-location criterion correspond to a trade-off between a small
913 enough distance between TIRVIM and MCS data (in order to limit the effects of mete-
914 orological variability over these spatio-temporal scales), and a large enough amount of
915 co-located data. Given the local time coverage of MCS data, this validation exercise will
916 be based on "near-3 PM" and "near-3 AM" observations. Several MCS profiles can match
917 one TIRVIM profile, and conversely, a MCS profile can be found co-located with several

918 TIRVIM profiles. As an example, for the near-3 PM observations in the first 45 sols pe-
919 riod, this selection process results in 10,386 TIRVIM profiles being co-located with 6,201
920 unique MCS profiles. Figure 15 shows the coverage, as a function of latitude and local
921 time, of all TIRVIM-MCS co-located observations for these first 45 sols. We note that
922 TIRVIM data south of 55°S are mostly missing at all local times: those have been fil-
923 tered out at the pre-processing stage and correspond to bad-quality flagged interferograms.
924 Poor quality data at cold surface temperatures seem to be more frequent. This might
925 reflect a poorer quality of the response of the instrument to low signal levels. The longitude-
926 latitude coverage of these two co-located data sets is illustrated in Fig. 15 for the 3 PM
927 data near $L_s=150^\circ$, revealing a dense and nearly uniform coverage for both instruments.

928 In the following, we estimate the quality of the match between MCS and TIRVIM
929 retrieved temperature profiles in several ways:

- 930 • We compute statistics based on MCS-TIRVIM pairs of co-located individual tem-
931 perature profiles, for strict co-location criteria.
- 932 • We compare latitude-pressure sections of zonally-averaged temperatures, for strict
933 co-location criteria.
- 934 • We also compare latitude-longitude sections of temperature at given pressure lev-
935 els, acquired at similar dates and local times, but without considering spatial co-
936 location.

937 5.2 Comparison of individual temperature profiles

938 Comparison of TIRVIM and co-located MCS temperature profiles allows us not only
939 to assess potential biases between the two sets of retrievals, but also to evaluate the im-
940 pact of the different vertical sensitivity in comparing a nadir with a limb sounder. We
941 present two selected cases of the direct comparison between TIRVIM and MCS temper-
942 ature profiles in Figure 16. In one case, near 65°N and 3 AM, the comparison is excel-
943 lent between these two instruments. In the second example, a significant mismatch (up
944 to 10K) is found over the range 1–10 Pa. Here, the difference in vertical resolution and
945 sensitivity is striking, with TIRVIM profiles being much smoother than those from MCS.
946 In particular, TIRVIM does not capture the sharp vertical oscillation seen by MCS in
947 the range 1–10 Pa. As mentioned in section 3, this is consistent with the broad TIRVIM
948 functional derivatives in that pressure range. To further investigate this, we can apply

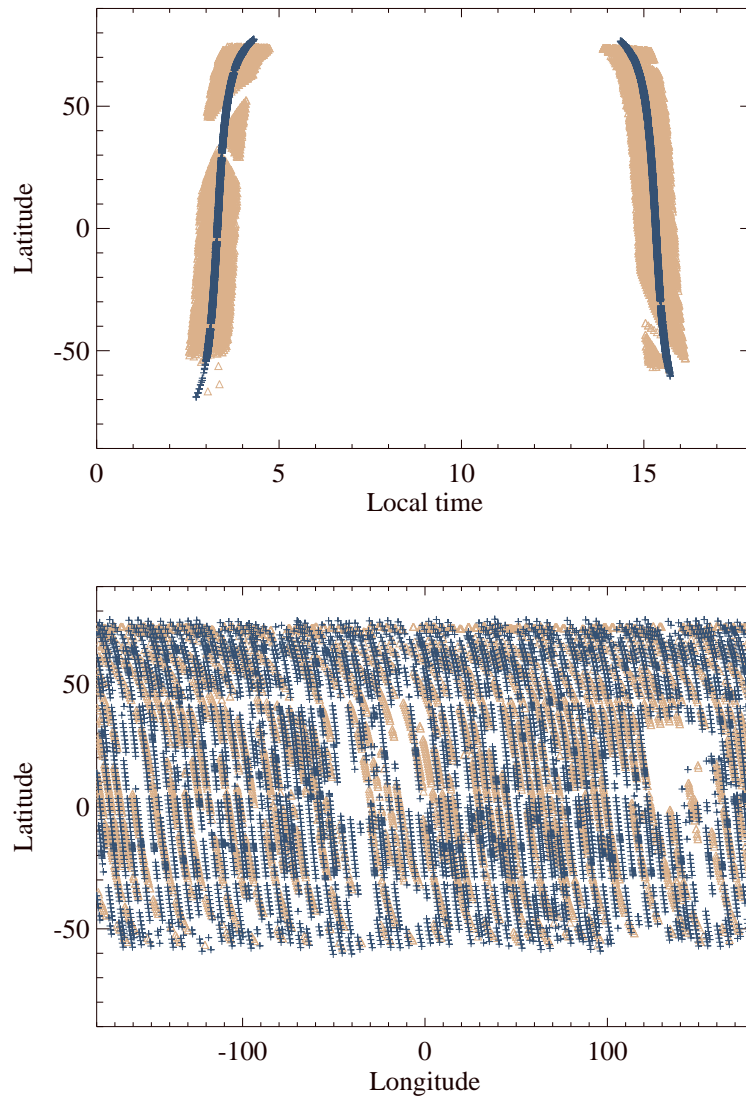


Figure 15. Coverage of TIRVIM (orange triangles) and MCS (dark blue crosses) co-located observations over the course of the first 45 sols of TIRVIM science phase ($L_s \sim 150^\circ$). Top: latitude–local time coverage ; bottom: East longitude–latitude coverage for the near 3PM data only. Here we display existing MCS data co-located with TIRVIM, irrespective of whether the MCS profiles extend to near-surface altitudes or not.

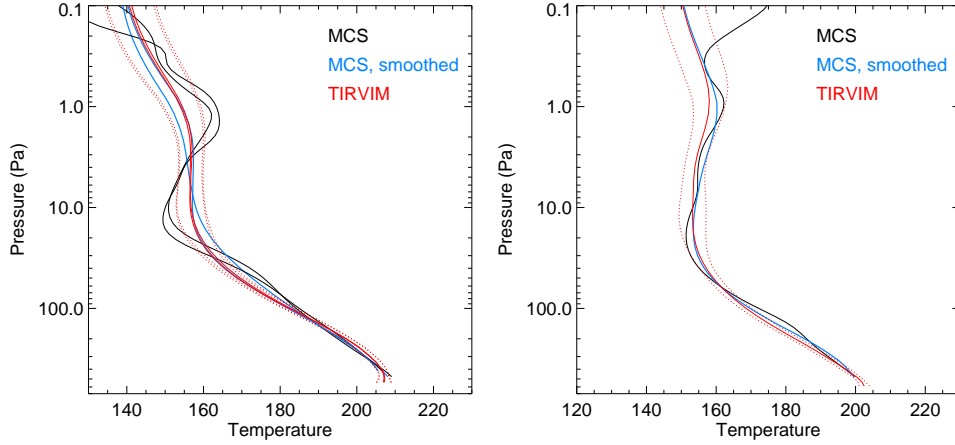


Figure 16. Retrieved temperature profiles from TIRVIM (in red, with error envelop in dot-dashed lines) compared with co-located MCS profiles (in black) and smoothed versions of the MCS profiles (in blue) taking into account TIRVIM averaging kernels and the influence of its *a priori* profile, as described in the text. The example on the left is for latitude 45°N, the one on the right is for 65°N; both were acquired near 3 AM. Note that the vertical axis ranges till 0.1 Pa for context, to display the behavior of MCS temperature profiles at higher altitudes, but TIRVIM data are sensitive only up to ~ 2 Pa.

949 TIRVIM averaging kernels to MCS profiles to emulate the coarser vertical sensitivity of
 950 TIRVIM on MCS profiles and to account for the fact that when TIRVIM information
 951 content is low, the temperature smoothly goes back to an *a priori* profile. In a fashion
 952 similar to the smoothing of the MCD profiles done in our OSSE described in section 4.3,
 953 we thus replace \mathbf{T}_{true} by \mathbf{T}_{MCS} in equation 7 to derive a smoothed MCS profile, noted
 954 $\hat{\mathbf{T}}_{\text{MCS}}$. This procedure follows the methodology for inter-comparing profiles retrieved from
 955 different instruments documented in Rodgers and Connor (2003). By employing equa-
 956 tion 7 in such an inter-comparison exercise, we assume that the MCS profiles are not in-
 957 fluenced by their own *a priori* (which holds true on the pressure range considered here,
 958 1–500 Pa) and that the MCS vertical resolution significantly exceeds that of TIRVIM,
 959 which is also satisfied. When we apply equation 7, the emulated $\hat{\mathbf{T}}_{\text{MCS}}$ profiles are now
 960 much closer to the retrieved TIRVIM profiles (see Figure 17), as can be expected. In-
 961 dividual differences that previously reached 10K in the direct comparison are now smaller
 962 than 3K. In the following, we thus focus on the comparison between TIRVIM and the
 963 smoothed MCS profiles, as this is more relevant to validate our results.

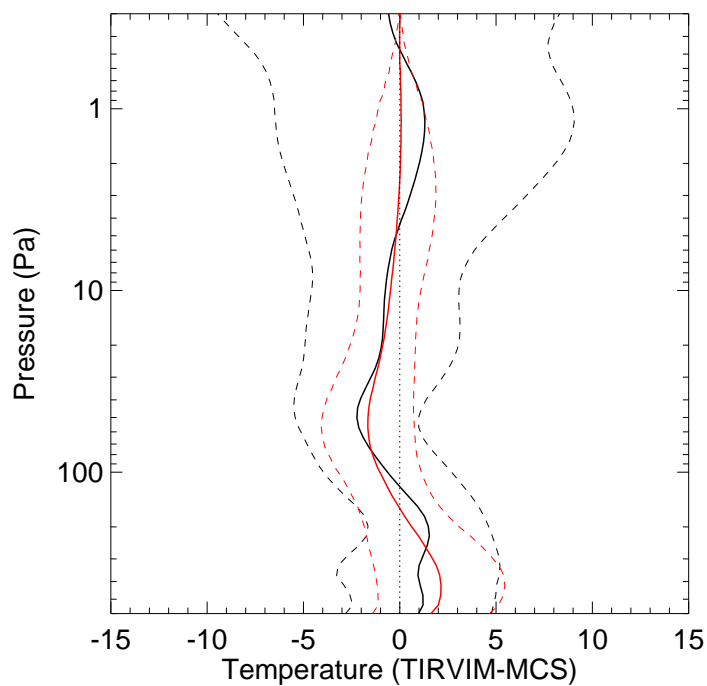


Figure 17. Statistics of the $\text{TIRVIM}-\hat{\text{T}}_{\text{MCS}}$ difference based on thousands of co-located temperature profiles near 3 AM, $L_s \sim 150^\circ$. The red solid line shows the average of this difference, the red dashed line is the $1-\sigma$ standard deviation of this difference. Black lines are the same but considering the difference between TIRVIM and the raw MCS profiles.

964 We then compute statistics based on all pairs of MCS-TIRVIM co-located profiles.
 965 Figure 17 displays the average and $1\text{-}\sigma$ standard deviation of the $\text{TIRVIM}-\hat{\text{T}}_{\text{MCS}}$ differ-
 966 ence for all co-located profiles acquired near 3 AM. Both the bias and standard devia-
 967 tion of the difference tend to be zero at high altitudes, which simply results from the fact
 968 that the smooth MCS profiles go back to the same *a priori* profile as the one used for
 969 TIRVIM retrievals. This tendency starts between 1 and 2 Pa, which is consistent with
 970 the information content in nadir observations and remind the fact that TIRVIM retrievals
 971 should not be interpreted at pressures lower than 1–2 Pa. Over the range 2–500 Pa, the
 972 average of the difference between the two datasets is within $\pm 2\text{K}$, which we take as an
 973 estimate of TIRVIM accuracy. The standard deviation of the $\text{TIRVIM}-\hat{\text{T}}_{\text{MCS}}$ difference
 974 is in the range to 2–3 K, which is then an estimate of TIRVIM precision. These figures
 975 are of the order of magnitude of the typical formal retrieval error of either TIRVIM or
 976 MCS temperatures. Hence, this shows that when differences in vertical sensitivities are
 977 taken into account, TIRVIM and MCS are in excellent agreement. For completeness, we
 978 include in Figure 17 the same statistics should the raw MCS temperature profiles be taken
 979 in consideration. This illustrates the precision that would be (wrongly) derived if one
 980 were to disregard differences in vertical resolution between instruments. Similar results
 981 are obtained for the 3 PM case.

982 *5.2.1 Comparison of the zonally-averaged temperature*

983 We now focus on the comparison of the latitude-pressure thermal structure from
 984 TIRVIM and MCS near 3 AM and 3 PM, considering zonal averages of the co-located
 985 measurements, in bins of 5° latitude. One word of caution regarding the computation
 986 of zonal averages: while TIRVIM (nadir) retrievals are sensitive to almost down to the
 987 surface (except in extreme dusty or cloudy conditions not encountered here), MCS pro-
 988 files often display a limited vertical coverage, extending only down to 80 Pa (20 km), for
 989 instance. This occurs when the optical depth of water ice and/or dust was too high at
 990 lower tangent altitudes to allow a reliable temperature retrieval from the MCS limb data.
 991 We thus have to be careful and avoid comparing a TIRVIM zonal average obtained from
 992 a rather uniform longitudinal sampling with a MCS "zonal average" for which the lon-
 993 gitudinal coverage could be uneven and vary with altitude. For each 5° -wide latitudinal
 994 bin considered, we thus proceed by browsing one by one the MCS pressure grid and search
 995 for co-located MCS-TIRVIM data only among a subset of the MCS database, where tem-

996 perature was indeed retrieved at that level, before averaging the temperatures. In the
 997 following, for simplicity, we call zonal average the average over observed longitudes.

998 The resulting latitude-pressure cross-sections of the zonal-mean temperature are
 999 shown in Figure 18 for TIRVIM and \hat{T}_{MCS} for 3AM and 3PM, along with the cross-sections
 1000 of the TIRVIM– \hat{T}_{MCS} difference. Similar figures for MCS temperature (on their own re-
 1001 trieval pressure grid, without vertical smoothing) are shown in Figure A8 in Supplemen-
 1002 tary Material. We also display the day/night temperature difference (3 PM–3 AM) for
 1003 TIRVIM, \hat{T}_{MCS} and MCS in the bottom panels of Figure 18. The agreement between
 1004 the two data sets is very satisfactory, both qualitatively and quantitatively. Before ap-
 1005 plying the averaging kernels to MCS profiles, temperature differences between TIRVIM
 1006 and MCS data sets are already mostly in the range ± 4 K except at high altitudes (pres-
 1007 sures lower than 10 Pa) where it can reach 12K. These larger discrepancies between TIRVIM
 1008 and MCS can be explained by differences in their inherent vertical sensitivity, as discussed
 1009 previously. Indeed, when comparing TIRVIM and \hat{T}_{MCS} , these differences decrease and
 1010 become smaller than 4K everywhere, except at 3AM in the lower atmosphere. The TIRVIM–
 1011 \hat{T}_{MCS} temperature differences at pressures greater than 200 Pa at 3 AM is not well un-
 1012 derstood and may partly reflect an artefact of applying equation 7 on the lower portion
 1013 of MCS profiles and/or partly result from an actual bias of either TIRVIM or MCS re-
 1014 trievals at these pressures.

1015 The main features of the temperature field seen by MCS are well captured by TIRVIM,
 1016 both at 3 AM and 3 PM. At this season (end of summer in the northern hemisphere)
 1017 and in the lower atmosphere (pressures greater than 200 Pa), the meridional tempera-
 1018 ture structure is characterized by warmer temperatures in the northern hemisphere com-
 1019 pared to the southern hemisphere. The temperature decreases rapidly towards high south-
 1020 ern (winter) latitudes, from typically 210K at 30°S to 180K at 50°S, at the edge of the
 1021 cold polar vortex. At lower pressures, the meridional thermal structure is more symmet-
 1022 ric about the equator, as the dominant feature is the thermal tide pattern.

1023 The diurnal mode of the thermal tide is well visible in the day/night temperature
 1024 difference shown in the bottom panels of Figure 18. These figures highlight the well-known
 1025 pattern of positive and negative temperature anomalies vertically stacked, at the equa-
 1026 tor and 45° latitude (with an opposite sign). These patterns have been well documented
 1027 in the past, for instance by Lee et al. (2009) and Kleinböhl et al. (2013) from the anal-

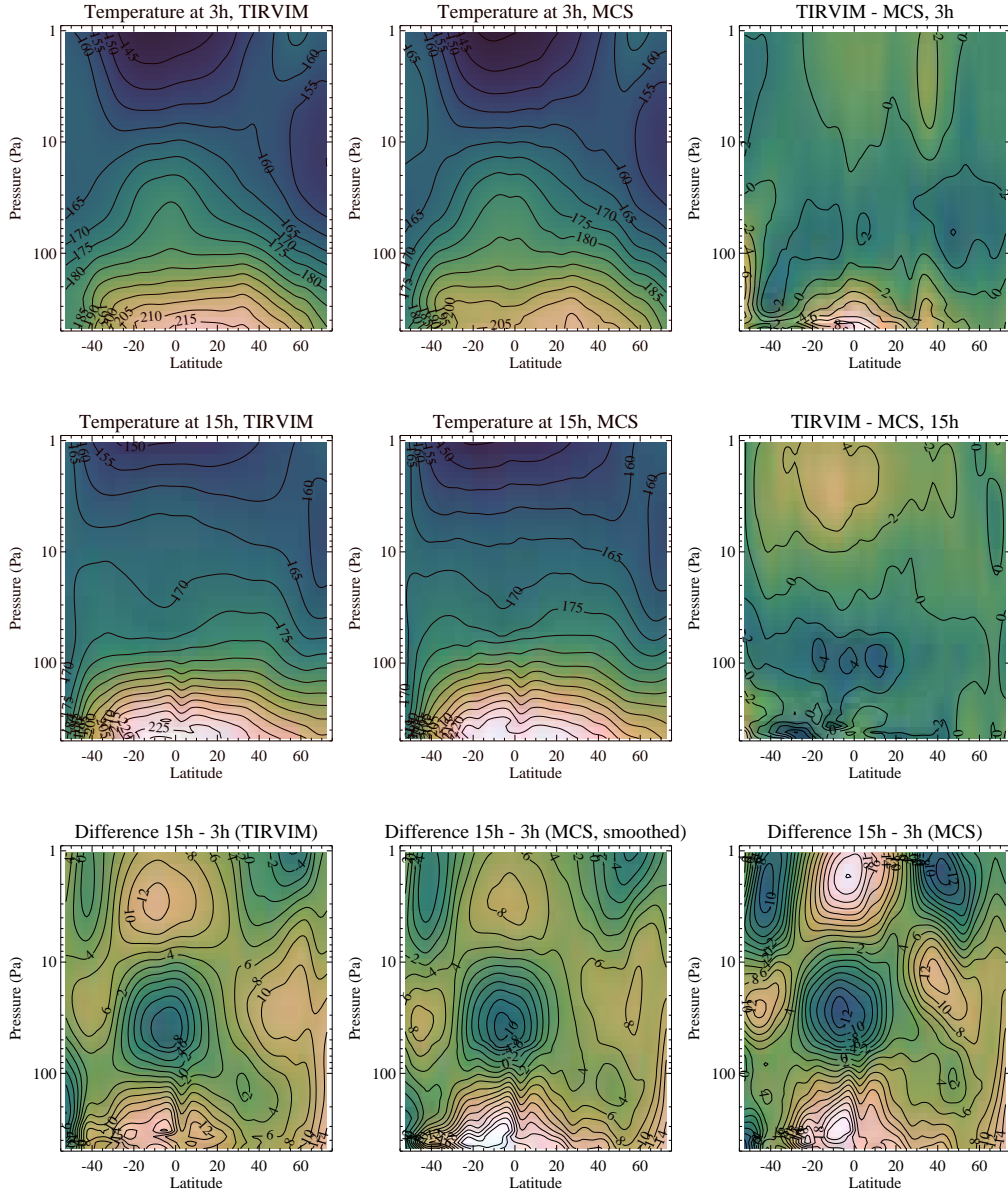


Figure 18. Pressure-latitude sections of the zonally-averaged temperature near 3 AM (top), 3 PM (middle), and the difference between 3 PM and 3 AM (bottom). In the two top rows, left panels correspond to TIRVIM, middle panels to \hat{T}_{MCS} and the difference between the two datasets is shown in the right panels. In the bottom row, TIRVIM results are shown on the left, smoothed \hat{T}_{MCS} in the middle and raw MCS ones on the right. These figures highlight the diurnal mode of martian thermal tides. Bins of 5° wide in latitude are used. In each panel, zonal averages are performed for a subset of the available TIRVIM and MCS data that meet co-located criteria, as described in the text.

1028 ysis of MCS data. TIRVIM captures well the signs and locations of these temperature
 1029 extrema, and the amplitude of these extrema are similar to that of the smoothed MCS
 1030 temperature profiles ($\hat{\mathbf{T}}_{\text{MCS}}$). For instance, near the equator, the 30 Pa afternoon tem-
 1031 perature is found by TIRVIM to be ~ 8 K colder than at night (10K in the $\hat{\mathbf{T}}_{\text{MCS}}$ field),
 1032 and the 3 Pa afternoon temperature is found to be ~ 12 K warmer than at night (8K in
 1033 the $\hat{\mathbf{T}}_{\text{MCS}}$ field). The actual amplitudes of the thermal tides are known to increase even
 1034 more with decreasing density, as can be seen in the raw MCS day-night temperature dif-
 1035 ference in Figure 18. Indeed, in the raw MCS data, the amplitude of the 3 PM–3 AM
 1036 difference reaches +20K at the equator at 2 Pa, and +10–12K near 45° latitude at 2 Pa
 1037 as well. These large extrema value are linked with sharp vertical gradients or oscillations
 1038 of the temperature profile at these altitudes (see for instance the local temperature min-
 1039 imum seen in the MCS profiles at 3 AM and 45°N in Figure A8) that TIRVIM cannot
 1040 capture properly. The fact that TIRVIM provides a muted version of the actual ther-
 1041 mal tide signal at 1–10 Pa despite a moderate sensitivity in this region and a growing
 1042 influence of the *a priori* profile (which is not based on any prior knowledge on how the
 1043 thermal tide should look like) complies with its coarse vertical resolution – as shown from
 1044 the good comparison with $\hat{\mathbf{T}}_{\text{MCS}}$ – and is thus very satisfactory.

1045 *5.2.2 Comparison of longitude–latitude sections*

1046 We also investigated the robustness of the retrieved temperature field in terms of
 1047 longitudinal variations. Here we consider the retrieved temperature binned in latitude
 1048 and longitude with bin width of $3.75^\circ \times 5.625^\circ$, a resolution typical of GCM simulations
 1049 or the MCD. We consider all TIRVIM or MCS data acquired near 3 AM or 3 PM (± 1 h)
 1050 and restrict the date between $\text{Ls}=149^\circ$ and 155° (sols 316–329). Hence, we do not im-
 1051 pose strict co-location between the two datasets, except for similar season and local times,
 1052 and each of the resulting temperature map reflects the inherent latitude/longitude cov-
 1053 erage of each instrument. We detail below two examples: the longitude/latitude cross-
 1054 section of temperature at 288 Pa, 3 PM and that at 30 Pa, 3 AM, shown in Figure 19.

1055 Firstly, we highlight that MCS coverage features significant gaps in the equatorial
 1056 region regarding the afternoon temperature at 288 Pa. This is linked to enhanced cloud
 1057 opacity, as this corresponds to the end of the aphelion belt season, which hampers limb
 1058 retrievals. TIRVIM has the advantage to provide a more uniform coverage at these al-
 1059 titudes. A prominent wavenumber-3 feature is seen at 30 Pa and 3 AM, well captured

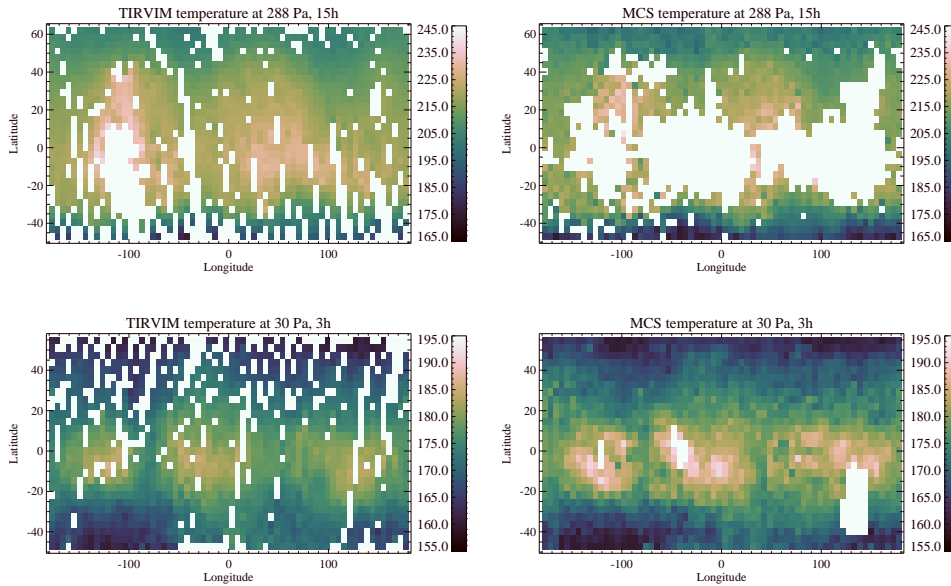


Figure 19. Temperature maps as derived from TIRVIM (left column) and provided by MCS (right column) at $L_s \sim 150^\circ$, at 3 PM and 288 Pa (upper row) and at 3 AM and 30 Pa (lower row). Both TIRVIM and MCS feature similar longitudinal wave patterns.

1060 by TIRVIM. The better coverage of TIRVIM data in the lower atmosphere allows a more
 1061 precise characterization of a similar wave seen at 3 PM, 288 Pa. As these wave signa-
 1062 tures are visible in a constant local time framework, this indicates that they are non-migrating
 1063 thermal tides. An apparent wavenumber 3 can correspond to the diurnal Kelvin wave
 1064 with zonal wavenumber 2, already reported eg. by Banfield et al. (2003); Wilson (2000)
 1065 from TES and Guzewich et al. (2012); Forbes et al. (2020) from MCS observations. The
 1066 analysis of these waves and of the 4-D structure of the thermal tides is deferred to fu-
 1067 ture work. The local time coverage of TIRVIM will be an asset to better characterize,
 1068 for instance, the amplitudes and phases of different modes of the thermal tides.

1069 Hence, we conclude that TIRVIM temperature retrievals are reliable, whether zonally-
 1070 averaged temperature fields or individual temperature profiles are considered, as long
 1071 as their coarse vertical resolution are kept in mind. The main features of the diurnal mode
 1072 of the thermal tides and longitudinal waves are well reproduced, compared to MCS ob-
 1073 servations. This validation exercise performed near 3 AM and 3 PM is a necessary step
 1074 before the scientific exploitation of temperature variations at all local times, which will
 1075 be addressed in subsequent publications.

1076 5.3 A first assessment of dust total column opacity retrievals

1077 In section 3.2.4, we have defined a quality filter for dust that is satisfied if the deriva-
 1078 tive of the radiance at 1100 cm^{-1} over a relative change in dust opacity is greater than
 1079 the $1\text{-}\sigma$ NER estimated at 1100 cm^{-1} . In other words, we retain dust opacity values for
 1080 which the estimated error is less than 100%. The fraction of dust retrievals that passed
 1081 this quality (or sensitivity) filter is shown as a function of local time and latitude in fig-
 1082 ure 20, for all TIRVIM data acquired between $L_s=142^\circ$ and 167° . As expected and al-
 1083 ready noted in section 4, two blind zones exist near 7AM and 7PM when retrieving dust
 1084 is not possible due to the lack of sufficient temperature contrast between the surface and
 1085 the lower atmosphere, where dust lies. During daytime (10AM – 5PM), 100% of dust
 1086 retrievals pass our quality filter due to a high sensitivity to dust (a combination of warm
 1087 surface and cold atmosphere) except at high southern winter latitudes, where there is
 1088 a low surface/atmosphere thermal contrast even during daytime. At nighttime, most dust
 1089 retrievals (60–80%) pass our quality filter, however, the uncertainty associated with those
 1090 nighttime retrievals is quite large, as we will see later.

1091 Validation of the retrieved dust opacity is evaluated near 3 AM and 3 PM by com-
 1092 parison with co-located MCS data, with the same co-location criteria as for the valida-
 1093 tion of atmospheric temperature. We exploit the data product called *coldust* provided
 1094 by the MCS team, which is total dust extinction at $21\text{ }\mu\text{m}$ obtained from extrapolation
 1095 of the dust profile down to the surface. This extrapolation was done under the assump-
 1096 tion that dust is well-mixed below the level of the last valid measurement (Montabone
 1097 et al., 2020). We multiply this value by 2.7 to estimate the MCS dust extinction at $9.3\mu\text{m}$
 1098 and further divide it by 1.3 to get from dust extinction to dust absorption, as recommended
 1099 by Montabone et al. (2015, 2020) and based on the work by Smith (2004); Wolff and Clancy
 1100 (2003). Indeed, we recall that we neglect scattering effects and only derive an effective
 1101 dust absorption. Dust absorption derived from TIRVIM and MCS data are compared
 1102 in figure 21 for daytime and nighttime observations during the first 45 sols. Overall, TIRVIM
 1103 daytime retrievals are in excellent agreement with MCS, and the associated $1\text{-}\sigma$ stan-
 1104 dard deviation of that difference for individual dust opacity retrievals (not shown) is about
 1105 10%. Dust opacity (in absorption, at $9.3\mu\text{m}$) is low, of the order of 0.1, which is expected
 1106 at this season.

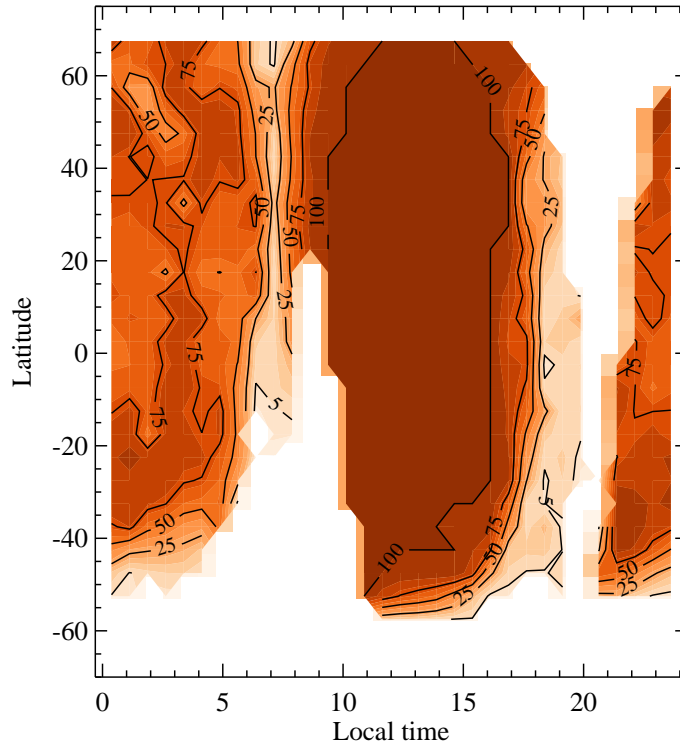


Figure 20. Percentage of retrievals that pass our quality flag for dust retrievals, for all first 45 sols of TIRVIM observations (Ls 142° to 167°), as a function of latitude and local time. White areas are missing data (the latitude - local time coverage after 45 sols is not complete).

Figure 21. Retrieved dust absorption opacity from TIRVIM near 3 PM (top) and 3 AM (bottom) as a function of latitude, for $L_s \sim 150^\circ$. Black dots stand for individual retrieved values, while red stars indicate zonal averages for 5° -wide latitude bins. For validation purpose, blue triangles are zonal averages of MCS retrieved dust absorption scaled at $9.3 \mu\text{m}$, for data co-located with TIRVIM measurements. Vertical bars illustrate the variance of each data set within a latitudinal bin.

1107 At night, we note a significant scatter in the derived dust opacities from TIRVIM.
1108 This is actually consistent with the rather poor S/N ratio and individual errors that are
1109 near 40% (hence a $1\text{-}\sigma$ error of 0.08 for a 0.2 dust opacity). More worrying is a nearly
1110 systematic overestimation of nighttime dust opacity by TIRVIM, except at latitudes 15°N –
1111 40°N . The reason behind this bias is highly similar to one of the cases described in our
1112 OSSE and illustrated in figure A3: our assumed profile for dust vertical distribution over-
1113 estimates the dust loading above the first scale height, which happens to be at the same
1114 atmospheric temperature as the surface. Indeed, we compared the MCS vertical profiles
1115 of dust opacity to our assumed one and confirms that the observed dust (by MCS) de-
1116 creases more steeply with altitude above the first scale height. In this example, we are
1117 blind to dust located near 1.5 scale height (as it emits at a similar brightness temper-
1118 ature as the surface) and we are mostly sensitive to dust in the first scale height above
1119 the surface (where the surface-atmosphere temperature contrast is high enough). As we
1120 only derive a scaling factor to a profile that has too much dust at higher altitudes, this
1121 results in an overestimated total opacity.

1122 To overcome this problem, we will have to improve our assumptions about the ver-
1123 tical distribution of dust in a future version of our algorithm. This is not trivial, as pre-
1124 vious studies have shown that the dust vertical distribution can vary quite dramatically
1125 with latitude, season, and with local time in MCS data (Heavens et al., 2011; Kleinböhl
1126 et al., 2020). As MCS only provides constraints near 3 AM and 3 PM, it appears dif-
1127 ficult to set up a robust vertical profile that would be relevant for any local time observed
1128 by TIRVIM. However, as we have previously shown that our retrieval performs well dur-
1129 ing the day (even if our assumed vertical distribution is wrong), and because dust re-
1130 trievals from a nadir sounder are not possible at evening and morning times anyway, it
1131 might be sufficient to assume the nighttime MCS profile as a baseline for all our retrievals.
1132 This will be investigated in future work.

1133 6 Summary and Conclusions

1134 In this paper, we have documented and evaluated a retrieval algorithm tailored to
1135 ACS/TIRVIM thermal infrared spectra acquired in nadir viewing geometry, with the goal
1136 of providing the best estimates of Mars' surface temperatures, vertical profiles of its at-
1137 mospheric temperature (between 5 and 50 km) and the integrated infrared optical depths
1138 of dust and water ice clouds.

1139 This algorithm was first tested on a set of synthetic spectra in conditions chosen
1140 to be representative of the variability of the martian atmosphere at various seasons, lat-
1141 itudes and local times extracted from the Mars Climate Database. This constitutes our
1142 Observing System Simulation Experiment (OSSE). The precision and accuracy of these
1143 synthetic retrievals were carefully evaluated, and in parallel, the information content of
1144 the data was studied in detail. Regarding surface temperature and aerosol opacity re-
1145 trievals, we find that our algorithm performs very well for the most favorable scenes, i.e.
1146 scenes with a warm surface temperature and featuring a large contrast between the sur-
1147 face and the atmospheric layer where aerosols reside. We caution that there are frequent
1148 conditions when this temperature contrast is low, for which the optical depth of aerosols
1149 cannot be constrained. This mostly (but not solely) occurs for observations acquired near
1150 dawn and dusk. For intermediate cases, for which we have a moderate sensitivity to dust
1151 and/or clouds, the retrievals can be significantly biased due to wrong assumptions on
1152 the vertical distribution of aerosols and/or a wrong estimate of the temperature in the
1153 lower atmosphere. Uncertainty values on dust optical depth are highly variable. They
1154 are of the order of 5-20% when the surface-atmosphere temperature contrast is high (typ-
1155 ically, daytime observations) and of 20 to 60% when this contrast is moderate (night-
1156 time conditions). Error on retrieved surface temperature is of the order of 1K for warm
1157 surfaces ($>220\text{K}$), and 3K for colder surfaces. However, significant biases (up to 10K)
1158 are reported, in particular linked with a wrong determination of retrieved dust or ice opac-
1159 ity, as there are situations where there is a high level of degeneracy between these quan-
1160 tities. Future work should thus focus on a more realistic representation of the vertical
1161 distribution of dust and water ice clouds in our algorithm, either with the help of mod-
1162 els or other independent observations. In order to improve our aerosol estimates, we also
1163 envision in the future to co-add spectra acquired at close locations (in particular for low
1164 surface temperatures) to increase their signal-to-noise ratio.

1165 The retrieval of atmospheric temperature is found to be very robust. Most of the
1166 differences found between retrieved temperatures and the input temperatures used to
1167 generate synthetic spectra in our OSSE can be explained by the coarse vertical resolu-
1168 tion of TIRVIM, especially in the 2–10 Pa range where the width of the functional deriva-
1169 tives is of the order of two scale heights. These differences can locally reach 10K. How-
1170 ever, when TIRVIM vertical resolution is taken into account (through the use of aver-
1171 aging kernel matrices), our retrieved temperatures agrees with the input ones within 2–

1172 3K, which is taken as an estimate of uncertainty in our retrieved profiles and supports
1173 the good performance of our algorithm. We report some difficulties in retrieving atmo-
1174 spheric temperatures in the first scale height when there are optically thick clouds at low
1175 altitudes. These thick clouds limit our sensitivity to the lower atmosphere as the result
1176 of the degeneracy between surface temperature, cloud opacity and/or low atmospheric
1177 temperature retrievals. Important biases are also found when there is a very steep tem-
1178 perature inversion in the first scale height, also linked with the rather coarse vertical res-
1179 olution of TIRVIM. However, these cases remain rare.

1180 We then applied our algorithm to the first 45 days of TIRVIM operations, corre-
1181 sponding to $L_s=142\text{--}167^\circ$ of Martian Year 34. Retrieved temperature profiles were val-
1182 idated against co-located measurements by the Mars Climate Sounder near 3 AM and
1183 3 PM. As for the OSSE, we find that most of the differences between the thermal struc-
1184 ture derived from TIRVIM and MCS can be attributed to differences in vertical reso-
1185 lution and sensitivity. Local temperature extrema (vertical oscillations of the temper-
1186 ature profile) seen by MCS at pressures lower than 10–20 Pa are not well captured by
1187 TIRVIM, consistently with its coarse vertical resolution. As a consequence, the signa-
1188 ture of the diurnal mode of the thermal tide, well visible in the day-night temperature
1189 difference, appears severely muted in TIRVIM retrievals at these low pressure levels. On
1190 the positive side, TIRVIM retrievals are highly comparable to MCS temperatures in the
1191 range 300–20 Pa (within 2–3K). Furthermore, they have the advantage of a more homo-
1192 geneous spatial coverage at higher pressures, where MCS is frequently blind due to larger
1193 aerosol opacity along the limb-viewing light path. We also showed that several wave pat-
1194 terns are well visible in longitude-latitude cross-section of the retrieved temperature from
1195 TIRVIM.

1196 These results are promising and open the way to future detailed studies of atmo-
1197 spheric dynamics at the diurnal scale in Mars' lower atmosphere. Indeed, the strength
1198 of the TIRVIM dataset lies in its sampling of the diurnal cycle, with all local times be-
1199 ing sampled on the planet every 54 sols. As an example, full local time coverage is an
1200 asset to better characterize the amplitudes and phases of the different modes of the ther-
1201 mal tides.

1202 **Appendix A Supplementary figures**

1203 **A1 Quality of dust retrievals**

1204 Figure A1 shows the "true" versus retrieved dust opacity at different latitudes and
 1205 local times, highlighting a subset of Figure 8 in the main text.

1206 **A2 Examples of synthetic retrievals**

1207 In this appendix we display five detailed examples (out of the 440 test case retrievals
 1208 of our OSSE) showing fits to synthetic TIRVIM spectra ; functional derivatives (Jaco-
 1209 bian) for the retrieval of atmospheric temperature ; and the comparison between "true"
 1210 and retrieved quantities. These examples are chosen as they exhibit significant errors on
 1211 dust opacity, water ice opacity, surface temperature and/or atmospheric temperature de-
 1212 spite satisfactory fits to the spectra. These figures are discussed in the main text.

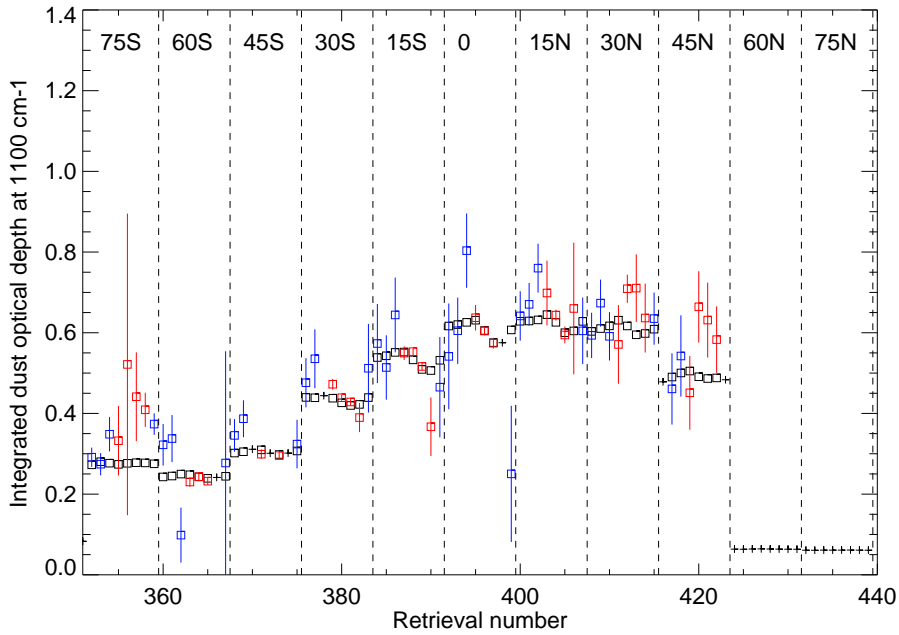


Figure A1. Same as Figure 8 but only for data at $L_s=270^\circ$, with labels for different latitudes. For a given latitude, data is sorted by local time (from midnight to 9 PM, every three hours). No satisfactory dust retrievals were obtained at latitudes 60N and 75N (winter) due to cold surface and poor signal-to-noise ratio.

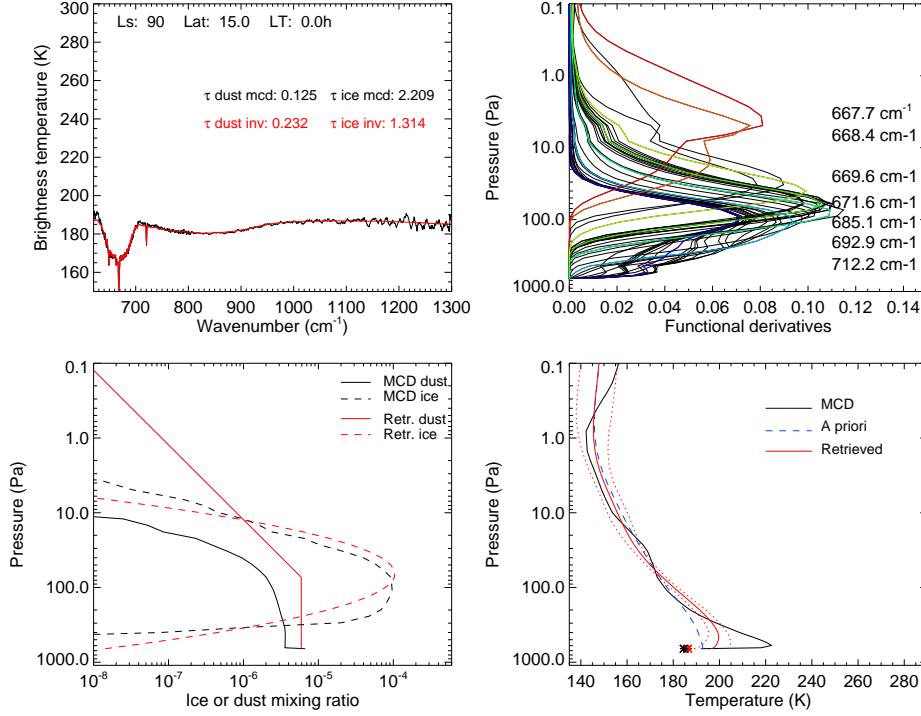


Figure A2. Example of a synthetic retrieval for a MCD scenario extracted at $L_s=90^\circ$, latitude 15°N , local time 0 AM. Top, left: Synthetic TIRVIM spectrum (black) along with the best fit (red). Retrieved and MCD dust and water ice cloud integrated opacities are indicated. Top, right: functional derivatives of the temperature as a function of pressure, for 50 different wavenumbers within the CO_2 band. Several wavenumbers are highlighted in different colors and labeled. Bottom, left: Mixing ratio vertical profiles for dust and water ice as taken from the MCD (used to generate the synthetic spectrum, in black) and as derived from the retrieval process (in red ; note that only a scaling factor to a generic *a priori* profile is retrieved). Bottom, right: Temperature vertical profile from the MCD (used to generate the synthetic spectrum, in black), *a priori* profile built from the synthetic spectrum (dashed blue line), and retrieved profile (red), with error bars in red dotted lines. The black and red stars stand for the MCD and retrieved surface temperature, respectively.

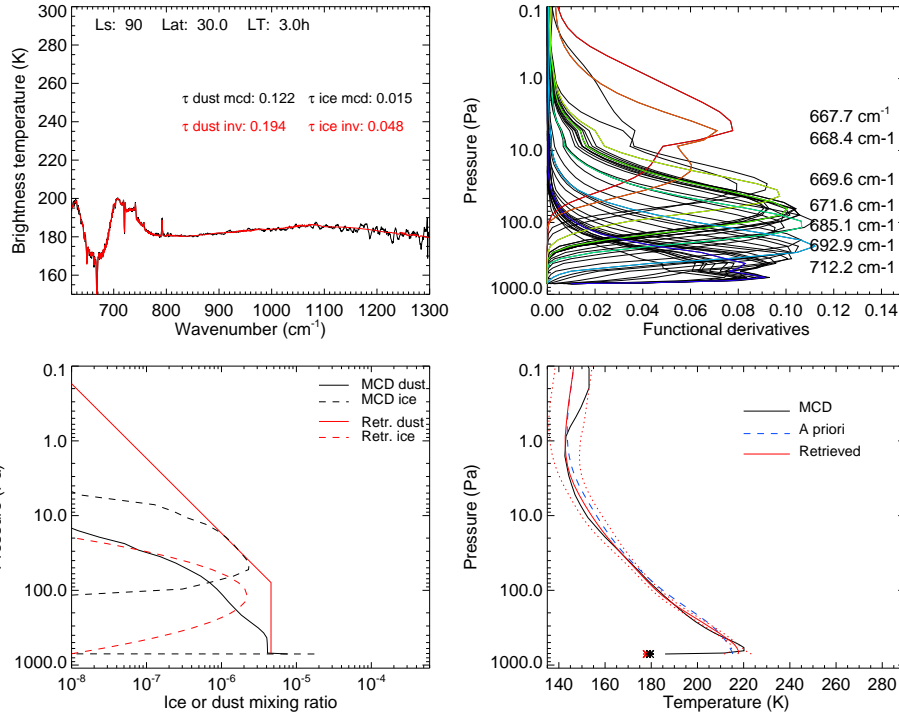


Figure A3. Same as figure A2 for $L_s=90^\circ$, latitude 30°N , local time 3 AM.

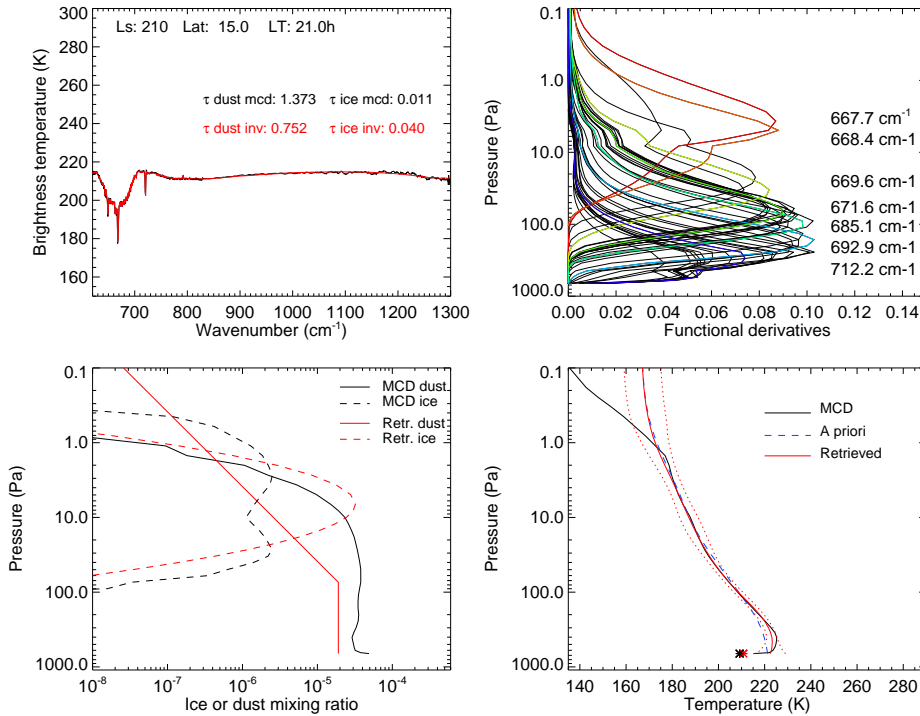


Figure A4. Same as figure A2 for $L_s=210^\circ$, latitude 15°N , local time 9PM.

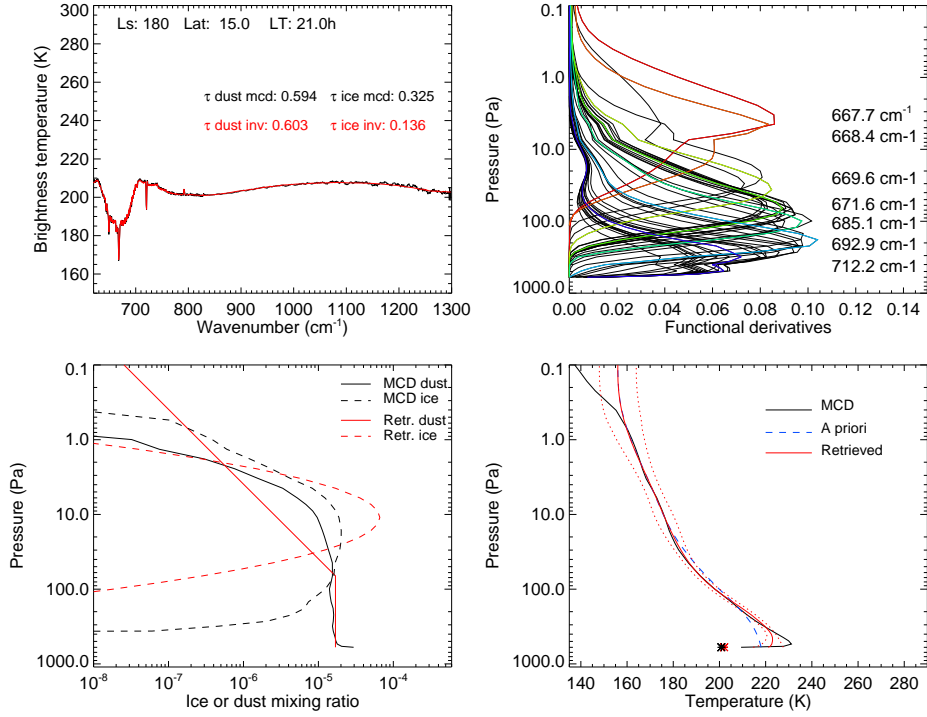


Figure A5. Same as figure A2 for $L_s=180^\circ$, latitude 15°N , local time 9 PM.

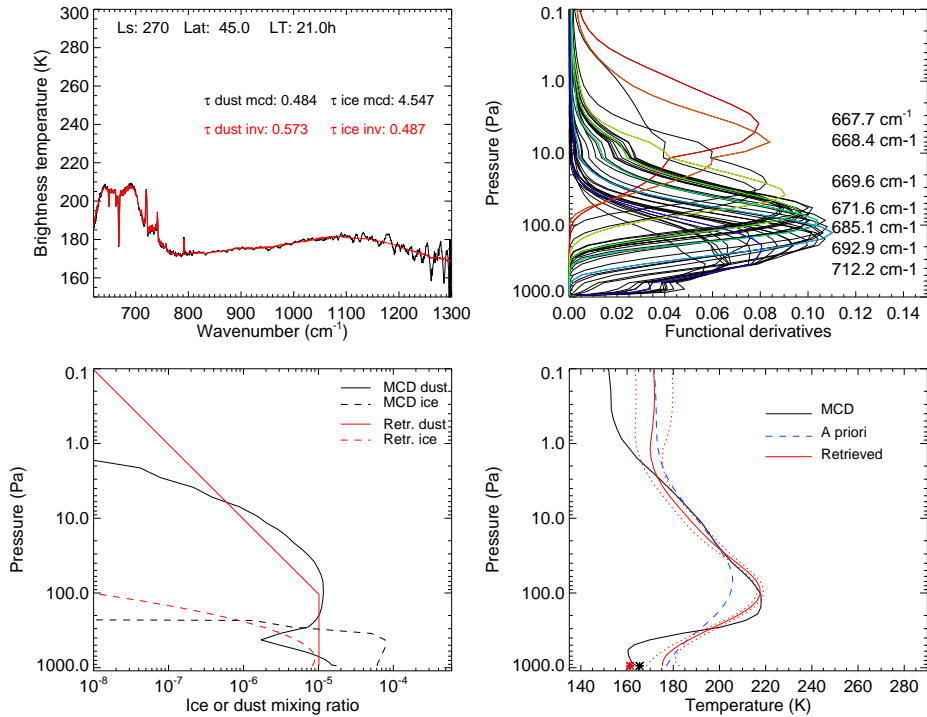


Figure A6. Same as figure A2 for a MCD scenario extracted at $L_s=270^\circ$, latitude 45°N , local time 9PM.

1213 **A3 Impact of using different *a priori* temperature profile**

1214 Figure A7 demonstrates the good performance of our atmospheric temperature re-
1215 trieval starting from different *a priori* profiles (see main text).

1216 **A4 TIRVIM-MCS comparison**

1217 Figure A8 shows the comparison of the zonally-averaged temperature near 3 AM
1218 and 3 PM as retrieved from TIRVIM and MCS, for co-located measurements. No av-
1219 eraging kernels were applied to the MCS temperature fields in that figure.

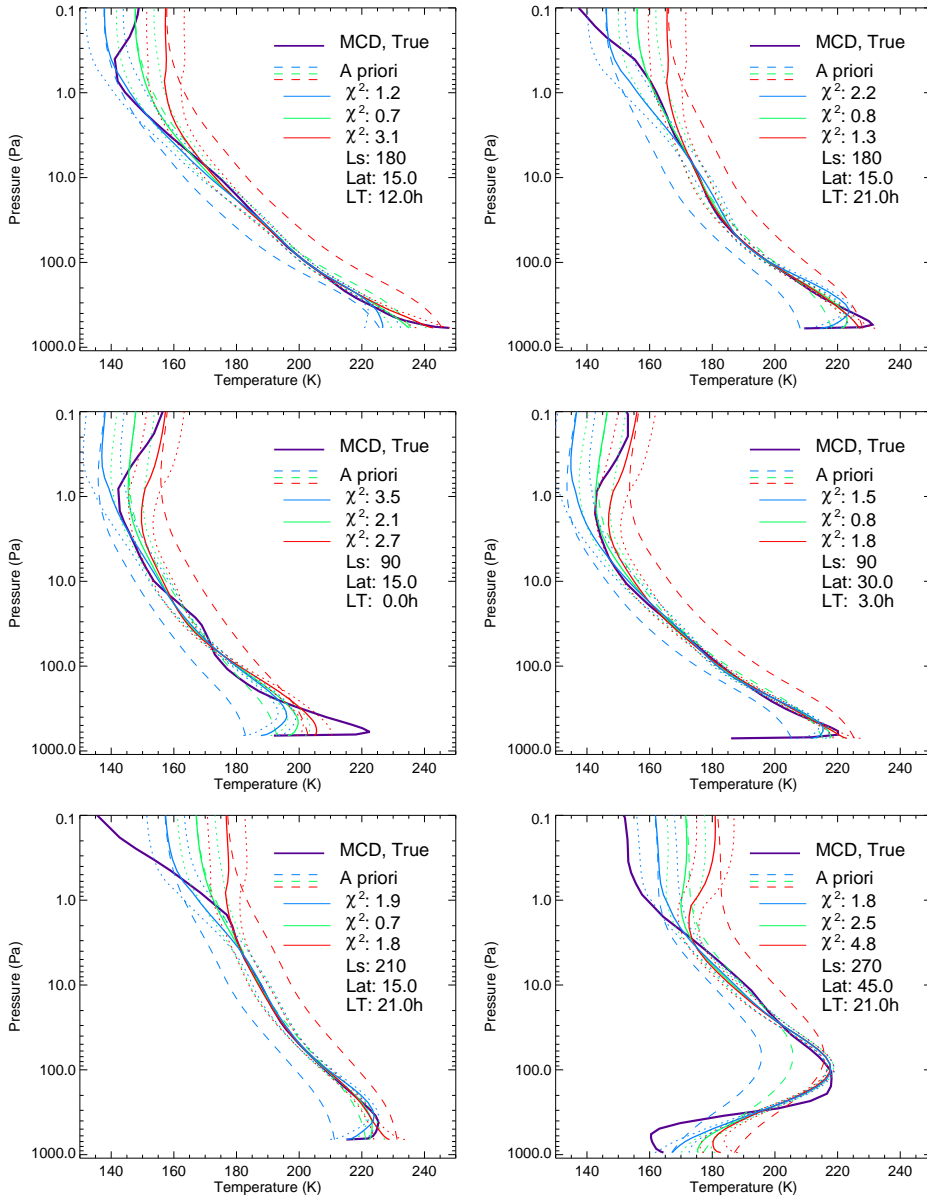


Figure A7. Retrieved temperature profiles (color solid lines) for different *a priori* profiles (dashed lines): in green our nominal *a priori* profile, in blue a profile 10K colder, in red a profile 10K warmer. Quality of the fit in the CO₂ band is given for each retrieval (χ^2). These examples are for 6 out of 440 synthetic retrievals of our OSSE, with the "true" temperature profile in purple. Dotted lines highlight the error envelopes. These six examples correspond to local times, season and latitudes of the cases shown in Figures 6 and A2–A6.

Figure A8. Pressure-latitude sections of the zonally-averaged temperature near 3 AM (top) and 3 PM (bottom). Left panels correspond to TIRVIM, middle panels to MCS and the difference between the two datasets is shown in the right panels. Bins of 5° wide in latitude are used. In each panel, these zonal averages are performed for a subset of the available TIRVIM and MCS data that meet co-located criteria, as described in the text.

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