

Validation of the Reference Forward Model's Radiative Transfer Simulation by Comparison with IASI Observations



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Abstract

Accurate radiative transfer modelling is crucial for supporting Earth observation through remote sounding, with benefits for climate modelling and weather prediction. This study uses radiance closure to validate simulations by the Reference Forward Model (RFM), a general-purpose line-by-line radiative transfer model, of spectral observations in the mid-infrared by the Infrared Atmospheric Sounding Interferometer (IASI), a nadir-viewing Fourier transform interferometer operating aboard EUMETSAT's MetOp satellites. During adjustment of internal RFM parameters, inclusion of CO₂ line-mixing and χ –factor modification of the Voigt lineshape were deemed essential to decreasing residuals in the CO₂ ν_2 and ν_3 bands, although increasing overall computation time. When comparing with IASI observations, the RFM's input atmosphere was iteratively adjusted using retrievals of temperature and gas concentrations. The residuals were decreased to the order of IASI noise in some regions, whilst this was not possible especially for parts of the H₂O ν_2 band and the CO₂ ν_2 and ν_3 bands. This was caused by limitations in vertical resolution of retrievals which failed to capture tropospheric H₂O concentration. CO₂ line-coupling effects and errors in specifying the temperature profile at high altitudes were deemed probable causes, with implications for future RFM development.

Introduction

Uncertainties in knowledge of spectroscopic line parameters and continua are the primary limitations on the accuracy of computed radiances. Reducing these uncertainties is an important part of improving the accuracy of radiative transfer modeling for both short-term weather forecasting and long-term future climate predictions.

Objectives

The first objective of this study was to optimise RFM modelling parameters for accurate simulation of IASI spectra. The second objective was to iteratively improve the atmosphere profile (radiance closure), with the goal of minimising residuals and their root mean square error (RMSE) to within IASI noise. From this, regions of the spectrum which could not be adequately fit were identified.

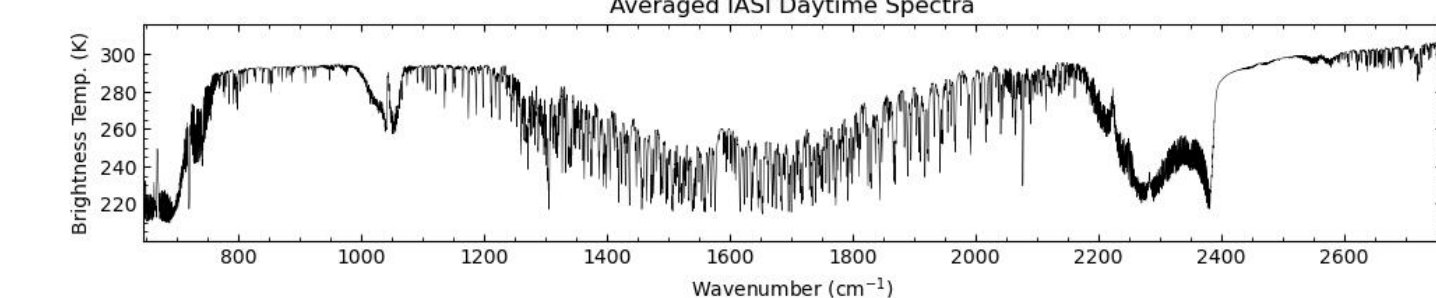
Methods

The Reference Forward Model (RFM) is a general-purpose line-by-line radiative transfer model developed by the Earth Observation Data Group (EODG) at the University of Oxford, solving the radiative transfer equation for each spectral channel.

$$L_{\nu\uparrow} = L_{\nu}(z_s)\tau(z_s, z_{obs}) + \int_{z_s}^{z_{obs}} B_{\nu}(T(z)) \frac{d\tau}{dz} dz$$

It considers by default a 1D atmosphere profile, with a vertical grid specifying pressure, temperature, and gas fractions at each level. The RFM is run using a driver table which reads 1D atmospheric profiles under the ATM flag as well as other flags which control e.g. spectral resolution, and incorporate certain physical effects. CO₂ line-mixing (MIX), applying a χ -factor to modify the lineshape (CHI) and relaxing the assumption of local thermodynamic equilibrium (NTE) were examined by the taking residuals and comparing computation speed from RFM runs without these flags. The RFM can simulate IASI spectral data by performing spectral convolution with the apodised instrument line shape (ILS).

```
*HDR      ! text for headers of output spectra
Example of nadir brightness spectrum
*FLG      ! flags defining type of calculation:
NAD       ! nadir-viewing, plane-parallel atmosphere
BBT       ! output Brightness Temperature spectra
SFC       ! default surface temperature, emissivity=1
AVG       ! apply triangular instrument line-shape
*SFC      ! define spectral range/resolution of output
1200 1300 0.25
*GAS      ! list of absorbing molecules to consider
CH4 H2O N2O
*ATM      ! atmospheric profile: T,p,VMRs on height grid
./atm/usa.atm
*SEC      ! Viewing angle, sec(theta)=1 is nadir
1.0
*HIT      ! HITRAN data, in RFM binary format
./hit/hitrان_2012.bin
*END
```



IASI is a nadir-viewing Fourier transform interferometer which records the mid-infrared region in three bands between 645 and 2760 cm⁻¹ with 0.5 cm⁻¹ apodised resolution and 0.25 cm⁻¹ spectral channel width. Three IASI instruments — A (2006), B (2012), C (2018) — operate aboard EUMETSAT's MetOp satellites. These are in sun-synchronous, polar orbits with an orbital period of 101 minutes allowing near-global coverage.

Suitable IASI pixels were in cloud-free, mid-latitude subtropical, and over-ocean. The ocean can be approximated as a black body since its emissivity ≈ 1 . This study focused on two IASI-C observations from January 13th 2022: 0144 -- 0326 GMT and 1332 -- 1514 GMT, giving a cluster of 49 daytime pixels and 24 nighttime pixels within a 3° × 3° grid box centred on 26.5° S, 91.5° E over the Indian Ocean. The radiance and brightness temperature spectra of suitable pixels was averaged to reduce noise.

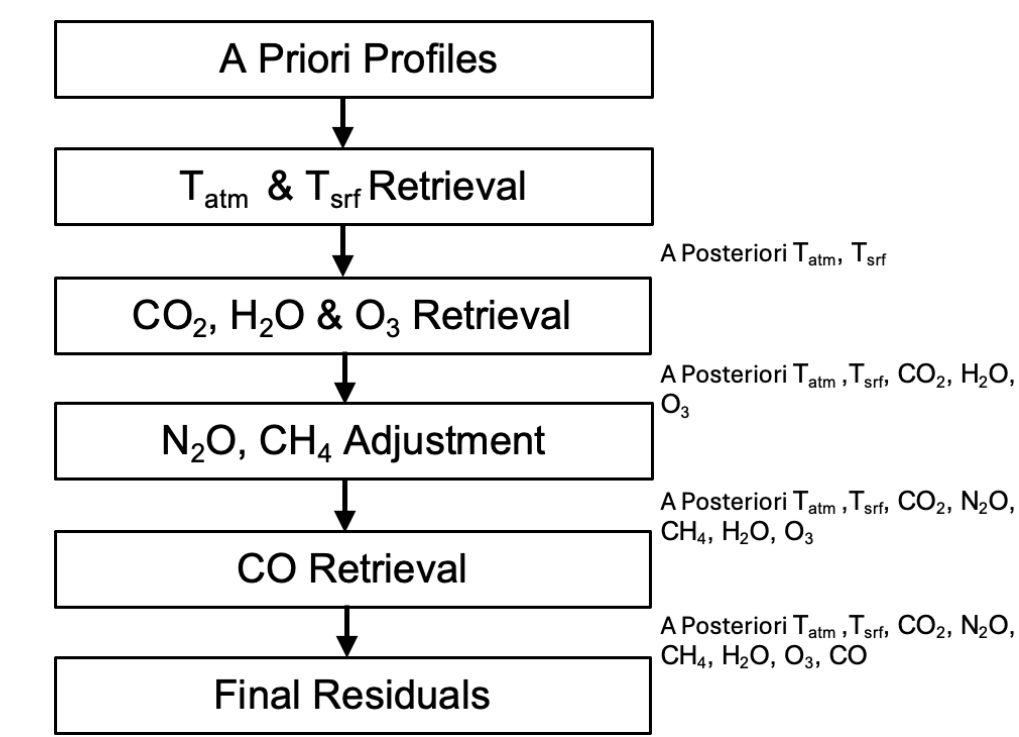
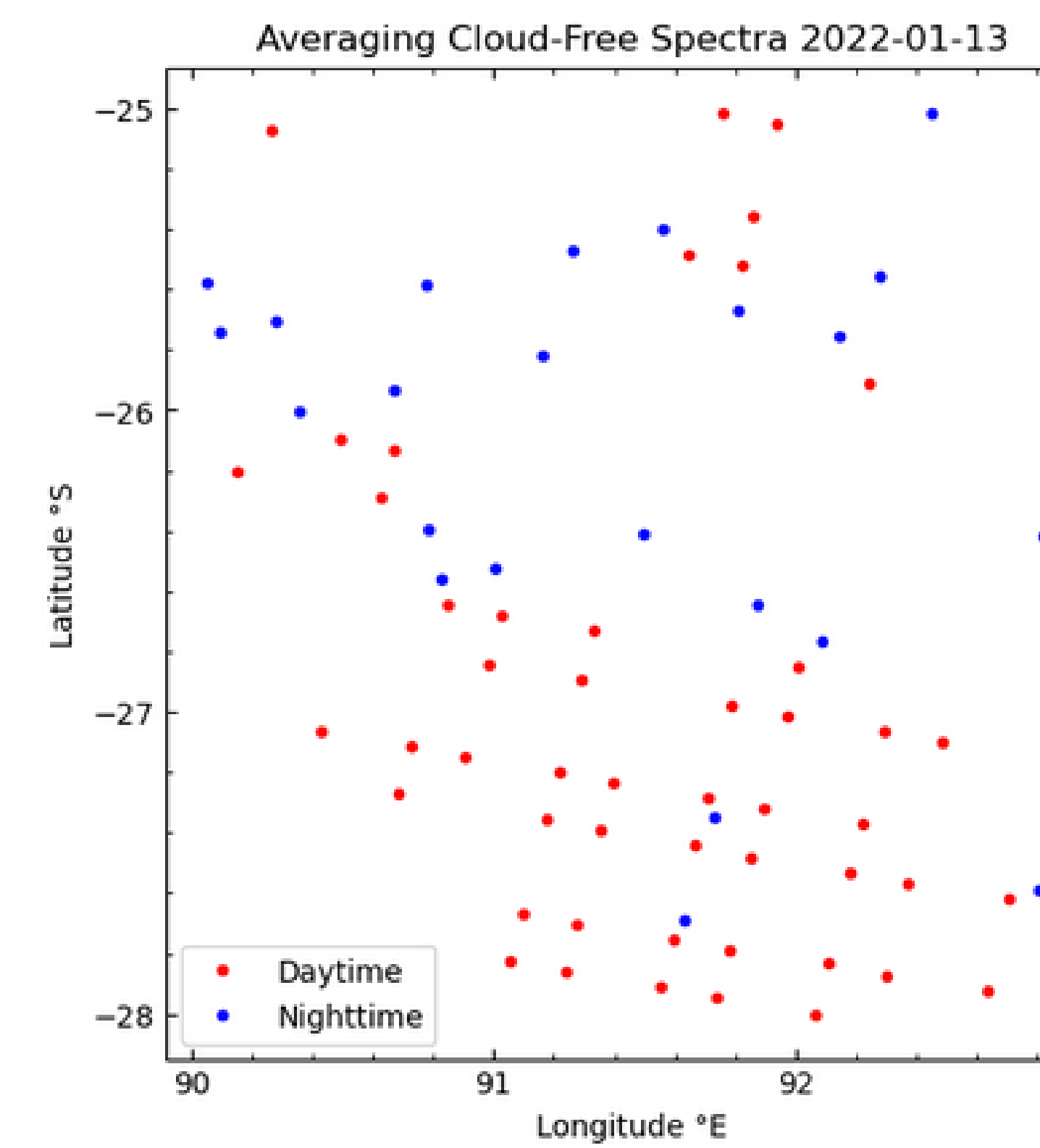
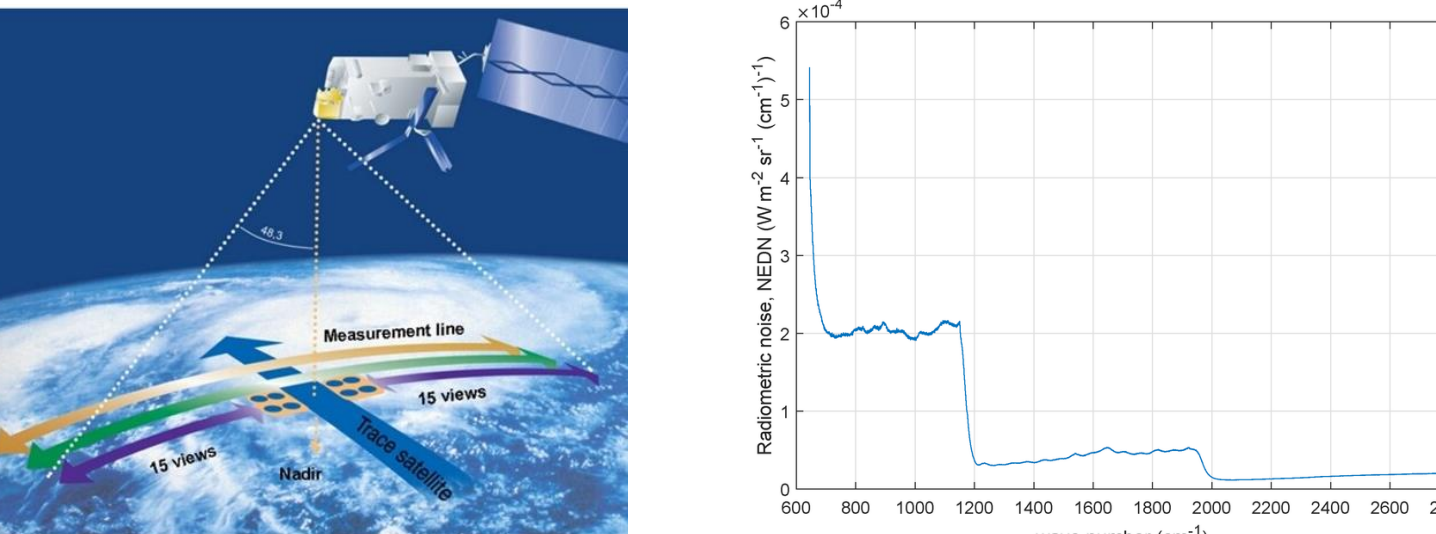
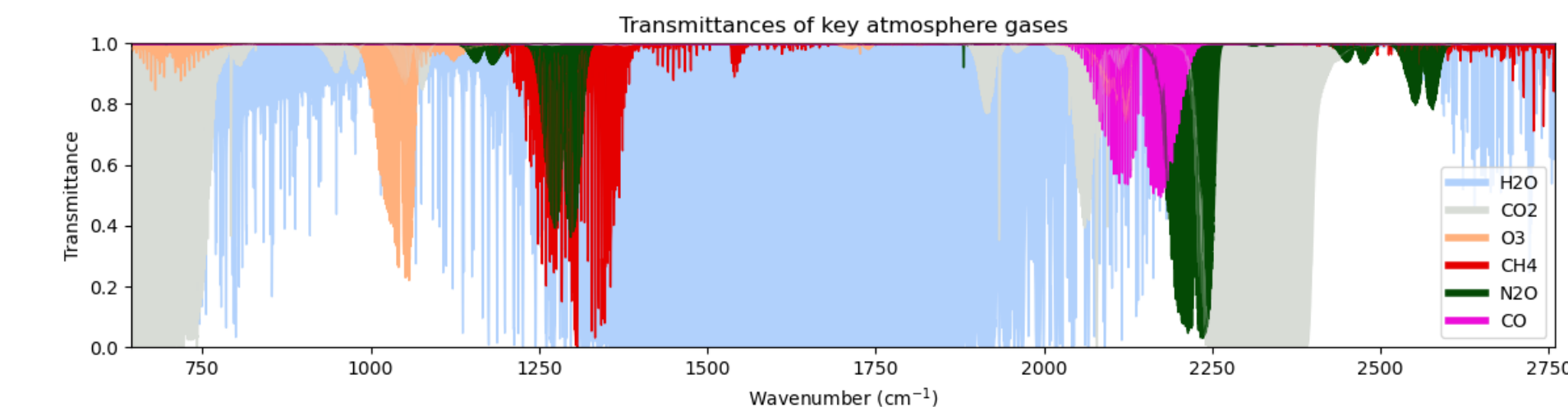


Table 1: Summary table of RFM parameters necessary for accurate modelling of IASI spectra

Parameter (Flag)	Optimum setting
Vertical resolution (ATM)	50 levels up to 120 km
Fine mesh resolution (FIN)	0.001 cm ⁻¹
CO ₂ line-mixing (MIX)	Necessary for ν_2 R-branch
CO ₂ χ -factor (CHI)	Necessary for ν_3 R-branch
Non-LTE (NTE)	Necessary for daytime only

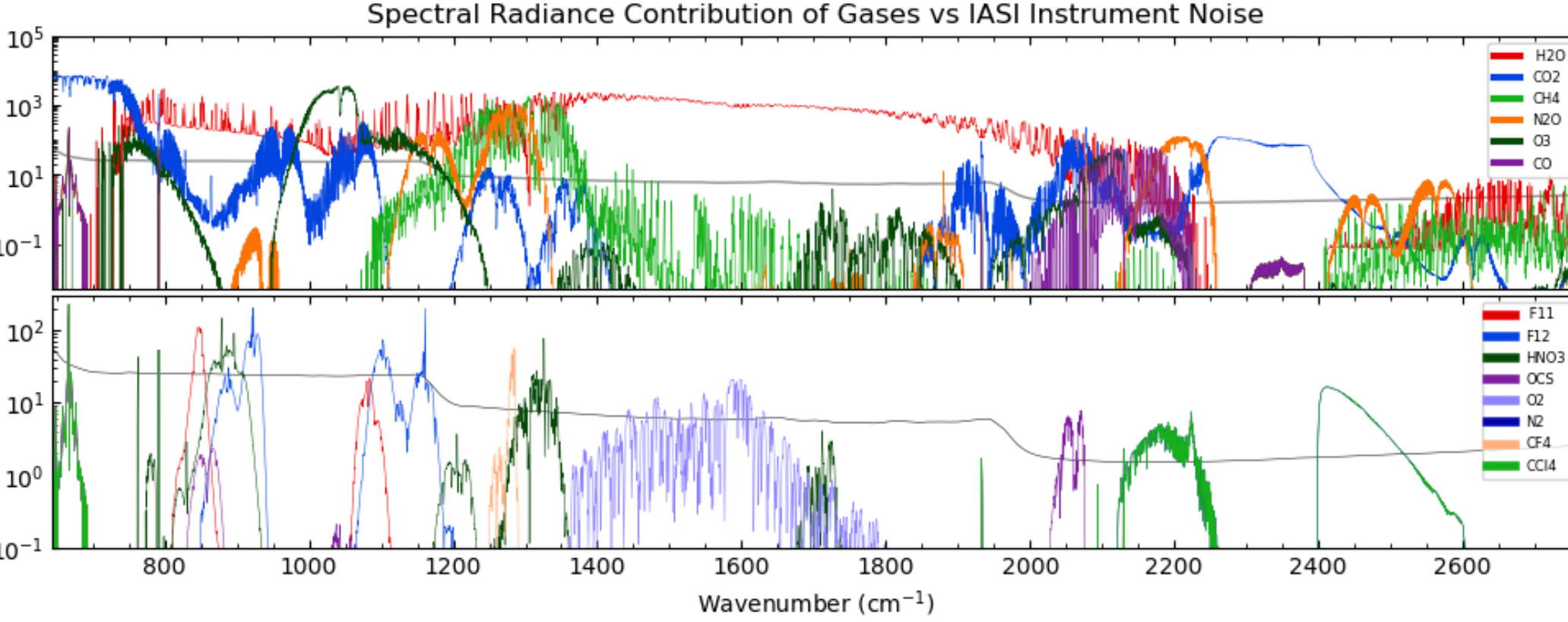


Radiance closure began with an a priori atmospheric profile from 2001 which was iteratively improved to identify anomalous features. Since 2001, atmospheric concentrations of the six greenhouse gases most optically thick in the mid-infrared have all increased – water vapour (H₂O), carbon dioxide (CO₂), methane (CH₄), ozone (O₃), nitrous oxide (N₂O), and carbon monoxide (CO) – have all increased steadily. This led to systematic residuals in initial comparisons between IASI observations and RFM calculations. Since CO₂, N₂O, and CH₄ are all long-lived, homogeneously-distributed absorbers, the atmospheric profile was adjusted using NOAA observation data for January 2022 by taking the average tropospheric concentration for each gas and applying a multiplier to the concentration at each level.

Meanwhile, O₃ and H₂O tend to concentrate in the stratosphere and troposphere respectively, necessitating their concentrations to be optimised via MORSE retrieval instead. A retrieval step is crucial in to solving the inverse problem, inferring gas concentrations and temperature from spectral measurement. For this, the study used Multispectral Orbital Retrievals using Sequential Estimation (MORSE), a constrained iterative optimal estimation retrieval algorithm developed by EODG. Two metrics were used to assess accuracy, an error parameter ϵ_{ν} , and root mean square error (RMSE):

$$\epsilon_{\nu} = \frac{\Delta L_{\nu} \sqrt{N_{\text{pixels}}}}{\text{NESR}_{\nu}} \quad \text{RMSE} = \sqrt{\frac{N_{\text{channels}} \sum_{i=1}^{N_{\text{pixels}}} (\text{IASI}_{i,j} - \text{RFM}_{i,j})^2}{N_{\text{channels}}}}$$

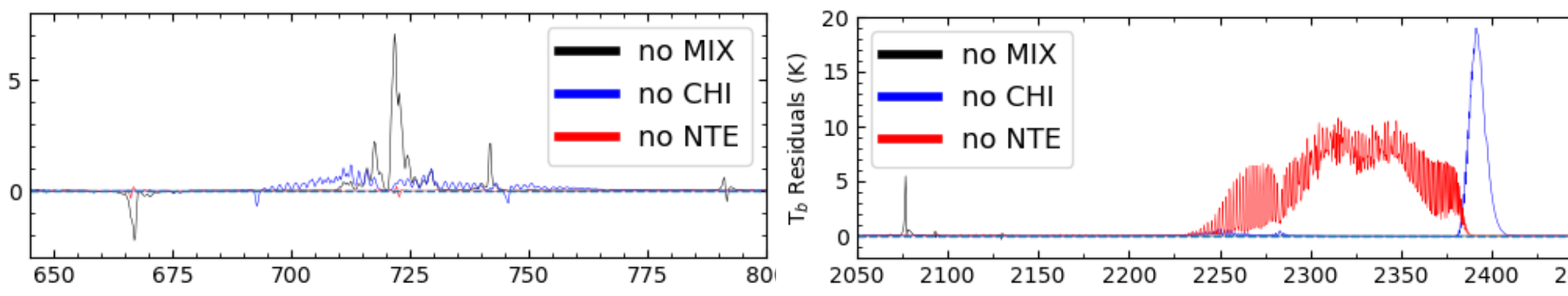
RFM Adjustment: Results & Discussion



Other trace gases were added onto the baseline atmosphere of CO₂, N₂O, CH₄, CO, O₃, and H₂O. The radiance residual of this modified atmosphere was taken and compared with the IASI NESR spectrum. Only gases greater than IASI noise were necessary for retrieval, as inclusion of more gases is computationally expensive.

In the lower atmosphere there is a significant temperature gradient, and absorption is stronger, varying more rapidly with height. The vertical grid spacing had to be fine enough to capture this. The default MIPAS 2001 profile contains 121 levels from sea level up to an altitude of 120 km. A coarsened vertical resolution of 50 levels up to an altitude of 100 km, with level spacing decreasing exponentially with altitude, led to no significant difference in output and this was used subsequently.

FIN: At higher altitudes, the spectral line shape is dominated by Doppler broadening although this is usually finer than IASI resolution, especially with nadir-viewing. To fully capture these features, the RFM had to be run at sufficiently fine resolution before ILS convolution. The RFM's default 'fine mesh' calculation is run with a resolution of 0.0005 cm⁻¹ spacing (2000 points per cm⁻¹). With this baseline, the residuals for running at 0.0001 cm⁻¹, 0.001 cm⁻¹, 0.005 cm cm⁻¹, and 0.01 cm⁻¹ were taken and compared with IASI instrument noise. 0.001 cm⁻¹ was found to be sufficient, although care should be taken when using averaged datasets as this reduces noise.



MIX: CO₂ line-mixing is a non-linear effect where the absorption coefficient cannot be represented as the sum of individual lineshapes. Without the MIX flag there were residuals of ~5 K in the CO₂ Q-branch at 667 cm⁻¹ and at 2075 cm⁻¹. Line-mixing effect is therefore essential to accurate modelling in these spectral regions.

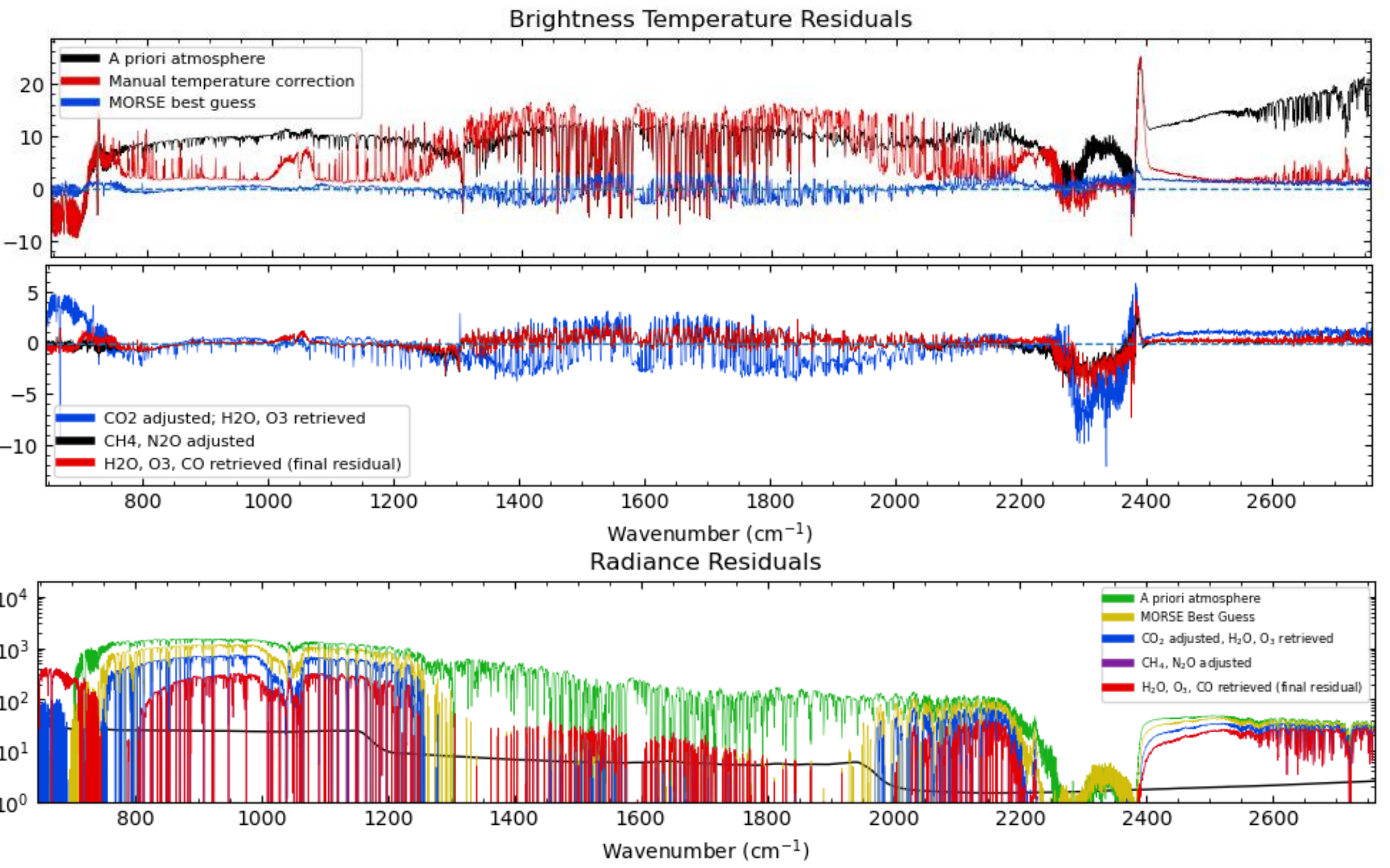
CHI: In prior studies, the absorption measured at wavenumbers beyond the CO₂ ν_3 R-branch has been less than that predicted by a Lorentzian profile. This is expressed using a corrective shape factor χ . Without the CHI flag, there was a large peak in residuals of ~18 K at 2390 cm⁻¹ making the χ -factor essential to accurate modelling in this region. Also notable were residuals in the CO₂ ν_2 R-branch, which were on the order of IASI instrument noise.

NTE: Initial RFM runs assumed local thermodynamic equilibrium (LTE), where energy levels of gas molecules are in equilibrium with the local radiation field, but this is disrupted by absorption of solar radiation, creating temperature gradients close to the surface. The non-LTE case was simulated using daytime vibrational temperature profiles. There was a significant underestimate of the brightness temperature in the CO₂ ν_3 band of ~10 K, although other parts of the spectrum were not affected. However, when using a nighttime vibrational atmosphere profile, the residuals were negligible across the IASI spectral range.

Table 2: Summary table of residuals for each iterative improvement of the atmospheric profiles, giving RMSE for both brightness temperature and spectral radiance, as well as the maximum value for the error parameter ϵ_{ν} and the wavenumber ν_{max} where this occurs.

Radiance Closure Stage	Brightness Temp. RMSE (K)	Spectral Radiance RMSE (nW/(cm ² sr cm ⁻¹))	$\epsilon_{\nu_{max}}$	ν_{max} (cm ⁻¹)
A priori atmosphere	10.35	634.4	561.8	1204.5
Best guess T _{surf} , H ₂ O, O ₃	1.273	418.5	446.7	1204.5
CO ₂ adjusted, H ₂ O, O ₃ retrieval	1.273	254.3	280.1	1204.5
CH ₄ , N ₂ O adjusted	0.7726	149.3	284.8	1367.25
H ₂ O, O ₃ , CO retrieval (final residuals)	0.7594	149.3	284.8	1367.25

IASI Comparison: Results & Discussion



Initial IASI-RFM residuals had a RMSE of 10.35 K, indicating a systematic difference between actual and modelled values of surface temperature T_{surf}. This was modified manually using the SFC flag, leading to decreased residuals except in the H₂O ν_2 band (1350—2050 cm⁻¹), where they remained the same.

A MORSE retrieval was then performed to get an updated best-guess T_{surf} of 295.1 K, which was used in subsequent RFM runs. Given the large variation in initial residuals in the H₂O ν_2 band, the retrieval was also used to update H₂O and O₃ concentrations. This was successful in reducing the overall residuals, with only a spike of ~1 K in the O₃ ν_3 band (950—1150 cm⁻¹), just outside of instrument noise.

The high final residuals (~4 K) in the CO₂ ν_3 band (2250—2400 cm⁻¹) were due to line-coupling effects and errors in specifying the temperature profile at high altitudes. As CO₂ is long-lived and therefore well-mixed, concentration errors were not likely to cause systematic residuals. Apart from for line-coupling, CO₂ spectroscopic parameters are well-known and unlikely to be the source of any detectable error.

CH₄ and N₂O profiles were also adjusted but failed to yield an improvement on residuals, indicating that concentration errors were not significant. A final retrieval was performed for CO, H₂O, and O₃ concentrations, but there was no significant improvement in the final residuals in the CO band (2050—2250 cm⁻¹).

Overall, RMSE brightness temperature improved from 10.35 to 0.7594 K and RMSE radiance from 634.4 to 149.3 nW/(cm² sr cm⁻¹).

Conclusion

In summary, RFM parameters must include CO₂ line-mixing and CO₂ χ -factor for accurate modelling in the ν_2 and ν_3 bands respectively. The non-LTE case was also found to have a much greater effect on residuals in daytime than nighttime, which was expected given its increased insolation.

Except for the H₂O ν_2 band and CO₂ ν_3 band, final residuals from radiance closure were within IASI noise. Certain regions featured residual outliers that even the optimised atmosphere was still unable to account for. In the CO₂ ν_3 band, residuals near 2200 cm⁻¹ remained even after profile optimisation. Since CO₂ is long-lived and well-mixed, concentration specification errors were likely insignificant. Persistent errors were likely due to line-coupling effects and errors in specifying the temperature profile at high altitudes. For the H₂O ν_2 band, a lack of sufficient vertical resolution in the MORSE retrievals picking up lower atmosphere temperature and variation in H₂O concentration in the lower troposphere also led to greater errors. Usually, with IASI's high radiometric accuracy, the dominant limitation in RT calculations lies in errors specifying the atmospheric state and spectroscopic line parameters.

The work of this study will contribute to the RFM's ongoing development in incorporating scattering effects as part of the Ox-HARP retrieval scheme, improving the RFM's forward modelling capability for a wider range of atmosphere retrievals, enabling enhanced climate and weather prediction.

Major References

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