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Progress in ozone monitoring and assimilation



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# Progress in ozone monitoring and assimilation

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Since the launch of the Environmental Satellite (Envisat) in March 2002, the number of remote sensors with the capability of performing measurements of atmospheric gas composition (in particular ozone) has progressively increased. These new instruments, on one hand, provide the much-wanted constraint to the corresponding model fields, whilst on the other hand they represent a real challenge. Apart from the technical issues such as data handling, complex observing systems require continuous monitoring of the ozone information derived from each of its components, as well as an assessment of their potential benefits to the operational ozone analyses.

This article describes the ozone observing system currently used in the ECMWF operational suite. It briefly discusses the quality of the ECMWF ozone analyses, and shows the potential benefits of using ozone products as well as ozone-sensitive radiances from these new instruments. Results from a number of Observing System Experiments (OSEs) are presented.

A full list of the instruments referred to in this article and their acronyms is given in Table 1.

# The ozone observing system used at ECMWF

Table 2 presents the ozone observing system currently used at ECMWF. It includes a variety of instruments from both lower orbiting polar (LEO) and geostationary (GEO) satellites. These instruments provide information about total column ozone (TCO), ozone partial columns and ozone profiles.

The operational ozone assimilation at ECMWF includes the following.

- **SBUV/2.** Near-real-time ozone retrievals from the Solar Backscatter Ultra Violet (SBUV/2) instrument flying on board the NOAA-16 satellite have been assimilated since April 2002. Starting from 6 November 2007, the ECMWF ozone analyses also benefited from the active assimilation of ozone partial columns from the SBUV/2 instruments on board NOAA-17 and NOAA-18.
- SCIAMACHY. TCO produced in near-real-time by KNMI from the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) nadir measurements has been assimilated since 28 September 2004. The SCIAMACHY retrievals, which are distributed via the ESA funded PROMOTE-2 consortium, are pre-thinned to a horizontal resolution of 1°×1° before the assimilation. This approach is taken to limit the contribution of the horizontal error correlations, as no account is taken of these.

In addition to the actively assimilated ozone products, ECMWF also monitors ozone data from a number of different remote sensors on an operational basis. Currently (as in cycle Cy32r3 of ECMWF's Integrated Forecast System), the set of passively monitored ozone data includes:

- GOMOS. Ozone profiles from GOMOS (Global Ozone Monitoring by Occultation of Stars) on board Envisat.
- **SEVIRI.** TCO retrieved from the SEVIRI (Spinning Enhanced Visible and Infra-Red Imager) 9.7 μm channel on board Meteosat 9.
- · OMI. TCO from OMI (Ozone Monitoring Instrument) on board AURA.

Monitoring statistics plots are available on-line for all the ozone products at www.ecmwf.int/products/ forecasts/d/charts/monitoring/satellite/o3/.

	Instrument	Satellite		
AIRS	Advanced Infrared Sounder	AQUA		
GOME-2	Global Ozone Monitoring Experiment-2	MetOp-A		
GOME-1	Global Ozone Monitoring Experiment-1	ERS-2		
GOMOS	Global Ozone Monitoring by Occultation of Stars	Envisat		
HIRDLS	High Resolution Dynamic Limb Sounder	EOS-AURA		
MIPAS	Michelson Interferometer of the Passive Atmospheric Sounding	Envisat		
MLS	Microwave Limb Sounder	EOS-AURA		
ОМІ	Ozone Monitoring Instrument	EOS-AURA		
SBUV/2	Solar Backscatter Ultra Violet/2	NOAA-16, NOAA-17 and NOAA-18		
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography	Envisat		
SEVIRI	Spinning Enhanced Visible and Infra-Red Imager	Meteosat 9		
TOMS	Total Ozone Mapping Spectrometer	ADEOS and Earth Probe		

Sensor	Satellite	Satellite type	Data provider	Product type
SCIAMACHY	Envisat	LE0	KNMI	TCO
SBUV/2	NOAA-16, -17,-18	LEO	NOAA	0 <sub>3</sub> partial columns
SEVIRI	Meteosat-9	GEO	EUMETSAT	TCO
0MI	AURA	LE0	NASA	TCO
GOMOS	Envisat	LE0	ESA	0 <sub>3</sub> Profile

**Table 2** The ozone observing system currently usedat ECMWF. The satellite types are lower orbiting polar(LEO) and geostationary (GEO).

 Table 1
 Instruments on board satellites referred to in this article.

# The quality of the operational ozone analyses

At the time this article was written, the ECMWF operational ozone analyses were only constrained by the SCIAMACHY TCO and the three SBUV/2 partial column ozone products. The bottom layer of the assimilated SBUV/2 data spans the atmosphere from surface up to about 16 hPa so that it can be almost regarded as a total column. The combination of these data generally provides a good constraint to the TCO analyses. Figure 1 shows the comparison between the time series of the zonal mean TCO analyses produced operationally at ECMWF and the retrieved TCO from OMI for January 2007 to February 2008. The level of agreement between the operational TCO analyses and OMI is generally good in terms of distribution, seasonal variability, and total ozone amount.

Although important, the ozone products that are currently assimilated are often not able to provide the information required to constrain the ozone vertical distribution. This is worse in regions where nadir ultraviolet instruments – largely used for ozone retrieval – cannot make measurements, such as the polar winter hemisphere.

Figure 2 shows the monthly mean comparisons between ozone sondes launched from the McMurdo station during the 2007 Match campaign in Antarctica (*Mercer et al.*, 2007), and their model equivalent derived from the operational ozone analyses during August. During the polar winter, the maximum of the ozone analyses is generally placed at a higher vertical level than that measured by the ozone sondes. In addition, the ozone analyses show deeper depletion in the mid-stratosphere just below the ozone maximum. This shortcoming is known and can be addressed by improving the quality of the ozone first guess as well as by assimilating ozone data retrieved from remote sensors employing different geometries and sounding different ozone-sensitive spectral regions.

The ozone first guess used at ECMWF is derived from an updated version of the *Cariolle & Deque* (1986) scheme. In this scheme the ozone continuity equation is expressed as a linear relaxation towards a photochemical equilibrium for the local value of the ozone mixing ratio, the temperature, and the overhead ozone column. An ozone destruction term is used to parametrize the heterogeneous chemistry as a function of the equivalent chlorine content for the actual year. Although this parametrization has undergone significant upgrades in recent years thanks to collaboration with Daniel Cariolle (Météo-France), undoubtedly the ozone analyses would benefit from any further increase in their accuracy (e.g. by using improved coefficients in the linear expansion of the ozone continuity equation).

As far as the assimilation of ozone observations is concerned, ozone profiles retrieved from a limb sounder could improve, for example, the vertical distribution of the ozone analyses. Infrared and microwave sounders can provide the required constraint where the ultraviolet sensors are practically blind. *Dethof* (2003) showed that the assimilation of ozone profiles from the Michelson Interferometer of the Passive Atmospheric Sounding (MIPAS) into the ECMWF system can substantially improve the quality of the ozone analyses. This is particularly apparent in the tropical lower stratosphere, where the ozone peak value is usually underestimated, as well as inside the winter vortex, where the stratospheric ozone transport and depletion are, in general, difficult to model accurately. Furthermore, microwave sounders offer the added advantage of providing measurements that are not affected by cloud contamination. The Microwave Limb Sounder (MLS), launched on the NASA's EOS-AURA satellite on July 2004, is a potential candidate to provide this kind of information. In addition to the standard level 2 ozone products, an investigation into the assimilation of the ozone-band in the infrared spectral range (about the 9.7 µm channel) has also started.



**Figure 1** Comparison between the time series of the zonal mean of (a) ECMWF TCO analyses and (b) OMI TCO retrievals for 1 January 2007 to 29 February 2008.



**Figure 2** Comparison between the monthly mean operational ozone profiles (red) and co-located ozone sondes (black) launched from the McMurdo station (77.8°S, 166.7°E) in August 2007 as part of the 2007 Match campaign. Dotted lines limit the one standard deviation range about the mean. The Norwegian Institute for Air Research (NILU) provided the Match ozone sonde data.

#### **Observing System Experiments (OSEs)**

The potential benefits of assimilating four ozone products will now be discussed.

- We first present some results from the assimilation of TCO from the ultraviolet nadir sounder OMI on board EOS-AURA.
- There follows a discussion of the monitoring and assimilation of TCO from the ultraviolet nadir sounder GOME-2 on board MetOp-A.
- Then, we will show some preliminary results from the assimilation of ozone profiles retrieved from MLS on board EOS-AURA.
- Finally, we will present some results from the assimilation of radiances in the infrared O3-channels as measured by the Advanced Infrared Sounder, AIRS, on board AQUA.

Each OSE includes two experiments: a control experiment (always referred to as CTRL) used as reference, and a perturbation experiment which has the same configuration as CTRL except for the element under study. All the OSEs were performed using the 12-hour 4D-Var data assimilation scheme. Unless otherwise stated, the experiments were run at resolution T159 L91 using the current operational cycle (Cy32r3). In the following discussion an indication is given of when a different set up was used.

#### Assimilation of the OMI TCO

TCO retrieved from OMI has been passively monitored in the operational suite since 6 November 2007 (Cy32r3). The monitoring statistics shows that the agreement between these observations and the ECMWF analyses of TCO is generally within 3 DU.

The first assimilation trial of OMI TCO was performed using the current operational system at a resolution of T255L60 (from surface up to 0.1 hPa) for 1 July to 31 August 2006. With the exception of only the ozone data, both the control (CTRL) and the perturbation experiment (Exp/OMI) used the same observations as were assimilated operationally. As far as the ozone assimilation is concerned, SCIAMACHY TCO was used to constrain the CTRL ozone analyses. OMI TCO was added to that reference in Exp/OMI. The active assimilation of the SBUV/2 partial columns was, instead, turned off in both CTRL and Exp/OMI. Owing to data redundancy of a complex GOS, such as that used at ECMWF, performing impact studies using the full operational dataset can only show very limited impact and does not necessarily highlight the intrinsic benefit of the element under study. Furthermore, having switched off their active assimilation, the three SBUV/2 instruments can be used for the ozone analysis validation.

It is found that there are small but statistically significant differences between the CTRL and Exp/OMI ozone analyses in the region of the atmosphere between 10 and 80 hPa. Comparisons with independent, unassimilated observations show improved levels of agreement of the Exp/OMI analyses. Figure 3 presents the global mean relative differences between MLS ozone profiles and the ozone analyses from CTRL and Exp/OMI averaged over the two month period July-August 2006. Overall, the assimilation of OMI TCO leads to a better level of agreement of the ozone analyses with MLS data in the region between 20 and 150 hPa.

Comparisons of the ozone analyses with ozone profiles from HIRDLS (HIgh Resolution Dynamic Limb Sounder on AURA) and the SBUV/2 data from NOAA-16, NOAA-17 and NOAA-18 (not shown here) also confirm these results by showing a better fit to the independent observations when OMI TCO is actively assimilated. Finally, comparisons with ozone sondes show a neutral or positive impact of the OMI data. The active assimilation of OMI TCO will start with the next operational cycle (Cy33r1).



**Figure 3** Relative ozone difference between MLS ozone profiles and their model equivalent obtained from CTRL and Exp/OMI. The plotted profiles were computed as 100×(MLS-A)/MLS, where A is the ozone analysis. The profiles were obtained as global mean over the period 1 July to 31 August 2006.

# Monitoring and assimilation of GOME-2 TCO

On October 2006, the first of three satellites of the EUMETSAT Polar System (EPS), MetOp-A, was launched. On board this satellite was an ozone monitoring sounder, the second Global Ozone Monitoring Experiment, GOME-2. This instrument benefits from the inheritance of GOME-1, launched on board of ERS-2 in 1995, as well as from more recently launched sensors, such as SCIAMACHY and OMI. The passive monitoring of GOME-2 TCO is currently in a pre-operational status, and will start operationally with the next ECMWF cycle (Cy33r1). Preliminary comparisons between GOME-2 TCO and their model equivalent show a high level of agreement. As an example, Figure 4 shows the distribution of the first-guess departures (namely observations minus first-guess) for one-day's worth of GOME-2 data.

In addition to the passive monitoring, preliminary assimilation experiments of GOME-2 TCO have already started covering the period between 1 January and 28 February 2008. In the baseline experiment (CTRL), the SCIAMACHY TCO was the only ozone data actively assimilated. In the perturbation experiment (Exp/ GOME2), the TCO from GOME-2 was also assimilated.

A complete assessment of the impact of GOME TCO on the ECMWF ozone analyses is not yet available. Comparisons with ozone sondes show some limited improvements in the upper troposphere and lower stratosphere when GOME-2 observations are assimilated. Two examples of monthly mean comparisons for January 2008 are shown in Figure 5 for one station at mid-latitudes in the northern hemisphere. The impact of the mean scores is generally negative, in particular in the southern hemisphere. Such a negative impact determined by the GOME-2 TCO assimilation contradicts, somehow, the good level of agreement found in the passive monitoring between these data and the ECMWF ozone analyses. However, if confirmed, these preliminary results seem to suggest that some extra care has to be taken before the assimilation. A potential problem in the assimilation, that requires further investigation, is the presence of systematic biases between different ozone products that have not yet been corrected.



**Figure 4** Distribution of the GOME-2 TCO firstguess departures over 24 hours for 25 July 2007. Values are in DU.

**Figure 5** Comparison between the monthly mean ozone sonde profile launched from the Madrid station (40.5°N, 3.7°W) in January 2008 (blue) and co-located mean ozone profile from CTRL (black) and Exp/GOME2 (red).

#### Assimilation of MLS ozone profiles

There are a number of studies which have shown the potential benefit of assimilating the off-line ozone profiles retrieved from MLS data. For example, at the NASA Goddard's Global Modeling and Assimilation Office (GMAO), assimilation trials of MLS ozone profiles in the GEOS-5 (Goddard Earth Observing System 5) data assimilation system produced a more realistic Antarctic ozone hole than, for example, SBUV/2 ozone data (*Sienkiewicz & Stajner,* 2007). Also *Feng et al.* (2008) found that the assimilation of MLS data using the ECMWF system had a positive impact on the stratospheric ozone analyses. However, the unavailability of MLS data in near-real-time, which is required by NWP centres, has enormously limited their usage. With the start of the near-real-time dissemination of this product, a further investigation of the potential benefits of MLS ozone profiles on the ECMWF ozone analyses using the most recent model is both timely and needed.

An assimilation trial of off-line MLS ozone profiles was performed for the period 1 July to 31 August 2007. In the CTRL experiment, SCIAMACHY TCO was the only ozone data actively assimilated. In the perturbation experiment (Exp/MLS), the MLS ozone profiles were also used to constrain the ozone analyses. Preliminary results are encouraging.

Figure 6 shows the comparison between the monthly mean ozone profiles obtained from the McMurdo ozone sondes and the corresponding mean ozone analyses from CTRL and Exp/MLS in August 2007. A similar comparison using the operational ozone analyses was shown in Figures 2. For clarity, Figure 6 does not show the one standard deviation range about each mean profile. As expected, the assimilation of MLS ozone profiles strongly improves the ozone vertical distribution, both in terms of vertical localization of the ozone maximum and its values, especially in a critical region like Antarctica.



**Figure 6** Comparison between the monthly mean ozone sonde profile launched from the McMurdo station (77.8°S, 166.7°W) in August 2007 (blue) and co-located mean ozone profile from CTRL (black) and Exp/MLS (red), respectively. All the ozone sondes were launched as part of the 2007 Match campaign.

# Assimilation of AIRS infrared channels in the ozone-band

In addition to the traditional assimilation of ozone products, some attempts of assimilating radiances from the ozone-band in the infrared spectral region from infrared sounders, such as AIRS, are also under investigation. A huge amount of data is available from infrared sounders, currently not sufficiently exploited.

Two three-month long assimilation experiments (from 15 September to 14 December 2006) were run with cycle Cy31r2. CTRL made use of the operational set-up (i.e. all data used operationally in Cy31r2). In the perturbation experiment (Exp/AIRS), thirty-six channels in the spectral range between 1003 and 1286 cm<sup>-1</sup> were also actively assimilated. Owing to emissivity problems, all radiances over land were blacklisted, and therefore not actively assimilated.

Comparisons between the two sets of ozone analyses showed little differences up to 7 to 8 DU in the total ozone. In the vertical, the assimilation of AIRS channels produces differences within –1 and +1 ppmm (parts per million mass), mainly in the lower stratosphere between 6 and 100 hPa. Comparisons with ozone sondes show negligible differences between the two experiments at mid-latitudes. In contrast, the assimilation of AIRS infrared channels generally leads to an improved level of agreement between

the ozone sonde profiles and the collocated analyses in the tropics and at high latitudes in both hemispheres. As an example, Figure 7 shows the November monthly mean comparison for the sondes launched from Syowa (69°S), San Cristobal (0.9°S), and Eureka (80°N). The contribution of AIRS to the ozone analyses is particularly noticeable in the upper troposphere and lower stratosphere. Comparisons with MLS ozone profiles also exhibit some improvements in the upper troposphere.

The impact of AIRS assimilation on the mean scores is generally positive, as shown by the mean geographical normalized rms (48-hour) forecast error difference between Exp/AIRS and CTRL for the total column ozone (Figure 8). Negative values (green) have to be regarded as an improvement determined by the assimilation of AIRS radiances over the CTRL analyses.

Table 3 summarises the mean normalized rms difference of the 24-, 48-, 72-, 96-, 120- and 240-hour forecast error of TCO between Exp/AIRS and CTRL for different regions. Indeed, the assimilation of AIRS channels in the ozone-band leads to improvements in the ozone field, especially within the first 96 hours of the forecasts. Particularly noticeable is the improvement in the mean scores over the southern hemisphere that still shows a positive impact (negative value) at day 10.



**Figure 7** Comparison between the November monthly mean ozone sonde profile (blue) and co-located mean ozone profile from CTRL (black) and Exp/AIRS (red) for (a) a station at high latitudes in the southern hemisphere (Syowa, 69°S), (b) a station in the tropics (San Cristobal, 0.9°S), and (c) a station at high latitudes in the northern hemisphere (Eureka, 80°N).



**Figure 8** Mean normalized rms difference of the 48-hour forecast error between Exp/AIRS and CTRL for the total column ozone. Negative values (green) indicate an improvement due to the assimilation of AIRS radiances over the CTRL analyses.

	T+24	T+48	T+72	T+96	T+120	T+240
Northern hemisphere	-0.17	-0.11	-0.06	-0.03	-0.01	0.02
Southern hemisphere	-0.09	-0.06	-0.05	-0.03	-0.03	-0.01
Europe	-0.20	-0.14	-0.09	-0.04	-0.03	0
East Asia	-0.15	-0.08	-0.03	-0.01	-0.01	0.02
North America	-0.11	-0.09	-0.04	-0.02	0	0.01
Tropics	-0.12	-0.05	-0.02	0	0.02	0.08
North Atlantic	-0.18	-0.11	-0.07	-0.05	-0.03	0
North Pacific	-0.19	-0.10	-0.05	-0.01	0	0

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**Table 3** Summary of the mean normalized rms difference of the 24-, 48-, 72-, 96-, 120and 240-hour total ozone forecast errors between Exp/AIRS and CTRL for different regions. Negative values (black) refer to a reduction (i.e. improvement) of the rms forecast error when AIRS radiances are actively assimilated. Positive values (blue) refer to an increase of the rms forecast error when AIRS radiances are actively assimilated. Zero values (red) correspond to neutral impact of the AIRS assimilation on the total ozone forecast error.

# **Ozone bias correction**

Observations (and models) are prone to be affected by biases which, if uncorrected, can introduce systematic errors in the final analyses. In addition, non-negligible inter-instrumental biases can make the simultaneous assimilation of data from different sensors highly inefficient; the contribution from one instrument can, in principle, cancel that of another one. When increasing the number of sensors that provide the same data product, it becomes crucial to account for and correct these mutual biases. An operational bias correction for ozone (and retrieved products, in general) is not yet available at ECMWF, but development work is currently ongoing.

Based on the adaptive scheme of *Derber & Wu* (1998), a variational bias correction for radiances, VarBC, was introduced in the ECMWF operational suite (Cy31r1) on 11 September 2006 (*McNally et al.*, 2006). This scheme successfully corrects for systematic biases in the Level-1 data. In VarBC the bias correction is computed as a linear regression of a number of predictors. These predictors have to be carefully defined for each sensor and according to the data type. As far as the radiance bias correction is concerned, the predictors may include correction for air-mass or scan angle dependence, in addition to a global offset. The coefficients of the linear regression are included in a modified state vector, and therefore they are computed during the assimilation minimization. VarBC has recently been extended to correct for systematic errors in retrievals. This feature is currently being tested but is not yet operational.

The monitoring of satellite ozone products, which is routinely performed at ECMWF, shows that the observational systematic biases can vary in amplitude with season and location (with a strong latitudinal dependence), and with the vertical level for profiles. Using the solar elevation at the location and time of the observations, in addition to a global constant offset as a bias predictor, a two-month long ozone bias correction experiment (Exp/SOE) has already been completed. A second experiment with no ozone bias correction (CTRL) has been run for reference. The period under study is January and February 1997. The ozone products actively assimilated in both experiments were TOMS TCO retrieved from the ADEOS and Earth Probe measurements, SBUV/2 ozone partial columns from NOAA-9 and NOAA-14, and GOME ozone profiles from ERS-2. All the ozone data were simultaneously bias corrected in Exp/SOE.

Preliminary results show that for the ozone products both the first-guess and analysis departures are generally reduced in Exp/SOE compared with those of CTRL. In some cases this results in an increase of the number of data actively assimilated. Improvements were also found in the mean scores. Figure 9 shows the mean normalized difference of the rms error of the 24-hour forecasts of TCO between Exp/SOE and CTRL averaged over January and February 1997. Negative values (green) refer to a reduction (i.e. improvement) of the rms error of the 24-hour forecast when the ozone bias correction is applied. These preliminary results highlight some problems at high latitudes in the southern hemisphere – these require further investigation. Here the various sources of ozone information seem to be less consistent with each other when the bias correction is applied. In contrast, the consistency between the various sources of ozone information is substantially improved in the tropics due to the ozone bias correction.



**Figure 9** Mean normalized difference of the rms of the 24-hour forecast error between Exp/SOE and CTRL the total column ozone. Negative values (green) indicate a reduction (i.e. improvement) of the rms error of the 24-hour forecast when the ozone bias correction is applied.

# Improving ozone products

A number of OSEs have been performed to assess the potential benefits of ozone products from a number of recently launched remote sounders on the ECMWF ozone analyses. Indeed, all the sensors and data products used in these studies have shown that they can potentially improve the quality of the ozone analyses. TCO retrieved from ultraviolet nadir sensors, such as OMI, showed a small but statistically significant positive impact on the ozone analyses especially in the lower stratosphere where there is improved agreement with independent, unassimilated observations.

Despite of this potential enhancement, constraining the ozone vertical distribution with such sensors is generally still a challenge. Comparisons of the operational ozone products with ozone sonde profiles clearly show that the ozone observations that are currently assimilated at ECMWF (mainly TCO from ultraviolet sounders) can provide an appropriate constraint to the analysis of total column ozone. However, they are still inadequate to fully constrain the ozone vertical distribution. In addition, the high latitude region in the winter hemisphere can also suffer from a lack of data, as at this time of the year nadir ultraviolet instruments – largely used for ozone retrieval – cannot make measurements. Preliminary results from the assimilation of MLS ozone profiles using the latest suite are very promising.

An additional source of information in critical regions, such as the high latitudes in the winter hemisphere, and yet not fully exploited is represented by infrared sensors. A first attempt of assimilating radiances in the infrared ozone-band from the AIRS sounder has also been performed. Preliminary results show that, although small, the assimilation of the AIRS ozone-band has a positive impact on the ozone analyses. There is an improvement in the comparison with independent observations (ozone sondes and MLS) mainly in the upper troposphere and lower stratosphere, as well as improving the mean forecast scores. As for future plans, the investigation of the potential benefits of the assimilation of infrared ozone-channels from AIRS will be completed and extended to other sounders, such as IASI.

As the number of ozone instruments actively used increases, systematic inter-instrumental biases start to be important, and in some cases the potential benefits of one instrument are cancelled by the assimilation of another one. Work on limiting, if not completely removing, these biases in the ozone observations is currently ongoing. Preliminary results from the first ozone bias correction trial performed within the reanalysis framework are encouraging. Some problems were seen at high latitudes in the southern hemisphere that require further investigation. However, the preliminary results show a general reduction of the first-guess and analysis departures of all the ozone products, as well as a substantial reduction in the rms error of the 24-hour forecast in the tropics.

#### **Further reading**

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