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**RESEARCH ARTICLE**

# Use of variable ozone in a radiative transfer model for the global Météo-France 4D-Var system

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Région Occitanie**Abstract**

Nowadays, the assimilation of satellite observations, particularly radiances from infrared sounders, into numerical weather prediction (NWP) models plays a dominant role in improving weather forecasts. One of the keys to make optimal use of radiances is to simulate them with a radiative transfer model (RTM). At Météo-France, the RTTOV RTM is used for NWP models. Currently, simulations are carried out taking into account single chemical profiles. However, neglecting the spatial and temporal variability of these gases can affect the accuracy of the simulations and thus the quality of the subsequent analyses and forecasts. To reduce the impact of this assumption on weather forecasts, we use a variational bias correction but it would be more appropriate to correct the bias directly at the source. Ozone is one of the atmospheric constituents with significant impacts on spectral radiances measured by hyperspectral infrared sounders. Thus, the objective of this paper is to replace the use of a single ozone profile with a realistic and variable ozone field in RTTOV for the simulation of infrared observation. The results show that the use of a variable ozone allows us to further reduce biases in simulation of ozone-sensitive channels but also of channels sensitive mainly to other parameters such as CO<sub>2</sub> for example. This has positive effects on the analyses and improves the fit of the short-range forecasts (or analyses) to other observations such as radiosondes, microwave radiances, GNSS-RO bending angles, etc. All of these positive impacts allow us to significantly improve weather forecasts.

**KEYWORDS**

4D-Var data assimilation, chemistry transport model, numerical weather prediction, ozone, radiative transfer model.

## 1 | INTRODUCTION

Since the advent of data assimilation for numerical weather prediction (NWP), models have continued to evolve in order to produce increasingly accurate weather forecasts. One of the major evolutions for the ARPEGE (Action de Recherche Petite Echelle Grande Echelle)

global model at Météo-France has been the implementation of four-dimensional variational data assimilation (4D-Var; Gauthier and Thépaut 2001) which takes into account time in addition to the three dimensions of space. This technique has allowed us to assimilate a greater quantity of observations, particularly those from satellites. Indeed, the 4D-Var method corrects a background state

from a short-time forecast (Lorenc 1986; Courtier *et al.*, 1994) using observations along an assimilation window. This state is thus used as an initial condition in the NWP models. In this paper, the notation used for data assimilation will be as in Ide *et al.* (1997).

At Météo-France, 90% of the observations assimilated in the ARPEGE model come from satellite instruments. Currently, 75% of the observations used to estimate meteorological analyses come from infrared instruments. They mostly come from the Infrared Atmospheric Sounding Interferometer (IASI; Guidard *et al.*, 2011), the Cross-track Infrared Sounder (CrIS) and the Atmospheric InfraRed Sounder (AIRS; Auligné *et al.*, 2003). These instruments are respectively on board the polar satellites MetOp-A, B and C, SUOMI-NPP and NOAA-20, and Aqua. The Spinning Enhanced Visible and Infrared Imager (SEVIRI) on board geostationary satellites METEOSAT-8 and 11 also provides useful information for weather forecasting. These instruments do not directly measure geophysical parameters but spectral radiances at the top of the atmosphere. The radiation reaching the various sensors is subject to emission, absorption and scattering processes that depend on the structure of the atmosphere (temperature, water vapour, pressure, etc.) as well as its chemical composition.

To extract information useful for meteorological analysis, satellite radiances are simulated from model profiles using a radiative transfer model (RTM). The difference between the simulated and actual observations is called the first-guess (FG) departure or innovation as:

$$\mathbf{d}_b^o = \mathbf{y} - H(\mathbf{x}^b), \quad (1)$$

where  $\mathbf{y}$  is the observation,  $\mathbf{x}^b$  is the background and  $H$  is the observation operator. At Météo-France, the ARPEGE global model uses the RTTOV RTM. This fast model is developed and maintained by the Satellite Application Facility (SAF) within the EUMETSAT consortium. It is used to simulate spectral radiances from instruments measuring in the visible, infrared and microwave ranges given an atmospheric profile of temperature, variable gas concentrations, cloud and surface properties (Saunders *et al.*, 2018). The only mandatory variables for RTTOV are pressure, temperature and water vapour; if not provided by the user, other constituents such as  $O_3$ ,  $CO_2$ ,  $CH_4$ ,  $CO$ , etc. are prescribed using a single profile, constant in space and time for each constituent. These profiles are derived from the mean of 83 diverse profiles extracted from chemical fields reanalyzed from the Composition Integrated Forecasting System (C-IFS) model of the Copernicus Atmosphere Monitoring Service (CAMS) program (Matricardi, 2008). In real life, gases such as ozone, carbon dioxide, methane and carbon monoxide are variable in the atmosphere both spatially and temporally. Therefore, the

approximation made by using single chemical profiles in RTTOV can impact significantly the simulation of channels sensitive to these constituents.

In order to limit systematic errors made by the observations or the observation operator, it is important to correct inconsistencies between different satellite instruments. At Météo-France, we use a variational bias correction called VarBC (Auligné *et al.*, 2007). This method attempts to estimate the systematic bias correction for radiances while preserving the differences between the background and the other observations in the analysis system. The bias correction results from the linear combination of model state-dependent predictors and coefficients included in the 4D-Var control variable so that they are adjusted along with the other variables in the analysis at each assimilation window to ensure optimal consistency between all sources of information. Thus, VarBC is capable of correcting large-scale biases induced by the use of single chemical profiles in RTTOV, but it does not allow correcting biases arising from the small-scale variability of some atmospheric constituents such as  $CO_2$ ,  $O_3$ ,  $CH_4$  and  $CO$ . However, it would be more efficient to correct the biases at the source in order to better model the radiative transfer and thus improve the data assimilation system.

Engelen *et al.* (2001) has shown, for example, that neglecting the variability of  $CO_2$  has a strong impact on the quality of temperature retrievals from the radiance data provided by AIRS instrument. Subsequently, Engelen and Bauer (2014) showed that the use of realistic  $CO_2$  treated as a tracer in the European Centre for Medium-Range Weather Forecasts (ECMWF) Integrated Forecasting System (IFS) model has a positive impact on the simulation of AIRS and IASI radiances from the RTTOV RTM by reducing the bias correction for almost all sensitive channels in the  $CO_2$  absorption band. Although the impact on analyses and forecasts was found to be neutral, because  $CO_2$  channels are used to extract temperature information, there is the potential for errors in the  $CO_2$  profile to induce temperature errors in the analysis and subsequent forecast.

For a long time, ozone-sensitive infrared observations were not used in the data assimilation process for the ARPEGE global model. However, the work of Coopmann *et al.* (2018) has shown that ozone-sensitive IASI channels are also sensitive to temperature and humidity which could be beneficial for analyses. In addition, this work has also shown that the use of a realistic ozone field instead of constant  $O_3$  reduces errors in the simulation of  $O_3$ - and  $CO_2$ -sensitive channels. Indeed, many of the  $CO_2$ -sensitive channels used for atmospheric temperature information are also slightly sensitive to  $O_3$ . Therefore, by taking into account the variability and realism of  $O_3$ , more accurate simulations and temperatures retrievals can be obtained

(Lahoz *et al.*, 2007). Then, Dragani *et al.* (2018) explains that recent results showed that using climatological O<sub>3</sub> can degrade the system, for example in the fit to other used observations. Finally, Derber and Wu (1998) and John and Buehler (2004) have also shown that the use of realistic O<sub>3</sub> can improve the simulation of the O<sub>3</sub>-sensitive satellite radiances of the High-resolution Infrared Radiation Sounder (HIRS) and the Advanced Microwave Sounding Unit-B (AMSU-B) respectively.

In this study, our objective is to replace the single ozone profile in the RTTOV RTM with realistic and variable O<sub>3</sub> fields from the MOCAGE (MODèle de Chimie Atmosphérique à Grande Echelle) Chemistry Transport Model (CTM), available at Météo-France, in the observation operator in order to improve infrared satellite data simulations, to optimize bias correction and to improve meteorological analyses and forecasts. Section 2 describes the methodology of the experiments, then Section 3 presents the main results and impacts on observations, analyses and forecasts. Finally, a summary of the conclusions and short-term prospects is provided in Section 4.

## 2 | METHODOLOGY

### 2.1 | MOCAGE model

MOCAGE is an off-line global three-dimensional chemistry transport model (Josse *et al.*, 2004; Guth *et al.*, 2016). The operational version of MOCAGE simulates the atmospheric chemistry without data assimilation. It provides the time evolution of the chemical air composition from the surface to the stratosphere (top at 5 hPa).

This model is used for operational daily forecasts (e.g., Marecal *et al.*, 2015) and also for research studies (e.g., Boussez *et al.*, 2007; Anderson *et al.*, 2017; Morgenstern *et al.*, 2017; Guth *et al.*, 2018). The meteorological fields (temperature, wind, specific humidity, pressure, cloud and precipitation) used in this study for MOCAGE come from outputs of ARPEGE. The advection of chemical species in MOCAGE follows the semi-Lagrangian approach of Williamson and Rasch (1989). Subgrid-scale convection and diffusion are represented using Bechtold *et al.* (2001) and Louis (1979), respectively. Dry deposition comes from Wesely (2007) parametrization modelling. Scavenging of trace gases by stratiform and convective precipitation follows Giorgi and Chameides (1986) and Mari *et al.* (2000), respectively. Gas chemistry is based on the Regional Atmospheric Chemistry Mechanism chemical scheme (RACM; Stockwell *et al.*, 1997) for the troposphere, and Reactive Processes Ruling the Ozone Budget in the Stratosphere (REPROBUS; Lefevre *et al.*, 1994; 1998) for

the stratosphere. This leads to a total of 115 gas species and 372 reactions.

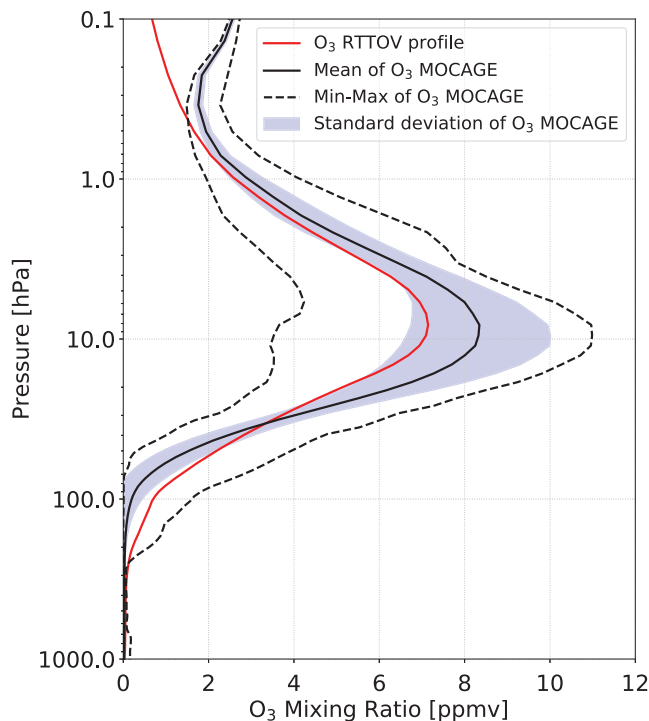
All thermal reaction rates were updated following the latest version of JPL (Jet Propulsion Laboratory) recommendations (Burkholder *et al.*, 2015). Photolysis rates are calculated in MOCAGE via a look-up table computed off-line. This table was updated using TUV (The Tropospheric Ultraviolet and Visible) software version 4.6 (Madronich, 1987). Also the photolysis of PAN (Peroxyacetic Nitric Anhydride) was added. All these changes provide improvements to ozone in MOCAGE, particularly in the Upper Troposphere and Lower Stratosphere (UTLS) where ozone plays an important role on the radiation.

For this study, we carried out a simulation from the MOCAGE model on 60 hybrid vertical levels, from the ground up to 0.1 hPa and a global domain with a horizontal resolution of 0.1° (11 km). Indeed, as mentioned above, the ARPEGE model has its top at 0.1 hPa while that of the operational MOCAGE model is at 5 hPa. For the purpose of consistency, we used a research version of the MOCAGE model with a top at 0.1 hPa. The research version of MOCAGE was run from September 2015 to April 2017, with the first 6 months being considered as spin-up. Figure 1 illustrates the differences between the ozone profile provided by RTTOV (red line) and the actual ozone variability from MOCAGE, for two days in summer and winter. The ozone profile of RTTOV is obtained as the average of typical and extreme ozone profiles from the Chevallier *et al.* (2006) database, used to compute RTTOV coefficients. The profiles described in Chevallier *et al.* (2006) have a variability which is consistent with statistic profiles computed with MOCAGE ozone fields.

Even though the mean ozone profiles are similar, there are still significant differences. Indeed, the ozone profile from RTTOV appears to overestimate the concentration (by up to 0.75 ppmv) between 300 and 40 hPa, while it underestimates it (by up to 2.50 ppmv) between 30 and 0.1 hPa compared to the mean of realistic ozone from MOCAGE. Thus, these differences can affect the calculation of the layer-to-space transmittances, the accuracy in the simulation of channels sensitive to these constituents and possibly on the quality of the information extracted from these observations for data assimilation. An important part of the atmospheric temperature information provided to the model comes from CO<sub>2</sub>-sensitive channels in the spectral band around 15 μm, some of which, as previously stated, have sensitivity to ozone.

### 2.2 | ARPEGE model and assimilation system

The global NWP model ARPEGE is an essential tool for operational weather forecasting at Météo-France. The



**FIGURE 1** Ozone profile from RTTOV and statistics (Min, Max, Mean and standard deviation) using CTM MOCAGE on two days (July 12 and November 12, 2016)

initial conditions of the ARPEGE model are based on a 4D-Var assimilation which incorporates a very large and varied amount of conventional and satellite observations with a 6 hr assimilation window centred on 0000, 0600, 1200 and 1800 UTC. ARPEGE uses a set of primitive equations with a triangular spectral truncation on the horizontal, with a finite-element representation on the vertical and a sigma-pressure hybrid vertical coordinate. The horizontal resolution of the ARPEGE model is on variable grid at truncation 2,635 over France and 544 at the antipole (about 7.5 and 36 km horizontal resolution, respectively). It has 105 vertical levels, with the first level at 10 m above the surface and an upper level at 0.1 hPa. The Météo-France ARPEGE NWP global model uses a 4D-Var data assimilation scheme whose objective is to minimize both the observational and background deviation by minimizing a cost function  $\mathcal{J}$ . In order to reduce computation time, the incremental formulation which solves the problem in terms of departure from the background fields at low resolution is considered (Veersé and Thépaut, 1998). This formulation is adapted to the mesh size of the observation network. Moreover, it allows us to solve a quadratic problem, which, through the trajectory updates, allows us to take into account nonlinear effects. Finally, making corrections on low-resolution increments in a 4D assimilation with the time dimension also makes it possible to free oneself from the linearization of the complete model, and

to have a simplified model in particular of the physical process which cause difficulties when linearizing them. Thus the incremental vector is such that:

$$\delta\mathbf{x} = \mathbf{x} - \mathbf{x}^b, \quad (2)$$

where  $\mathbf{x}$  is the model state and  $\mathbf{x}^b$  is the background state. This minimizes the cost function

$$\mathcal{J}(\delta\mathbf{x}) = \mathcal{J}_b(\delta\mathbf{x}) + \mathcal{J}_o(\delta\mathbf{x}) + \mathcal{J}_c(\delta\mathbf{x}), \quad (3)$$

where the  $\mathcal{J}_b(\delta\mathbf{x})$  term refers to the background cost function

$$\mathcal{J}_b(\delta\mathbf{x}) = \frac{1}{2}(\delta\mathbf{x})^T \mathbf{B}^{-1}(\delta\mathbf{x}) \quad (4)$$

and the  $\mathcal{J}_o(\delta\mathbf{x})$  term refers to the observation cost function

$$\mathcal{J}_o(\delta\mathbf{x}) = \frac{1}{2} \sum_{i=1}^n (\mathbf{d}_{b,i}^o - \mathbf{H}_i[\delta\mathbf{x}(t_i)])^T \mathbf{R}_i^{-1} (\mathbf{d}_{b,i}^o - \mathbf{H}_i[\delta\mathbf{x}(t_i)]), \quad (5)$$

where  $n$  is the total number of observations at time  $i$ ,  $\mathbf{d}_{b,i}^o$  is FG departure as expressed in Equation (1),  $\mathbf{H}_i$  is the tangent-linear observation operator in the vicinity of the background and it includes an atmospheric model, interpolation and observation simulations by RTTOV. Finally, the  $\mathcal{J}_c(\delta\mathbf{x})$  term in Equation (3) represents the dynamic constraint on the analysis,  $\mathbf{R}_i$  is the observation-error covariance matrix and  $\mathbf{B}$  is the background-error covariance matrix.

### 2.3 | Experimental set-up

In the data assimilation process, any change taking place in the calculation of FG departure (Equation (1)), will influence the observation cost function term (Equation (5)) and thus the minimization. Two experiments were therefore carried out:

- The first one (CONTROL), used the version of the 4D-Var ARPEGE system operational in year 2016 using constant ozone from RTTOV for the calculation of simulations in the observation operator.
- The second one (O3EXP) is similar to the previous one but with the difference that, instead of using a constant ozone, we use the ozone background variable in time and space from the MOCAGE CTM in the forward observation operator.

The ozone background used in the O3EXP experiment from MOCAGE are forecasts valid at the centre of the 4D-Var ARPEGE assimilation window. The minimizations are performed at low resolution and with two outer loops

on a regular grid, at truncation 149 (135 km) and 399 (50 km), respectively, and the FG departures are calculated at truncation 1,198 on the variable grid. The set-up of the data assimilation system used for this study does not assimilate channels whose main sensitivity is to ozone, methane or CO. The fields from MOCAGE were interpolated onto the geometry of the ARPEGE model both horizontally on a variable grid and vertically on 105 hybrid vertical levels. Finally, the CONTROL and O3EXP experiments were carried out over a summer period from 01 July to 10 September and a winter period from 01 November to 31 December 2016.

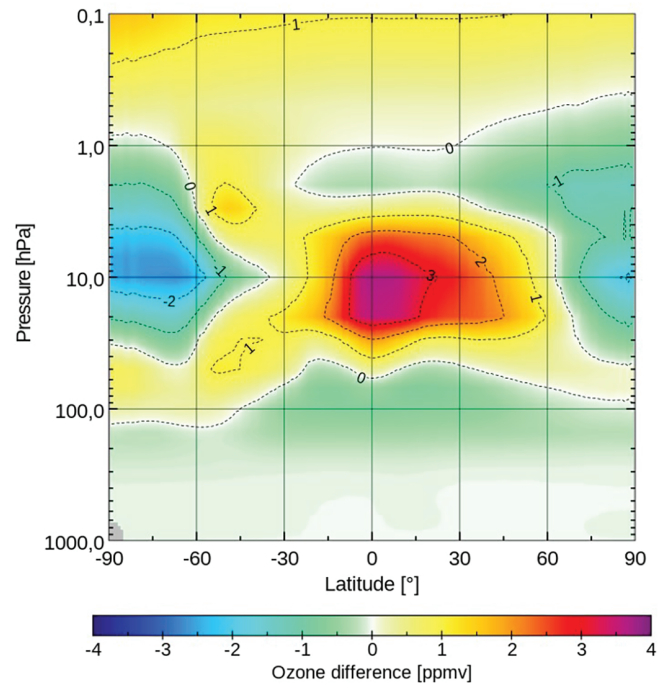
In order to illustrate this work and to highlight the differences between the use of a single constant profile and the realistic variability of ozone, we have plotted in Figure 2 the difference between the monthly mean zonal mean cross-section of ozone in the ARPEGE model for July 2016 interpolated from the CTM MOCAGE model and the single ozone profile from RTTOV. There are significant horizontal (not shown) and vertical differences. In particular, the single profile tends to underestimate the concentration of ozone (by up to 4 ppmv) in the Tropics in the mid-stratosphere between 100 and 1 hPa, and on the contrary to overestimate it (by up to  $-2$  ppmv) at high latitudes in the same part of the atmosphere. It is also noted that the differences are more or less significant at midlatitudes depending on the season of the year and that the single profile underestimates the ozone concentration in the upper stratosphere above 1 hPa at all latitudes.

### 3 | RESULTS

#### 3.1 | Impact on infrared radiance simulation

In a first step, we have chosen to evaluate the impact of the use of a realistic  $O_3$ , in the observation operator RTTOV on simulated radiances from four main infrared instruments: IASI, CrIS, AIRS and SEVIRI. Table 1 summarizes for these instruments, the number of channels monitored, assimilated, as well as their description and spectral range at the period of the study. It is important to note that all monitored channels of these instruments have one or more channels for which the primary sensitivity is ozone (band around  $9.6 \mu\text{m}$ ) but none of them are assimilated.

We calculated the differences of the global mean and standard deviation of the FG departures between the O3EXP and CONTROL experiments during the first assimilation on the first assimilation cycle of each experimental period. These differences are equivalent to comparing the values of the simulations between the two experiments. Figure 3 shows the results of these differences for the



**FIGURE 2** Difference between the monthly mean zonal mean cross-section of ozone background (6 hr forecast) in the ARPEGE model for July 2016 interpolated from the CTM MOCAGE model and the single ozone profile from RTTOV

monitored channels of the IASI, CrIS, AIRS and SEVIRI instruments in July 2016. Statistics were calculated on FG departures before bias correction from 78,491 observations for IASI, 77,160 for CrIS, 16,619 for AIRS and 5,129 for SEVIRI.

As expected, the largest impact is obtained for ozone-sensitive channels; between  $1,014.5$ – $1,091.25 \text{ cm}^{-1}$  for IASI with differences in average up to  $-9.5 \text{ K}$ , between  $982.5$  and  $1,095 \text{ cm}^{-1}$  for CrIS ( $-9.2 \text{ K}$ ), between  $979.02$  and  $1,135.43 \text{ cm}^{-1}$  for AIRS ( $-9.8 \text{ K}$ ) and for the channel  $9.66 \mu\text{m}$  for SEVIRI ( $-9.8 \text{ K}$ ). We also notice that the use of a more realistic  $O_3$  has an impact on some  $\text{CO}_2$ -sensitive channels simulation; between  $704.5$  and  $781.25 \text{ cm}^{-1}$  for IASI with differences in averages of up to  $-0.4 \text{ K}$ , between  $705$  and  $770 \text{ cm}^{-1}$  for CrIS ( $-0.8 \text{ K}$ ), between  $704.359$  and  $759.486 \text{ cm}^{-1}$  for AIRS ( $-1.1 \text{ K}$ ) and for the SEVIRI channel  $13.4 \mu\text{m}$  ( $-0.4 \text{ K}$ ). There is also an impact on the  $8.70 \mu\text{m}$  SEVIRI channel sensitive to the surface with a mean difference of  $-0.4 \text{ K}$ . Similar results are found for the winter period experiments on 01 November 2016 at 0000 UTC (not shown here). The results obtained for  $\text{CO}_2$ -sensitive channels are expected because ozone is also an active gas in the v2 band at  $14.3 \mu\text{m}$  ( $701 \text{ cm}^{-1}$ ), which is superimposed on the  $\text{CO}_2$  v2 band (Liang, 2017).

Once we have illustrated the impact of the use of realistic  $O_3$  on the simulations of the four main infrared instruments during the first assimilation, we evaluate the

**TABLE 1** Number of channels monitored and assimilated, description and spectral range for IASI, CrIS, AIRS and SEVIRI instruments in the ARPEGE NWP process

Instruments	Number of channels		Application and spectral range of assimilated channels		
	Monitored	Assimilated	Temperature	Surface	Water Vapour
IASI	314	124	99 (657–759 cm <sup>-1</sup> )	4 (773.5–962.5 cm <sup>-1</sup> )	23 (1,320–2015.5 cm <sup>-1</sup> )
CrIS	331	68	58 (650–792.5 cm <sup>-1</sup> )	5 (847.5–872.5 cm <sup>-1</sup> )	5 (1,363.75–1,538.75 cm <sup>-1</sup> )
AIRS	324	72	72 (649.55–721.46 cm <sup>-1</sup> )	—	—
SEVIRI	8	6	1 (13.4 μm)	3 (8.7, 10.8, 12.0 μm)	2 (6.25, 7.35 μm)

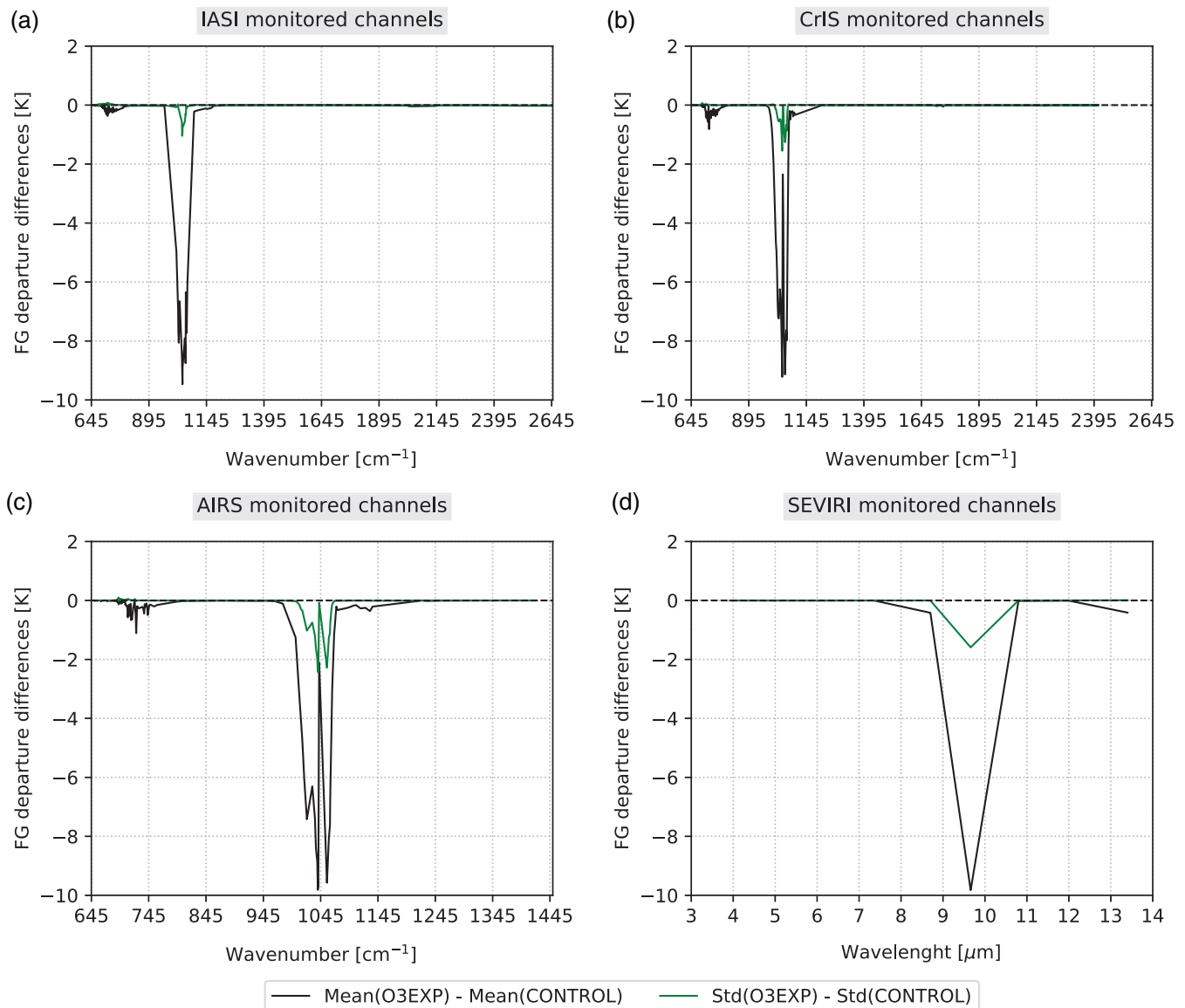
long-term impact on the assimilation suite, taking into account the variational bias correction. For this, we have examined the time required for the VarBC to adapt to the new ozone information for the different channels. This bias correction takes about 8 days (not shown here) to reach a new equilibrium. Thus, the first 12 days of each period are discarded from the evaluation of the experiments. Figure 4 shows the global mean of bias-corrected FG departures for CONTROL (black line) and O3EXP (red line) experiments from 12 July to 10 September 2016 (from 12 November to 31 December 2016 in Figure 5) on the assimilated channels of observations from IASI, CrIS, AIRS and SEVIRI. Overall, there is a positive impact of the use of realistic O<sub>3</sub> on the bias in the radiance simulation for the each instrument. Thus, it is observed that it is possible to reduce the bias further than Var-BC is able to correct. These improvements are observed on CO<sub>2</sub>-sensitive channels, surface and water vapour channels. There is a bias increase for the O3EXP experiment for H<sub>2</sub>O-sensitive channels for IASI in Figure 4a; 2,951 and 5,583 (1,382.5 and 1,990.5 cm<sup>-1</sup> respectively), for CrIS in Figure 4b; 837, 853, 865, 913 and 977 (1,363.75, 1,383.75, 1,398.75, 1,458.75 and 1,538.75 cm<sup>-1</sup> respectively) and for SEVIRI in Figure 4d; channel 3 at 7.35 μm. Similar results are observed over the winter period (Figure 5) for the O3EXP experiment except for the H<sub>2</sub>O-sensitive channels of the CrIS and AIRS instruments which have biases close to those of the CONTROL experiment. For both periods, the main differences are observed for the H<sub>2</sub>O-sensitive channels of the IASI (2,951 and 5,583) and SEVIRI (3) instruments. These channels have Jacobians whose maximum values are in the middle troposphere between 750 and 450 hPa. Meteorological forecasts still have biases in humidity, which can translate into biases in the simulation of some water vapour-sensitive infrared channels. One explanation for having higher biases in O3EXP than in CONTROL is that these biases for humidity compensate for biases induced by a poor ozone description in CONTROL, which is not now the case in O3EXP.

In general, it can be seen that the use of a realistic O<sub>3</sub> in the observation operator instead of a single ozone profile

reduces the bias in addition to the Var-BC of the radiances of the infrared instruments. In our case, the CO<sub>2</sub>-sensitive channels in the O3EXP experiment can see their corrected biases reduced by up to 0.04 K for IASI compared to the CONTROL experiment. SEVIRI and IASI H<sub>2</sub>O-sensitive channels can have their bias reduced by up to 0.05 K and the surface-sensitive channels by up to 0.02 K. The gain in simulation accuracy may seem small, but as information useful to the data assimilation process is extracted from the FG, even small reductions in bias can have an impact on meteorological analyses. In addition, we noted that the global reduction in bias for the channels of the infrared instruments affects the quality control of the observations. Indeed, the difference in assimilated observations between the two experiments shows that sometimes more observations are assimilated while at other times fewer are assimilated. The percentage variations in infrared data usage are summarized in Table 2. At the time of this study, IASI represented 50% of observations assimilated in the system. As a result, a variation of 1% in the IASI data used can have significant impacts compared to the full observing system.

### 3.2 | Impact on analyses

Once we assessed the impact of using realistic O<sub>3</sub> on infrared radiance simulations, we evaluated the impact on meteorological analyses and more specifically on temperature, relative humidity and the zonal wind component. We averaged the differences in analysis between the O3EXP and CONTROL experiments over both periods of the study. The results are represented by zonal mean cross-sections of temperature, relative humidity and zonal wind analysis differences from 12 July to 10 September 2016 in Figure 6 and from 12 November to 31 December 2016 in Figure 7. There are differences in analysis between the two experiments with more impact in the summer hemisphere. Figure 6a shows that the differences in temperature analysis are mainly located in the upper stratosphere and lower mesosphere in the Tropics and high latitudes.

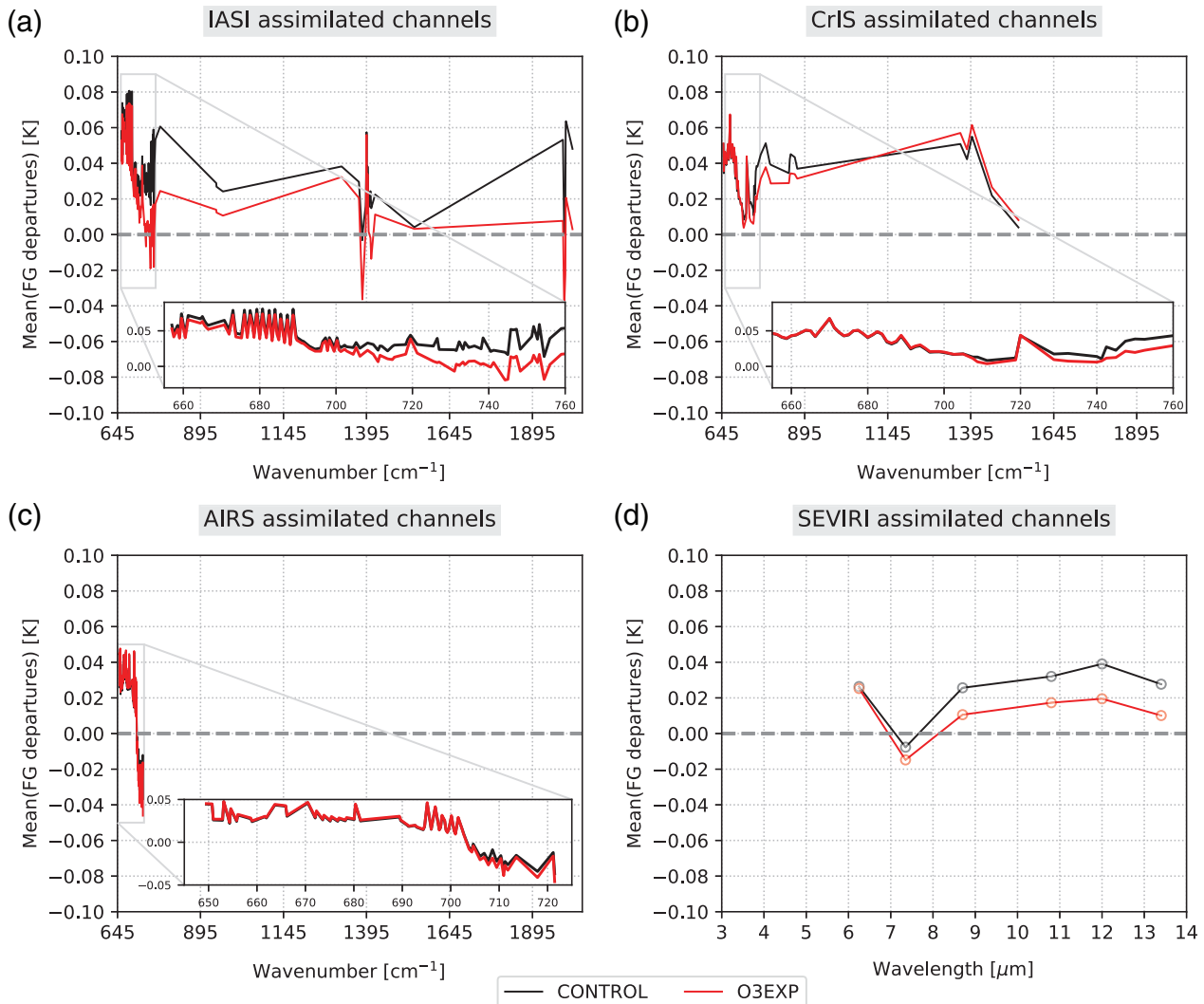


**FIGURE 3** Difference of the global mean (black line) and standard deviation (green line) of the first-guess (FG) departures between O<sub>3</sub> experiment (O3EXP) and control experiment (CONTROL) for the first analysis at 0000 UTC on 01 July 2016 on the monitored channels of observations from (a) IASI, (b) CrIS, (c) AIRS and (d) SEVIRI

The use of realistic O<sub>3</sub> in the O3EXP experiment tends to cool the upper stratosphere in the Tropics and to warm it at high latitudes with minimum and maximum values of  $-2.0$  and  $2.2$  K, respectively. The same trend is observed for the winter period in Figure 7a, except for warming in the Northern Hemisphere with minimum and maximum values of  $-1.8$  and  $1.8$  K respectively. Then, in Figure 6b, differences in relative humidity analysis are mainly located in the lower troposphere on either side of the Equator and at high latitudes. The use of realistic O<sub>3</sub> in the O3EXP experiment tends to moisten the atmosphere in the Tropics and high latitudes around 700 hPa in the Northern Hemisphere and between 200 and 500 hPa in the Southern Hemisphere and to dry out above, with minimum

and maximum values of  $-2.1$  and  $2.5\%$  respectively. The same overall trend is observed for the winter period in Figure 7b, but moistening reaches the upper troposphere in the Tropics and a dryness takes place over Antarctica observed between 300 and 500 hPa with minimum and maximum values of  $-3.4$  and  $2.6\%$  respectively. Finally, Figure 6c shows the differences in zonal wind analysis. The differences are mainly located in the middle and upper stratosphere and in the lower mesosphere. We observe that the use of realistic O<sub>3</sub> in the O3EXP experiment tends to increase the zonal wind in the mid-stratosphere at the Equator and decrease the zonal wind in the upper stratosphere in the tropical Southern Hemisphere and in the mid-latitude Northern Hemisphere with minimum and





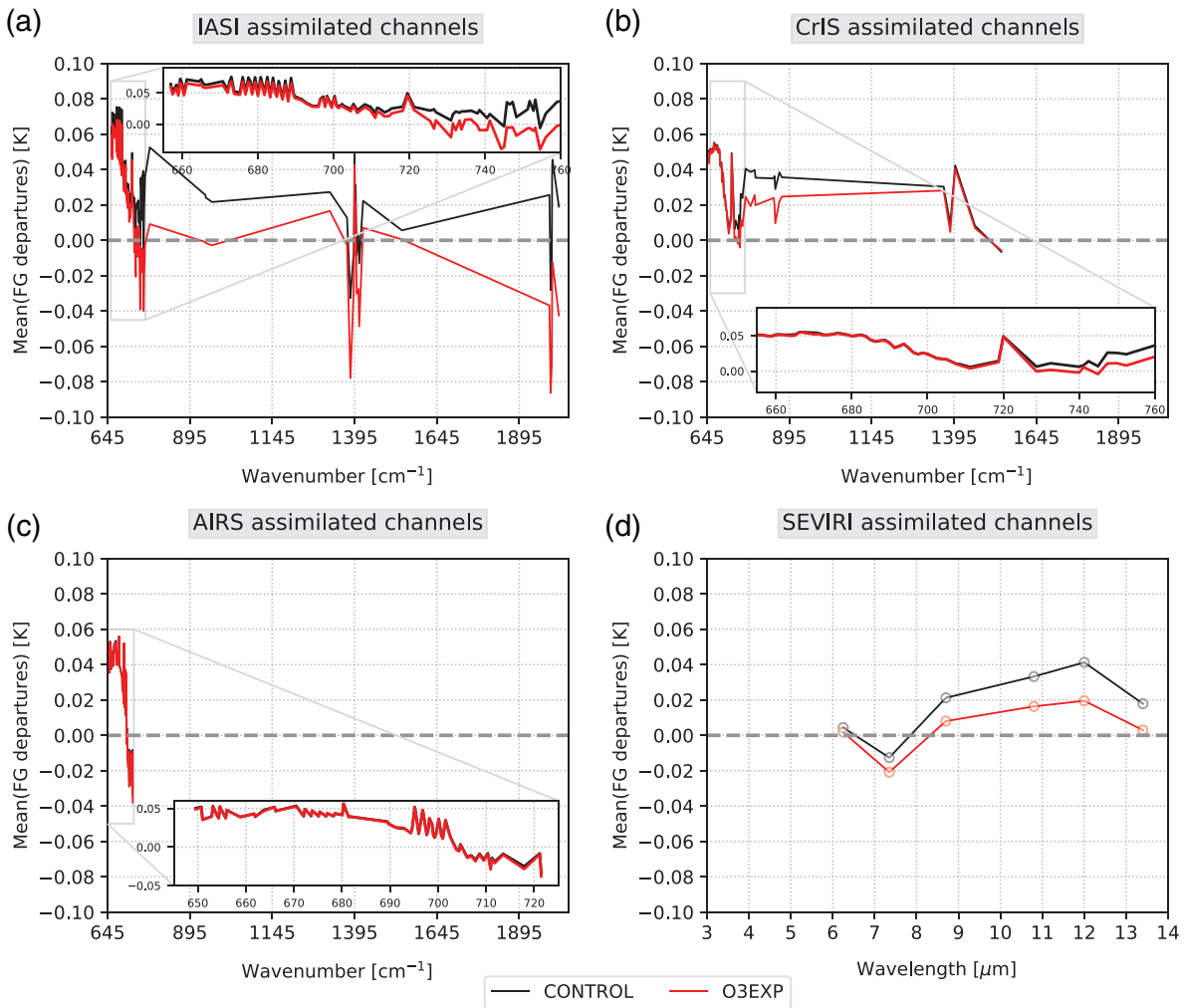
**FIGURE 4** Global mean bias corrected first-guess (FG) departures for O3EXP (red line) and CONTROL (black line) from 12 July to 10 September 2016 on the assimilated channels of observations from (a) IASI, (b) CrIS, (c) AIRS and (d) SEVIRI. Note that zoom has been made for the CO<sub>2</sub>-sensitive channels for the IASI, CrIS and AIRS instruments

maximum values of  $-1.6$  and  $0.3 \text{ m}\cdot\text{s}^{-1}$  respectively. The same trend can be seen for the winter period in Figure 7c with a shift towards the Southern Hemisphere with minimum and maximum values of  $-1.7$  and  $0.5 \text{ m}\cdot\text{s}^{-1}$ .

It can be assumed that the channels of the infrared instruments, which are sensitive to ozone in the CO<sub>2</sub> band, are simulated more accurately and provide additional information to the temperature analysis. The higher values observed for differences in relative humidity analysis in the Tropics can be explained by the fact that, at constant specific humidity, cooling can increase the relative humidity. Indeed, lower values for differences in temperature analysis are observed in this part of the atmosphere. In addition, lower values of the differences in temperature analysis in the upper troposphere can also be observed in the Tropics and midlatitudes. However, this cooling can lead to a reduction in baroclinicity and thus to a decrease

in zonal wind values. This is observed in the differences in zonal wind analyses in this part of the atmosphere. This hypothesis suggests that the differences observed for the humidity and zonal wind analyses are indirect impacts of the modifications on the temperature analysis induced by the use of a more realistic ozone for the simulations.

We have previously shown that the use of a realistic O<sub>3</sub> in the observation operator further reduces bias in the infrared radiance simulations of the IASI, CrIS, AIRS and SEVIRI instruments. Even if the mean differences between the global mean FG departures between the O3EXP and CONTROL experiments are small, it appears that the impact on the analyses is not negligible. Even slight bias reduction can assist quality control in the observation selection process to more accurately screen for observations that may or may not contribute information to the system. For example, during the summer



**FIGURE 5** As Figure 4, but from 12 November to 31 December 2016

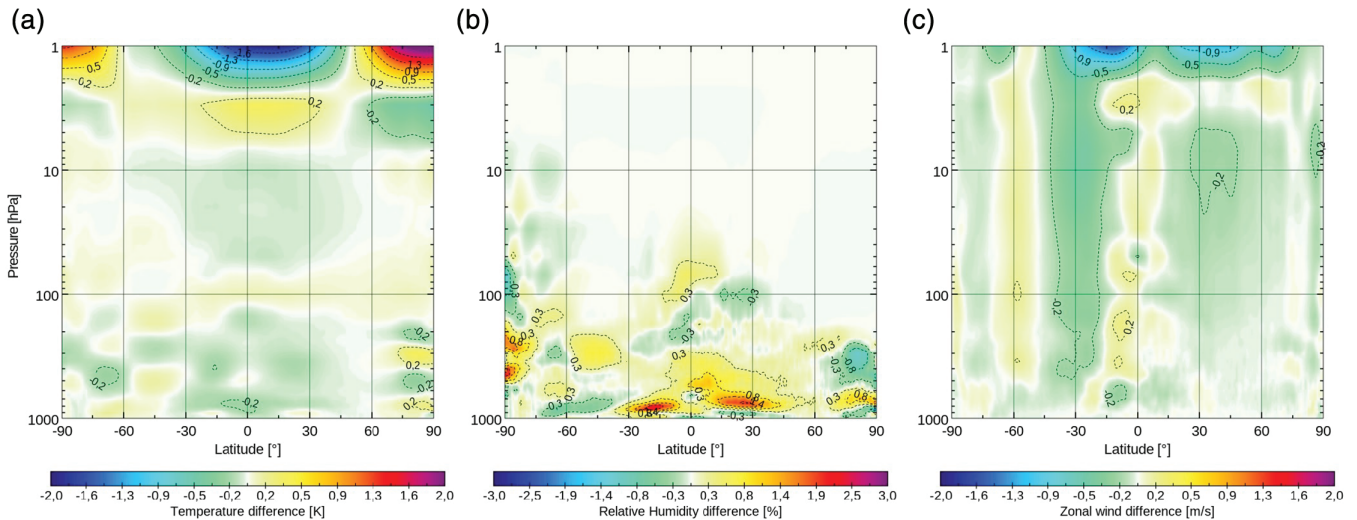
**TABLE 2** Percentage difference of data usage of infrared sensors. (A positive value means more data are assimilated in O3EXP, and a negative value means more data are assimilated in CONTROL.)

Instrument	Period	Temperature	Surface	Water Vapour
IASI	Summer	+1.0	+0.5	+1.4
	Winter	-0.05	-0.2	-2.9
CrIS	Summer	-0.5	-0.7	—
	Winter	+1.0	+1.1	—
AIRS	Summer	-0.06	—	—
	Winter	+0.07	—	—
SEVIRI	Summer	+0.01	+0.01	+0.002
	Winter	+0.003	-0.01	-0.008

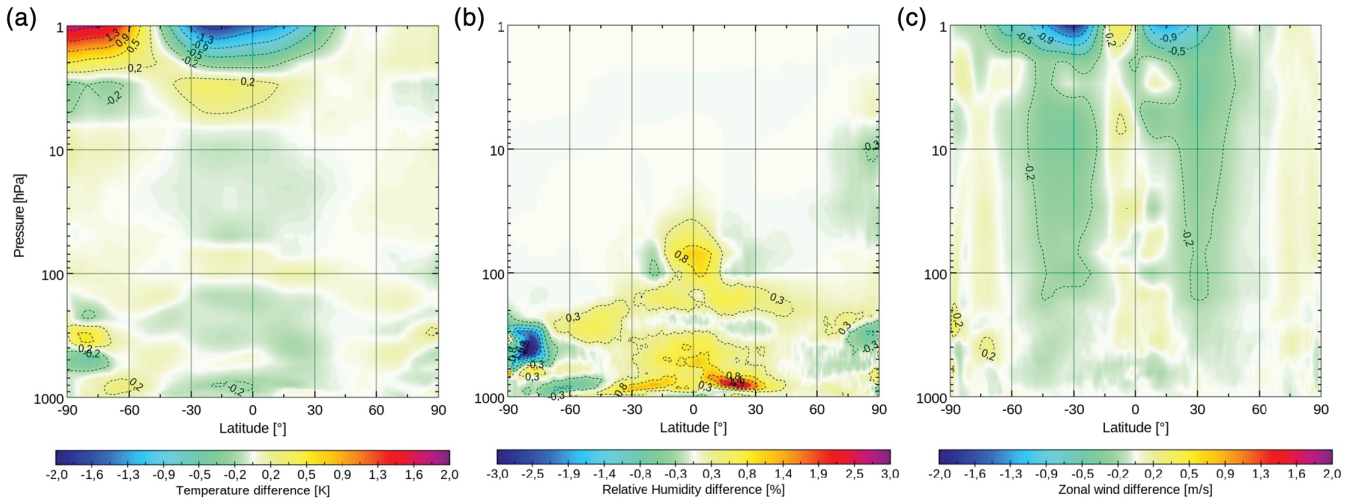
period, the use of realistic ozone allows us to use 1.0% more observations for temperature (Table 2), which may seem quite low but represents more than 3 million more assimilated channels. Moreover, when the O3EXP experiment assimilates fewer observation, this is not necessarily negative but may, for example, be the result of a better

identification of cloud observations than was previously the case.

To summarize, for the two periods considered, we observe that means of analysis differences between the two experiments range from  $\pm 2.0$  K in the upper stratosphere,  $\pm 0.1$  K in the lower stratosphere and  $\pm 0.25$  K



**FIGURE 6** Zonal mean cross-section of (a) temperature, (b) relative humidity and (c) zonal wind analysis differences between O3EXP and CONTROL from 12 July to 10 September 2016



**FIGURE 7** As Figure 6, but from 12 November to 31 December 2016

in troposphere for the temperature,  $\pm 3.0\%$  in the lower troposphere and  $\pm 1.0\%$  in UTLS for the relative humidity and  $\pm 2.0 \text{ m}\cdot\text{s}^{-1}$  in the upper stratosphere,  $\pm 0.2 \text{ m}\cdot\text{s}^{-1}$  in the lower stratosphere and  $\pm 0.1 \text{ m}\cdot\text{s}^{-1}$  in troposphere for the zonal wind component. It is interesting to note that the patterns and observed areas of differences in temperature and zonal wind analyses are similar to those presented in the work by Allen *et al.* (2018) on the use of ozone for temperature and wind information extraction.

### 3.3 | Indirect impacts on other observations

We then investigated whether the use of realistic  $\text{O}_3$  in the observation operator during the data assimilation process has an impact on other observations that are not sensitive

to ozone. Overall, there is a positive impact of the use of realistic  $\text{O}_3$  in the O3EXP experiment on the simulations of the other observations shown in Figures 8 and 9 over the two study periods. Significant improvements up to  $-0.5\%$  at 400 hPa and  $-0.35\%$  at 50 hPa for the summer period and up to  $-0.5\%$  at 100 hPa and  $-0.25\%$  at 50 hPa for the winter period are found for temperature radiosondes (Figures 8a and 9a). Only one significant improvement up to  $-0.85\%$  at 850 hPa is found for humidity radiosondes for the winter period (Figure 8b). Significant improvements up to  $-0.3\%$  between 30 and 20 hPa and up to  $-0.55\%$  between 150 and 70 hPa are found for zonal wind radiosondes for the summer period and up to  $-0.8\%$  between 100 and 5 hPa and up to  $-0.85\%$  at 500 hPa for the winter period. Significant improvements up to  $-0.65\%$  between 150 and 50 hPa are found for meridional wind radiosondes for the summer period and up to  $-0.3\%$  between

150 and 30 hPa and up to  $-0.8\%$  at 500 hPa for the winter period. Then, the Advanced Technology Microwave Sounder (ATMS) shows significant improvements in the humidity-sounding channels (20, 21 and 22) up to  $-0.5\%$  and in these temperature-sounding channels (10, 11, 12, 13 and 14) up to  $-0.75\%$  for the summer period and only for the temperature-sounding channels (10, 11, 12 and 14) up to  $-1.2\%$  for the winter period. Finally, Global Navigation Satellite System Radio Occultation (GNSS-RO) data show significant improvements up to  $-0.6\%$  between 45 and 50 km, up to  $-0.5\%$  between 31 and 38 km, up to  $-0.25\%$  between 37 and 39 km and at 11 km and then up to  $-0.8\%$  at 7 km for the summer period and up to  $-0.3\%$  between 35 and 50 km and up to  $-0.55\%$  at 10 km for the winter period. Very low significant degradation due to the O3EXP experiment can be noted except for ATMS channels 8 and 9 which are temperature-sounding for the summer period and ATMS channel 9 which is temperature-sounding and channels 18 and 19 which are humidity-sounding for the winter period.

Improved simulations of these observations are not due to the use of realistic  $O_3$  since they are not sensitive to it. In practice, successive improvements in the infrared radiance simulations slightly but positively affects the temperature, humidity and wind analyses and propagate through the assimilation cycles. Thus, more accurate analyses lead to more precise FG is provided to the RTM, thus allowing us to better simulate other observations such as radiosondes, micro-wave radiances or GNSS-RO bending angle. In addition, the differences in relative humidity analysis observed in the lower troposphere are consistent with improved simulations of humidity radiosonde in the same part of the atmosphere. Improvements are also present for wind radiosondes between the upper troposphere and upper stratosphere and GNSS-RO between 30 and 50 km (10 and 1 hPa). Thus, the use of realistic ozone upstream of the data assimilation process leads to a positive feedback allowing analyses to be modified to better assimilate all observations.

### 3.4 | Weather forecast scores

An essential aspect in assessing the effect of using realistic  $O_3$  in the data assimilation process is the control of the quality of the forecasts. Short-range forecast impact when evaluated against analyses should be treated with some caution, as the contribution from analysis errors is more significant and, in particular, the correlations between the analysis and short-range forecast errors play a more important role (Bormann *et al.*, 2016). Despite this, it seems that verifying against own analysis is the least worst option (Geer *et al.*, 2010). Forecast scores have also

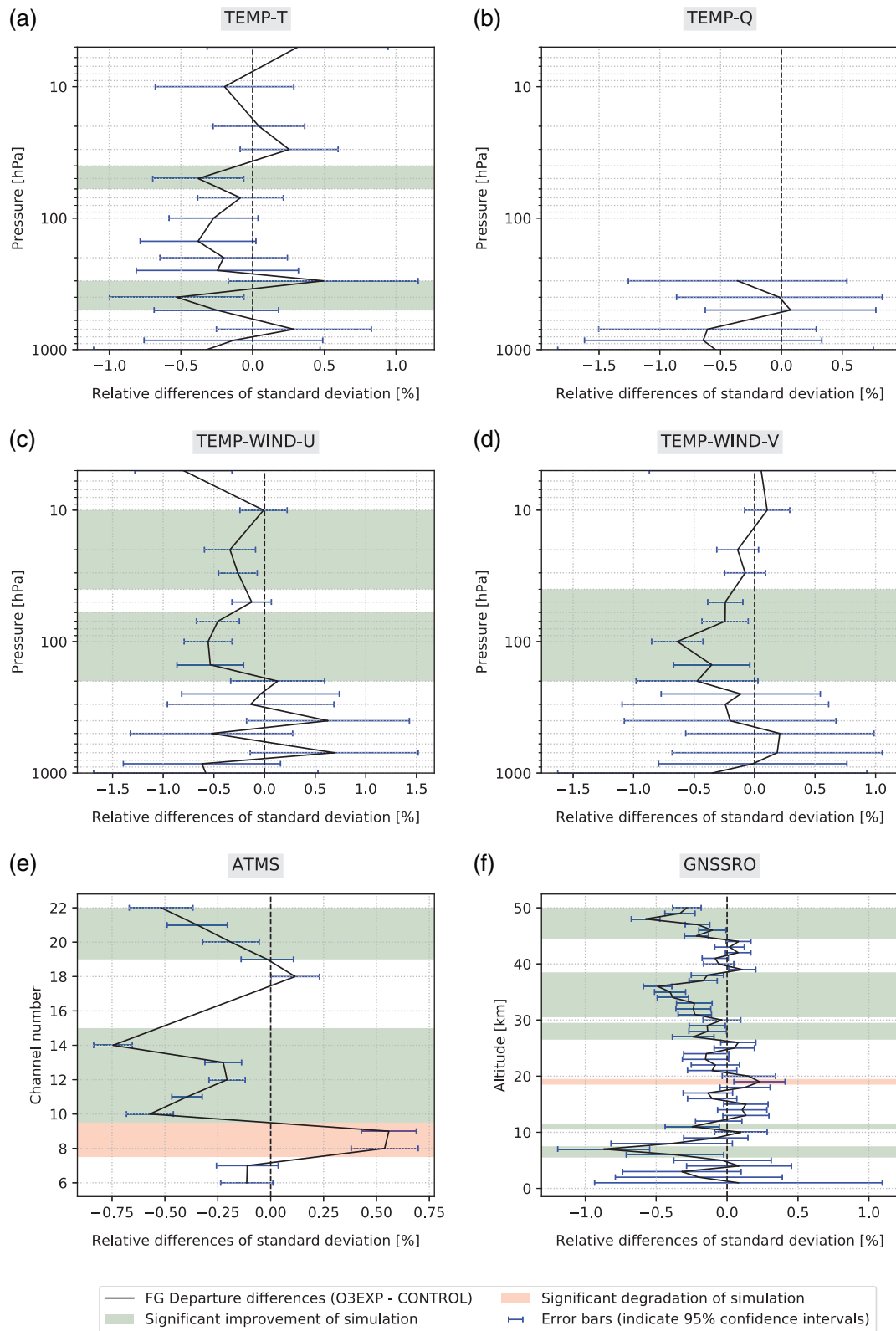
been computed with respect to radiosondes and ECMWF analysis and show consistency in improvement patterns with smaller values (not shown here).

Regardless of the study period, there is an overall improvement in temperature, humidity and wind forecasts (Figures 10 and 11) over the entire atmospheric column and forecast ranges, with certain specifics depending on the region being considered. Significant improvement in temperature forecasts is shown from 1,000 to 10 hPa with error reductions of up to 2.5% in the Southern Hemisphere for the summer period and 2.0% for the winter period. There is also a significant improvement in the lower troposphere between 1,000 and 800 hPa in the Tropics over all forecast ranges. The significant improvement in humidity forecasts is also observed over a large part of the troposphere over all forecast ranges with greater impacts in the lower and upper troposphere with error reductions of up to 2.0% in the summer period and 4.0% in the winter period. This higher impact observed for humidity in the summer period is consistent with the larger differences in humidity analysis observed for the same period at the same altitudes. Finally, the improvement is also significant for wind forecasts over large parts of the atmosphere, especially in the stratosphere with error reduction values up to 3.5% in summer and 2.0% in winter. Some significant degradations were observed for temperature and humidity forecasts mainly in the Tropics and in the Southern Hemisphere in the mid-troposphere. These degradations are observed only for the winter period. This can be related to the degradations of the humidity channel simulations (18 and 19) of the ATMS instrument whose channels are sensitive in the mid-troposphere and of GNSS-RO between 10 and 25 km altitude, again observed only for the winter period. Despite this, the impact on forecasts is very beneficial.

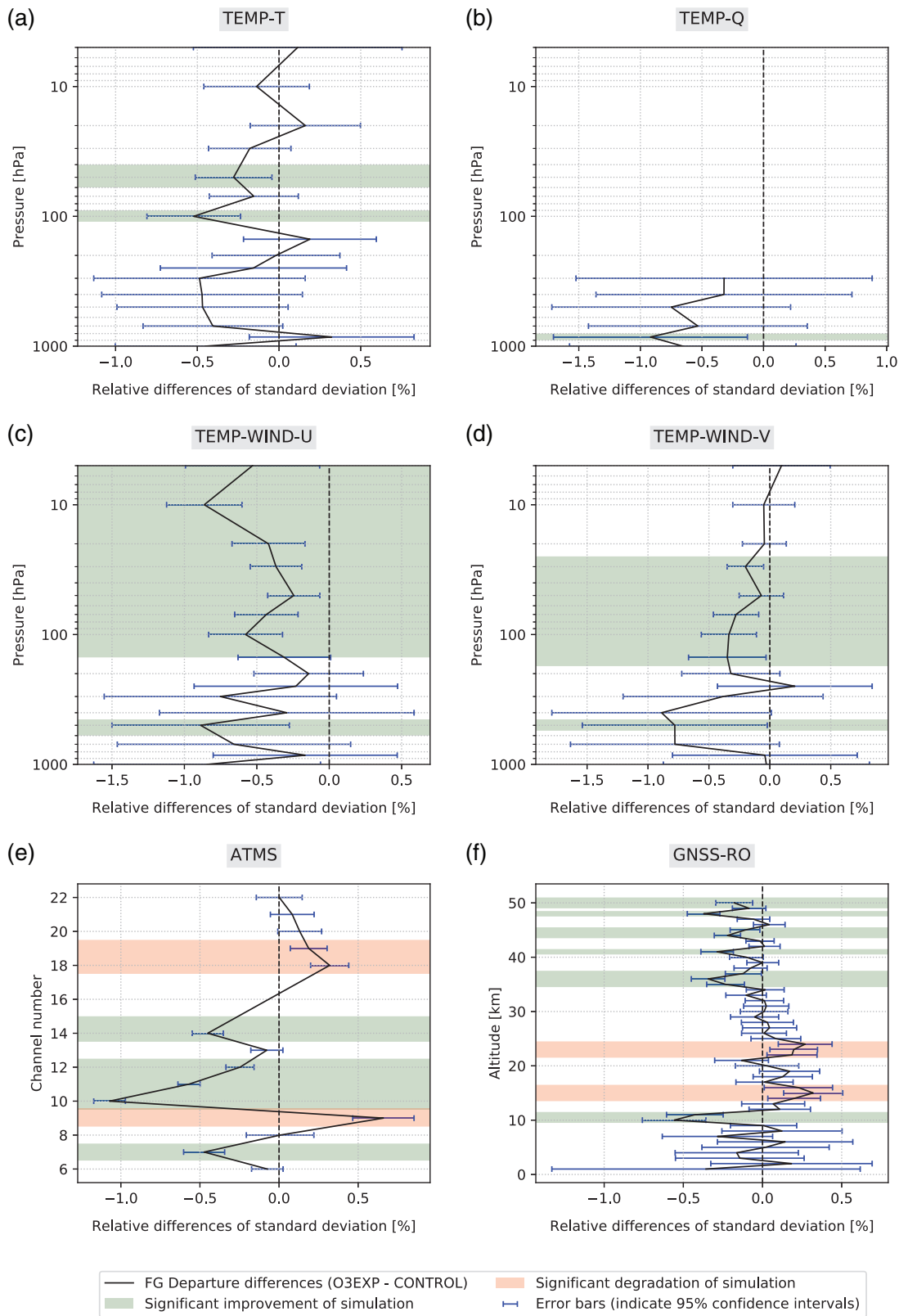
This positive impact of the use of realistic  $O_3$  in the observation operator for RTTOV on the forecast scores is exciting and unexpected. Usually, for NWP, forecast error reductions of the order of 0.5 to 1.0% are achieved on a particular variable, region, part of the atmosphere or time range. In our case, the O3EXP experiment allows us to improve the forecasts on all the parameters mentioned with substantial and significant error reduction values up to 4.0%. These results are really encouraging for the improvement of observation simulations, analyses and forecasts in the ARPEGE NWP system.

## 4 | CONCLUSIONS AND PERSPECTIVES

The radiative transfer model for the simulation of satellite radiances is one of the major ingredients of current data assimilation systems. At Météo-France, ozone is not



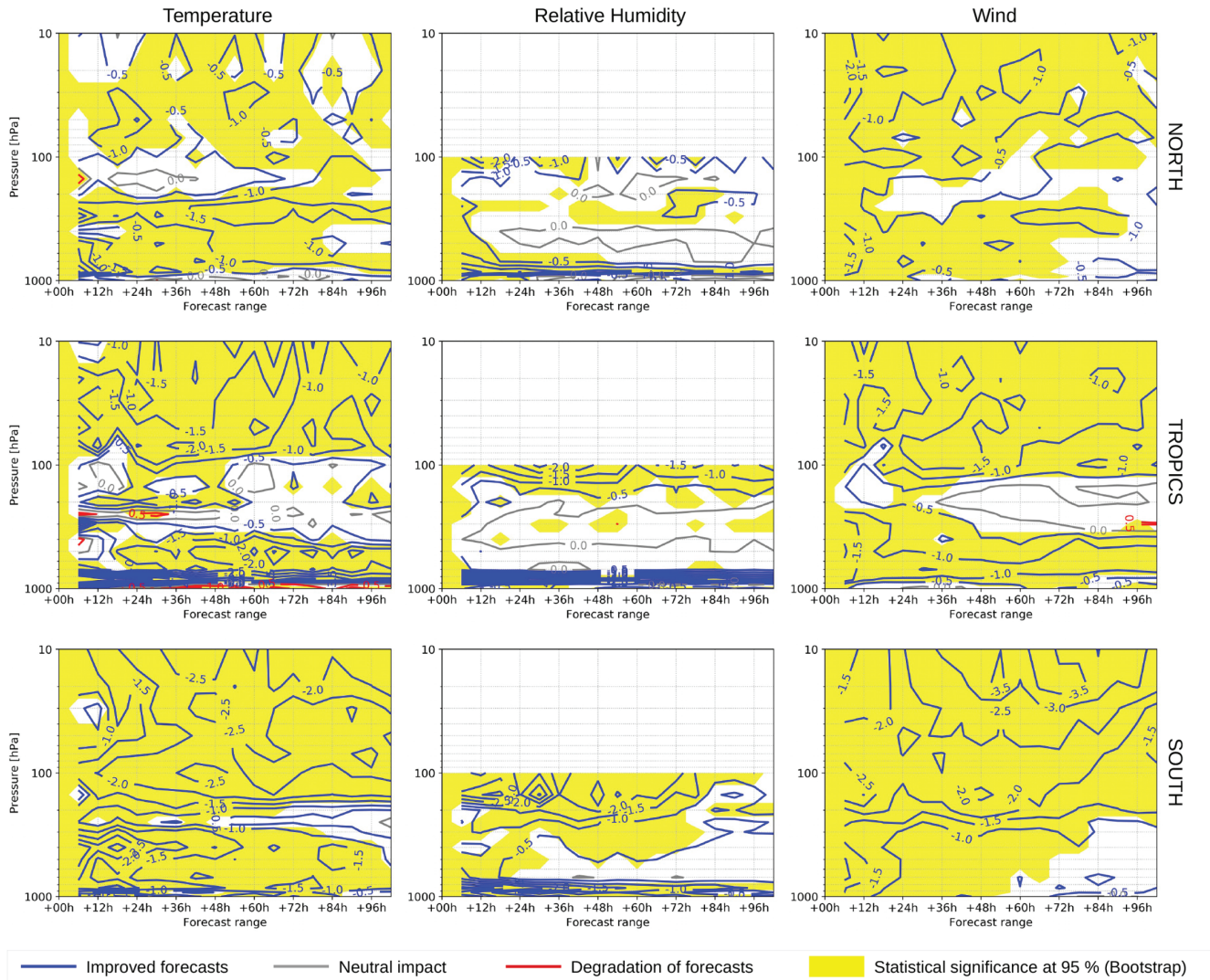
**FIGURE 8** Global relative differences in standard deviation of FG departures between O3EXP and CONTROL (black line) from 12 July to 10 September 2016 on the assimilated observations from (a) temperature radiosonde, (b) humidity radiosonde, (c) zonal wind radiosonde, (d) meridional wind radiosonde, (e) ATMS and (f) GNSS-RO bending-angle. Error bars (blue lines) give statistical significance intervals for differences at the 95% level. The green (red) shaded region indicate significant improvement (degradation) of simulation with the O3EXP experiment



**FIGURE 9** As Figure 8, but from 12 November to 31 December 2016

included in the prognostic variables of the ARPEGE global NWP model. As a matter of fact, only the temperature and humidity fields are considered as input variables to the

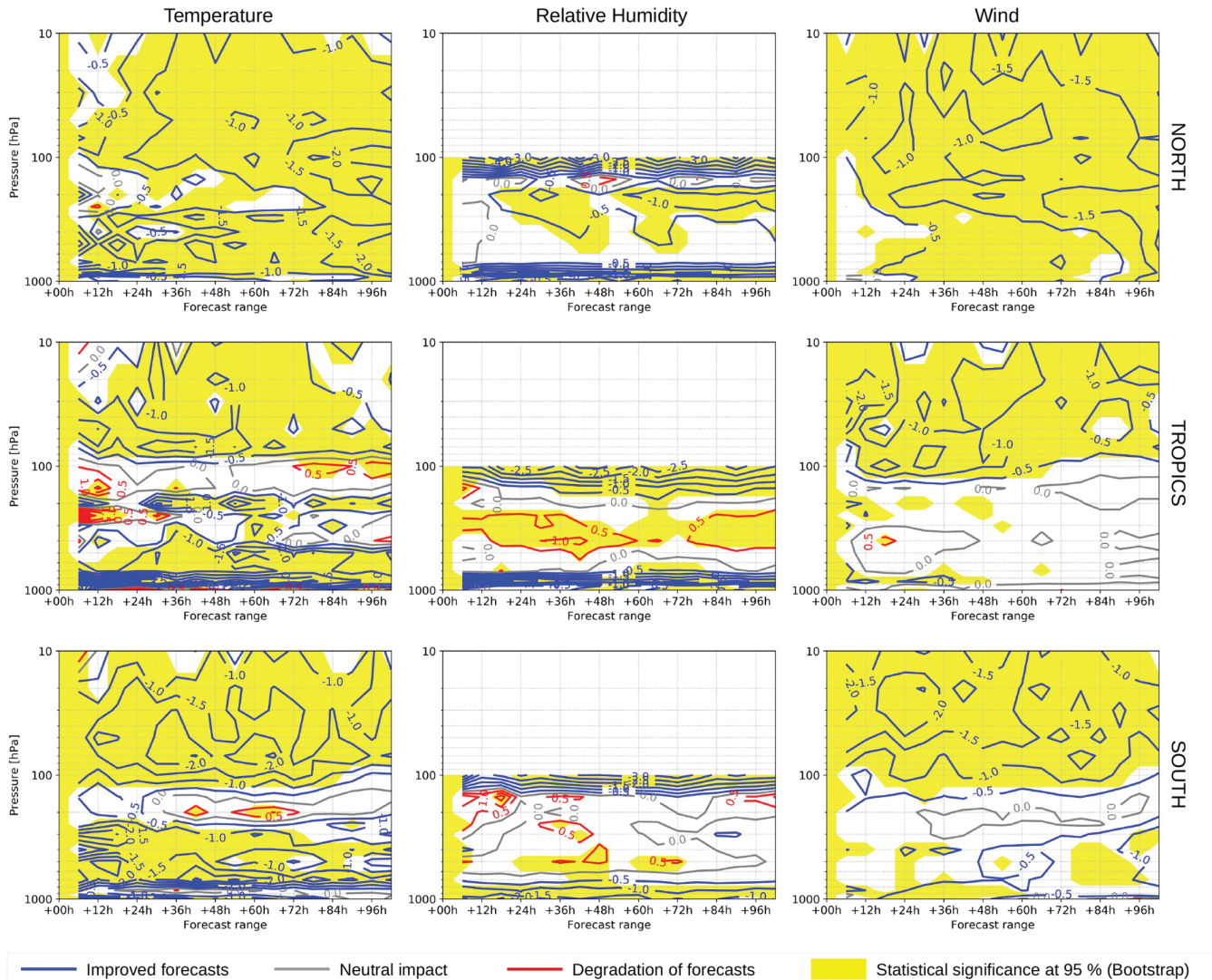
RTTOV RTM. We therefore assume that trace gases such as O<sub>3</sub>, CO<sub>2</sub>, CH<sub>4</sub>, CO, etc. are constant. Many studies have shown the positive impact of improving this assumption



**FIGURE 10** Normalized differences (%) of the standard deviation forecast error of temperature (left), relative humidity (centre) and wind (right) between O3EXP and CONTROL experiments versus forecast range from 0 to 102 hr. Statistics are computed over 57 simulations from 12 July to 10 September 2016 and verified against its own analysis. The top row shows scores over the Northern Hemisphere, the middle panels over the Tropics and the lower row over the Southern Hemisphere. The blue (red) contours indicate that the O3EXP experiment has improved (degraded) the forecasts. The yellow shaded region indicates 95% statistical significance computed from a bootstrap test

by using more realistic chemical fields, especially in the context of infrared satellite data where information on atmospheric temperature and humidity is extracted from the difference between observations and simulations. Ozone can have a significant impact both on simulations of radiative transfer, particularly in the infrared, and on the modelling of atmospheric dynamics due to its radiative contribution. Thus, the objective of this study was to evaluate the impact of using a realistic  $O_3$  in the observation operator RTTOV instead of the single  $O_3$  profile. As ozone is not analysed or forecasted by ARPEGE, we used realistic ozone fields from the MOCAGE CTM. This work is a first step towards integrating ozone into the 4D-Var data assimilation system for the ARPEGE model.

First, the impact of a realistic  $O_3$  in RTTOV was evaluated in the observation operator for the simulation of the four main infrared instruments used for ARPEGE. The results show significant differences in the simulation of ozone-sensitive channels (not bias corrected) between the experiment using variable ozone (O3EXP) and the experiment using constant ozone (CONTROL). However, these channels are currently not assimilated in the 4D-Var. Nevertheless, small simulation differences of channels also exist that are mainly sensitive to  $CO_2$ . After allowing the variational bias correction (Var-BC) to converge, we illustrated the impact of O3EXP on the global mean of first-guess departures of channels assimilated in the 4D-Var over long periods (summer and winter). The results



**FIGURE 11** As Figure 10, but from November 08 to December 31, 2016

indicate that the Var-BC is capable of reducing a large part of the bias but it is preferable to improve upstream the realism of the atmospheric fields provided to RTTOV. Indeed, the use of a realistic  $O_3$  can lead to modest further reductions in the biases of some  $CO_2$ , surface and  $H_2O$ -sensitive channels.

Secondly, we have shown that these slight modifications made by the O3EXP experiment on simulations affect the analyses. Indeed, the results over the two periods of interest show differences in analysis of temperature of the order of  $\pm 2.0$  K, in humidity of  $\pm 3.0\%$  and in wind of  $\pm 2.0$  m·s<sup>-1</sup> in the regions of highest difference (upper stratosphere for temperature and wind; troposphere for humidity). These modifications during the analysis cycles also have a positive and indirect impact on the simulations of other non-ozone-sensitive observations such as radiosondes and microwave instruments like

ATMS and GNSS-RO, allowing a better assimilation of these observations.

Finally, we evaluated our experiments in terms of forecast scores. The results achieved with the O3EXP experiment are surprising since the slight reduction of the bias obtained at the beginning of the data assimilation process translates into significant improvements in terms of standard deviation in forecasts over a large part of the atmosphere and over forecast ranges. The reduction in forecast errors for temperature can reach 2.5%, for humidity 4.0% and for wind 3.5%. We suggest that the use of more realistic ozone in RTTOV allows more accurate simulation, especially of  $CO_2$ -sensitive channels, some of which are also sensitive to ozone. Reducing the bias in the observations provides better quality control which seems to be beneficial in terms of the temperature information brought to the analysis. This impact on temperature analysis appears to



propagate positively to humidity and wind analysis, allowing an improvement cycle that also leads to better simulation of other observations. These major improvements could be beneficial to the ARPEGE global model, especially since the use of realistic O<sub>3</sub> in the observation operator does not require any additional computational cost.

This work is a first step towards a possible coupling or integration of ozone in the 4D-Var data assimilation for the ARPEGE model. Since 2017 and the first work on ozone-sensitive sensors used in NWP at Météo-France, we have been operationally assimilating five ozone-sensitive IASI channels. Recent work on the operational use of diagnosed observation-error covariance matrices for infrared instruments has led to a new selection of IASI channels taking into account inter-channel error correlations. This work provides a new selection of 31 ozone-sensitive IASI channels which we will soon evaluate in the global 4D-Var ARPEGE system.

Experiments adding ozone to the 4D-Var control variable in ARPEGE are also currently being evaluated. In the work to include ozone as a prognostic variable in the ARPEGE model, we plan to investigate the assimilation of additional ozone-sensitive observations from infrared sounder instruments (IASI, CrIS, AIRS, etc.), as well as imagers such as SEVIRI. Ozone observations in terms of geophysical variables should also be used and can be derived from the level 2 products provided by EUMETSAT. We will also investigate the impact that the use of realistic ozone can have on the coefficients used to simulate microwave observations mainly for channel 18 (183.31 ± 1.00 GHz) which seems to be sensitive to ozone.

Finally, in the mid-term, we will evaluate the possibility of adding ozone as a prognostic variable in the global ARPEGE model using a linear ozone scheme describing chemical processes, sources and sinks. This step would provide the opportunity to perform analyses and forecasts directly in the model and thus take advantage of the improvement of ozone fields by data assimilation to improve the entire system and thus improve meteorological forecasts, and assess the impact on the forecasts of using realistic ozone in the radiation scheme.

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