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Olivier Coopmann, Vincent Guidard

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Preparation for the assimilation of the future IRS sounder in MOCAGE CTM



Olivier COOPMANN (olivier.coopmann@meteo.fr) & Vincent GUIDARD
CNRM, Université de Toulouse, Météo-France & CNRS



1) The future MTG-IRS (Infra-Red Sounder)

- Planned launch in 2025 onboard geostationary sounding satellite MTG-S
- Measurement with 4 Local Area Coverage (LAC) zones and Earth disc covered with ~ 313 Dwells. LAC 4 covering Europe every 30 minutes
- Each Well is taken in 10 s and covers about 640 x 640 km² at nadir with 160 x 160 spatial samples
- Each Pixel covers ~ 4 x 7 km² over Europe (4 x 4 km² at nadir)
- 1960 channels between 680 - 1210 cm⁻¹ and 1600 - 2250 cm⁻¹
- Spectral sampling of ~ 0.6 cm⁻¹ for both bands

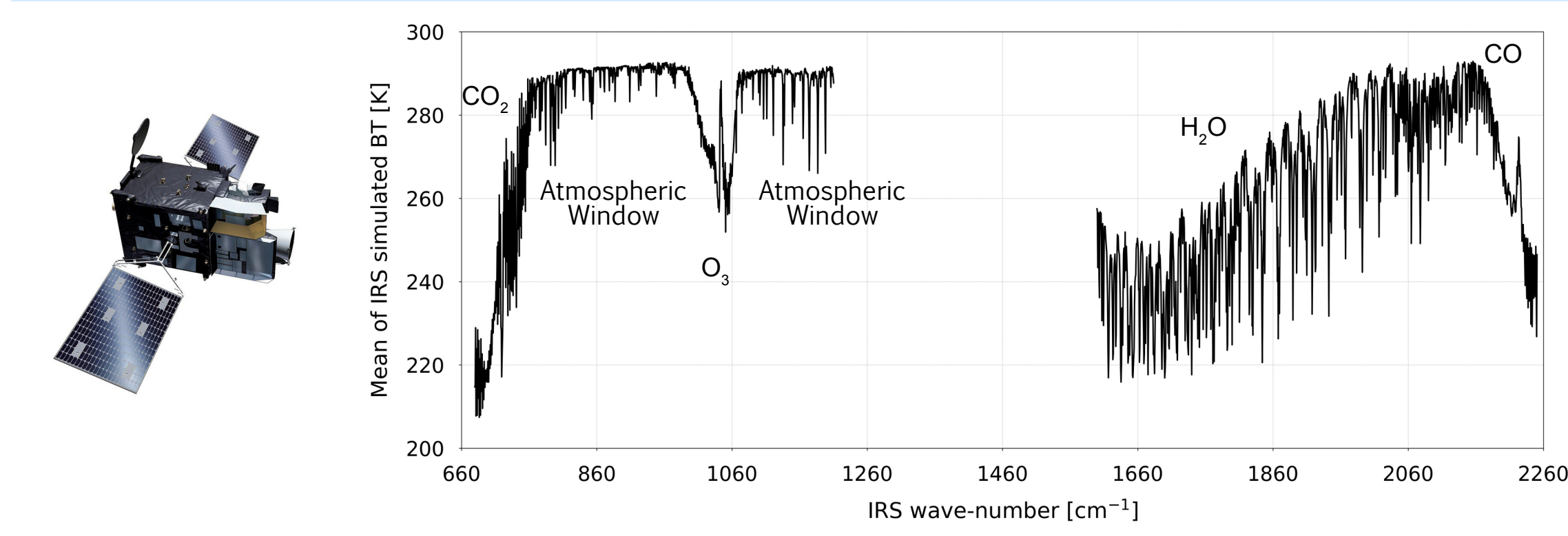


Fig.1 MTG-S satellite Fig.2 IRS brightness temperature spectrum

2) Objective of this study

- Continuation of Francesca Vittorioso's thesis (2023) work on the preparation of IRS assimilation in the MOCAGE regional (0.1°x0.1° - 60L) Chemistry-Transport Model (CTM)
- Improve the assessment framework (OSSE) and add assimilation for carbon monoxide in addition to ozone
- Evaluate IRS sensitivity to O₃ and CO and select the channels most sensitive to these gases

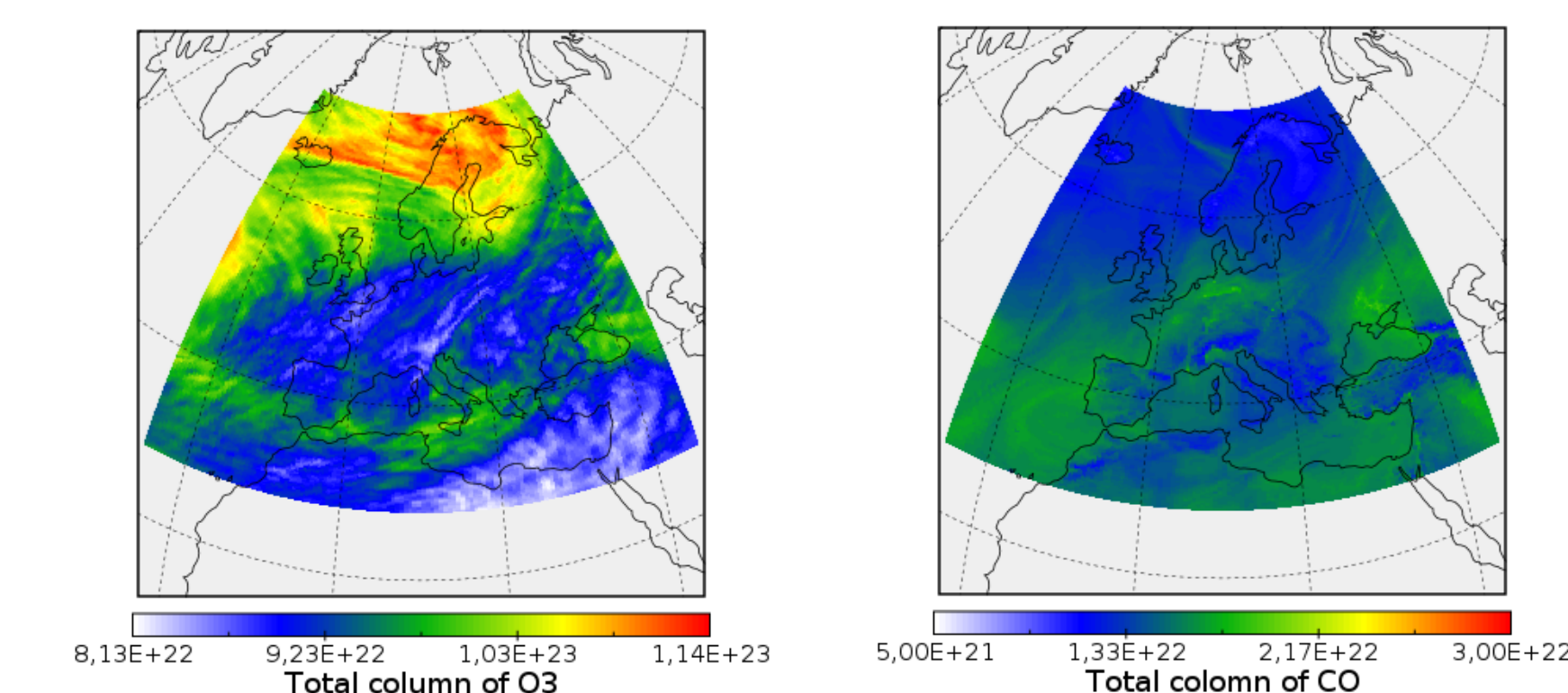


Fig.3 Example of a total column field for ozone (left) and carbon monoxide (right) over the day 2019-05-22 in the MOCAGE regional domain. Unit [molecule.cm⁻²]

3) The OSSE framework

- OSSE (Observing System Simulation Experiment) tests the impact of future observations in an assimilation system in terms of analysis and forecasts
- Based on our atmospheric reality (Nature Run), we simulate IRS observations using a radiative transfer model (RTTOV), then add the instrumental noise of the instrument to these simulations, thus constructing a synthetic IRS observation (see Fig.4)
- Compared with Francesca Vittorioso's study, I have chosen to remove pixels located at the lateral boundaries of the domain in order to eliminate border effects. Then I simulated all IRS (1960) channels. Finally, to construct the synthetic observations by adding the full observation error covariance matrix from a previous study

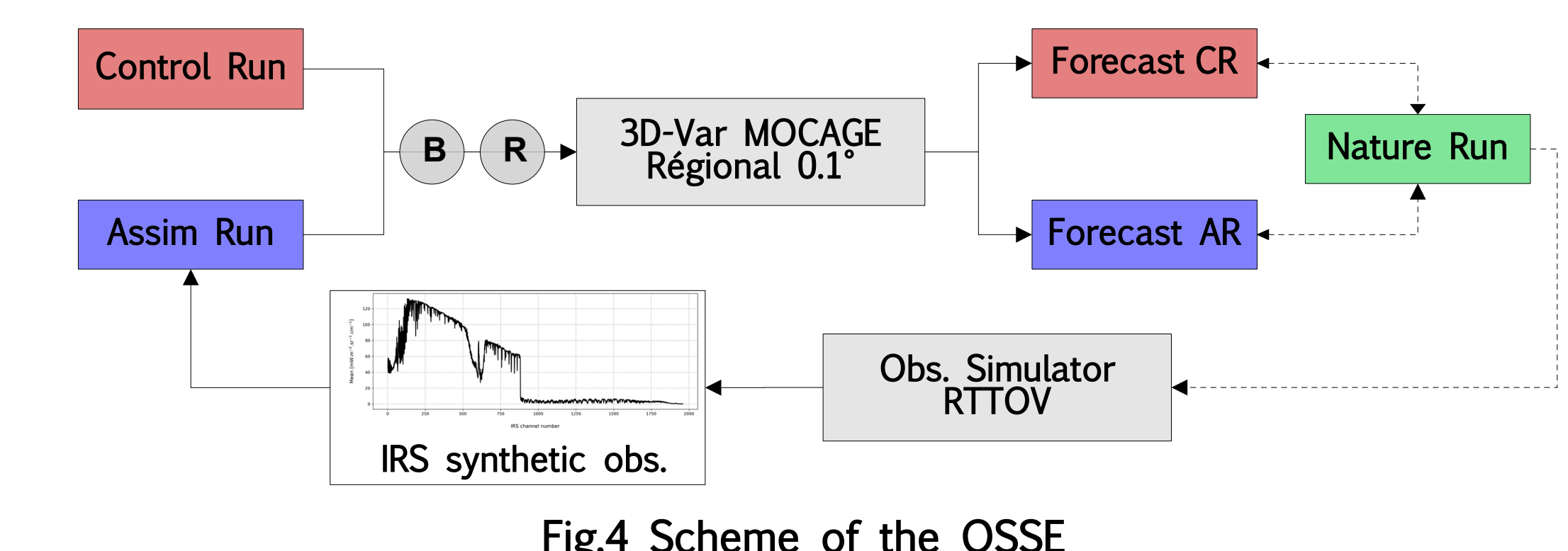


Fig.4 Scheme of the OSSE

4) IRS sensitivity analysis

- We used the method using RTTOV which consists in evaluating the brightness temperature response ΔBT to a perturbation for each atmospheric constituent separately (O₃ and CO for this study)
- Typical perturbations → O₃ : 10 % & CO : 1 %

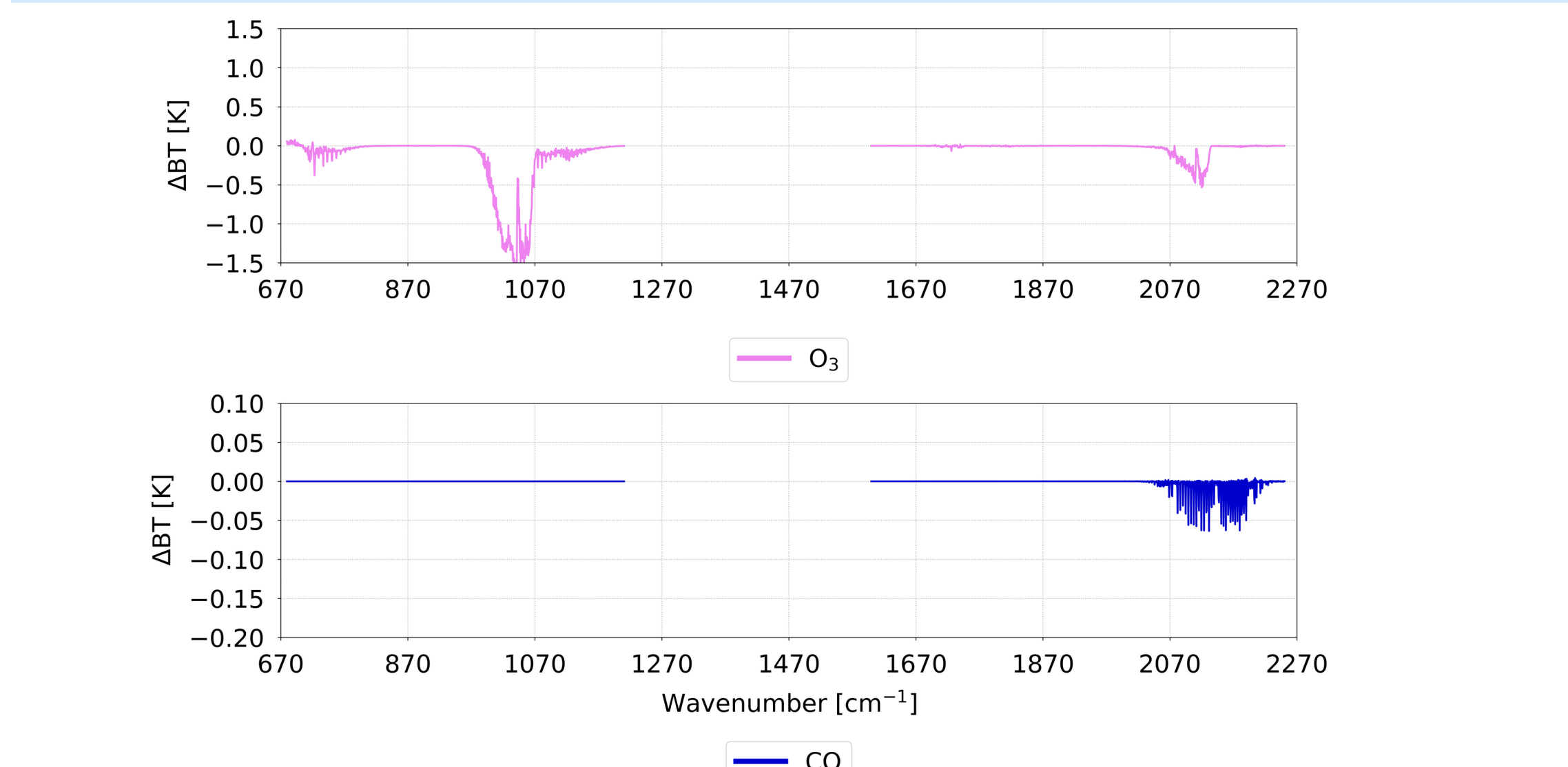


Fig.5 Differences in IRS brightness temperatures between raw and perturbed simulations for O₃ (top) and CO (bottom)

5) Channel selection

- Selection of the most sensitive ozone (143) and carbon monoxide (35) channels. Part of the CO absorption band is also sensitive to O₃, so these channels were not considered.

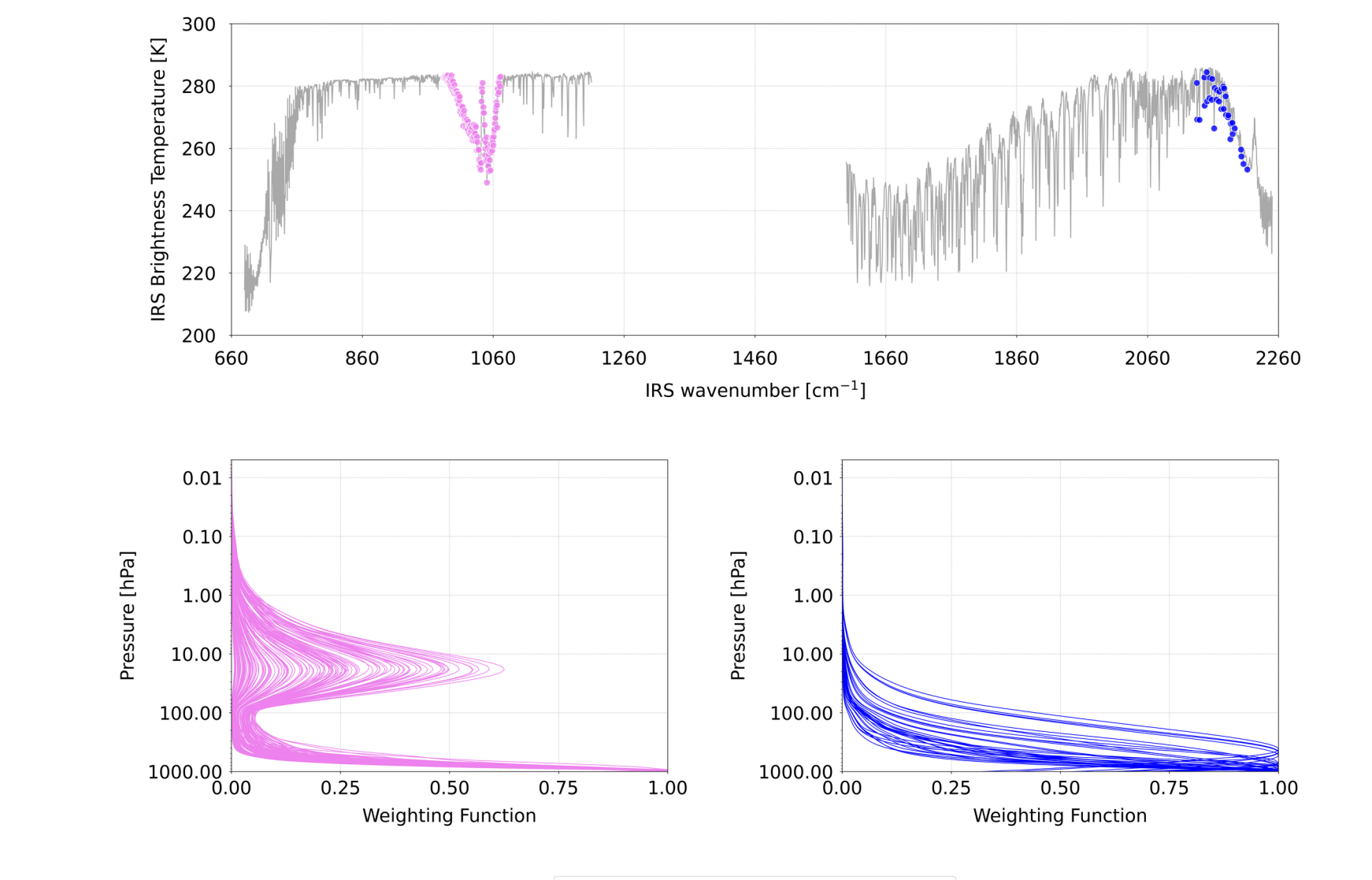


Fig.6 Illustration of selected channels on a typical spectrum (top) and weighting function associated with these channels in O₃ (bottom left) and CO (bottom right).

6) IRS synthetic observation

- In this study, the construction of the synthetic observations differs from the [Vittorioso, F., (2024), <https://doi.org/10.5194/amt-17-5279-2024>] study. Rather than just adding instrumental noise to the simulations, we decided to take into account a full and diagnosed observation error covariance matrix (taking inter-channel correlation into account). This matrix was derived from this study [Coopmann, O., (2023), <https://doi.org/10.1002/qj.4548>] for the preparation of IRS in the regional AROME model at Météo-France.
- Construction of synthetic observation:

- Before: $y_{IRS} = \mathcal{H}(x) + NEAT \times \eta$
- Version 1: $y_{IRS} = \mathcal{H}(x) + NEAT(T_{scene}) \times \eta$
- Present version: $y_{IRS} = \mathcal{H}(x) + R_{full} \times \eta$

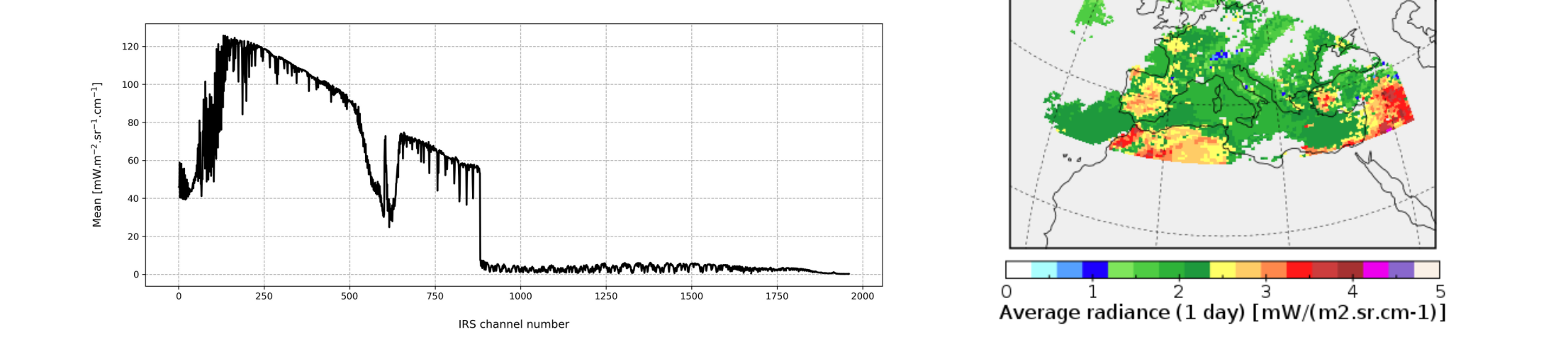


Fig.7 Average of IRS synthetic observations over the day 2019-06-01 (left) and representation of the average over the same day for the ozone-sensitive channel 577 (1027.1 cm⁻¹) (right)

7) IRS observation error

- Observation errors were diagnosed using the so-called top-down method, based on an initial assimilation experiment using a fixed observation error value, then at the end of this experiment, a [Desroziers, G., (2005), <https://doi.org/10.1256/qj.05.108>] diagnosis was performed. These diagnosed errors are then used in turn in a new assimilation experiment, and so on until convergence is achieved.
- Observation error standard deviation values are highly variable for O₃ channels, with strong correlations, whereas for CO channels the values are very low.

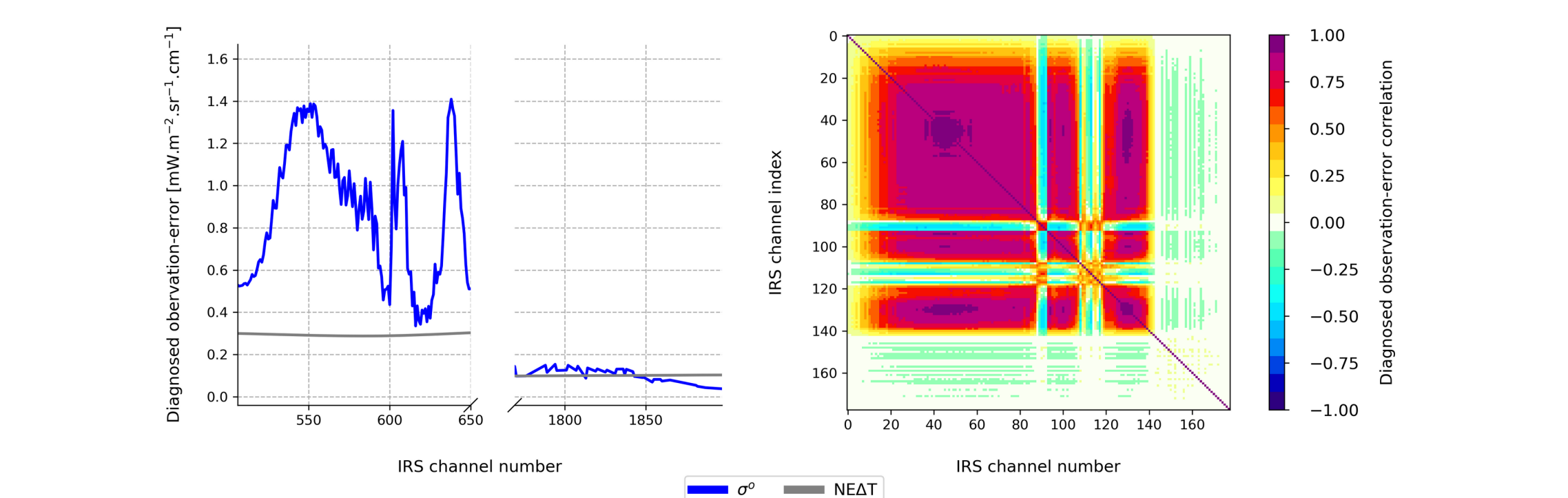


Fig.8 Diagnosed observation error standard deviation (blue) and instrumental noise (grey) (left) and diagnosed error correlation matrix (right)

8) Summary of experiments

XP	Control Run	Assim Run
Period	2019-05-22 → 2019-05-31 (spin-up) 2019-06-01 → 2019-07-31 (data used)	
Obs. assimilated	None	178 IRS channels
Control variable	None	O ₃ & CO
R error	None	Full & diagnosed R matrix
B error	None	Estimated standard deviation background error for O ₃ et CO vertical profile from NMC method
Verification	Nature Run	

9) Observation scores (temporal) for a specific O₃ channels

- Shown here is the temporal evolution of the daily mean and standard deviation for the ozone-sensitive channel 577 (1027.1 cm⁻¹). As before, the red curve for OmG and the blue curve for OmA. In the same way, we can see a reduction in bias thanks to assimilation over the whole period. We also note a reduction in standard deviations with assimilation, with a general tendency for values to increase as the period progresses.

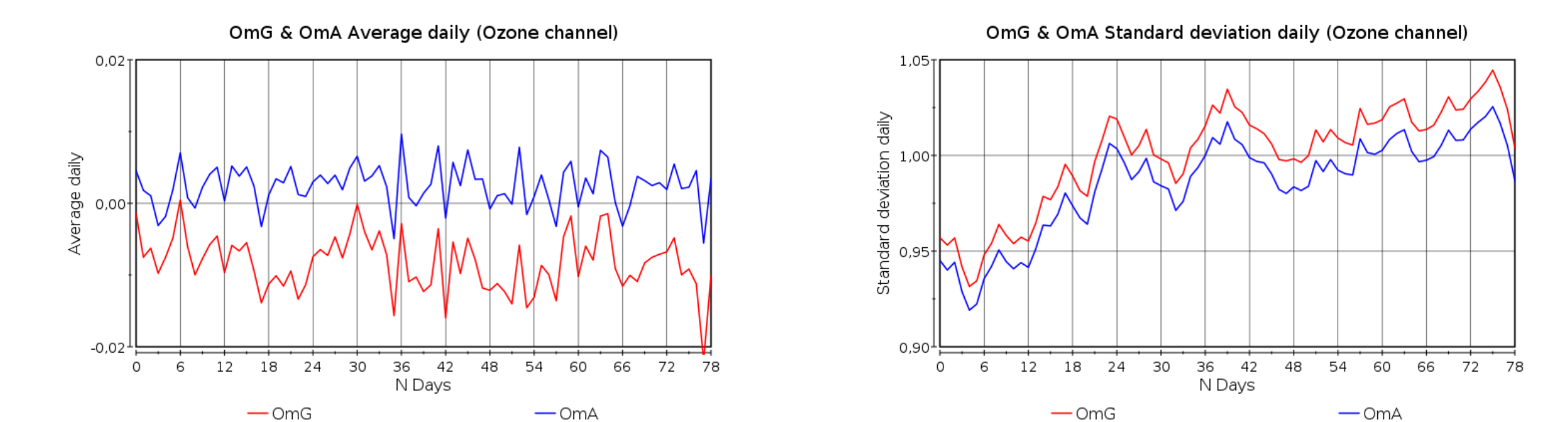


Fig.9 Temporal evolution of the daily mean (left) and standard deviation (right) for the ozone-sensitive channel 577 (1027.1 cm⁻¹)

10) Forecast error reduction (RMSE) for O₃ & CO

- These Figures show the forecast error reduction (RMSE) integrated over the atmospheric vertical for the 3 months of study (JJA) for the ozone (top) and carbon monoxide (bottom) fields of the control experiment (left) and the IRS assimilation experiment (right) compared with the Nature Run.
- The IRS assimilation experiment significantly reduced the forecast error in O₃ and CO over the regional domain (thinning of 0.4°), except at the edges of the domain. Indeed, we chose not to assimilate lateral boundary conditions to avoid edge effects. Moreover, the slightest reduction in RMSE in these areas is also linked to the coupler, which forces the domain boundaries with fields unconstrained by assimilation. Overall, assimilation of the 178 IRS channels reduces the forecast error by 0.1 ppv for the O₃ and CO fields.

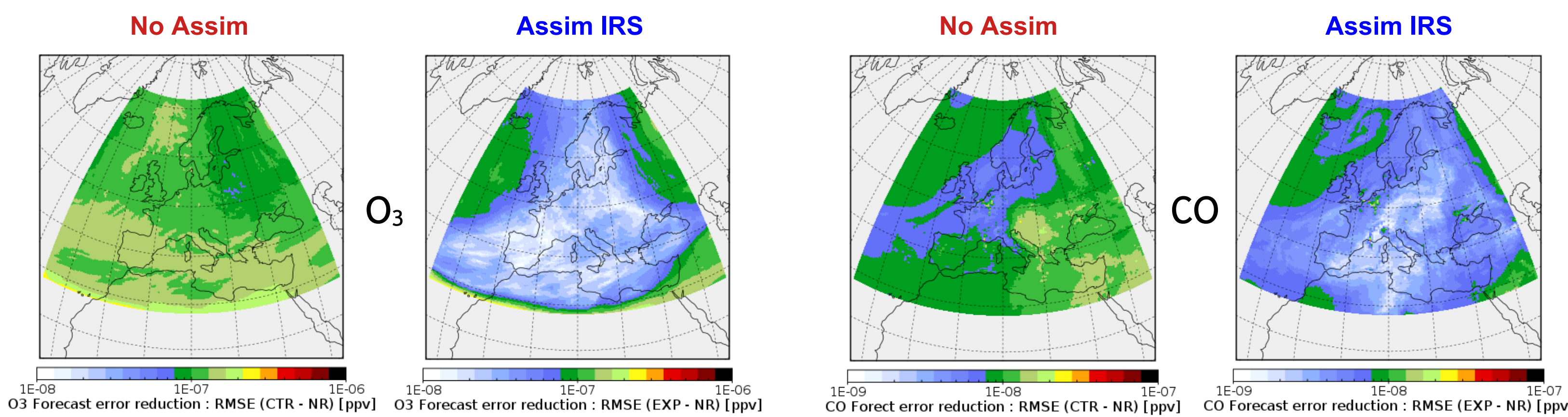


Fig.10 Forecast error reduction (RMSE) integrated over the atmospheric vertical for the 3 months of study (JJA) for the ozone (left) and carbon monoxide (right) fields of the control experiment and the IRS assimilation experiment compared with the Nature Run.

- We note a significant reduction in RMSE by assimilating IRS, mainly where the channels are most sensitive: troposphere and middle stratosphere for O₃ and troposphere for CO. The main reductions in error are observed at the bottom of the domain, where the frequency of observation is greatest. Degradation is nevertheless observed above 10 hPa for ozone and above 100 hPa for CO, due to the fact that the fields are not constrained by assimilation at these levels.

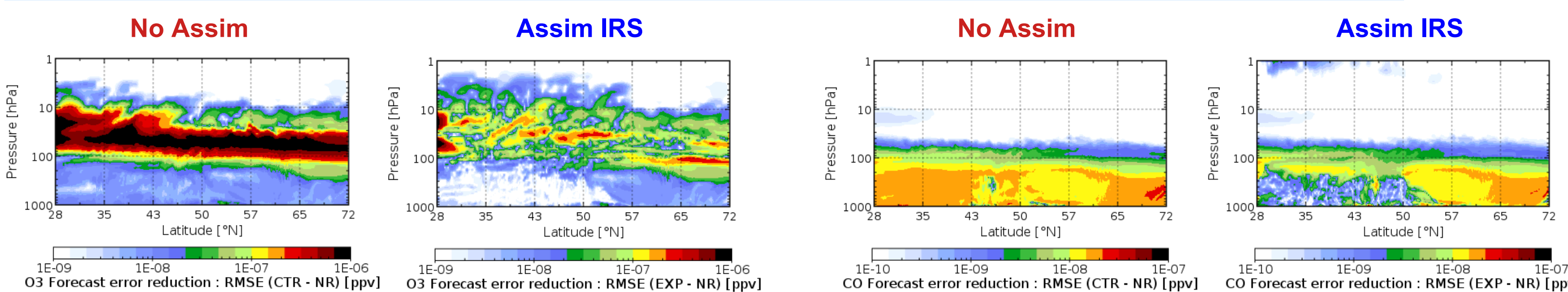


Fig.11 As the Figure 10, The forecast error reduction (RMSE) on the atmospheric vertical as a function of latitude (middle of the domain) for the 3 months of study (JJA) for the ozone (left) and carbon monoxide (right) fields of the control experiment and the IRS assimilation experiment compared with the Nature Run.

11) O₃ & CO forecast scores

- To assess the impact of assimilating the 178 IRS channels, we calculated the forecast scores for ozone (top) and carbon monoxide (bottom) over the full period. The graphs on the left represent the reduction in forecast error (RMSE) of the Control Run experiment compared with Nature Run (reality) on the atmospheric vertical as a function of forecast ranges up to +24h, in the middle the Assim Run experiment compared with Nature Run and on the right the relative differences between the two experiments compared with Nature Run. For the right-hand figures, blue curves indicate an improvement in forecasts for the Assim Run experiment compared with the Control Run, red indicates a degradation, grey indicates a neutral impact and yellow indicates the significance of the results.
- The results show that assimilation of the 178 IRS channels reduces the forecast error in ozone by up to 53 %, mainly from the surface to 10 hPa, and in carbon monoxide by up to 39 %, mainly in troposphere. This is in line with the sensitivity of the weighting functions shown in Figure 6.

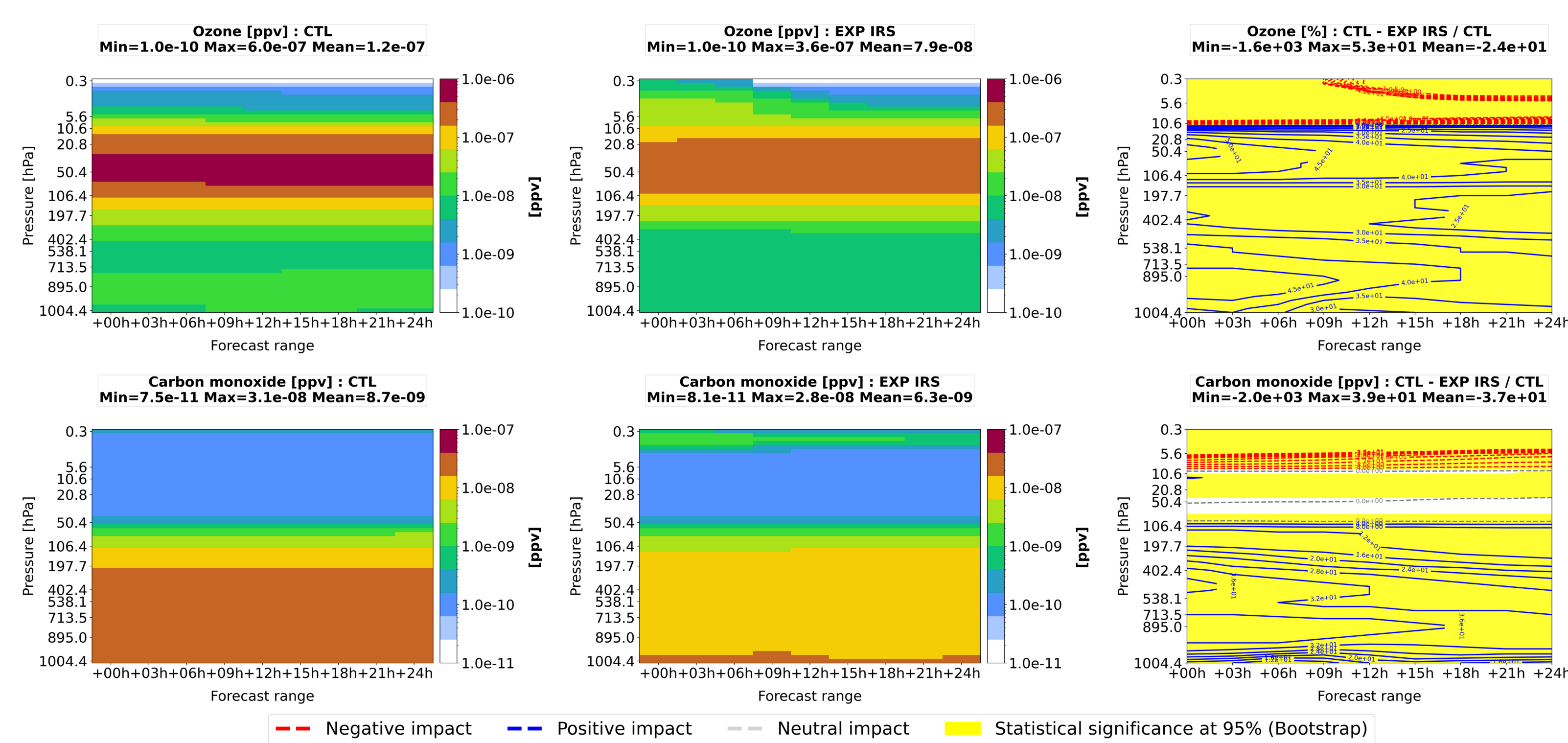


Fig.12 Forecast scores for ozone (top) and carbon monoxide (bottom) over the full period. The graphs on the left represent the reduction in forecast error (RMSE) of the Control Run experiment compared with Nature Run (reality) on the atmospheric vertical as a function of forecast ranges up to +21h, in the middle the Assim Run experiment compared with Nature Run and on the right the relative differences between the two experiments compared with Nature Run.

12) Conclusions

- Preparation for assimilation of IRS into the regional MOCAGE model → construction of a reproducible experimental framework (OSSE) that can be used for other geophysical parameters (simulation of 1960 channels)
- Significant improvements in 24-hour forecasts of O₃ (~ -50% error reduction) and CO (~ -40% error reduction) fields, mainly in the troposphere and part of the stratosphere. An article on this study is currently being written.

13) Perspectives

- Assessing the impact of IRS in the global MOCAGE model
- Studying the possibility of assimilating IRS observations for SO₂, Ammonia and N₂O, as well as for improving desert aerosol fields
- Research into the synergy between IRS and other infrared sounders in MOCAGE
- ! The recent change in IRS spectral resolution will force us to reassess the sensitivity of our observations, and new channel selections for NWP and atmospheric composition will have to be made.**

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