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]

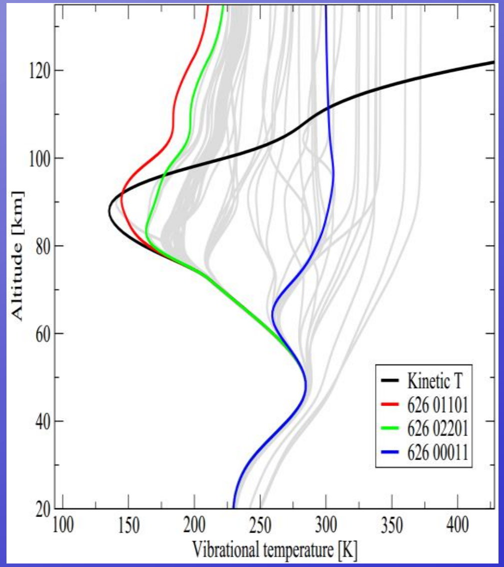
(1) CNRS/IPSL Laboratoire de Météorologie Dynamique, Ecole Polytechnique, Palaiseau, France
(2) Max Planck Institute for Solar System Research, Goettingen, Germany
(3) The Catholic University of America / NASA GSFC, Greenbelt, MD, USA
(4) GSMA, University of Reims, Reims, France
(5) QUAMER Laboratory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

April 13, 2016, IASI 2016 conference, Antibes, France

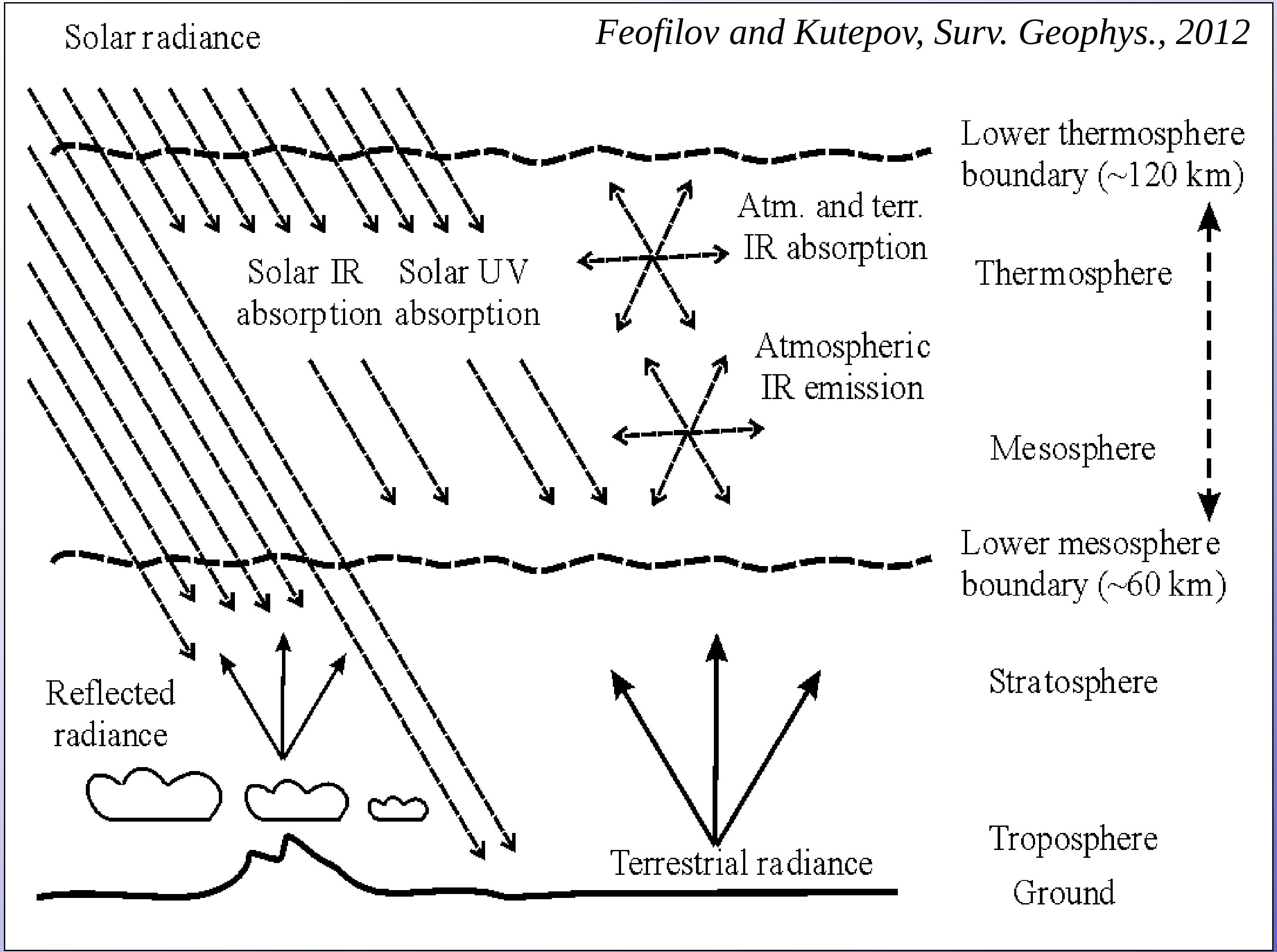
Middle and upper atmosphere – why bother?

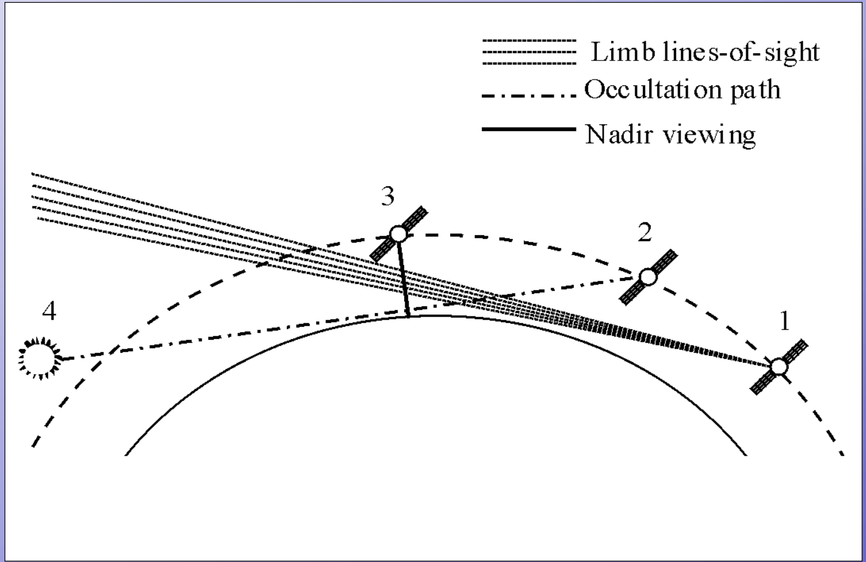
- This is a “gateway” between the lower atmosphere and space.
- It is sensitive to solar influence and to the inputs from below.
- Absorption and emission in molecular bands affect atmospheric observations of other areas.
- Anthropogenic changes in greenhouse gases may change the composition of middle/upper 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.

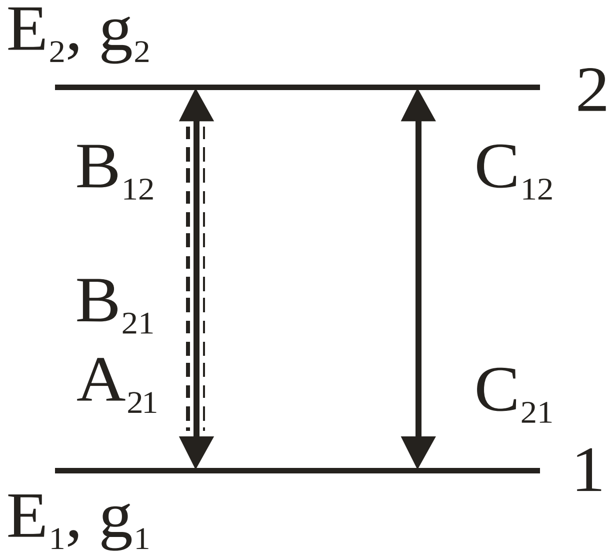
Formulation of the problem

- 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



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

$R << C$

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

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

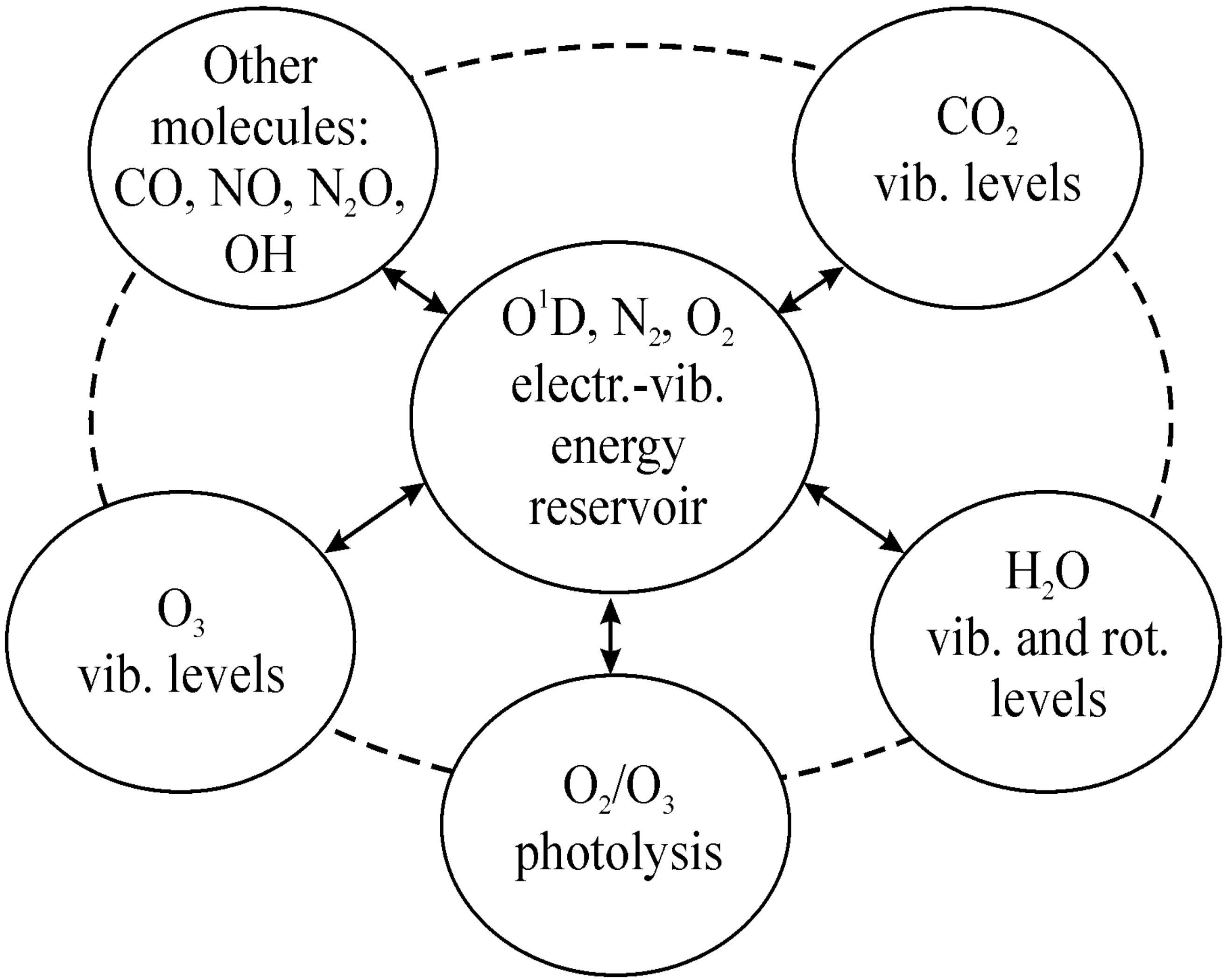
$$\frac{n_2}{n_1} = \frac{g_2}{g_1}\, e^{-\frac{E_2 - E_1}{kT}}$$

LTE

Otherwise - non-LTE !!!

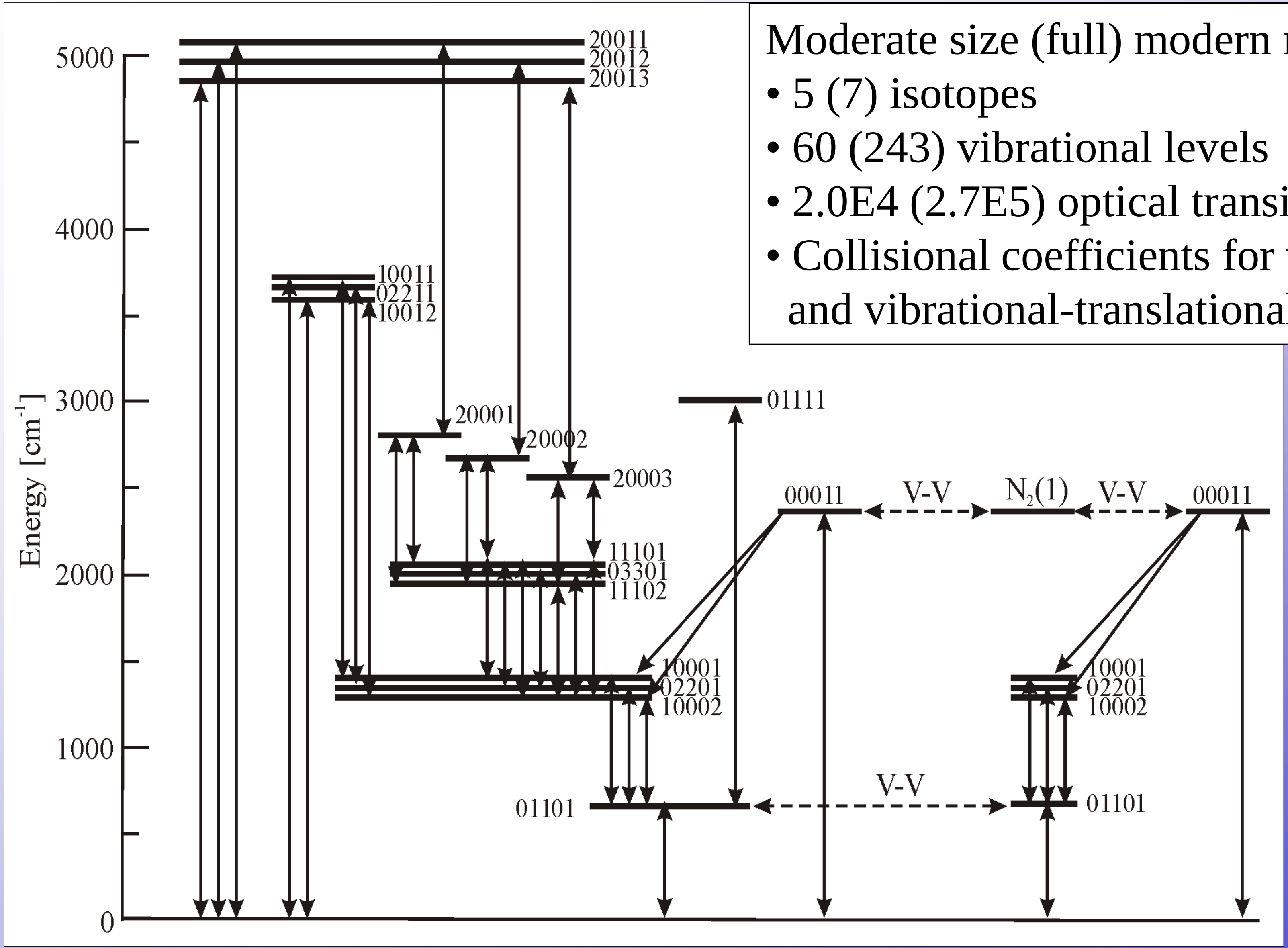
since J is non-local

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)

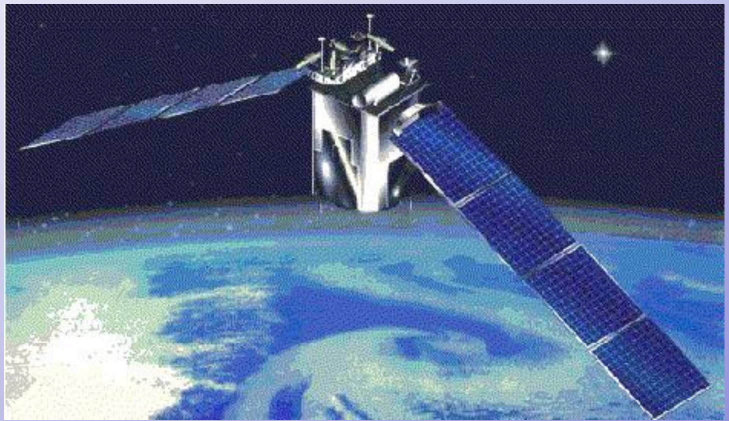
ALI-ARMS non-LTE research code

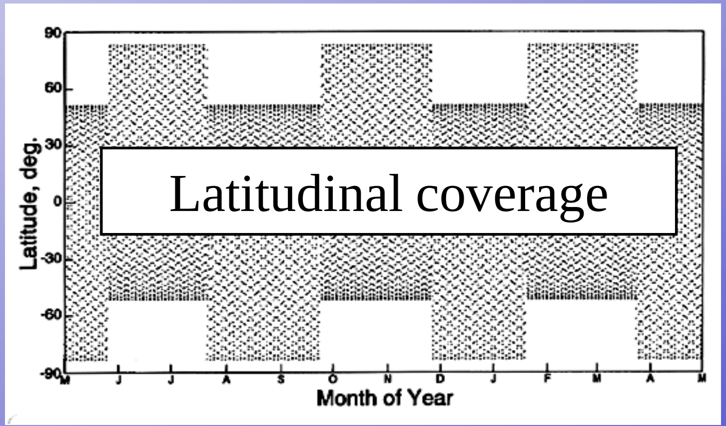
Retrieved/analyzed parameter(s)	Spectral band	Experiment/Model	References
CO_2 VMR, Earth	4.3 μm	CRISTA spectrometer	Kaufmann et al., 2002
CO_2 emissions, Mars	10 μm	MGS TES spectrometer	Maguire et al., 2002
O_3 VMR, Earth	9.6 μm	CRISTA spectrometer	Kaufmann et al., 2003
IR cooling/heating, Mars	15 μm	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

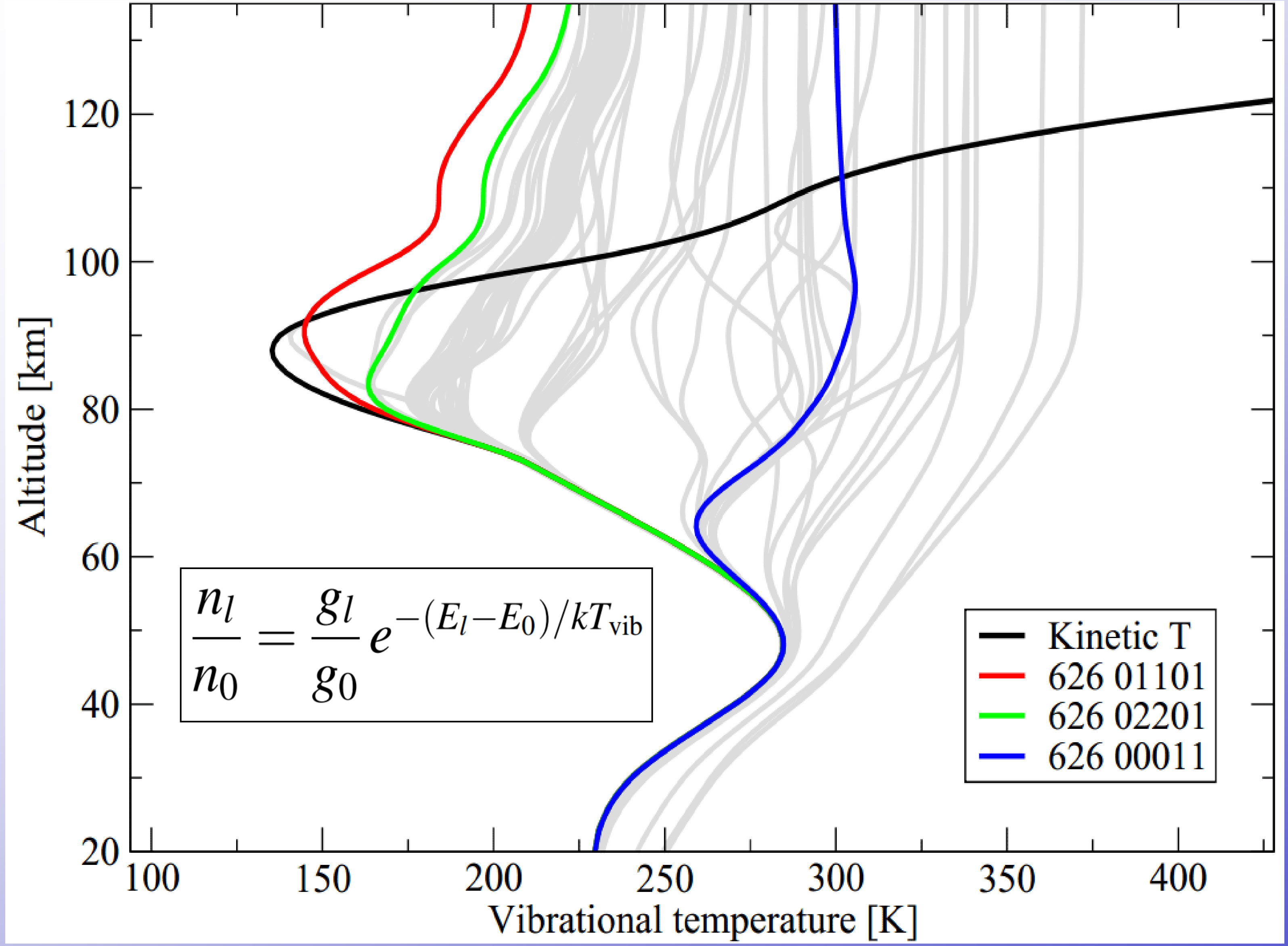
Ongoing mission launched on December, 7 2001





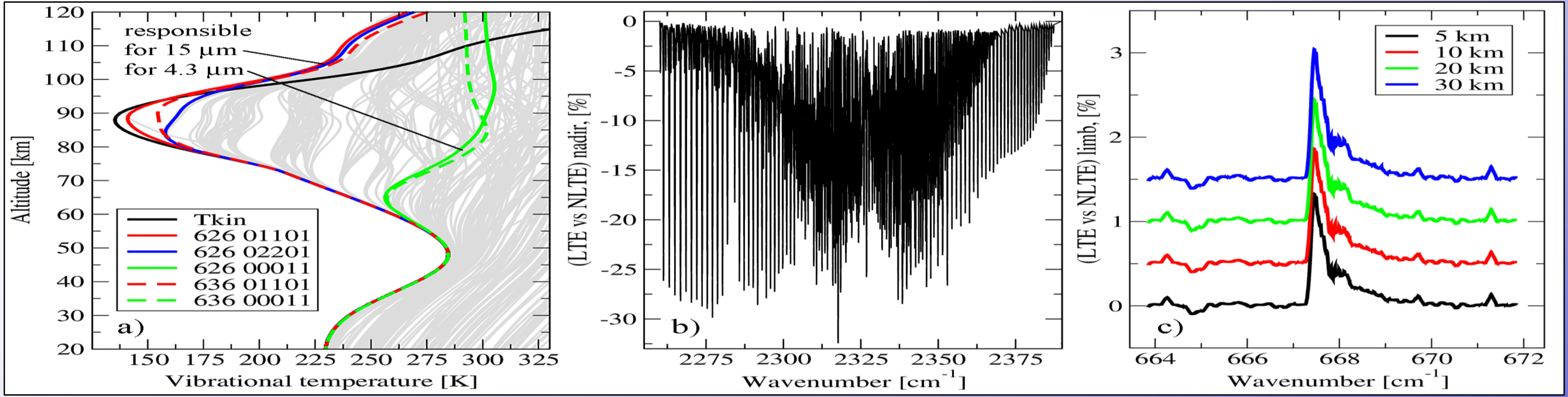
- SABER: limb scanning infrared radiometer (~13-110 km)
- 10 broadband channels (1.27-17μm)
- Products: T, CO_2, O_3, H_2O, NO, O_2, OH, O, H.
- Side products: vibrational level populations for main contributors.

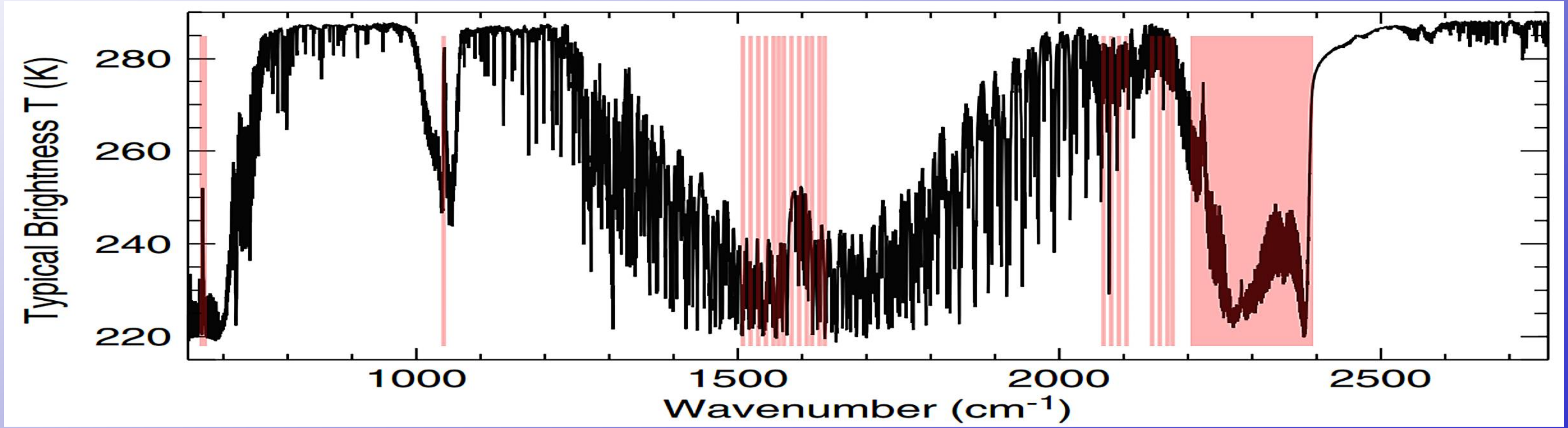
Non-LTE populations: vibrational temperatures



- 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

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

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

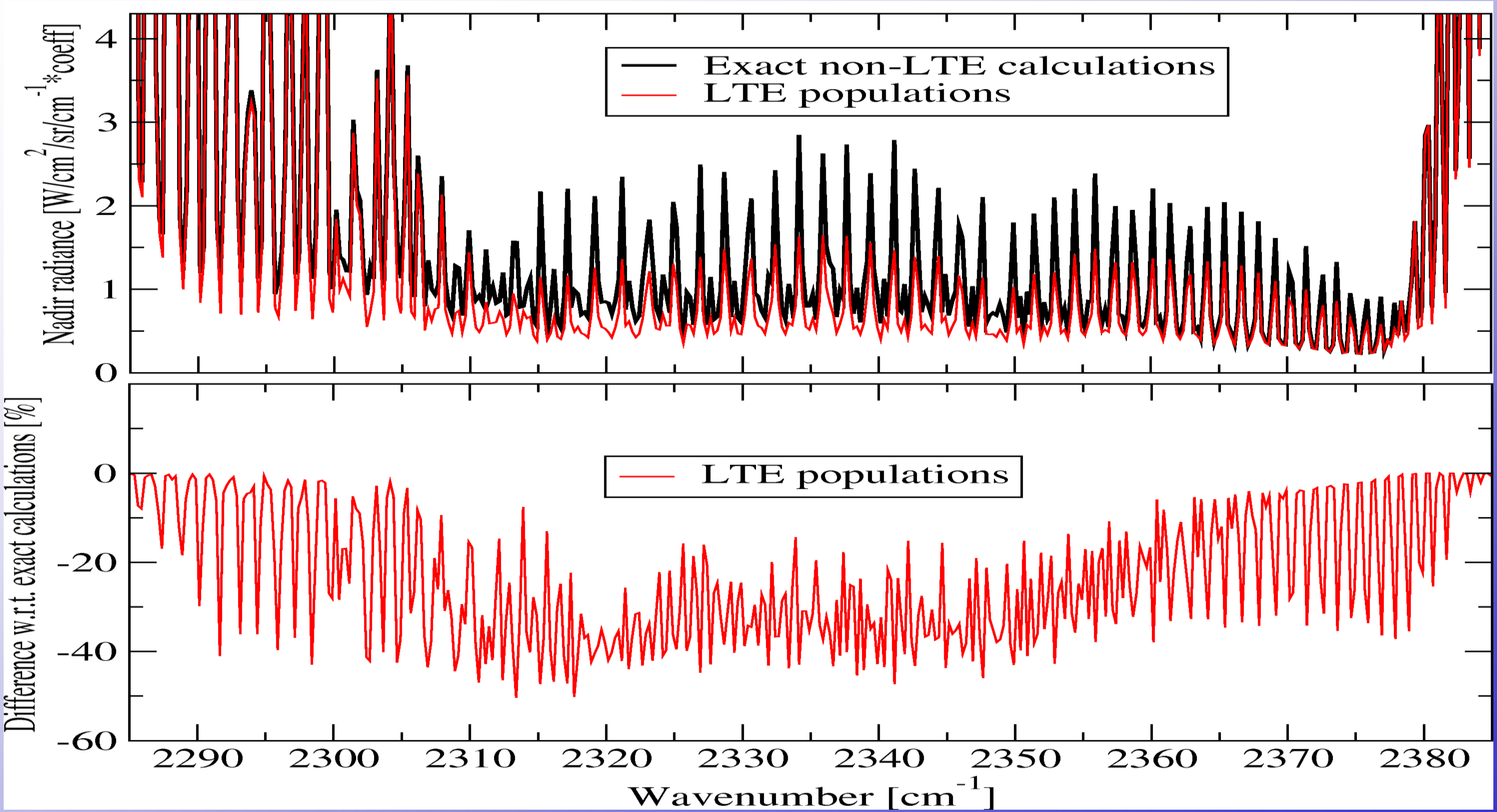
$$I_\lambda(s_1) = I_{\lambda 0} \exp(-\tau_\lambda(s_1,0)) + \int_0^{s_1} k_\lambda \rho r B_\lambda(T(s)) \exp(-\tau_\lambda(s_1,s)) ds$$

Typical representation in LTE-based codes

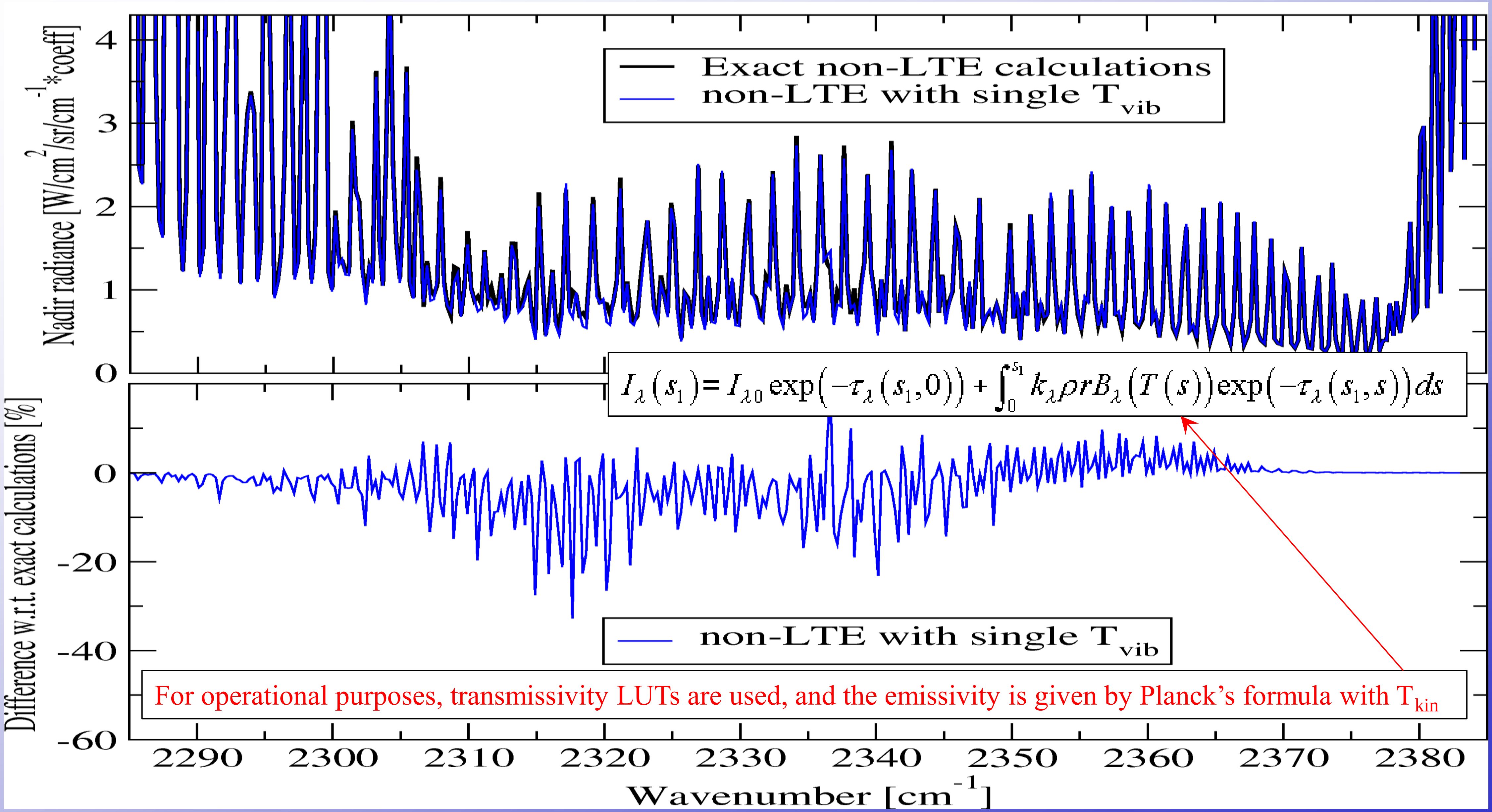
LTE-based codes assume that all populations are thermalized: how to bypass it ???

- 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.

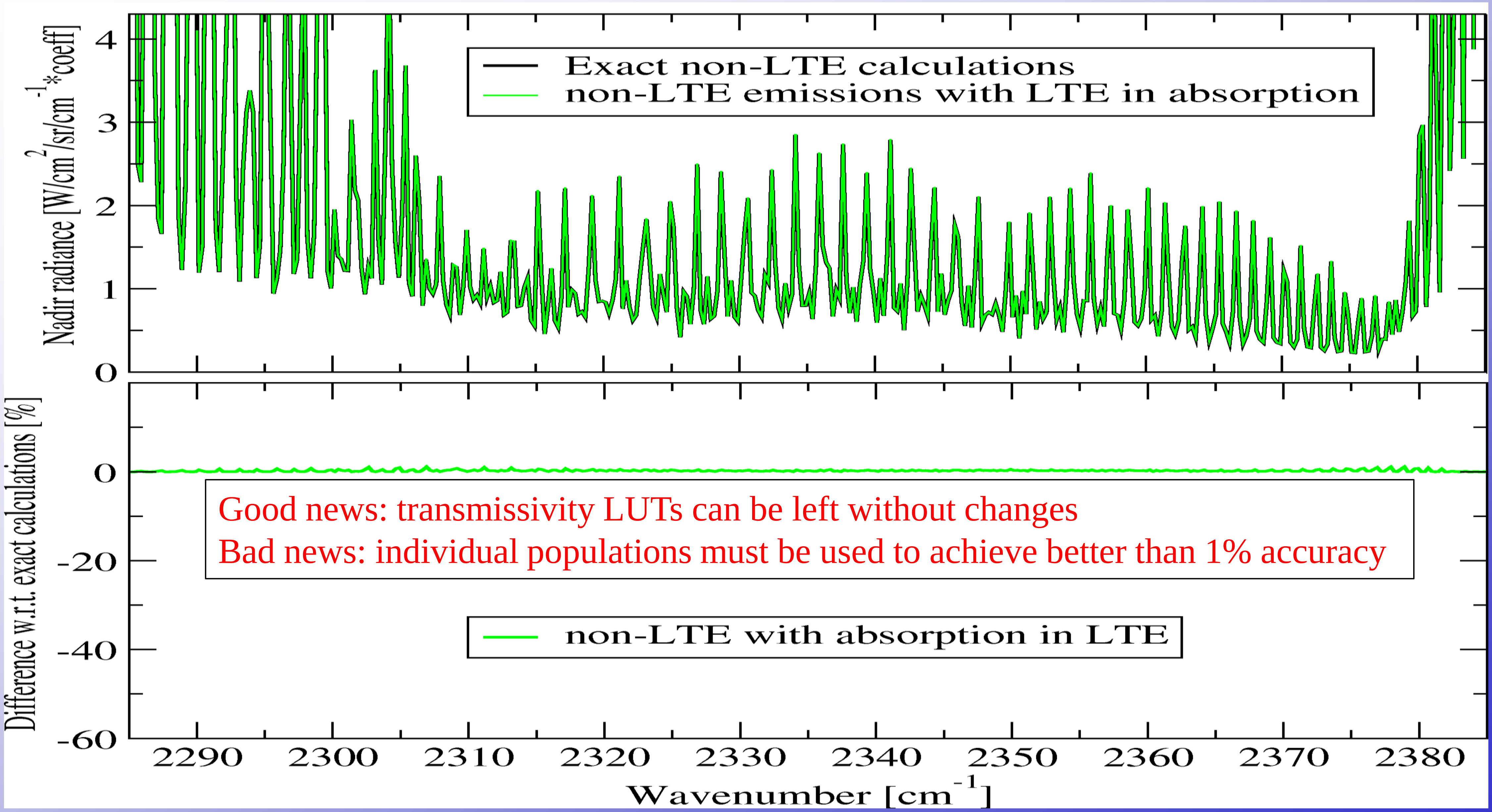
Implementing non-LTE populations: severity of the problem



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).