RADIATIVE TRANSFER IN THE MIDDLE AND UPPER ATMOSPHERE IN THE CONTEXT OF INFRARED SATELLITE OBSERVATIONS OF THE LOWER ATMOSPHERE

A.G. Feofilov[1], R. Armante[1], L. Rezac[2],
A. Kutepov[3], V. Capelle[1], M. Rey[4], A. Nikitin[5],
and V V. Tyuterev[4]

(1) CNRS/IPSL Laboratoire de Météorologie Dynamique, Ecole Polytechnique, Palaiseau, France
(2) Max Planck Institute for Solar System Research, Goettingen, Germany
(3) The Catholic University of America / NASA GSFC, Greenbelt, MD, USA
(4) GSMA, University of Reims, Reims, France
(5) QUAMER Laboratory of Tomsk University, Tomsk, Russia

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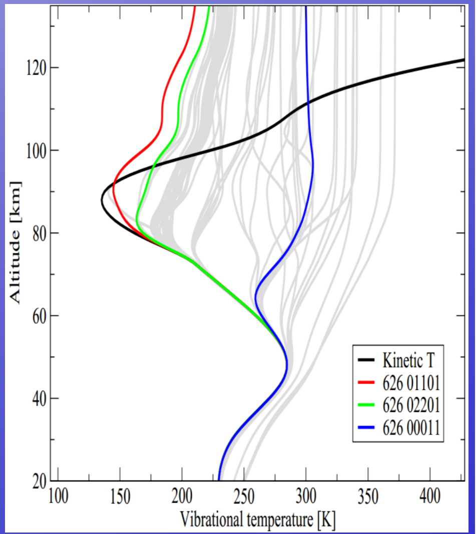
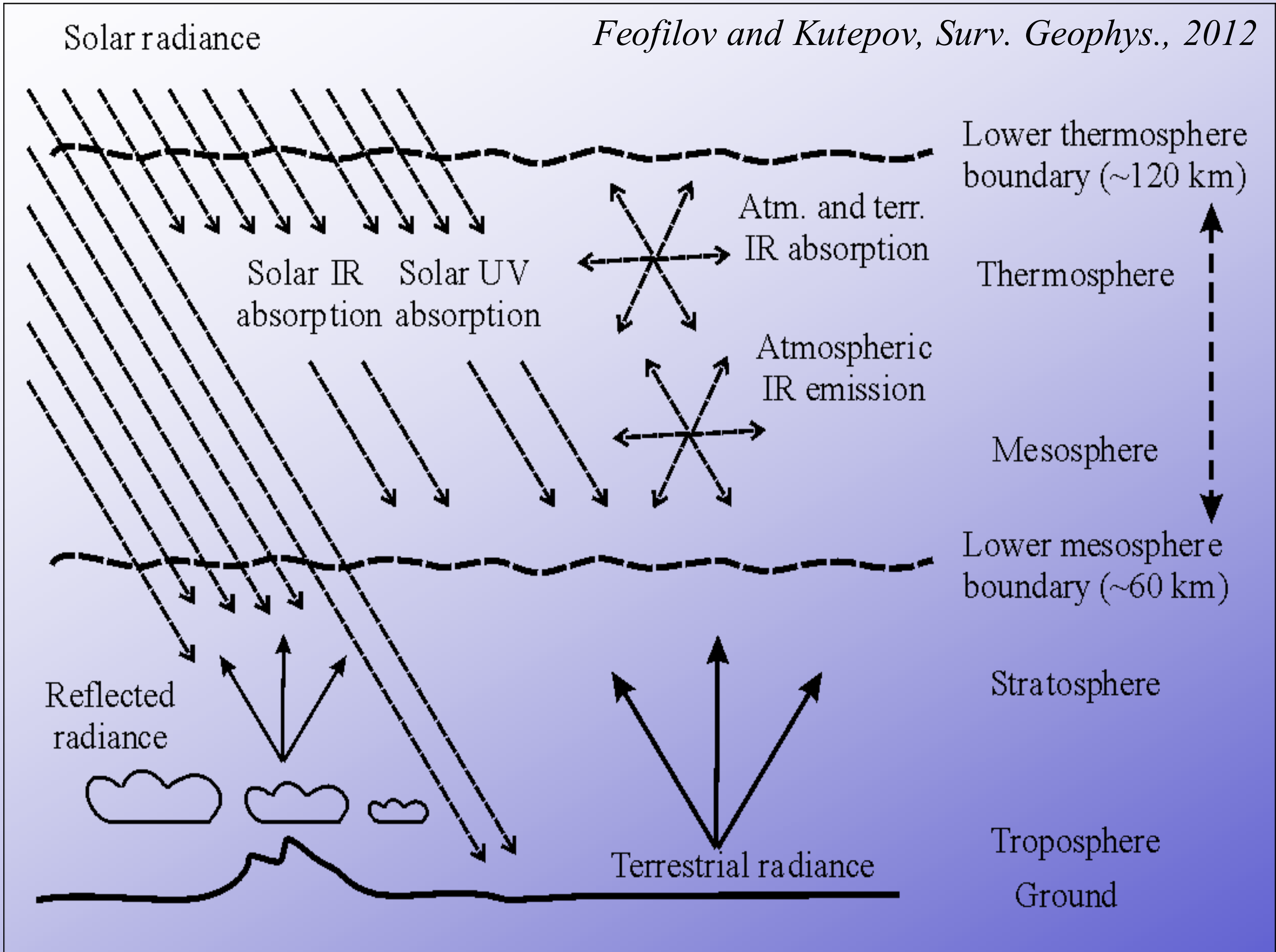
Middle and upper atmosphere – why bother?

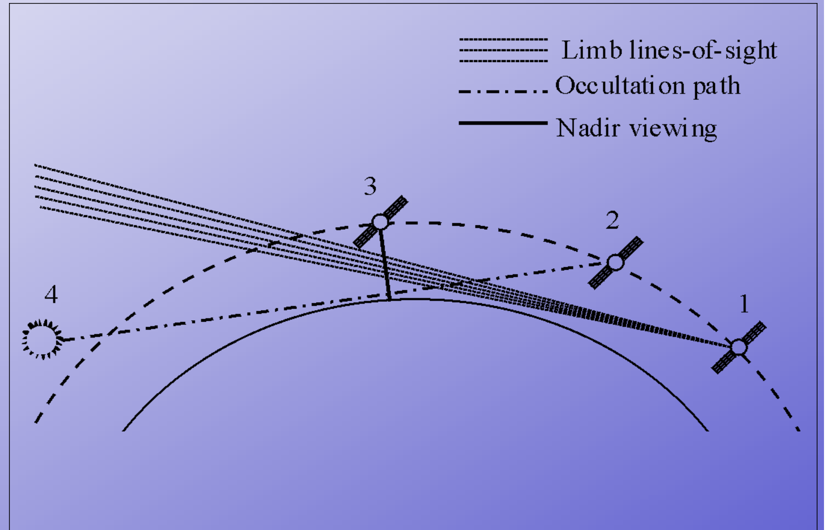
- This is a “gateway” between the lower atmosphere and space.
- It is sensitive to solar influence and to the inputs from below.
- Absorption and emission in molecular bands affect atmospheric observations of other areas.
- Anthropogenic changes in greenhouse gases may change the composition of middle/upper atm. and the input from below.
- Noctilucent clouds observed in polar summer mesosphere (80-83 km) are very sensitive to temperature changes.

Mesopause as a «miner's canary»



Satellite observations of the lower atmosphere: what's on the way?





- Downwelling radiance passes through the upper and middle atmosphere.
- Upwelling radiance is modified by atmospheric absorption and *emission*.
- All types of measurements affected.
- Absorption/emission in the infrared is associated with vibr. level pop-s.
- Important peculiarity in the MLT.

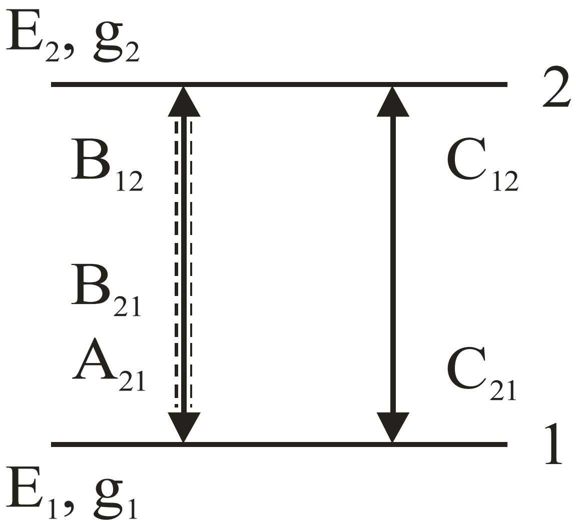
Formulation of the problem

- Infrared radiance absorption/emission correspond to vibrational excitation/de-excitation of the molecules.
- To estimate the energetic characteristics of the atmospheric layer and/or to interpret the infrared observations passing through / originating in the middle/upper atmosphere one needs to know the vibrational levels populations.

BUT !!!

- In the upper atmosphere the collisions between the molecules are **not** frequent and the populations are **not** defined by local T.
- Breakdown of Local Thermodynamic Equilibrium (LTE).
- Special methodology is applied (non-LTE modeling).

Explaining LTE and non-LTE:
2-level atomic gas in plane-parallel atmosphere



$$\begin{cases} (\underbrace{A_{21} + B_{21}\bar{J}}_{R_{21}} + C_{21})\, n_2 = (\underbrace{B_{12}\bar{J}}_{R_{12}} + C_{12})\, n_1 \\ n_1 + n_2 = n \end{cases}$$

$R \ll C$

$R_{21} n_2 \sim R_{12} n_1$

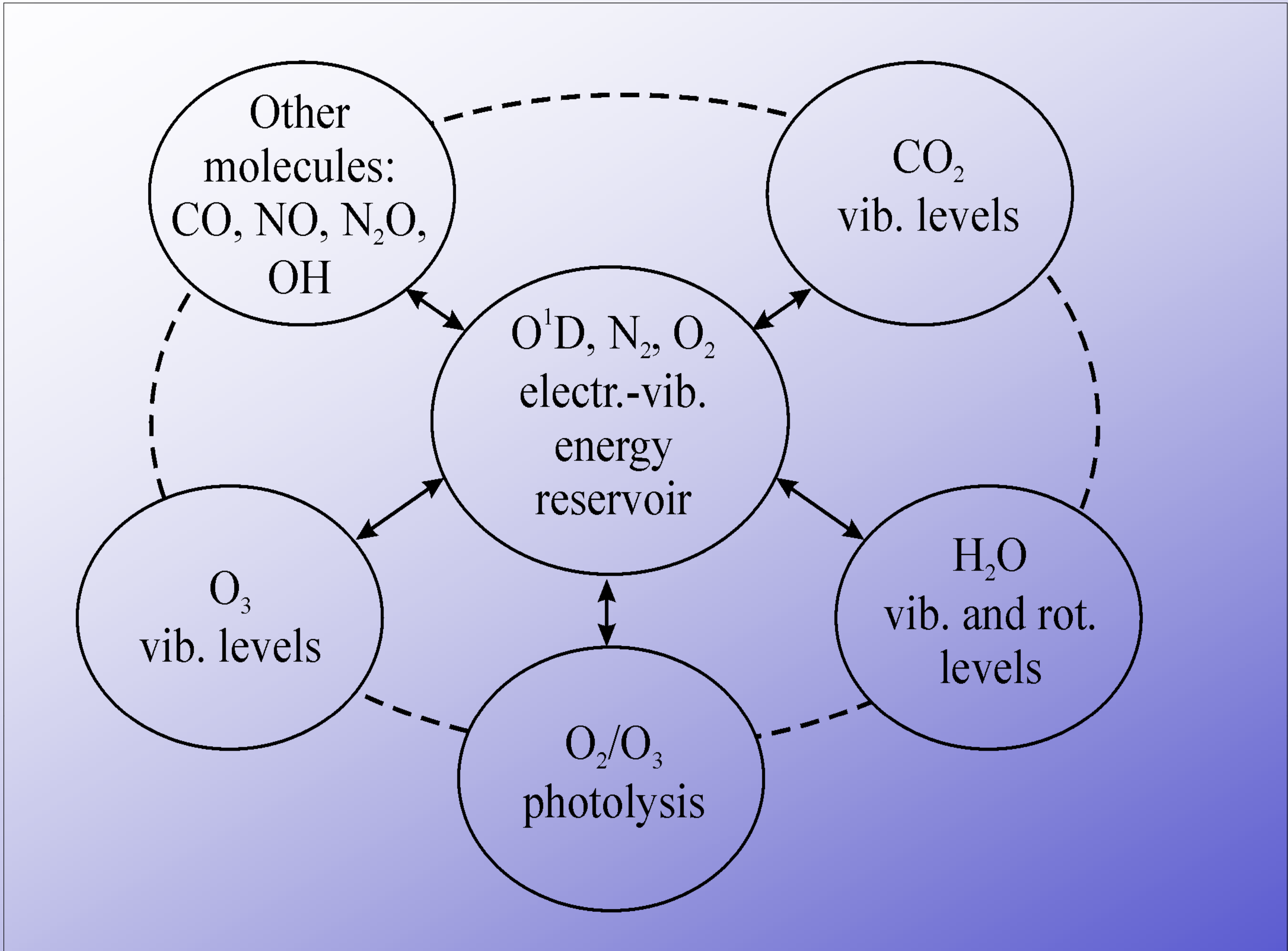
$$n_2 C_{21} = n_1 C_{12}$$

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-\frac{E_2 - E_1}{kT}}$$

LTE

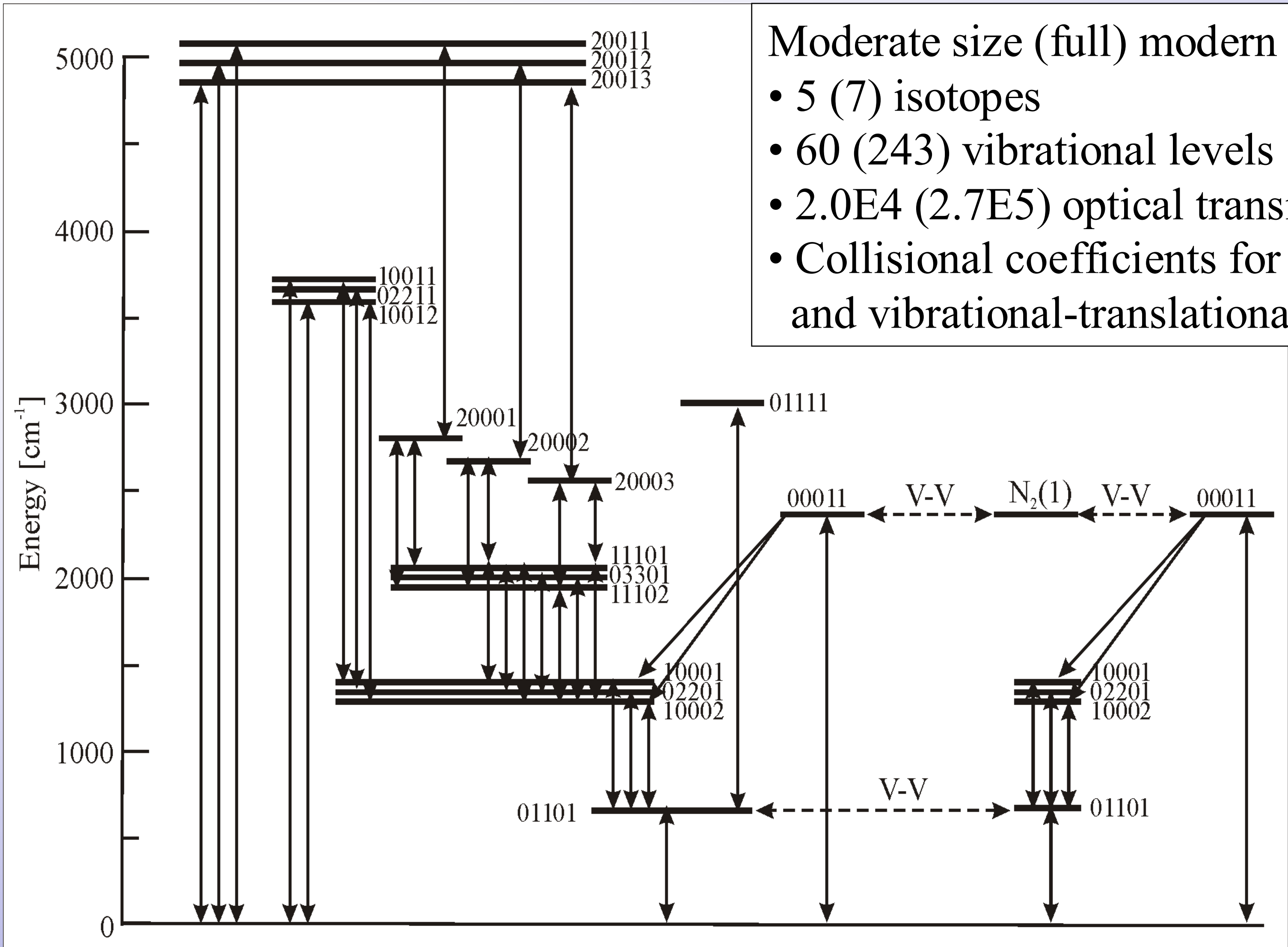
Otherwise - non-LTE !!!
since J is non-local

Energy exchange between atmospheric molecules



- each molecule has a system of vibrational levels and rotational-vibrational sublevels.
- collisional energy exchange: vibrational-vibrational and vibrational-translational (heat).
- Chemical/photochemical pumping.
- Solar and atmospheric radiance absorption.
- LTE breakdown height depends on a number of factors.
- rule of thumb: P<1Pa

Vibrational levels and transitions for CO_2



Moderate size (full) modern non-LTE model includes:
- 5 (7) isotopes
- 60 (243) vibrational levels
- 2.0E4 (2.7E5) optical transitions
- Collisional coefficients for vibrational-vibrational and vibrational-translational energy exchange processes.

Other molecules: O_3, H_2O, CO, CH_4 are modeled in the same way – levels, processes, transitions.

With this input information and atmospheric vertical profile (P(z), T(z), trace gases) one obtains the vibrational level populations at all heights: n(ivl,iz)

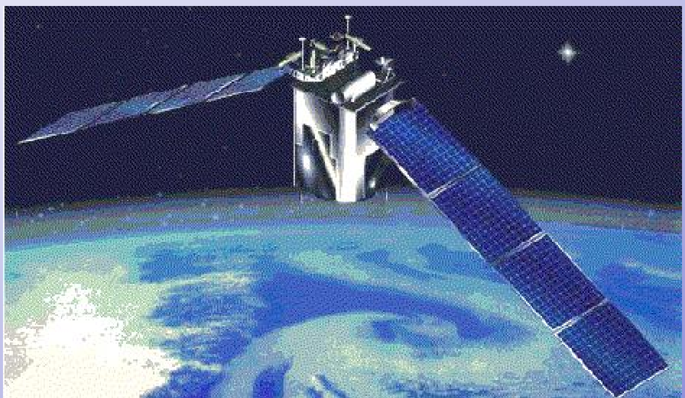
ALI-ARMS non-LTE research code

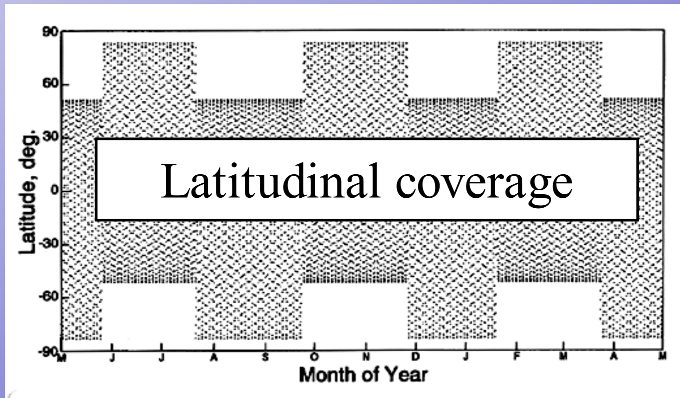
Retrieved/analyzed parameter(s)	Spectral band	Experiment/Model	References
CO_2 VMR, Earth	4.3 µm	CRISTA spectrometer	Kaufmann et al., 2002
CO_2 emissions, Mars	10 µm	MGS TES spectrometer	Maguire et al., 2002
O_3 VMR, Earth	9.6 µm	CRISTA spectrometer	Kaufmann et al., 2003
IR cooling/heating, Mars	15 µm	Mars GCM	Hartogh et al., 2005
Temperature, Earth	15 µm	CRISTA spectrometer	Gusev et al., 2006
Temperature, Earth	15 µm	SABER radiometer	Kutepov et al., 2006
H_2O VMR, Earth	6.3 µm	SABER radiometer	Feofilov et al., 2009
CO_2 VMR, temperature, Earth	4.7, 15 µm	SABER radiometer	Rezac, 2011, 2014
Temperature, Mars	15 µm	MGS TES spectrometer	Feofilov et al., 2012
HCN rotational cooling, Titan	100-1000 µm	Theoretical study	Rezac et al., 2013

- ALI-ARMS: Accelerated Lambda Iteration, Atmospheric Radiance and Molecular Spectra.
- Non-LTE methodology comes from stellar astrophysics.
- Solves the non-LTE task for large number of levels.
- Has numerous applications in planetary atmospheres.

The SABER Instrument Aboard the TIMED Satellite

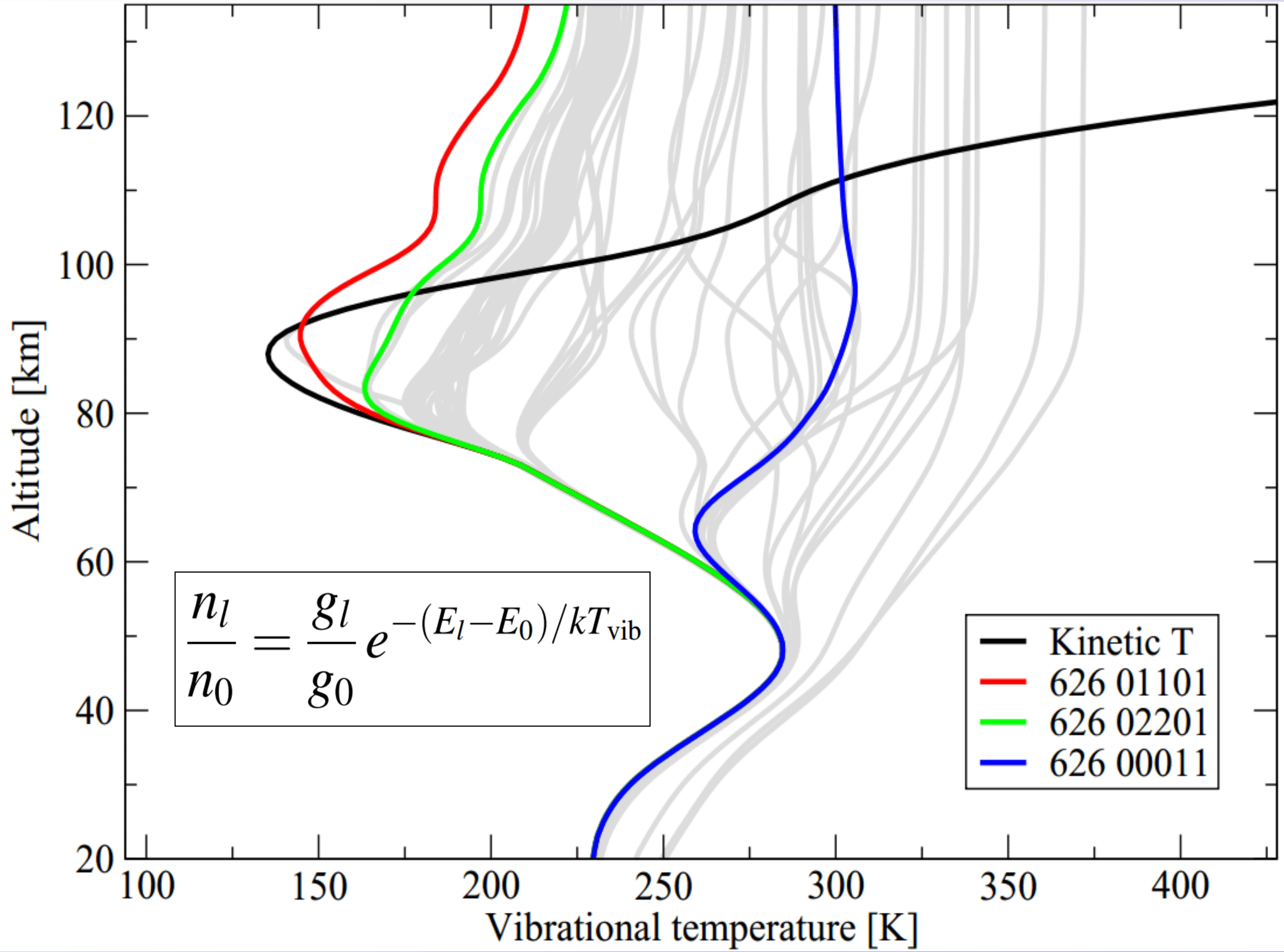
Ongoing mission launched on December, 7 2001





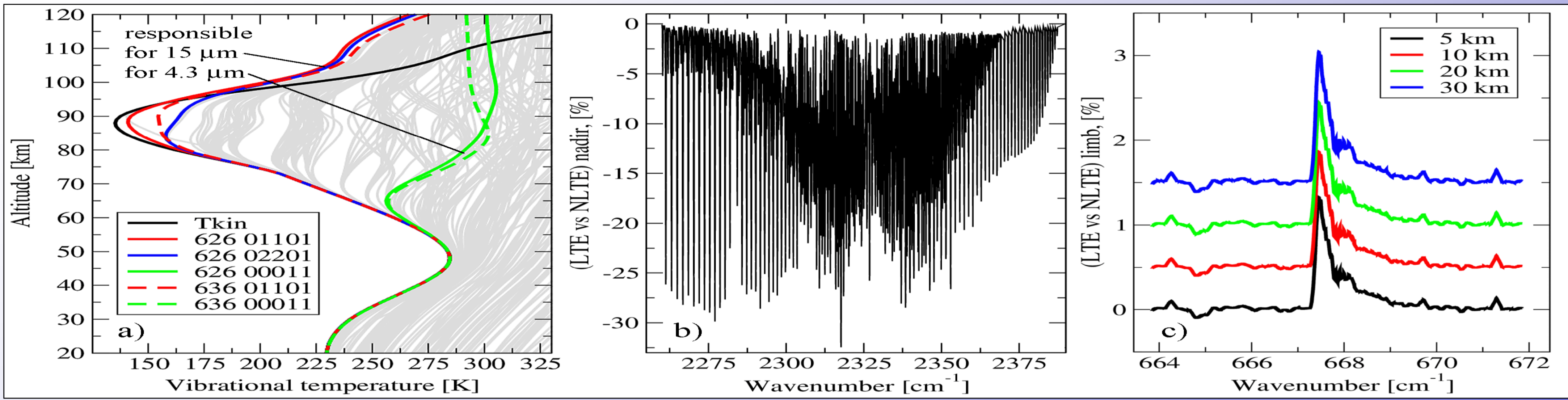
- SABER: limb scanning infrared radiometer (~13-110 km)
- 10 broadband channels (1.27-17µm)
- Products: T, CO_2, O_3, H_2O, NO, O_2, OH, O, H.
- Side products: vibrational level populations for main contributors.

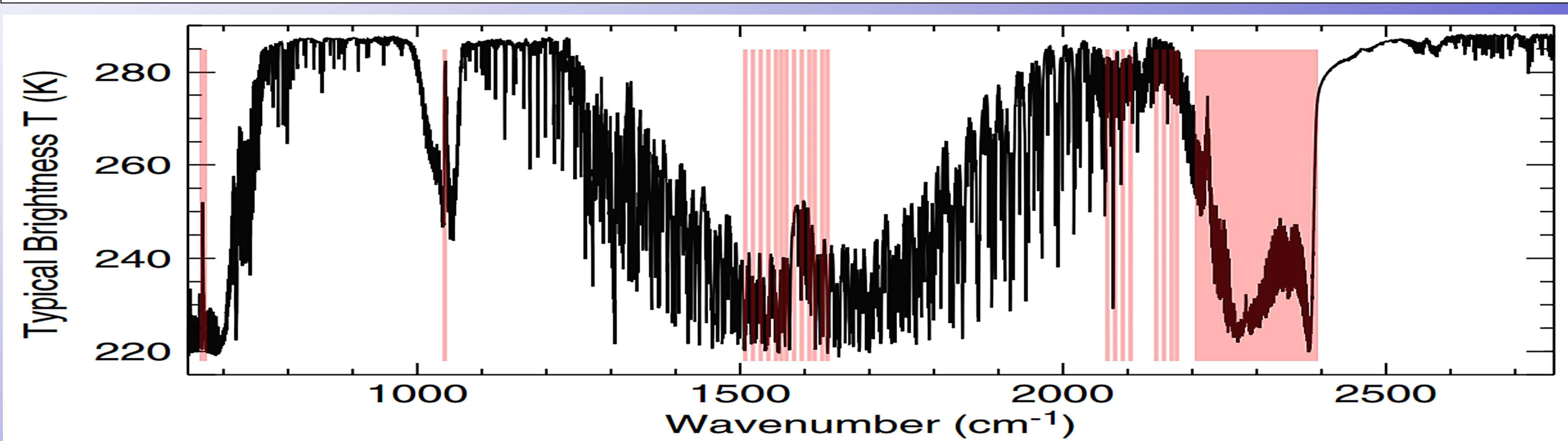
Non-LTE populations: vibrational temperatures



- convenient visualization method, not a physical T !
- T_{vib} is the temperature to be substituted to Boltzmann's equation to obtain a given population.
- $T_{vib} < T_{kin}$: cooling to space is not compensated by collisional pumping.
- $T_{vib} > T_{kin}$: solar or atmos. radiance or (photo)chemical pumping is not compensated by quenching.
- Levels responsible for 15µm radiance are thermalized up to ~80km, 4.3µm: 60km, some levels are not thermalized down to the ground.

Application to IASI channels





Implementing non-LTE populations to LTE-based operational retrieval codes

LEFE CHAT proposal,
PI: R.Armante

$$\mu \frac{\mathrm{d}I_{\mu\nu}(z)}{\mathrm{d}z} = -\chi_{\mu\nu}(z) I_{\mu\nu}(z) + \eta_{\mu\nu}(z)\,)$$

Radiative transfer equation for monochromatic line

$$\eta(z) = \frac{h\nu}{4\pi} n_2(z) A_{21} \qquad \chi(z) = \frac{h\nu}{4\pi}\left(n_1(z) B_{12} - n_2(z) B_{21}\right)$$

Emissivity and opacity terms

n_2 (upper state) is often in non-LTE and n_1 (lower state) can be out of equilibrium for hot transitions

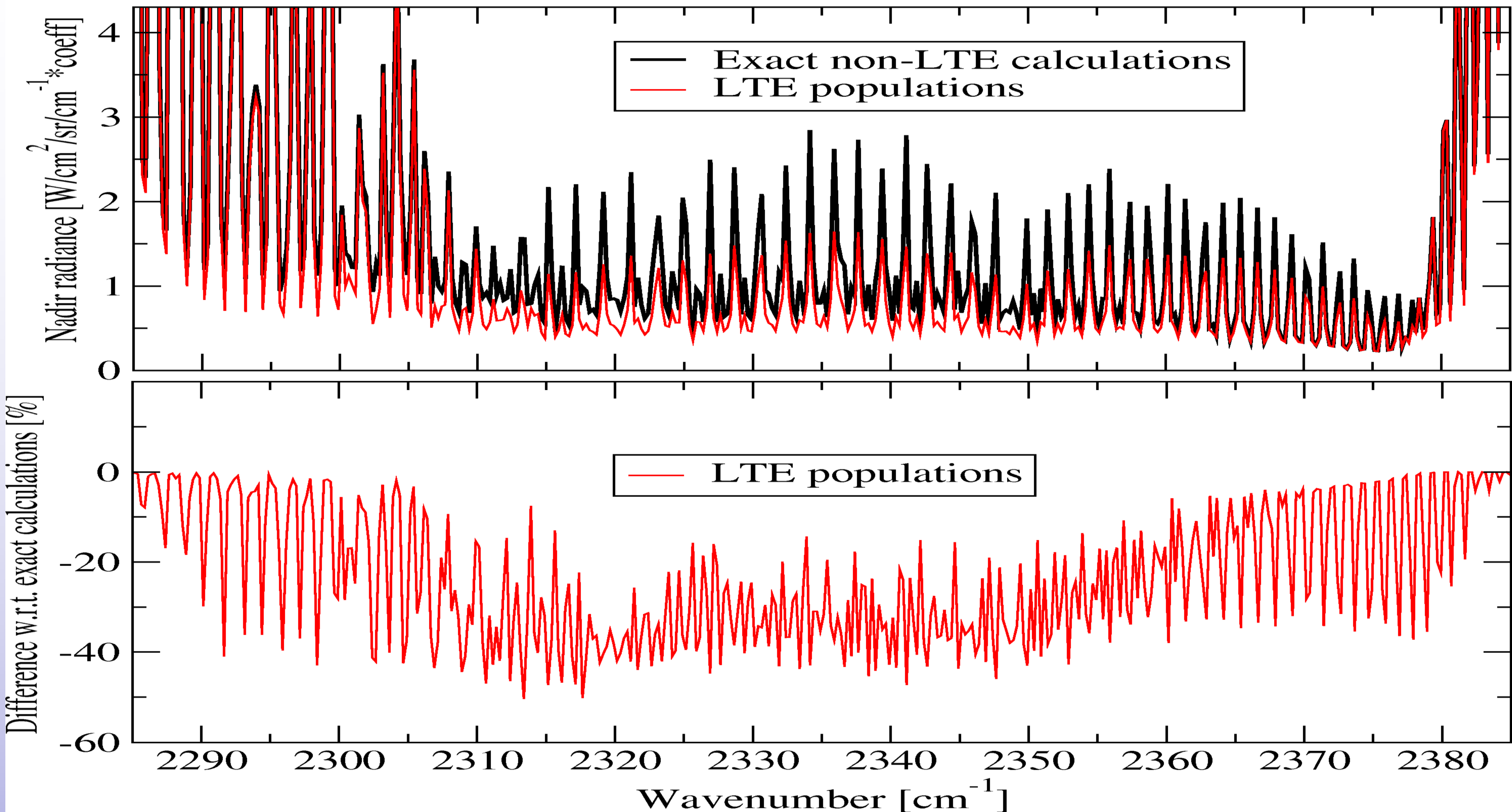
$$I_\lambda(s_1) = I_{\lambda 0} \exp\left(-\tau_\lambda(s_1, 0)\right) + \int_0^{s_1} k_\lambda \rho r B_\lambda\left(T(s)\right) \exp\left(-\tau_\lambda(s_1, s)\right) ds$$

Typical representation in LTE-based codes

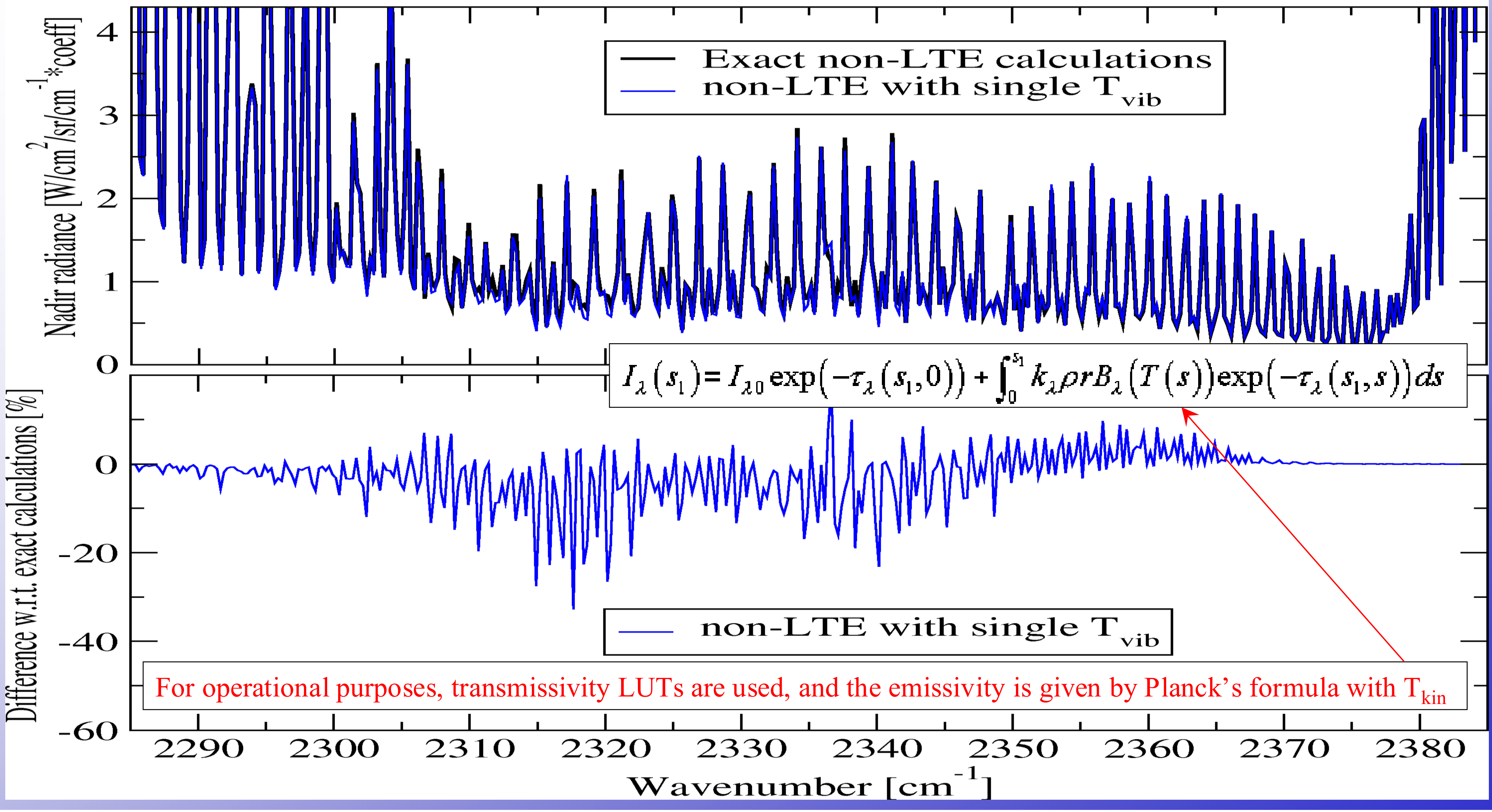
LTE-based codes assume that all populations are thermalized: how to bypass it ???

- The implementation depends on the way the radiative transfer is treated.
- If the populations of individual molecular levels can be traced, then the problem is solved – one has just read the output of the non-LTE code like ALI-ARMS (populations at all heights).
- Pre-calculating a look-up table of the residuals (atmospheric profiles, solar zenith angles, channel) [DeSouza-Machado et al., 2007]. Does the job, is instrument-specific, not portable.
- Getting inside the radiative transfer module to «intercept» the populations and replace them: more universal, more physical, more difficult to implement.

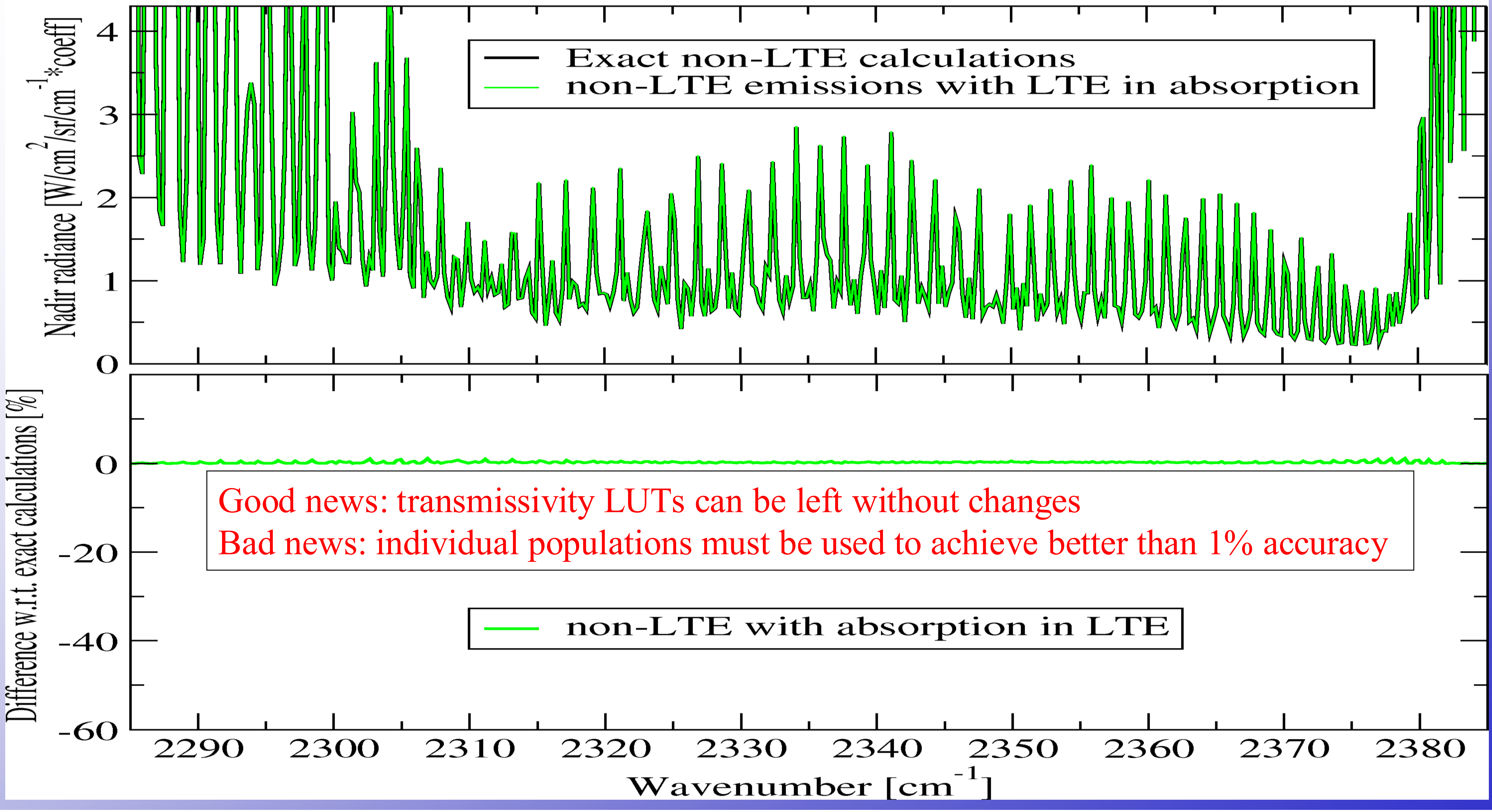
Implementing non-LTE populations: severity of the problem



Implementing non-LTE populations: all $T_{kin} \rightarrow T_{vib}$(626 00011)



Implementing non-LTE populations: LTE in absorption



Conclusions

- Above certain height (below certain pressure), the populations of molecular vibrational levels are not in local thermodynamic equilibrium.

- The strength of the effect depends on pumping (solar, chemical, photochemical, atmospheric) and quenching (collisional energy transfer to heat). Solar pumped 4.3 μm band of CO_2 – up to 40%.

- The state of the art in non-LTE modeling allows obtaining the vibrational level populations for any kind of atmosperic molecule given that the optical and collisional rates are known. Possible source of vibrational level populations: SABER instrument L2: 2002-now.

- Four ways of taking into account the non-LTE populations in the LTE-based operational codes:
  (1) direct usage of the populations – accurate, but requires a compelete change of the approach;
  (2) correction LUT per channel, atmosphere, SZA. Doable, not portable, less flexible;
  (3) replacing kinetic temperature with the vibrational one of the main contributor: 10% error;
  (4) calculating emissions in non-LTE and absorption in LTE: <1% error, implementation still not trivial though easier than (1).

- We are on the way from (3) to (4).