

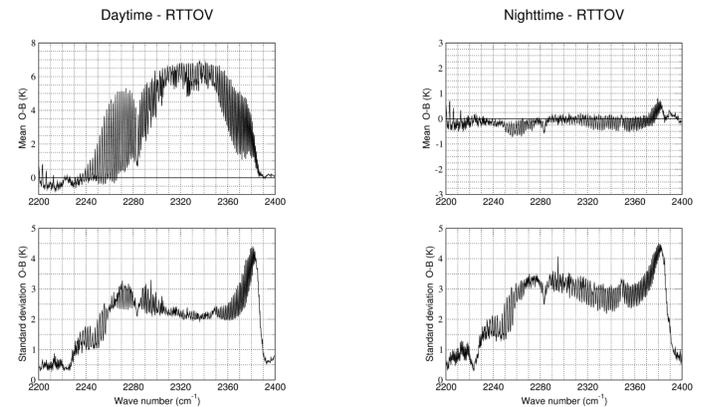
Modeling of nonlocal thermodynamic equilibrium effects in the classical and principal component based version of the RTTOV fast radiative transfer model

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1. Non Local Thermodynamic equilibrium emission

- Channels in IASI band 3 are currently underused compared to similar channels in the long-wave region for a number of reasons, which include day-night variations in data usability due to departures from Local Thermodynamic Equilibrium (LTE) and increased instrument noise.
- To avoid day/night sampling issues, the exploitation of short-wave IASI data requires the introduction of Non Local Thermodynamic Equilibrium (NLTE) effects in the simulation of the radiances.
- For IASI-like satellite nadir-sounding applications, NLTE effects occur primarily during daytime above altitudes of ~40 km in the CO₂ spectral region at 4.3 μm where the main mechanism responsible for the population of the excited states is the absorption of the strong solar radiation field. If not accounted for, NLTE effects can introduce significant errors in the simulation of daytime top-of-the-atmosphere (TOA) IASI radiances.



The mean value (upper panels) and the standard deviation (lower panels) of the difference between observed radiances and radiances computed using RTTOV. RTTOV simulations do not include NLTE effects.

2. The fast NLTE algorithm for IASI

- We have developed a computationally efficient algorithm that calculates the difference, ΔR_i^{NLTE} , between NLTE and LTE polychromatic line-by-line (LBL) radiances. The fast NLTE algorithm is trained using a limited set of diverse vibrational temperature profiles and allows the rapid estimation of ΔR_i^{NLTE} for any atmospheric profile for any nadir viewing angle and solar zenith angle geometry.
- The difference ΔR_i^{NLTE} in IASI channel i is expressed through a regression relation in which a set of profile-dependent predictors is governed by a set of channel-dependent coefficients:

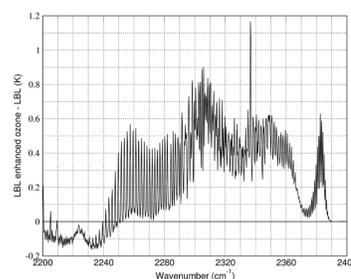
$$\Delta R_i^{NLTE} = \sum_{j=1}^n X_{i,j} b_j \quad (1)$$

where b_j are the predictors and $X_{i,j}$ are coefficients that have been estimated by fitting Eq. (1) to a dataset of ΔR_i^{NLTE} LBL radiances between 2200 cm⁻¹ and 2400 cm⁻¹. The predictors consist of various combinations of the solar zenith angle (θ_0), the sensor zenith angle (θ) and the average kinetic temperature in two broad atmospheric layers above 50 hPa, T_1 and T_2 .

Predictor number	Predictors
1	constant
2	$\cos(\theta_0)$
3	$(\cos(\theta_0))^{0.5}$
4	$\cos(\theta_0) \sec(\theta)$
5	$(\cos(\theta_0) \sec(\theta))^2$
6	$\cos(\theta_0) T_1$
7	$\cos(\theta_0) T_2$
8	$\sec(\theta) T_1$
9	$\sec(\theta) T_2$

The predictors used in the fast NLTE algorithm

- Although O₃ is an important parameter for the calculation of NLTE populations, our fast NLTE model does not yet include O₃ terms in the regression algorithm. This limits the skill of the model in presence of enhanced ozone concentrations in the mesosphere.



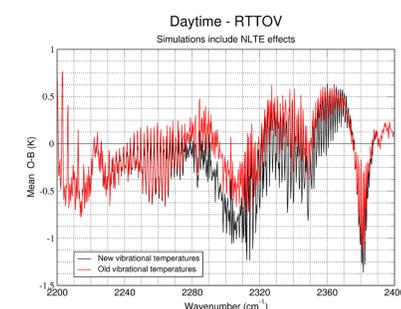
The difference between the NLTE spectrum corresponding to enhanced ozone concentrations in the mesosphere and the NLTE spectrum corresponding to the same atmosphere but with the ozone profile replaced by the ozone profile used for the training of the fast NLTE model.

3. Training of the fast NLTE model

- The training dataset of NLTE and LTE LBL spectra has been calculated using the LBLRTM [1] LBL model (version 12.2) utilising vibrational temperatures computed using the latest version of the GRANADA [2,3,4] NLTE population algorithm.
- To broaden the scope of the study, we have produced a supplementary set of regression coefficients using a pre-existing database of vibrational temperatures calculated with an older version of the GRANADA NLTE population algorithm [5]. This has allowed us to assess the relative merits of the old and new version of the GRANADA algorithm.

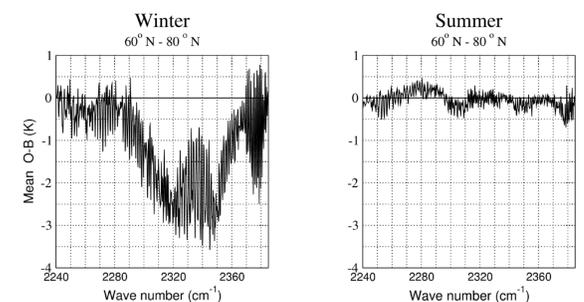
4. Validation against IASI observations

- The fast NLTE algorithm has been implemented in the classical version of the RTTOV [6] fast radiative transfer model and in the Principal Component based (PC) version of the same model (PC-RTTOV) [7].
- We have compared RTTOV simulations to daytime IASI spectra using global background (i.e. short-range forecast) fields of temperature, water vapour and ozone from version 41r2 of the ECMWF model.
- The introduction of NLTE effects in the RTTOV/PC-RTTOV simulations greatly reduces the daytime biases.
- The fast NLTE model based on the old GRANADA vibrational temperatures has a lower bias. However, because biases are generally small, it is difficult to conclude that the old vibrational temperatures are more accurate than the new ones due to the competing effects of biases from other sources.



The global mean value of the difference between daytime observed radiances and radiances computed using RTTOV. RTTOV simulations include NLTE effects

- While the performance of the fast NLTE model is overall very good, it is important to highlight its current limitations. Arguably the most important of these is the accuracy of the NLTE simulations at winter high latitudes (i.e. for large solar zenith angles).



The mean value of the difference between daytime observed radiances and radiances computed using RTTOV. Results are presented for the geographical region comprised between 60°N and 80°N.

- With regard to the origin of the biases at winter high latitudes, a possible explanation is that the pressure/temperature training profiles do not represent adequately the conditions found at winter high latitudes. There could also be an effect related to the representativeness of the vibrational temperatures at large solar zenith angles.

5. Conclusions

- We have developed a fast NLTE model based on state-of-the-art vibrational temperatures. The fast NLTE model has been implemented in the classical and PC based version of the RTTOV fast RT model.
- Testing against IASI observations shows that the computation of the daytime NLTE radiances is almost as accurate as the computation of the night-time radiances
- Current limitations of the fast NLTE model include the accuracy of the simulations at winter high latitude and the lack of an adequate representation of the ozone variability in the mesosphere.

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