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Extending MGS-TES Temperature Retrievals in the Martian Atmosphere up to 90 km: Retrieval Approach and Results

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Abstract

This paper describes a methodology for performing temperature retrievals in the Martian atmosphere in the 60–90 km altitude range using spectrally integrated 15 μm CO₂ limb emissions measured by the Thermal Emission Spectrometer (TES), the infrared spectrometer on-board the Mars Global Surveyor (MGS). We show that a limited number of limb-geometry sequences observed by this instrument are characterized by a high enough signal-to-noise ratio (SNR) to allow extending the upper limit of the retrievals to ~ 90 km. Using the methodology described in the paper, we have retrieved ~ 1200 individual temperature profiles from the MGS TES limb observations in the altitude range between 60 and 90 km. The set of retrieved temperature profiles is available for download in supplemental materials of this paper. The temperature retrieval uncertainties are mainly caused by noise in the observed radiance, and are estimated to be about 3 K at 60 km and below, 4 K at 70 km, 7 K at 80 km, 10 K at 85 km, and 20 K at 90 km. We compare the retrieved profiles to the Martian Year 24 (MY 24) dataset of the Mars Climate Database (MCD) and SPICAM measured temperature profiles for MY 27 and find good qualitative agreement. Quantitatively, our retrieved profiles are in general warmer and demonstrate strong profile-to-profile variability. The warm bias is explained by the selection of high SNR limb scans and can be estimated and taken into account (values in brackets below correspond to corrected TES). Overall, the average difference between the TES-retrieved temperatures and the MCD MY 24 dataset is: 7 (6) K at 60 km, 9 (7) K at 70 km, 10 (5) K at 80 km, and 13 (7) K at 90 km. The root-mean-square of the temperature variability caused by gravity waves estimated in this work is 7 K at 60 km, 8 K at 65 km, 11 K at 70 km, 15 K at 75 km, 18 K at 80 km, and 20 K at 85 km.

Keywords: temperature retrievals, middle atmosphere of Mars, remote sensing.

1. Introduction

The TES instrument on the MGS orbiter mapped the atmosphere of Mars for more than three Martian years allowing an unprecedented survey of the present Martian climate. The TES observations have been used to retrieve temperature profiles (Conrath et al. 2000), aerosol optical depth and physical properties (e.g. Pearl et al. 2001; Smith et al. 2001; Smith 2004; Clancy et al. 2003; Wolff and Clancy 2003), and water vapor abundance (Smith 2002; 2004). Most of the previously reported temperature retrievals from TES cover the atmosphere up to the ~ 0.01 mbar level, which corresponds to ~ 60 km altitude. The upper limit for the currently available TES retrievals was set in accordance with the signal-to-noise ratio of the observations used in the constrained linear inversion algorithm applied for temperature retrievals (Conrath et al., 2000). However, in the limb observation mode measurements were performed at higher altitudes, up to ~ 120 km altitude. In this work we used a forward-fitting temperature retrieval algorithm and applied it to a spectrally integrated CO_2 $15\text{ }\mu\text{m}$ limb radiance to extend the upper altitude of temperature retrievals to 90 km and to provide high-altitude temperature data for Martian Years (MY) 24 and 25. Temperature soundings in the middle atmosphere of Mars are of great significance since they can give an important insight into the dynamics of the region that is linked with convective instabilities and gravity wave (GW) propagation and dissipation (e.g. Heavens et al., 2010 and references therein) and can provide additional constraints on tidal and gravity wave drag needed for modeling work (e.g. Forget et al., 1999; Forbes and Miyahara, 2006; Hartogh et al., 2007; McDunn et al., 2010; Medvedev et al., 2011; Bougher et al., 2011).

The structure of this paper is as follows: Section 2 describes the TES instrument. In Section 3 we discuss the specifics of the CO_2 $15\text{ }\mu\text{m}$ emission in Martian atmosphere, define the integrated radiance that will be used for temperature retrievals, and introduce the radiance profile selection criteria. Section 4 describes the non-LTE code ALI-ARMS (see the Appendix for abbreviations not explained in the text), the temperature retrieval algorithm, and the retrieval uncertainties. In Section 5 we present the retrieved temperature profiles and compare them to averaged temperature profiles from the Mars Climate Database (MCD) dataset (Forget et al., 1999; Lewis et al., 1999; Gonzales-Galindo et al., 2005). A discussion of similarities and differences is also included into this section. Finally, we present our conclusions in Section 6.

2. TES instrument

MGS began mapping operations from Mars orbit on 1 March 1999 (MY 24, $\text{Ls} = 104^\circ$) and provided nearly continuous monitoring of conditions in the Martian atmosphere for over three full Martian years. The MGS mission ended on 2 November 2006 when the contact with the spacecraft

was lost. The TES instrument (Christensen et al. 2001) systematically measured and monitored the Martian surface and atmosphere throughout all phases of the mission. The imminent failure of a neon bulb required for calibration of the spectrometer forced spectrometer observations to end on 31 August 2004 (MY 27; Ls=81°), although observations continued using the TES bolometers. The near-polar solar-locked mapping orbit allowed 12 orbits per day of data at roughly 2:00 AM and 2:00 PM local time. A majority of observations were taken in the nadir geometry, but limb observations of the Martian atmosphere were included roughly every 10 degrees of latitude throughout the orbit (both day and night) throughout the mission. Each 8.3 mrad detector field-of-view had a projected size of about 13 km at the limb, allowing vertical resolution of just over a scale height. In a limb-geometry sequence, the 3x2 array of TES detectors scanned the atmosphere in overlapping steps from below the surface to about 120 km tangent height above the surface providing vertical sampling of about 1 to 5 km (see more details in (Christensen et al., 2001)). The total number of limb geometry spectra obtained during the mission is about 750,000. The spectral resolution of the TES instrument is 5 cm⁻¹ and 10 cm⁻¹. In this work we used 10 cm⁻¹ resolution spectra (Fig. 2). We show that a limited number of limb geometry spectra taken during the first two Martian years have SNR that allows an extension of temperature retrievals up to 90 km altitude. The selection criteria for these spectra are described in Section 3.2.

3. CO₂ 15 μm radiance measured by TES

In the gas phase, carbon dioxide (CO₂) molecular vibrations involve combinations of symmetric stretch (ν_1), covalent bond bending (ν_2), and asymmetric stretch (ν_3) modes. The diagram in Fig. 1 shows the ground state and various excited vibrational levels of the main CO₂ isotope (¹⁶O¹²C¹⁶O) up to an energy of 3900 cm⁻¹. The vibrational structure of minor isotopes is similar to that of the main isotope and is not shown in Fig. 1. The levels in Fig. 1 are marked in accordance with the Herzberg notation $\nu_1\nu_2^l\nu_3$ where ν_1 , ν_2 , and ν_3 denote the number of the corresponding vibrational quanta and the l symbol refers to the orbital quantum number. The 15 μm radiance measured by the TES instrument and used for temperature retrievals in this study arises from the optical transitions from vibrationally excited states with $\Delta\nu_2 = l$, where $\Delta\nu_2$ denotes the change in the ν_2 vibrational quanta number.

3.1. CO₂(ν_2) vibrational levels populations in the Martian atmosphere

The interpretation of TES 15 μm limb radiance profiles requires knowing the populations of the corresponding CO₂(ν_2) vibrational levels at the altitudes of the limb observations. In general, in the lower atmosphere of planets the frequency of inelastic molecular collisions is sufficiently high that these collisions overwhelm other population/depopulation mechanisms of the molecular vibrational

97 levels. This leads to a local thermodynamic equilibrium (LTE), and the populations follow the
 98 Boltzmann distribution governed by the local kinetic temperature. In the middle and upper
 99 atmosphere, where the frequency of inelastic collisions is much lower than that at lower altitudes,
 100 other processes also influence the vibrational levels population. These include: a) the direct
 101 absorption of solar radiance; b) absorption of the radiance coming from the lower atmosphere;
 102 c) radiative de-excitations; d) vibrational-translational (V–T) energy exchanges by collisions with
 103 molecules and atoms of other atmospheric constituents; and e) collisional vibrational-vibrational
 104 (V–V) energy exchange with other molecules. As a result, LTE no longer applies in this altitude
 105 region and the populations must be found by solving the self-consistent system of kinetic equation
 106 and radiative transfer equation, which express the balance relations between various excitation/de-
 107 excitation processes described above. Our calculations show that for the $\text{CO}_2(\nu_2)$ vibrational levels
 108 in the Martian atmosphere the LTE-breakdown is observed at heights greater than ~ 80 km and that
 109 $\text{CO}_2(\nu_2)$ populations depend mainly on the balance between processes b) – e) and the most
 110 important rate coefficient that influences the population of $\text{CO}_2(\nu_2)$ vibrational levels in the upper
 111 atmosphere of Mars is $k_{\text{VT}}\{\text{CO}_2\text{-O}\}$, the quenching rate coefficient for V–T energy exchange
 112 process at $\text{CO}_2\text{-O}$ collisions (Feofilov et al, 2011 and references therein). The sensitivity of the
 113 retrieval to this coefficient will be discussed below.

114 **3.2. TES spectra selection and processing**

115 In this work we used a spectrally integrated $15\ \mu\text{m}$ CO_2 band radiance in the retrievals to increase
 116 SNR and to extend the upper limit of the retrieved temperature profile. In a sense, using the
 117 integrated radiance converts the spectrometer to a broadband radiometer like, for example, the
 118 SABER instrument (Russell et al., 1999) that was successfully used for temperature retrievals in the
 119 Earth’s atmosphere up to ~ 110 km altitude from the $15\ \mu\text{m}$ broadband radiance profiles. Spectra
 120 selection for integration and processing was based on two criteria: a limb sequence should
 121 a) provide a sufficient number of measured points above 60 km altitude and b) SNR for the
 122 integrated signal should be greater than unity up to at least 85 km. The calculations performed in
 123 this work show that both during the day and night in the Martian atmosphere, the $15\ \mu\text{m}$ CO_2 band
 124 radiance is confined within the $560\text{--}770\ \text{cm}^{-1}$ spectral range. Below we will refer to this range as to
 125 “spectral window A”. Besides this window, we have also defined windows B ($510\text{--}560\ \text{cm}^{-1}$) and
 126 C ($770\text{--}830\ \text{cm}^{-1}$) that were used to estimate the noise and offset in the observed signal. The
 127 calculations show that all spectral line intensities in windows B and C are less than 1% of the line
 128 intensities in the maximum of the $15\ \mu\text{m}$ manifold. For the purpose of the present work we fit for a
 129 second order polynomial using the spectral points in windows B and C, and then subtract the
 130 corresponding offset values from the spectral intensities in window A. Examples of the resulting

131 spectra in the 61–89 km altitude interval are shown in Fig. 2a–f. As one can see, the suggested
132 procedure efficiently removes the offsets at all considered altitudes.

133 The integrated values of the 15- μm radiance in the 560–770 cm^{-1} spectral range with offset
134 removed are shown in Fig. 2g. This panel also contains the NER (noise equivalent radiance) value
135 estimated from windows B and C. As one can see in Fig. 2g, for a given limb sequence the NER
136 becomes comparable to the integrated signal at ~ 86 km altitude. The number of measurements for
137 which the NER allows retrievals up to 90 km altitude is small compared with the total number of
138 limb measurements. There are two reasons for that. First, the altitude coverage of limb
139 measurements differs and not all limb sequences provide valid data points up to 90 km altitude.
140 Second, the increasing noise in TES observations as the mission went on limited the limb scans
141 with “good SNR” up to 90 km to the first two Martian years of the mission. We also note that
142 selecting high SNR scans may introduce a positive offset to the average retrieved temperature
143 profile as we will show below in Sect. 5.2. However, the selection routine does not modify any
144 individual temperature profile used in the study nor does it add to the retrieval errors. We will
145 estimate the systematic error caused by the high SNR scan selection in Sect. 5.2. Overall, we have
146 identified 1410 limb sequences that satisfy the SNR and altitude coverage criteria. The
147 latitudinal/seasonal distribution of the selected measurements is presented in Fig. 3. As one can see,
148 most of the selected observations correspond to nighttime cases. This needs some explanation. The
149 day-night temperature difference at 85 km altitude due to diurnal thermal tide is ~ 7 K (McCleese et
150 al., 2008) and the expected 15 μm radiance increase due to that temperature change is $\sim 20\%$.
151 Another 15–20% increase in 15 μm radiance comes from the redistribution of the absorbed solar
152 energy (see Fig. 1). However, this 40% radiance increase is compensated by the higher daytime
153 TES noise level that leads to filtering out more measurements during daytime than during
154 nighttime.

155 All of the selected limb sequences were processed using the retrieval procedure described in the
156 next section.

157 **4. ALI-ARMS research code and retrieval algorithm**

158 **4.1. ALI-ARMS research code**

159 All of the calculations performed in this work were made using the ALI-ARMS computer code (see
160 Kutepov et al., 1998; Gusev, 2003; Gusev and Kutepov, 2003; and references therein) that solves
161 the multi-level problem using the Accelerated Lambda Iteration (ALI) technique developed for
162 calculating non-LTE populations of atomic and ionic levels in stellar atmospheres (Rybicki and
163 Hummer, 1991). The code iteratively solves a set of statistical equilibrium equations and the

radiative transfer equation. The algorithm efficiency is ensured by the ALI technique, which avoids the expensive radiative transfer calculations for the photons trapped in the optically thick cores of spectral lines. The ALI-ARMS model was successfully applied by Kaufmann et al. (2002; 2003) and Gusev et al. (2006) to the non-LTE diagnostics of spectral observations of the Earth's limb from the CRISTA instrument (Offermann et al., 1999; Grossmann et al., 2002). Kutepov et al. (2006) used ALI-ARMS to validate temperature retrievals from the 15 μm CO₂ emissions measured by the SABER instrument onboard the terrestrial TIMED satellite. This code was also used for the H₂O non-LTE model validation (Feofilov et al., 2009) and for the $k_{VT}\{\text{CO}_2\text{-O}\}$ rate coefficient estimate from the atmospheric observations (Feofilov et al., 2011 and references therein).

In this work we used the CO₂ non-LTE model developed in our group (Gusev, 2003; Kutepov et al., 2006). The full model includes 350 vibrational levels of 7 CO₂ isotopes but as Gusev (2003) showed, for most of the applications it is enough to include five CO₂ isotopes, 60 vibrational levels, and 20,000 optical transitions from the HITRAN 2004 database (Rothman et al. 2005) so we used this optimized model. The retrieval method implemented in the ALI-ARMS code is similar to the iterative onion-peel technique using the relaxation method described in Gordley and Russell (1981) for LTE. We will describe here the algorithm for non-LTE temperature retrieval but this approach is applicable also for trace gas retrievals. The process starts with the initial temperature profile combined with pressure, VMRs of CO₂ and atomic oxygen distributions taken from the MCD. The non-LTE populations are estimated and used for monochromatic limb radiance calculations. These radiances are integrated for each limb path and an integrated profile is convolved with the TES field of view. The resulting simulated radiance I is compared to the measured radiance at each tangent height, and the temperature profile is iterated using the following relaxation scheme:

$$T_{i+1} = T_i + (I_{meas} - I_i) / (\partial I / \partial T)$$

where T_{i+1} and T_i are the temperature values at the $i+1$ -th and i -th iterations, respectively, I_{meas} is the integrated limb radiance measured by TES (see Section 3.2 above), I_i is the simulated limb radiance at the i -th iteration, and $(\partial I / \partial T)$ is the numerically calculated derivative of the radiance produced by the forward model with respect to temperature. Finally, a new temperature profile is produced, pressure profile is adjusted using the hydrostatic law, the new non-LTE populations of CO₂ molecular levels are calculated, and the radiance is simulated again. The iterations are repeated until the differences between the simulated and measured radiances become equal to or smaller than the radiance noise in the observed integrated limb radiance. It is important to note that if iteration is allowed to proceed indefinitely, then it will converge to an “undesirable exact solution” or quickly is getting unstable (Houghton et al, 1984, p.148). However, a convergence analysis demonstrates that broad-scale features converge rapidly,

198 and the fine-scale features (often associated with the signal noise) converge slowly, so the
199 reasonable “physical solution” may be found if the iteration is stopped at the right point (see
200 below).

201 In this work we ran the retrievals up to 100 km altitude even though the estimates show that the
202 upper limit for SNR=1 in TES temperature retrievals is 90 km. This was done deliberately. Even
203 though the individual radiance values in 90–100 km layer are comparable to NER, the integrated
204 radiance of the layer has SNR larger than 1 and, therefore, still carries the information about the
205 area. Temperature values retrieved in this layer combined with the model temperature profile above
206 ensure proper radiance add-on for the line-of-sight of the instrument in limb observation mode.
207 These temperatures cannot be considered as true ones since they compensate for the difference
208 between the model atmosphere and the real one above 100 km. However, as a result of using the
209 90–100 km layer the temperature retrievals below are less affected by the uncertainties of the
210 atmosphere above (see the self-consistency tests in the next section).

211 ***4.2. Self-consistent retrievals, convergence of the method, and retrieval uncertainties***

212 To illustrate the convergence of the method we have performed a self-consistent retrieval using 10
213 Martian atmospheric profiles corresponding to seasons and latitudes shown in Fig. 25 and Fig. 28
214 of (Kleinböhl et al., 2009). We have selected three representative cases for demonstrational
215 purposes. Atmosphere #1 corresponds to tropical case (latitude = 0°) and the atmospheres #2 and
216 #3 represent high latitudes in the Northern and Southern hemispheres, respectively
217 (latitude = 80°N and 80°S) for $L_s=330-340^\circ$. Temperature distributions up to 0.01 Pa level were
218 taken from (Kleinböhl et al., 2009) and supplemented with the MCD atmospheric profiles available
219 for download at <http://johnson.lmd.jussieu.fr:8080/las/servlets/dataset>. We used
220 pressure/temperature, CO₂, and O VMR profiles covering the 0–200 km altitude range. To simulate
221 the GW-induced temperature variations we combined the average temperature deviations for the
222 corresponding models from (Kleinböhl et al., 2009) with the temperature variations estimated from
223 the RMS wind values from (Medvedev et al., 2011) above 0.01 Pa level assuming the
224 proportionality of these parameters (Medvedev, private communication, 2012). As a result, we
225 obtained the temperature RMS profile $\langle \Delta T(z) \rangle$ up to the turbopause altitude. Then we “generated”
226 a GW for each test atmosphere by combining two harmonics with random wavelengths and phases
227 (17 and 25 km for the examples shown in Fig. 4). The GW amplitude was modulated by
228 $\langle \Delta T(z) \rangle \cdot \sqrt{2}$ producing waves with up to ± 35 K amplitude at 85–100 km. The “random” pattern of
229 the wave was kept the same for all cases to simplify tracing noise induced effects in retrieved
230 temperatures. The obtained waves were applied to the corresponding average temperature

231 distributions. The top of the atmosphere (TOA) was set at 200 km, and $k_{VT}\{\text{CO}_2\text{-O}\}$ was set to
 232 $6 \cdot 10^{-12} \text{cm}^3 \text{s}^{-1}$, the value that is typically retrieved from the atmospheric observations on Earth
 233 (Sharma and Wintersteiner, 1990; Ratkowski et al., 1994; Gusev et al., 2006; Feofilov et al., 2011).
 234 First, we calculated the non-LTE populations of the CO_2 vibrational levels at all heights and then
 235 calculated the limb radiance for each spectral line in window A and at each tangent height. After
 236 that, the radiance was spectrally integrated, convolved with the vertical field of view (FOV) of the
 237 TES instrument, and the resulting integrated $15 \mu\text{m}$ radiance formed the reference profile $I_{ref}(z)$
 238 for the corresponding atmospheric model. Three retrievals were performed for each of the test
 239 atmospheres: two noise-free retrievals that started from temperature profiles that were 25 K warmer
 240 and colder than the original one, and one retrieval starting from the 25 K warmer profile with noise
 241 added to the reference radiance. The noise was estimated from real TES spectra for the
 242 corresponding season and locations using spectral information in windows B and C. The
 243 hydrostatic adjustment of the pressure-temperature profile was performed at each of the iterations
 244 as it is done in the standard ALI-ARMS temperature retrieval process. It is convenient to define an
 245 additional convergence criterion for the retrieval process as a weighted relative radiance deviation
 246 in the 60–90 km altitude range: $(\Delta I_i / I)_{R.M.S.} = \left[\sum_{id=60}^{90} ((I_{ref}^{id} - I_i^{id}) / I_{ref}^{id})^2 / (90 - 60 + 1) \right]^{1/2}$ where I_{ref}^{id} is
 247 a “reference” limb radiance for tangent height id and I_i^{id} is the radiance simulated at the i -th
 248 iteration for the same tangent height. We remind here that in real retrievals the reference radiance
 249 profile $I_{ref}(z)$ is substituted with measured radiance profile $I_{meas}(z)$. The behavior of $(\Delta I / I)_{R.M.S.}$
 250 for all three test atmospheres is shown in Fig. 4a. As one can see, noise-free retrievals demonstrate
 251 rapid convergence up to the 6–7th iteration. After that the convergence continues but at a slower
 252 rate. The corresponding temperature profiles obtained at the 11th iteration are close to the original
 253 profile (see the temperature deviation from the original profile in Fig. 4b–d). However, further
 254 iterations do not lead to better agreement between the retrieved and original profiles. This is
 255 explained by a) large vertical FOV of the instrument that “mixes” the effects of different heights;
 256 b) hydrostatic adjustment that redistributes the changes occurring in the lower part to the whole
 257 atmosphere. Overall, the uncertainties caused by the retrieval methodology are within $\pm 4\text{K}$ limits
 258 for all three test atmospheres. One can trace the GW-induced temperature variation pattern (beating
 259 frequency) in the residuals in Fig. 4b–d but its magnitude is less than 1 K at heights up to 90 km.
 260 Naturally one should expect larger errors in retrieving GWs with a wavelength shorter than doubled
 261 value of FOV. Adding noise complicates the situation. The convergence becomes slower (see the
 262 corresponding solid lines with circles in Fig. 4a) and there is almost no improvement in
 263 $(\Delta I / I)_{R.M.S.}$ after the 6th iteration (the NER level is reached). Solid lines with circles in Fig 4b–d

show the discrepancy between the retrieved temperature profile and the reference one for the 6th iteration. Note the similarity of the response of all three retrievals to adding the same noise pattern to the reference radiance profile.

Another important factor that might affect the retrievals is the uncertainty of the atmospheric profile below and above the retrieval area. The lower part may affect the retrieval through hydrostatics while the upper part may change the absorption and emission along the line of sight in the limb observation mode. To estimate these effects we performed a set of retrievals for the same three model Martian atmospheres. For simplicity, we demonstrate them on noise-free, GW-free retrievals starting from the original temperature distributions. For these tests we only changed the temperature profiles above and below the retrieval area by ± 20 K and ± 5 K, respectively. All the other combinations (0 K change below 50 km, ± 20 K above 100 km and so on) have demonstrated smaller effects on the retrieval and are not shown here. Figure 5 demonstrates that ± 5 K changes below 50 km altitude do not significantly affect the retrievals in 50–90 km area (overall offset caused by these changes is less than ± 1 K). On the other hand, ± 20 K modification of temperature profile above 100 km leads to ± 6 K offsets at 90 km altitude for Atmosphere #3 and smaller offsets for other two test atmospheres.

Changing $k_{VT}\{\text{CO}_2\text{-O}\}$ to $1.5 \cdot 10^{-12} \text{cm}^3 \text{s}^{-1}$, the value obtained in laboratory measurements (Pollock et al., 1993; Khvorostovskaya et al., 2002; Castle et al., 2006; Huestis et al., 2008) modifies the retrieved profile in the entire range of the retrieval. This is explained by the non-LTE effects in CO_2 : reducing the collisional rate coefficient leads to less efficient thermalizing of the vibrational levels that become more populated by radiance coming from the warmer and denser layers below. This leads to overestimating the radiance and, therefore, to underestimating the temperature. The temperature uncertainty caused by the $k_{VT}\{\text{CO}_2\text{-O}\}$ change from “atmospheric” to “laboratory” value is about 3 K above 65 km. Finally, “removing” the 110–200 km part of the atmosphere (TOA 110 in Fig. 5) doesn’t significantly affect the 60–90 km retrieval area since missing radiance is compensated in the retrieval process by increasing the temperature in the 90–100 km layer. However, lowering TOA introduces positive offset so we opted not to lower TOA. Overall, running the retrievals with random noise profiles and summing up all the uncertainties listed in this section provides the following estimate for the uncertainty of the single profile retrieval: 3 K at 60 km, 4 K at 75 km, 7 K at 80 km, and 10 K at 85 km altitude.

5. Temperature retrievals from TES measurements

5.1. Input data and retrieval procedure

296 All the retrievals performed in this study utilized the retrieval algorithm described in Section 4. For
 297 each of the 1410 integrated TES radiance profiles (see Section 3.2 and Fig. 3) the initial guess
 298 atmospheric profile was assembled from pressure/temperature profiles in the 10–60 km altitude
 299 range retrieved by the TES team using nadir geometry observations (Conrath et al. 2000; Smith
 300 2004), and from pressure/temperature, CO₂ and O VMRs taken from the MCD in the 60–200 km
 301 interval. The retrieval was performed over the 50–100 km range. The upper 10 km layer of this
 302 interval was used to damp the effects of uncertainties in the upper atmosphere (see Section 4.2) and
 303 is included in the retrieved temperature dataset only for quality control purposes (the larger the
 304 gradient in the 90–100 km layer, the larger the difference between the model atmospheric profile
 305 above 100 km, and the real one). The 50–60 km interval was included in the retrieval to allow for
 306 temperature profile adjustment in this area due to changes in the upper part. The retrieval procedure
 307 was described in Sect. 4.1. For the majority of the profiles the $(\Delta I / I)_{R.M.S.}$ calculated for 60–90 km
 308 altitude range reached the value calculated with the corresponding NER (estimated using windows
 309 B and C) between the 7th and 10th iteration. Approximately 14% of the processed profiles were
 310 filtered out due to poor convergence (compare small filled and large empty circles and triangles in
 311 Fig. 3).

312 In the next section we present 1214 temperature profiles that satisfied these convergence criteria.

313 **5.2. Retrieved temperature profiles**

314 The complete set of individual temperature profile retrievals is available for download as an archive
 315 at http://cua-nasa-gsfc.info/feofilov/TES_HighAlt.zip or in the supplemental materials of the online
 316 version of the paper. For a description of the dataset see the file “readme.txt” inside the archive. In
 317 this work we present some examples of individual retrievals and compare the averaged profiles
 318 with those from the MCD (using the standard MY 24 dust and average flux scenario) and with
 319 temperature distributions obtained from stellar occultation observations by the SPICAM instrument
 320 discussed in (Forget et al., 2009).

321 Three examples of individual temperature profiles retrieved from integrated TES radiance are
 322 shown in Fig. 6a–c. Below ~55 km the retrievals match the initial temperature profile. Above
 323 60 km, the retrieved temperature profiles differ from the original MCD profile and, in general,
 324 individual temperature retrievals show much higher variability than the model profiles. This may be
 325 explained by gravity waves in the Martian atmosphere, which are not present in the averaged model
 326 dataset.

327 Lack of temperature measurements in the Martian atmosphere for the period considered in the
 328 study hinders a direct profile-by-profile comparison with other instruments. Therefore, we compare

329 the TES temperature retrievals with the MCD MY 24 simulations for the corresponding seasons
330 and with the SPICAM temperature for MY 27. For the MCD comparison we used the zonally and
331 seasonally (with a 30° step over L_s) TES-retrieved temperatures. MCD temperature distributions
332 were averaged over the same period and for the same latitudinal belt and local time. For SPICAM
333 comparison we took the MY 27 dataset described in (Forget et al., 2009), which were retrieved for
334 top temperature of 175 K (top temperature value does not affect the SPICAM retrievals below
335 110 km). It is important to note here that these retrievals do not depend on non-LTE effects since
336 the SPICAM instrument observes the atmosphere in occultation mode and its high spectral
337 resolution allows tracking only the transitions from the ground state whose population can be
338 considered to be equal to the total CO_2 density.

339 Figure 7 shows six panels which correspond to six latitudinal/seasonal “boxes” defined in Fig. 3. In
340 this figure we compare MGS-TES retrievals for MY 24 with MCD simulated profiles and SPICAM
341 measured temperature distributions for MY 27. Figure 8 demonstrates the MY 24 and MY 25
342 temperature retrieval comparisons with MCD temperatures. The profiles are marked in the figure
343 captions with L_s counted from the year the mission started (MY 24) so that $L_s=390^\circ$ corresponds to
344 MY 25, $L_s=30^\circ$. The SPICAM distributions in Fig. 7 are shown down to ~ 60 km, the altitude below
345 which the airborne dust leads to overestimating the retrieved temperatures (Quemeralis et al., 2006;
346 Forget et al., 2009). The bins for the TES data correspond to SPICAM bins. Error bars for SPICAM
347 in the 60–90 km layer are almost constant and are equal to $\pm 10\text{K}$. They are not shown for the
348 readability of the figure. Lines with empty circles in Fig. 7 and Fig. 8 show standard variability of
349 TES-retrieved temperatures in the considered bin. Error bars for individual TES temperature
350 retrievals are given at the end of Sect. 4.2. The number of averaged TES profiles is indicated in
351 figure caption.

352 As one can see, there is a qualitative agreement between the TES, SPICAM, and the MCD
353 temperature profiles. However, the absolute temperature values differ. In general, MGS retrieves
354 higher than MCD and SPICAM retrieves lower temperatures than MCD above ~ 80 km. An analysis
355 of our entire retrieval set in comparison to the MCD profiles for the same seasons and locations
356 gives the following values for the offset: 7 K at 60 km, 8 K at 65 km, 9 K at 70 km, 10 K at 75 km,
357 10 K at 80 km, 11 K at 85 km, and 13 K at 90 km. One can also note large variability for TES-
358 retrieved temperature distributions. This is expected since our TES retrievals represent individual
359 profiles while the MCD profiles do not represent GW variability. The increase of TES profiles
360 variability with altitude can be explained by the growth of GW amplitudes in the Martian
361 atmosphere (Fritts et al., 2006). Accounting for the noise-induced variability, one obtains the
362 following values for the RMS of vertical temperature variability caused by GW: 7 K at 60 km, 8 K

363 at 65 km, 11 K at 70 km, 15 K at 75 km, 18 K at 80 km, and 20 K at 85 km. This is comparable
364 with the RMS of GW amplitude inferred from MCS observations and wind RMS (see Sect. 4.2).

365 Let us consider possible reasons for the positive temperature offset. First, there might be deviations
366 of the real atmospheric conditions for a given period from that modeled by the GCM and measured
367 by SPICAM 3MY later. It is known that there were at least two major dust storm events during the
368 considered time period (Smith, 2004): one at $L_s=225^\circ$ and one at $L_s=260^\circ$ that might be the cause
369 for large temperature deviation shown in Fig. 7d. Second, the retrieval algorithm and non-LTE
370 model uncertainties may be partially responsible for the offset (see Sect. 4.2). Third, the offset may
371 be caused by radiance calibration issues like the vertical field of view wing shape or by the spectra
372 selection procedure (see Sect. 3.2). A radiance leak from below would be barely noticeable if the
373 vertical radiance gradients are low. However, if an area with low temperatures and pressures is
374 observed then the contributions of lower layers become important (Rezac, 2011). And last but not
375 least, positive offset in our TES retrievals can be linked with the limb sequence selection criteria
376 described in Sect. 3.2 since using a selecting procedure that discards the observations with low
377 SNR may filter out the low temperature cases that are characterized by low radiance values. We
378 consider this as the most probable source of the observed systematic offset. To estimate its value
379 we performed the following study. For each of the time periods and locations shown in Fig. 7 we
380 have built a distribution of SNR maximal height using all available TES data. The maxima of these
381 distributions are centered at individual heights $H_{\text{SNR}=1}$ that are lower than 85 km SNR=1 cutoff used
382 for scans selection. The typical values of $H_{\text{SNR}=1}$ are about 70 km and the difference between
383 $H_{\text{SNR}=1}$ and 85 km can be used for characterizing the temperature offset introduced by our scan
384 selection criteria. Calculations performed with the help of ALI-ARMS show that the temperature
385 change required to compensate for low SNR at 85 km depends on the atmospheric scenario and
386 varies from 2 K to 4 K per 1 km of $(85 - H_{\text{SNR}=1})$ difference. The corresponding values are given in
387 Fig. 7 and Fig. 8 legends. We assume that the temperature profile variability is caused mainly by
388 gravity waves that penetrate these heights in Martian atmosphere (Medvedev et al., 2011 and
389 references therein) and that the scan selection routine only picks up “positive” waves with respect
390 to average temperature profile. Therefore, we assigned the estimated temperature offset to 85 km
391 with a linear decrease down to 50 km altitude. Solid curves with triangles in Fig. 7 and Fig. 8 show
392 the average temperature distributions compensated for scan selection effects.

393 As one can see, in 11 cases out of 12 shown in Fig. 7 and Fig. 8 the suggested correction leads to
394 better agreement between the MCD and TES retrievals above ~ 60 km and the averaged temperature
395 offset reduces to 6 K at 60 km, 7 K at 65 km, 7 K at 70 km, 6 K at 75 km, 5 K at 80 km, 6 K at
396 85 km, and 7 K at 90 km.

397 **6. Conclusion**

398 We have described a non-LTE model and algorithm that is applied to retrieve temperature profiles
399 in the Martian atmosphere using the 15 μm limb geometry CO_2 emissions measured by the TES
400 instrument. We used integrated limb radiance in the 560–770 cm^{-1} spectral range to increase the
401 SNR and to extend the retrievals up to ~ 90 km altitude. We showed that the temperature retrieval
402 algorithm provides a stable solution. The combined uncertainty of the temperature retrieval due to
403 noise, non-LTE model uncertainties, vertical FOV averaging, and algorithm properties for a single
404 retrieval is estimated to be 3 K at 60 km and below, 4 K at 70 km, 7 K at 80 km, 10 K at 85 km,
405 and 20 K at 90 km altitude. Overall, ~ 1200 individual limb sequences have been selected,
406 processed, and provided for download. The temperature profiles retrieved from TES at 60 – 90 km
407 altitude were compared to corresponding profiles obtained from the Mars Climate Database and
408 from the SPICAM observations. In general, a good qualitative agreement between the datasets is
409 observed. A positive offset of the TES retrieved temperatures with respect to the MCD
410 temperatures was found that varies from 7 K at 60 km to 13 K at 90 km. We explain this offset both
411 by natural atmospheric variability and by the filtering out of some of the low temperature profiles
412 in our signal selection routine. Compensating for the high SNR scan selection reduces the
413 difference between TES and MCD to 6 K at 60 km, 7 K at 65 km, 7 K at 70 km, 6 K at 75 km, 5 K
414 at 80 km, 6 K at 85 km, and 7 K at 90 km. The RMS of the gravity wave amplitude estimated from
415 the TES retrievals performed in this work is 7 K at 60 km, 8 K at 65 km, 11 K at 70 km, 15 K at
416 75 km, 18 K at 80 km, and 20 K at 85 km. In summary, this study extends the limits of the already
417 highly capable TES instrument, and validates the general concepts built in to the Martian GCMs.

418 **Acknowledgements**

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421 their helpful comments and recommendations. We also thank Dr. Francois Forget for providing the
422 SPICAM data and consultations regarding usage of the MCD data.

423 **Appendix: Abbreviations used in text**

424 ALI-ARMS: Accelerated Lambda Iterations for Atmospheric Radiation and Molecular Spectra

425 CRISTA: CRyogenic Infrared Spectrometers and Telescopes for the Atmosphere

426 FOV: field of view

427 GCM: General Circulation Model

428 GW: Gravity Wave

429 HITRAN: High-resolution TRANsmission molecular absorption database
430 LTE: Local Thermodynamic Equilibrium
431 MGS: Mars Global Surveyor
432 MY 24: Martian Year 24
433 NER: Noise Equivalent Radiance
434 RMS: Root Mean Square
435 SABER: Sounding of the Atmosphere using Broadband Emission Radiometry
436 SNR: Signal to Noise Ratio
437 TOA: Top of the Atmosphere
438 TES: Thermal Emission Spectrometer
439 TIMED: Thermosphere Ionosphere Mesosphere Energetics and Dynamics
440 VMR: Volume Mixing Ratio

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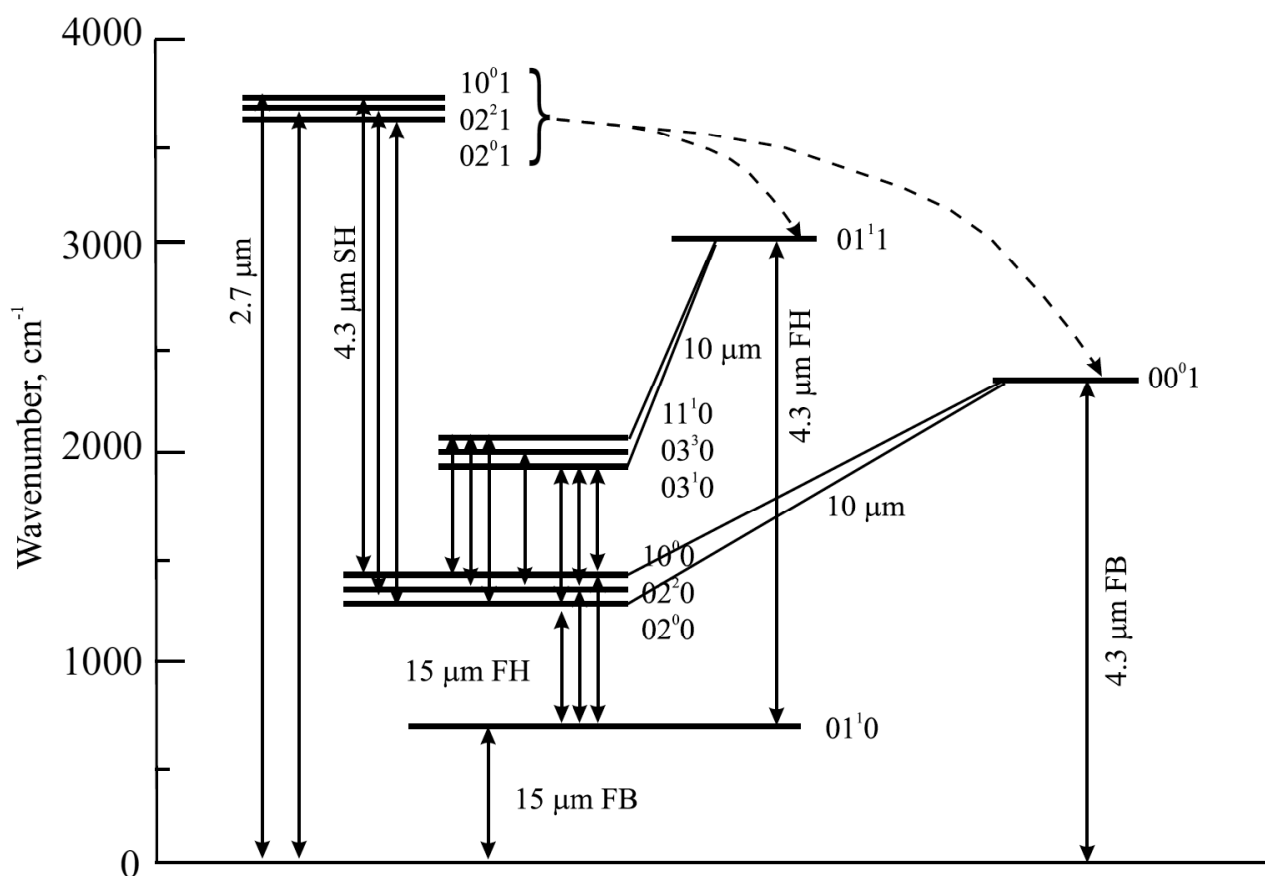
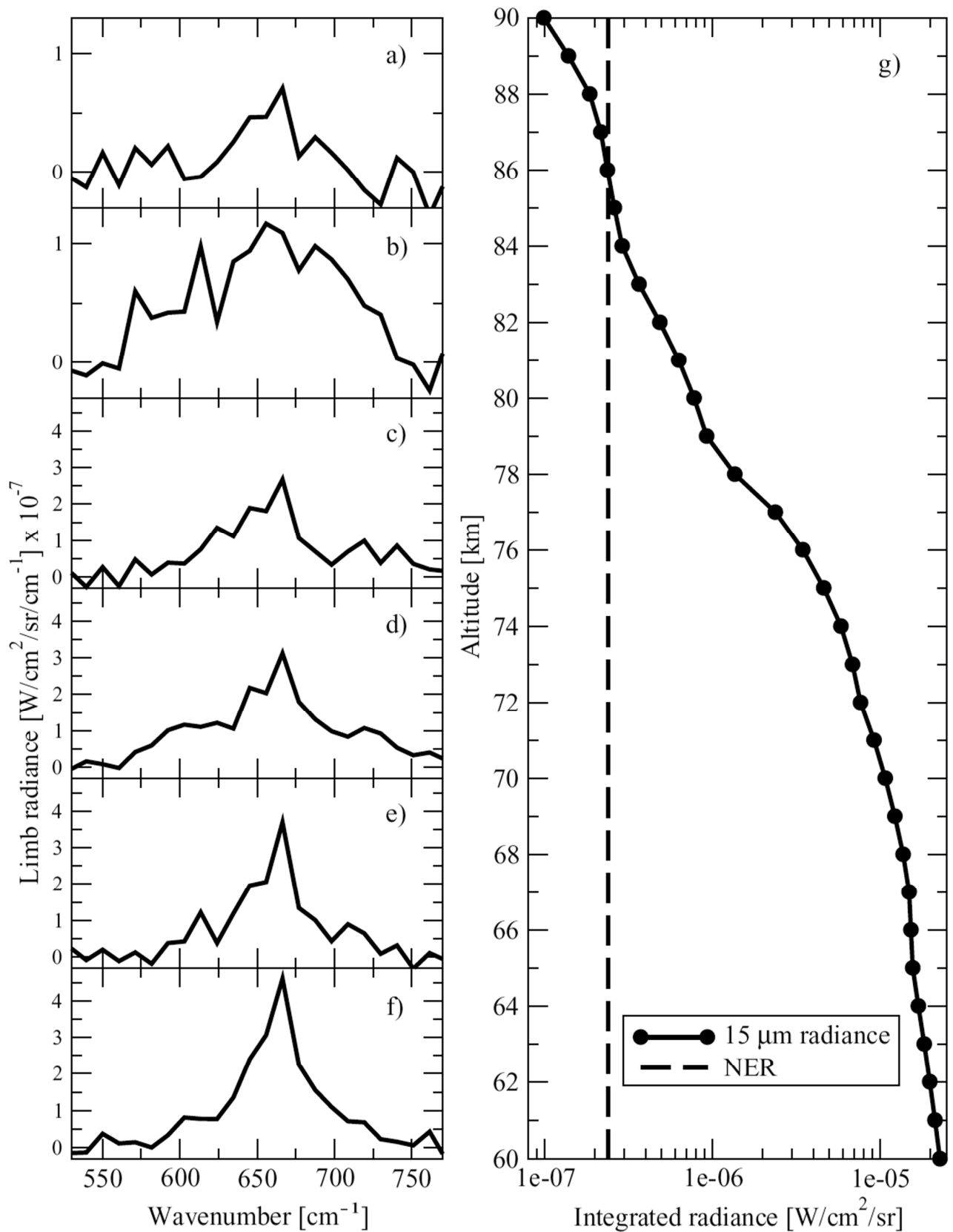
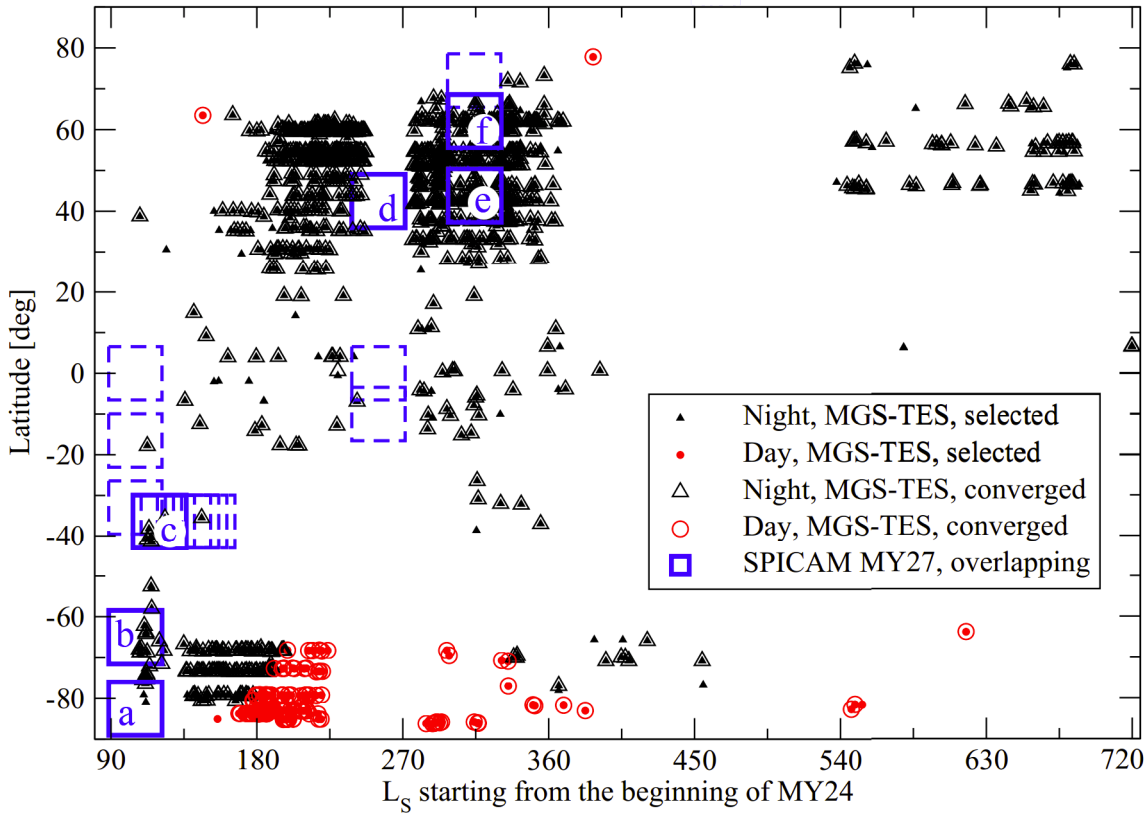


Fig. 1. Scheme of vibrational level and major energy exchange processes for CO₂ and its isotopes. Solid lines: radiative transitions, dashed lines: V–V energy transfer from solar pumped levels. V–T processes are not shown. FB: fundamental band; FH: first hot band; SH: second hot band.

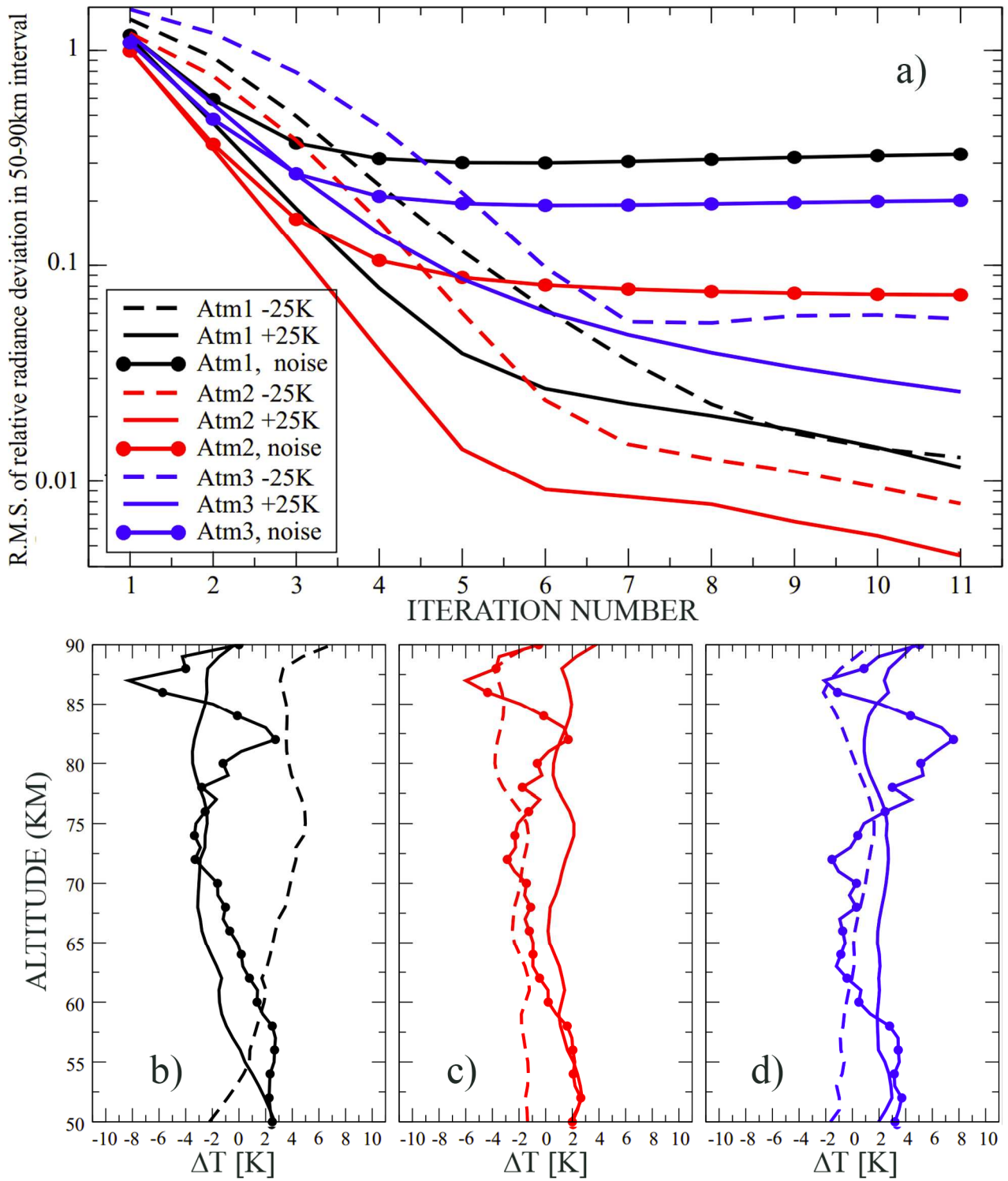


585
 586 Fig. 2. MGS TES spectra over 530–770 cm^{-1} at: a) 88.6 km; b) 82.6 km; c) 75.6 km; d) 71.4 km;
 587 e) 68.2 km; f) 60.8 km. Panel g) shows the 15 μm radiance integrated over the 560–772 cm^{-1}
 588 spectral range. Noise equivalent radiance (NER) was estimated from the points outside the
 589 integration interval: 508–560 cm^{-1} and 772–825 cm^{-1} .



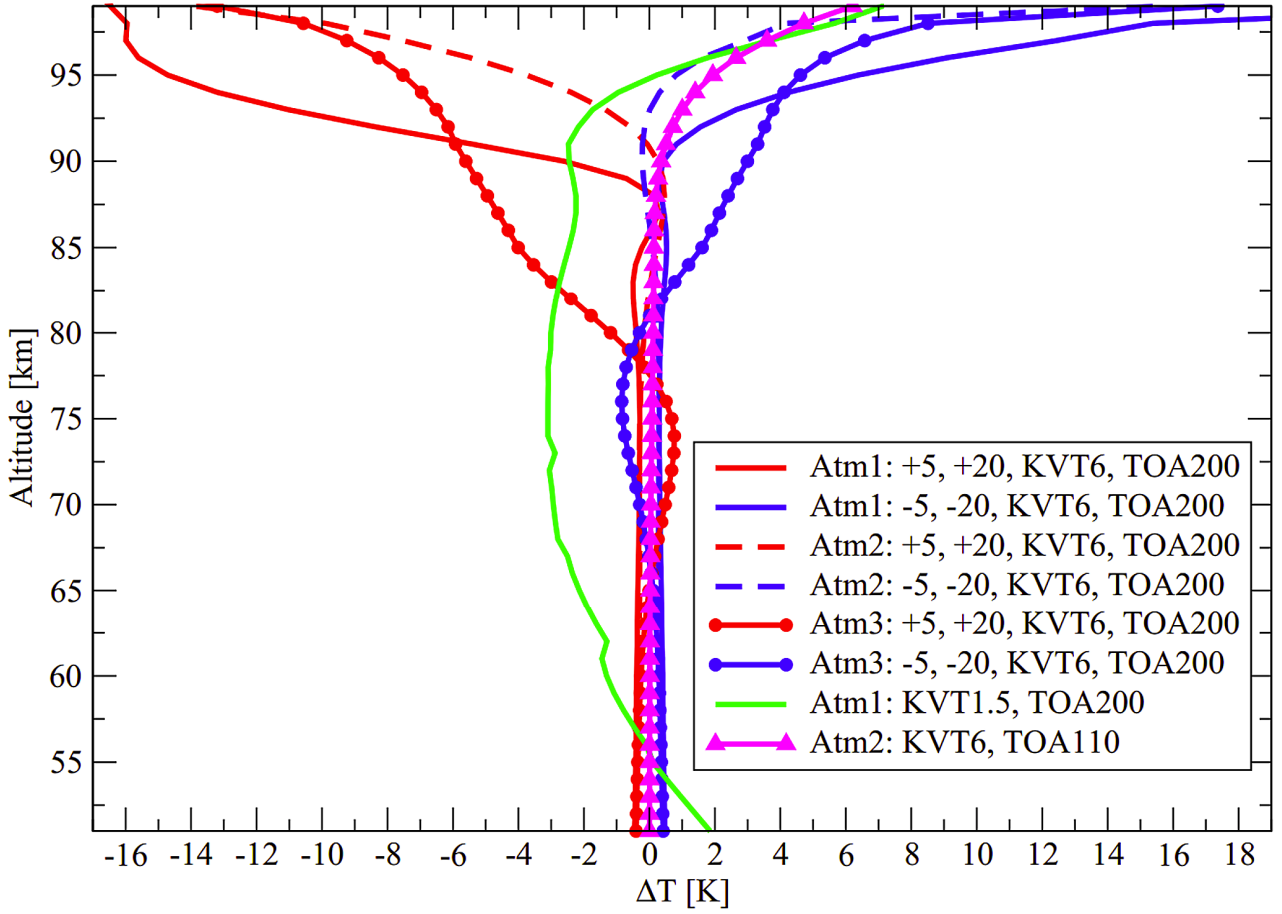
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591 Fig. 3. Seasonal and latitudinal coverage of the MGS TES limb sequences used in this work.
 592 Circles: daytime observations. Triangles: nighttime observations. Filled small circles and triangles:
 593 observations satisfying the selection criteria. Empty big circles and triangles: observations for
 594 which the retrieval algorithm converged. Small rectangles with dashed outline: SPICAM
 595 observations for MY27; rectangles with solid outline and a letter: SPICAM observations for MY27
 596 overlapping with TES retrievals and selected for intercomparison in Fig. 8.



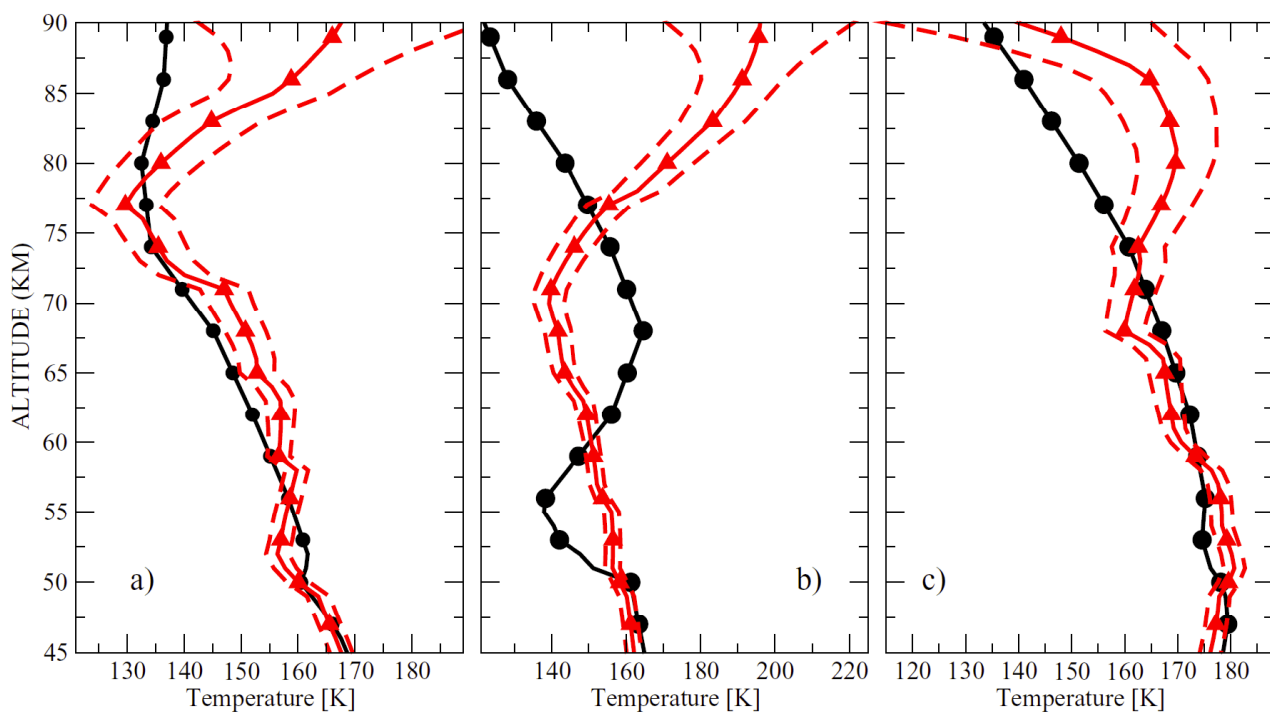
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598 Fig. 4. Self-consistent retrievals for the temperature profiles measured by MCS (Kleinböhl et al.,
 599 2009) with GW-perturbation applied: a) convergence of the method for the noise-free retrievals
 600 (solid and dashed curves) and retrievals with added noise (solid lines with circles); b)–d):
 601 temperature errors for the retrievals starting with 25 K warmer/colder temperature profile (solid and
 602 dashed curves, respectively), and for the 25 K warmer temperature profile with added noise.



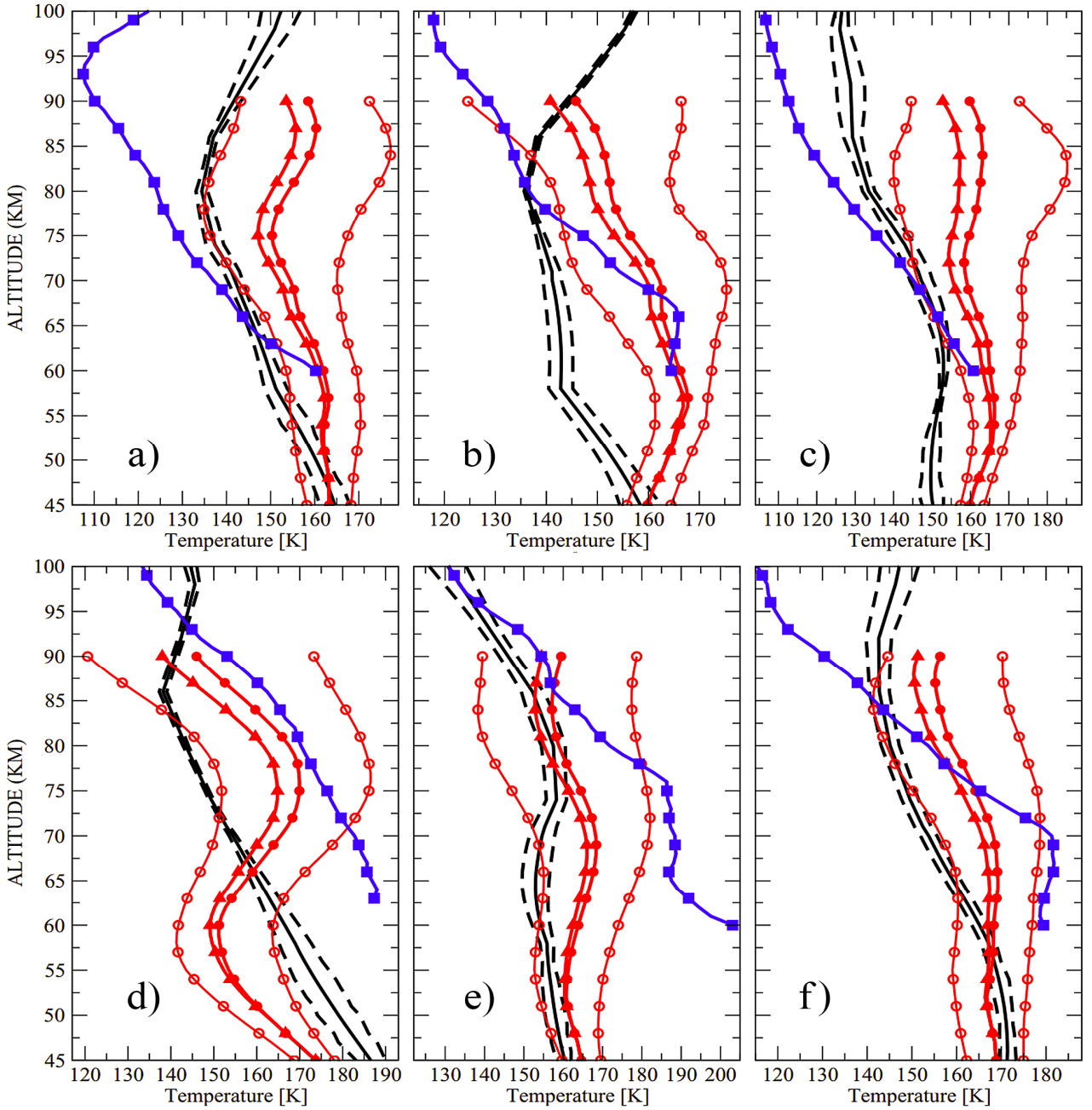
603

604 Fig. 5. Sensitivity of temperature retrievals to changes in temperature profile below and above the
 605 retrieval range, to $k_{VT}\{\text{CO}_2\text{-O}\}$ variations, and to top of atmosphere changes. The retrieved
 606 temperature profiles are compared to the “reference” one: no modification of temperature profile,
 607 top of atmosphere (TOA) at 200 km, $k_{VT}\{\text{CO}_2\text{-O}\}=6\cdot 10^{-12}\text{cm}^3\text{s}^{-1}$. The reference profile was used to
 608 obtain reference $15\ \mu\text{m}$ CO_2 radiance profile. Test atmospheres #1,2,3 are described in text. The
 609 first value in the legend refers to temperature profile change below 50 km altitude while the second
 610 value represents temperature profile shift above 100 km. KVT1.5 corresponds to retrieval
 611 performed with $k_{VT}\{\text{CO}_2\text{-O}\}=1.5\cdot 10^{-12}\text{cm}^3\text{s}^{-1}$.

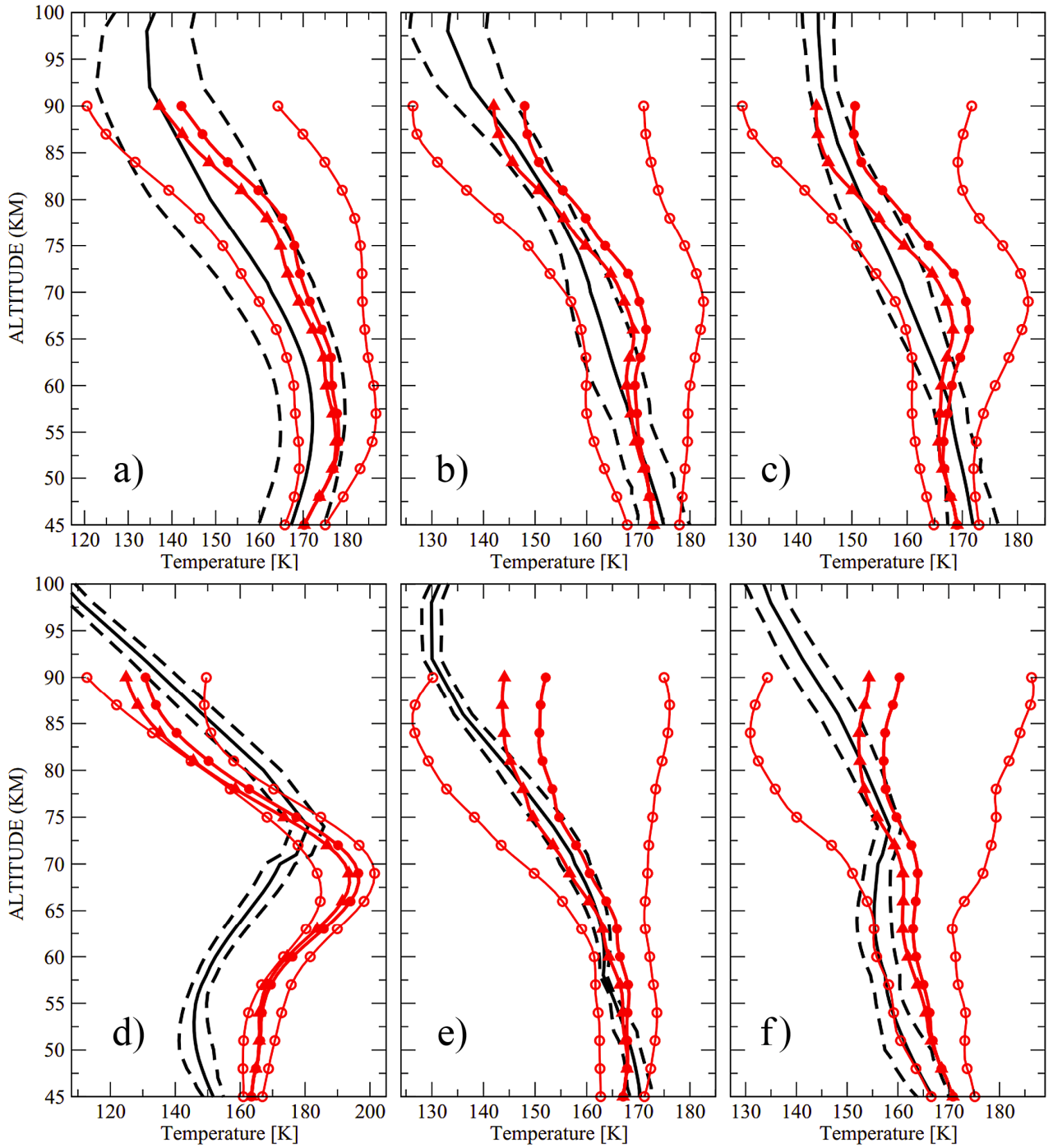


612

613 Fig. 6. Temperature retrieval examples: a) $L_s=110^\circ$, lat = 62S; b) $L_s=135^\circ$, lat = 6S; c) $L_s=180^\circ$,
 614 lat = 59N. Curves with circles: initial temperature profile (TES below 50 km; MCD above 50 km).
 615 Curves with triangles: temperature retrievals performed in this work. Dashed lines: error bars for
 616 temperature retrievals.



617
 618 Fig. 7. Comparing TES temperatures (this work) with SPICAM MY27 temperature distributions
 619 (Forget et al., 2009) for areas a)–f) defined in Fig. 3 and with MCD simulations. Solid lines: MCD;
 620 dashed lines: MCD standard deviations for given latitude and season; lines with filled circles:
 621 averaged TES retrievals (this work); lines with empty circles: TES profiles standard deviations (see
 622 text and Fig. 6 for TES error bars); lines with triangles: TES profile corrected for high SNR scan
 623 selection (see text); lines with filled squares: SPICAM retrievals (Forget et al., 2009): a) $L_s = 90$ –
 624 120° , lat= 60°S – 70°S , 9 profiles, 5 K compensation for high SNR selection; b) $L_s = 90$ – 120° ,
 625 lat= 70°S – 80°S , 7 profiles, 5 K; c) $L_s = 110$ – 130° , lat = 31°S – 41°S , 4 profiles, 7 K; d) $L_s = 240$ – 270° , lat
 626 = 30°N – 55°N , 23 profiles, 8 K; e) $L_s = 309$ – 319° , lat = 30°N – 55°N , 43 profiles, 5 K; f) $L_s = 309$ –
 627 319° , lat = 57°N – 67°N , 9 profiles, 5 K.



628
 629 Fig. 8. Same as in Fig. 7 but only for TES versus MCD profiles comparison: a) $L_s=165-195^\circ$,
 630 lat = $65-75^\circ\text{S}$, 49 profiles, 5 K compensation for high SNR selection; b) $L_s=180-225^\circ$, lat = $50-$
 631 65°N , 150 profiles, 6 K; c) $L_s=285-315^\circ$, lat = $55-65^\circ\text{N}$, 25 profiles, 7 K; d) $L_s=345-375^\circ$,
 632 lat = $20^\circ\text{S}-20^\circ\text{N}$, 5 profiles, 6 K; e) $L_s=345-375^\circ$, lat = $55-65^\circ\text{N}$, 16 profiles, 8 K; f) $L_s=650-685$,
 633 lat = $40-55^\circ\text{N}$, 14 profiles, 6 K.