Dynamical impact of total-ozone observations in a four-dimensional variational assimilation

By A. PEUCH*, J.-N. THÉPAUT and J. PAILLEUX
Météo-France, France

(Received 23 June 1999; revised 13 January 2000)

SUMMARY

Observing-system simulation experiments (OSSES) are performed to investigate the dynamical impact of total-ozone data used in a four-dimensional variational analysis in a numerical weather prediction (NWP) model. Ozone columns are generated by the model at the location of data retrieved by the National Environmental Satellite, Data, and Information Service, from the measurements of the TIROS (Television Infra-Red Observation Satellite) Operational Vertical Sounder (TOVS). They are assimilated over a 12-hour period. In the present experiments, ozone mixing ratio is considered to be a passive tracer, simply advected by winds. The initial three-dimensional ozone field is not analysed. An important positive impact is found in a fully idealized experiment, on the flow analysis as well as on the temperature analysis. The ability to derive thermodynamic information from ozone-column observations is confirmed by an OSSE performed in a more realistic context. Moreover, the information on wind fields supplied by ozone data may be in addition to the information already provided by observations currently assimilated in NWP models. Some conditions, needed to make the information provided by ozone columns effective, are discussed, such as the accuracy of the ozone measurements and the necessity of analysing ozone in addition to the usual model variables.

KEYWORDS: Four-dimensional variational assimilation Observing-system simulation experiment Total ozone

1. INTRODUCTION

Numerical weather prediction (NWP) models forecast the evolution of the atmospheric state from an initial point called analysis, the quality of the forecast depending to a large extent upon the accuracy of the analysis. The analysis is performed using different sources of information on the atmosphere, such as model outputs and observations. The data coverage is not homogeneous over all the atmosphere. Except for some aircraft measurements and some winds derived from cloud imagery from geostationary satellites, wind observations are scarce in the upper troposphere and in the stratosphere. Any indirect information on wind in these areas is of potential interest for assimilation in NWP models (Lorenc 1988).

Atmospheric ozone is attentively monitored, in particular through remote sensing, mainly because of its property of screening out ultraviolet radiation and its contribution to the greenhouse effect. For example, total-ozone measurements have been derived from the observations of the Total Ozone Mapping Spectrometer (TOMS) instrument on-board Earth Probe since 1976 (McPeters et al. 1998), and from the observations of the TIROS (Television Infra-Red Observation Satellite) Operational Vertical Sounder (TOVS) instrument on board the polar-orbiting satellites of the National Oceanic and Atmospheric Administration (NOAA) series since 1978 (Neuendorffer 1996). Several projects aim to increase the amount and the type of ozone data, such as, for instance, the Second Generation Meteosat or the Environmental Satellite.

The variability of ozone is dominated by transport processes in the upper troposphere and lower stratosphere (Carolile and Déqué 1986). In these areas, its photochemical lifetime is relatively long—typically of the order of months—and ozone can be considered to be a good tracer of the flow. Under these conditions, one can expect to be able to derive some information on the winds from successive observations of ozone structures (Karcher et al. 1998). The idea is quite similar to the principle which consists of deriving wind data from cloud-pattern movements, assessed with successive

* Corresponding author: Météo-France, CNRM/GMAP, 42 avenue G. Coriolis, 31057 Toulouse Cedex, France.
geostationary-satellite images; see for instance Buhler and Holmlund (1993). However, the purpose here is not to construct wind data from ozone-pattern movements and then to assimilate these wind products, but to assimilate directly ozone observations, with an adequate assimilation system, and to study whether information on winds is derived effectively.

The capability of estimating the wind field from chemical constituent observations has been explored, from a theoretical point of view, with an extended Kalman filter by Daley (1996); the necessity of having sufficient structure in the constituent field, as well as dense, frequent and accurate observations, was underlined. Riishojgaard (1996) pointed out the dynamical information present in the ozone data: he showed, with a barotropic-vorticity-equation model, that, when started from a purely zonal flow field, a four-dimensional variational (4D-Var) assimilation scheme could, to a large extent, reconstruct the flow field, using only observations of the mixing ratio of the tracer.

The purpose of this paper is to investigate the potential impact of ozone observations upon dynamical analysis, by using a pre-operational 4D-Var algorithm for the assimilation. The theory and the first applications of this assimilation method can be found in Lewis and Derber (1985), Le Dimet and Talagrand (1986), Courtier and Talagrand (1987) and Talagrand and Courtier (1987). Together with Kalman filtering, 4D-Var assimilation systems are particularly well adapted to the assimilation of satellite data which are asynoptic. They allow various types of data to be taken into account, and not necessarily measurements corresponding directly to prognostic variables of models. They are consequently well suited to our purposes.

The observations we are interested in are total-ozone columns, the linking of which with meteorology is well documented; see for example Dobson et al. (1929) or Vaughan and Price (1991). Ozone quantities present in the upper troposphere and lower stratosphere contribute significantly to total-ozone values. It should then be possible to derive wind information in these areas from total quantities. Moreover, several sensors work with horizontal resolutions quantitatively comparable to NWP model resolutions.

In the next section, a simple one-dimensional (1D) periodic advection model is used to show how a 4D-Var assimilation scheme is theoretically able to estimate the wind field from observations of a passive tracer; see also Thépaut (1993). The assimilation system used for the experiments is described in section 3, as well as the set-up common to all the runs performed. The rest of the paper is devoted to results and discussions. An assimilation experiment taking place in a fully idealized context is presented in section 4. A second set of experiments is described in section 5, to investigate the potential impact of ozone data in a more realistic context.

2. Theory

Let us consider a simple 1D advection model. Let us denote by $\mathbf{X}$ the state vector of the model, $\mathbf{X} = (u, R)$ with $u = u(x, t)$ the wind, and $R = R(x, t)$ the mixing ratio of any passive tracer simply advected by wind. Let us assume that the evolution equation for $u$ is given by Eq. (1), $\nu$ being a viscosity coefficient. The evolution equation for $R$ is Eq. (2). Moreover, $\mathbf{X}$ is assumed to be periodic in $x$, $L$ being the period.

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

(1)

$$\frac{\partial R}{\partial t} + u \frac{\partial R}{\partial x} = 0.$$  

(2)
Assuming now that $R$ is observed over the whole domain $(0, L)$ and over the time window $(t_0, t_n)$, a cost function, $\mathcal{J}$, can be defined, measuring the distance between the values of the tracer as predicted by the model and the observed values, $R_{\text{obs}}$:

$$\mathcal{J} = \frac{1}{2} \int_{t_0}^{t_n} \int_0^L (R - R_{\text{obs}})^2 \, dx \, dt. \quad (3)$$

The imposed constraint is that the forecast from $X_0$ at $t_0$ fits the observations, $R_{\text{obs}}$, in the best possible way. It is equivalent to finding $X_0$ which minimizes $\mathcal{J}$.

The tangent linear equations which describe, to first order, the time evolution of two perturbations, $\delta u$ and $\delta R$, in the vicinity of a trajectory, $X$, are:

$$\frac{\partial \delta u}{\partial t} + u \frac{\partial \delta u}{\partial x} + \delta u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 \delta u}{\partial x^2}$$

$$\frac{\partial \delta R}{\partial t} + u \frac{\partial \delta R}{\partial x} + \delta u \frac{\partial R}{\partial x} = 0. \quad (5)$$

A scalar product, $(\cdot, \cdot)$, is defined in Eq. (6); for the sake of clarity, the normalization factor is omitted.

$$\langle (u_1, R_1), (u_2, R_2) \rangle = \int_0^L (u_1 u_2 + R_1 R_2) \, dx. \quad (6)$$

Let $v$ and $w$ be two vectors from two spaces, $S_v$ and $S_w$, respectively. Let $M$ be a linear operator mapping from $S_v$ to $S_w$. There is a unique linear operator, $M^*$, called the adjoint of $M$, mapping from $S_w$ to $S_v$ such that, if $(\cdot, \cdot)$ denotes an inner product:

$$\langle Mv, w \rangle = \langle v, M^*w \rangle. \quad (7)$$

Using the definitions in Eqs. (6) and (7), and introducing the adjoint variable, $(\delta u^*, \delta R^*)$, the adjoint equations associated with Eq. (4) and Eq. (5) can be derived:

$$- \frac{\partial \delta u^*}{\partial t} - u \frac{\partial \delta u^*}{\partial x} + \delta u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 \delta u^*}{\partial x^2} + \frac{\partial R}{\partial x} \delta R^* = 0$$

$$- \frac{\partial \delta R^*}{\partial t} - u \frac{\partial \delta R^*}{\partial x} = 0. \quad (9)$$

Noting that the change, $\delta \mathcal{J}$, resulting from a perturbation, $\delta X$, is, to first order, equal to:

$$\delta \mathcal{J} = \int_{t_0}^{t_n} \int_0^L (R - R_{\text{obs}}) \delta R \, dx \, dt. \quad (10)$$

The ‘inhomogeneous adjoint equations’ (Talagrand and Courtier 1987) are deduced:

$$- \frac{\partial \delta u^*}{\partial t} - u \frac{\partial \delta u^*}{\partial x} + \delta u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 \delta u^*}{\partial x^2} + \frac{\partial R}{\partial x} \delta R^* = 0$$

$$- \frac{\partial \delta R^*}{\partial t} - u \frac{\partial \delta R^*}{\partial x} = R - R_{\text{obs}}. \quad (12)$$

As shown in Talagrand and Courtier (1987), the adjoint equations (8) and (9) allow changes in $\mathcal{J}$ at $t_n$ to be related to changes in the atmospheric state at $t_0$. In practice, the gradient of the cost function with respect to the initial conditions can be computed by integrating Eqs. (11) and (12) backward in time from $t_n$ to $t_0$, starting from Eqs. (13).
and (14)
\[ \delta u^*(x, t_n) = 0 \]  \hspace{1cm} (13)
\[ \delta R^*(x, t_n) = 0. \]  \hspace{1cm} (14)

The final values, \( \delta u^*(x, t_0) \) and \( \delta R^*(x, t_0) \), are the gradients \( \nabla_{u_0} \mathcal{J} \) and \( \nabla_{R_0} \mathcal{J} \) and are equal to:
\[ \delta u^*(x, t_0) = \int_{t_n}^{t_0} \frac{\partial R}{\partial x} (R - R_{\text{obs}})(t - t_0) \, dt \]  \hspace{1cm} (15)
\[ \delta R^*(x, t_0) = \int_{t_n}^{t_0} \left[ (R - R_{\text{obs}}) + u \frac{\partial (R - R_{\text{obs}})}{\partial x}(t - t_0) \right] \, dt. \]  \hspace{1cm} (16)

Equation (15) shows that \( \nabla_{u_0} \mathcal{J} \) is non-zero and contains information from the observations, \( R_{\text{obs}} \). As a consequence, it is possible to reduce the cost function by modifying the initial wind field, this modification being influenced by the tracer observations. In that way, we see that information on the tracer field will be transferred to the wind field during the minimization process.

3. EXPERIMENTAL DESIGN

(a) The 4D-Var assimilation system

The 4D-Var algorithm (Rabier et al. 1998) was developed jointly by the European Centre for Medium-Range Weather Forecasts (ECMWF) and Météo-France for the Integrated Forecasting System (IFS) of ECMWF and the global spectral NWP model of Météo-France, Action de Recherche Petite Echelle Grande Echelle (IFS/ARPEGE). The 4D-Var data-analysis problem can be seen as finding the starting point of a model trajectory which will best fit the data available over the assimilation period considered, \((t_0, t_n)\). A cost function, \( \mathcal{J} \), is defined, which measures the misfit between the model trajectory and the data. Since a model trajectory depends only on the initial state, \( \mathcal{J} \) can be written as a function of some chosen model variables at \( t_0 \), which form the control variable \( \mathbf{x} \). During the assimilation process, \( \mathcal{J} \) is minimized to get the ‘best’ \( \mathbf{x} \), through an iterative process involving the computation of the gradient of \( \mathcal{J} \) obtained with the adjoint model.

In our case, the data consist of the observations, and of a previous forecast valid at \( t_0 \) and called background. The diagnostic function, \( \mathcal{J} \), is thus written as the sum of two functions: \( \mathcal{J}^o \), relative to the distance between the model trajectory and the assimilated observations, and \( \mathcal{J}^b \), relative to the distance between the model initial state and the background. \( \mathbf{x} \) consists of wind, temperature and surface pressure. The minimization process is stopped when the gradient falls below a certain threshold or if a number of iterations have been performed (80 in our case). This number of iterations gives a satisfactory reduction of the cost-function gradient in our experiments; it is slightly superior to the number (70) used in the operational three-dimensional variational (3D-Var) system at Météo-France. Given the definition of \( \mathbf{x} \) in the present experiments, only the initial fields of wind, temperature and surface pressure are likely to be modified by the assimilation, to allow the subsequent forecast to fit the information better and reduce the cost function. Ozone is not included in \( \mathbf{x} \); in the simple case of the 1D advection model presented in section 2, it means that Eq. (16) is ignored.
$x^0$ is computed according to Eq. (17), where $y^0$ are the assimilated observations, $H$ the operators which convert forecast parameters into values homogeneous to observations, and $R$ the covariance matrix of the observational errors.

$$x^0(x) = [H(x) - y^0]^T R^{-1} [H(x) - y^0].$$

(17)

The ozone mixing ratio, $R_{O_3}$, is a prognostic variable of the model. Its evolution is governed by the passive tracer equation (Eq. (18), similar to Eq. (2) but in three dimensions (3D)), where $V$ is the wind vector. Over the time window of the assimilation, the ozone photochemical production and loss terms are neglected, as well as the other sources and sinks: convection, turbulent diffusion, dry and wet deposition ... 

$$\frac{\partial R_{O_3}}{\partial t} + V \cdot \nabla R_{O_3} = 0.$$  

(18)

When the observations consist of ozone columns, the $H$ operator is the sum over the model layers of the ozone mixing ratios, $R_{O_3}$, forecast at the times and locations of observations.

(b) Experimental procedure

The model horizontal resolution is T63. There are 31 levels in the vertical, with the top at 5 hPa. The date chosen for the study is 19 February 1997; it corresponds to a well documented case of the Fronts and Atlantic Storm-Track EXperiment (FASTEX) (Desroziers et al. 1999; Janisková et al. 1999).

The 3D ozone fields necessary to the experiments are obtained with the 3D chemical transport model REPROBUS (Lefèvre et al. 1994; Lefèvre et al. 1998), from a run of several months. REPROBUS is composed of a comprehensive chemical scheme for the stratosphere, involving more than 50 chemical species or transients, and a semi-Lagrangian advection scheme driven by four daily ECMWF analyses; the ozone columns computed from REPROBUS 3D fields compare quantitatively well with the measurements by the TOMS instrument over the month of February 1997. Fields were interpolated horizontally and vertically onto the T63L31 ARPEGE grid used for the present experiments. The use of more sophisticated techniques, involving the intermediate use of a two-dimension (2D) (potential vorticity equivalent latitude or passive tracer equivalent latitude, potential temperature) coordinate system (see, for instance, Lary et al. (1995) and Peuch et al. (personal communication)) to transfer ozone data from REPROBUS to ARPEGE, was tested; in our idealized experiments, the improved consistency of the initial ozone field with the dynamics of ARPEGE did not have a significant impact and the corresponding experiments are not reported here.

Observing-system simulation experiments (OSSEs) were performed. Two initial states are built, both valid on 19 February 1997, at 00 UTC. One is defined as the 'truth', the exact atmospheric state at that time. The other is taken as the background, starting point of the assimilation. The 3D ozone field of the background must be taken equal to the one of the 'truth': since ozone is not included in the control variable $x$, the initial ozone field cannot be modified by the minimization and is implicitly considered as perfect. In the present experiments, the assimilation time window is 12 hours long. Observations are generated beforehand over the period from 00 to 12 UTC, with a model run starting from the 'truth'. Except for the experiments presented in section 5(b), the values of the simulated observations are taken to be equal to the exact values predicted by the model, at times and locations of real observations; no noise is added: assimilated observations are thus supposed to be perfect (they are equal to the 'truth'), see Fig. 1.
Figure 1. Observing-system simulation experiment design: simulation and assimilation of observations, 19 February 1997. See text for further explanation.

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<th>TABLE 1. OBSERVATIONS ASSIMILATED IN EACH EXPERIMENT</th>
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<td>Context</td>
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<td>Fully idealized observing-system simulation experiment</td>
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<td>More realistic observing-system simulation experiment</td>
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In addition to ozone columns, the set of simulated observations is also composed of the conventional and satellite data normally used by assimilation systems of operational NWP models. Ozone observations are representative of TOVS ozone-data coverage, as deduced by the retrieval algorithm of the National Environmental Satellite, Data, and Information Service (NESDIS), on the specific date. With the TOVS instrument flying on board NOAA-12 and NOAA-14 satellites on that date, the globe is approximately covered every six hours. NESDIS total-ozone retrievals from TOVS are interesting for our purpose, since the data access is fast enough for an operational assimilation in NWP models. The coverage of conventional and other satellite data, referred to as 'operational data', is the same as that of data actually used for the operational analysis on the date considered. Depending upon the experiment, simulated ozone columns and/or 'operational’ observations are assimilated or not; Table 1 summarizes the data used for each experiment presented in this paper.

Given the experimental set-up, the difference between the ‘truth’ and the background corresponds to the ideal increments, i.e. the increments which perfectly correct the background. As a consequence, the impact of some simulated observations can be evaluated by comparing increments generated by their assimilation with the ideal increments: the closer to the ‘truth’ the 4D-Var analysed field, the more valuable the information contained in the observations. Statistical information about the difference
between the ‘true’ fields and the initial model fields, before and after the minimization process, is another way to assess the impact of assimilated data.

In the OSSEs performed, we are particularly interested in seeing if observations of a passive tracer can, in practice, provide information which can be used to analyse the wind field, as previously shown from a theoretical point of view (section 2). In addition, we focus on the impact on temperature, which is also included in the control variable. Although there is no direct link between ozone and temperature in our model, temperature increments are expected to be induced by wind increments, through the model equations.

4. AN OBSERVING-SYSTEM SIMULATION EXPERIMENT IN A FULLY IDEALIZED CONTEXT

In this section, a fully idealized experiment is presented. Figure 2 sketches the experimental procedure. The ‘truth’ is a two-day forecast valid on 19 February 1997 at 00 UTC, starting from the combination of an ARPEGE analysis and a REPROBUS ozone field both valid on 17 February 1997 at 00 UTC. In such a way, the balance between wind and ozone fields is assured. The three-day forecast from the ARPEGE analysis valid on 16 February 1997 at 00 UTC, is combined with the ozone field of the ‘truth’ to build the background. A first experiment, called OZONE, is performed: in this experiment, perfect ozone columns are the only observations assimilated; they are supposed to be very accurate, with standard deviations of the observational error of only 1% of the column values.

An experiment to investigate the sensitivity to initial conditions is performed, using the adjoint model as explained by Le Dimet and Talagrand (1986); the scalar product involved in the computations is the canonical scalar product. Detailed studies of the same kind can be found in Hall (1986) or in Rabier et al. (1996). The OZONE assimilation provides gradients of the cost function, $\mathcal{J}^o$ (Eq. (17)), with respect to initial vorticity or divergence, usually not equal to zero. See, for example, the gradients with respect to initial vorticity at 100 hPa in Fig. 3. This point illustrates the theoretical aspects recalled in section 2. Moreover, we see that the areas of strong gradients of $\mathcal{J}^o$ are domains with strong horizontal gradients in the total-ozone initial field; this field, deduced from the 3D distribution of the tracer mixing ratios, is presented in Fig. 4. The areas of strong gradients in the cost function denote high sensitivity to wind initial conditions: the modification of the initial state needed to get a given variation of the cost function is smaller if introduced in the areas of strong gradients than if introduced in domains of weak gradients. As a consequence, it is expected that the 4D-Var assimilation will tend to generate wind increments in the domains of strong gradients of $\mathcal{J}^o$. 

Figure 2. Construction of the ‘truth’ and the background in the fully idealized experiment.
Figure 3. Gradient of the cost function, $\mathcal{J}$, with respect to initial vorticity, at the 100 hPa level for 19 February 1997. The values have been normalized by their maximum. Contour intervals are 0.2 from $-0.4$ to 0.4, and 0.1 from 0.4 to 1.0 and from $-1.0$ to $-0.4$. The dashed lines correspond to negative values.

Figure 4. Total-ozone field for 00 UTC 19 February 1997, in Dobson units.

The study of increments indicates a positive impact of ozone columns upon wind analysis. Some reasonable agreement can be observed locally between ideal wind increments and wind increments generated by OZONE, especially over the northern hemisphere where the wave activity is more important and consequently the total-ozone gradients more pronounced. See, for example, 100 hPa ideal increments (Fig. 5(a)) and OZONE increments (Fig. 5(b)), over North America and the north-east part of the Pacific Ocean, or over Europe and Russia. At this level, the correlation between ideal and OZONE increments over the northern hemisphere ($30^\circ$N–$90^\circ$N) is equal to 0.73. OZONE increments over the southern hemisphere are also satisfactory, with a
Figure 5. Wind increments for 00 UTC 19 February 1997 at 100 hPa: (a) ideal increments, (b) increments of the OZONE experiment, and (c) increments of the OPER experiment. See text for further explanation.
Figure 6. Fit of wind background (bold) and analysis (thin) of the OZONE experiment (see text), to the 'true' fields, over the northern hemisphere, the tropical domain and the southern hemisphere, for the zonal and meridional components, at 00 UTC 19 February 1997: Biases (triangle) and standard deviations (circle) of the difference ('true' fields minus assimilation fields) are presented.

Figure 7. Fit of wind trajectory from the background (bold) and from the analysis (thin) of the OZONE experiment (see text), to the 'true' fields, at 12 UTC 19 February 1997. Symbols as in Fig. 6.
correlation coefficient between ideal and OZONE increments equal to 0.71. The wind is less correctly analysed over the tropics where the total-ozone field is more uniform (coefficient of 0.40 at 100 hPa). In comparison, the assimilation of simulated perfect 'operational' data, in an experiment called OPER, generates increments (Fig. 5(c)), whose correlations with ideal increments at 100 hPa are 0.92 over the northern hemisphere, 0.90 over the southern hemisphere and 0.65 over the tropical domain. It is interesting to notice that, at the level considered, the correlations between ideal and OZONE increments over the northern and southern hemispheres are similar to those between ideal and OPER increments over oceanic areas (Pacific and Indian Oceans) where remote-sensing data are almost the only data available.

The positive impact of ozone data spreads to a large fraction of the atmospheric column, as shown by Figs. 6 and 7 representing respectively at 00 and 12 UTC how wind fields, before and after the analysis, agree with the 'truth' in terms of biases and
standard deviations. Over the northern and the southern hemispheres, both zonal and meridional wind components are considerably improved over the whole column. At the end of the assimilation window, the standard deviations between initial and ‘true’ fields are reduced, for instance at the 250 hPa level, for the zonal (meridional) component, from 5.12 to 2.73 m s\(^{-1}\) (from 4.92 to 2.42 m s\(^{-1}\)) over the northern hemisphere, and from 7.81 to 5.64 m s\(^{-1}\) (from 9.13 to 5.76 m s\(^{-1}\)) over the southern hemisphere. Lastly the tropical wind fields are slightly improved by the analysis, except for a degradation of the zonal-wind bias at upper levels. It can be seen that the impact increases within the assimilation window: over the period from 00 to 12 UTC, the forecast from the guess undergoes an error growth, while the analysed trajectory takes advantage of the assimilated data. It can also be noted that an analysis of similar quality is produced at the beginning and at the end of the assimilation window. In the rest of the paper, comparisons between assimilation fields and ‘true’ fields will be presented at 12 UTC, considering that, if a forecast was to follow the analysis, it would start from the analysed fields at 12 UTC.

Concerning temperature analysis, increments generated by the 4D-Var assimilation are, as expected, in areas of strong wind increments (see Fig. 8(a)). They correspond rather well with ideal increments (Fig. 8(b)), but with a significantly smaller amplitude. Figure 9 presents the fit of temperature fields to the ‘truth’ at 12 UTC, before and after the assimilation process. A clear positive impact is found over the northern and the southern hemispheres, except for the bias at some levels, in particular at the top of the model over the northern domain. There is also an indication of an improvement in the initial state in the tropics, smaller than in the two other verifying areas, in relation to the weakness of the geostrophic relation over this domain.

In summary, an important positive impact was found in this OSSE, on the flow analysis as well as on the temperature. However, the experimental design is very much idealized: the OSSE context of course, but also the excellent accuracy of the observations. Moreover, the quality of the background is poorer than the one of an operational background, and hence provides more opportunities for assimilated observations to be useful. Next, another OSSE was performed in a context closer to an operational design.

5. **AN OBSERVING-SYSTEM SIMULATION EXPERIMENT IN A MORE REALISTIC CONTEXT**

Now, the ‘truth’ is based on an analysis valid on 19 February 1997 at 00 UTC, which was obtained with the 3D-Var system currently used operationally at Météo-France. A
Figure 10. Fit of wind trajectory from the background (bold solid), from the analysis of the OZONE10 experiment (see text) (thin solid), and from the analysis of the OZONE01 experiment (see text) (dashed), to the ‘true’ fields, at 12 UTC 19 February 1997. Symbols as in Fig. 6.

REPROBUS 3D ozone field valid at that time is added to the 3D-Var analysis to get the ‘truth’; it is added to a six-hour forecast to get the background.

(a) Perfect ozone observations

Two experiments in which only simulated perfect ozone columns are assimilated were performed. In the first experiment, the standard deviations of the observational error are assumed to be equal to 10% of the column values (OZONE10 experiment); in the second one, to 1% (OZONE01 experiment). In such a way we can assess the impact of total-ozone data for a wide range of measurement accuracy. It is admitted that the accuracy of current observations of total ozone is between these two limits. As far as TOVS retrievals from NESDIS are concerned, the accuracy is about 5% and, occasionally, worse.

The comparison with the ‘truth’, of the wind fields at 12 UTC, before assimilation, after OZONE10 analysis and after OZONE01 analysis, is presented in Fig. 10. A generally positive impact is found in both experiments. It is, however, smaller in OZONE10 than in OZONE01, according to the relative confidence given to observations. More precisely, in OZONE10 the definition of the initial flow state is improved principally over the northern hemisphere. Over this domain, the slight improvement extends over much of the atmospheric column, from 400 to 10 hPa. Over the tropics and the southern hemisphere, there is an indication of a very slight positive impact in the stratosphere only. OZONE01 results show a significant positive impact on both wind components over the northern hemisphere, particularly from 500 hPa to the top; the standard deviations between initial and ‘true’ fields at 12 UTC are thus reduced by 0.49 m s\(^{-1}\) for the zonal component at 300 hPa, and by 0.71 m s\(^{-1}\) for the meridional component at
200 hPa. Over the tropics, the improvement of the initial wind in the upper stratosphere, already observed in OZONE10, is greater with the assimilation of better data; over the southern hemisphere, it is not only more pronounced, but it also applies to most of the vertical. When measurements with 10% accuracy are considered, a marginal positive impact is seen over the whole globe, in the stratosphere, for the temperature fields (not shown). Although the positive impact is also small in OZONE01, it concerns a wide part of the atmospheric column over the northern and the southern hemispheres. For example, the maximum reduction in the standard deviation of the error at 12 UTC is from 0.78 to 0.64 K at 200 hPa over the northern hemisphere, and from 0.25 to 0.12 K at 20 hPa over the southern hemisphere. These runs provide a confirmation of the potential use of ozone data in a more realistic context than in section 4; however, assimilated observations have still been built to be perfect.

(b) Non-perfect ozone observations

In some additional experiments, ozone columns were simulated in a less optimistic way. Each simulated observation is now the sum of the ‘truth’ (exact model forecast) at the time and location of a real observation, and of a deviation. The added noise is distributed according to an unbiased Gaussian distribution. Firstly, its standard deviation is set to 1% of the ‘true’ column. Ozone data are then assimilated with standard deviations of the observational error equal to 1%; ‘operational’ observations are not used (OZ01-NOISE experiment). The positive impact on the flow analysis noticed in OZONE01 over the northern hemisphere is still observed in OZ01-NOISE, although the amplitude of the impact is smaller (not shown). Over the southern hemisphere, the impact contains more contrast, with a slight positive effect on the zonal component of the wind, but a marginal one on the meridional component. OZONE01 and OZ01-NOISE results seem to be most different over tropical areas, where a clear degradation in the initial definition of the meridional wind is induced by the noisy ozone columns, particularly around 150 hPa. A comparison (not shown) of OZ01-NOISE wind increments and ideal increments reveals that the negative impact is concentrated over an area without ozone observations during the 12-hour assimilation window and with the strongest flow for the tropical domain. The 4D-Var system appears to be insufficiently controlled when there is no other information than the background, and it tends to generate large inconsistent increments. Lastly, it can be added that the impact upon temperature analysis is marginal, sometimes positive and sometimes negative.

If the noise added to the ‘truth’ follows a Gaussian distribution, still with zero mean but with a standard deviation of 10% of the ‘true’ column (OZ10-NOISE experiment), the assimilation of ozone data leads to a significant negative impact on the analysis. During the minimization process, the gradient is correctly reduced but the value of the cost function remains nearly unchanged; the ratio of the final value to the initial one is equal to 0.9895. It happens as if there was no sensitivity to the initial wind. We have investigated the variation of the initial cost function, \( \mathcal{J}^0 \), according to different values of initial wind velocities, when ozone columns of varying quality are assimilated. In practice, values of \( \mathcal{J}^0(\alpha V) \) with \( V \) the 3D background wind and \( \alpha \) a coefficient varying from 0.5 to 1.5, were computed by considering five different sets of noise added to ‘true’ ozone columns; the five sets differ only by the standard deviation of the noise distribution equal to 1%, 2%, 3%, 5% or 10% of the ‘true’ columns. Figure 11 shows how the larger the standard deviation of the ozone column’s noise, the less sensitive to the winds \( \mathcal{J}^0 \). When the standard deviation of the noise is 3% of the ‘truth’ or more, the distance between the model total-ozone fields and the observed columns over the period from 00 to 12 UTC is not significantly modified, whatever the wind velocities at
Figure 11. Variation of the initial cost function, $g^0$, with wind velocities at 00 UTC 19 February 1997. Wind velocities tested are $uV$, with $V$ the three-dimensional background winds and $u$ a coefficient varying from 0.5 to 1.5. Observations considered in $g^0$ are simulated ozone columns, including Gaussian noise with increasing standard deviations.

00 UTC are within a wide range of values. In our experimental design, where the initial ozone field cannot be modified, a noise standard deviation of only 2% for the total-ozone observations can be considered as the threshold below which the assimilation has a globally positive impact on the wind analysis; it corresponds to standard deviations of the observational errors of the order of 5 to 10 Dobson units (DU).

(c) Complementary or redundant information?

With the previous experiments, it is not possible to conclude if the amount of information provided by total-ozone observations (under some conditions concerning the data accuracy) is complementary to information brought by data currently used in NWP models or if it is simply redundant. To investigate this point, both perfect ‘operational’ data and total-ozone columns were assimilated in an experiment called ALLDATA. The standard deviations of the observational errors are supposed to be equal to 1% of the columns. In an other experiment called OPER2, only perfect ‘operational’ data were assimilated; this experiment is similar to OPER (section 4), but in a more realistic context. The definition of the model initial state is improved by both assimilations, with a positive impact of assimilated data quantitatively rather similar in both experiments. The specific impact of ozone data can be assessed by comparing the fit of analysed fields, for both experiments, with the ‘truth’ (not shown). No additional information on the wind field is brought by ozone data over the northern hemisphere, where the existing operational observation coverage is rather satisfactory. In contrast, some information is provided in the stratosphere over the tropics and over the southern hemisphere; it induces an error reduction of 0.15 m s$^{-1}$ from 50 hPa to the top of the model. The additional information brought by ozone columns may be more important during more active meteorological periods of the southern hemisphere and may compensate for the scarcity of conventional observations over this domain. Concerning temperature analysis, there is no sign that ozone column observations provide additional information, whatever the geographical domain studied.
Figure 12. Fit of wind trajectory from the background (bold) and from the analysis (thin) of the observing-system experiment, to observations from radio soundings, over the northern hemisphere, for the zonal and meridional components, at 12 UTC 19 February 1997: Biases (triangle) and standard deviations (circle) of the difference (observations minus assimilation fields) are presented. The number of observations treated at each different level are given to the right of the diagrams.

6. LIMITATIONS

As shown by the OSSEs described in sections 4 and 5, total-ozone observations assimilated with a 4D-Var scheme can provide information for the analysis of thermodynamical fields, in the limit of sufficient accuracy. However, the experiments performed suffer from the general limitations of the OSSE approach (reviewed by Arnold and Dey (1986) or Atlas (1997)) and from limitations more specific to our experimental design. We can mention the fact that the same model is used to generate observations and to assess their impact. In addition, since all the observations have been generated with the same model run, ozone data are necessarily consistent with 'operational' data.

Lastly, an observing-system experiment (OSE) was performed in which real TOVS ozone columns from NESDIS are assimilated with prescribed standard deviations of errors of 10% of the columns. The starting point of the minimization is the background used in the experiments of section 5. A strong negative impact of ozone data is found. See Fig. 12 showing how wind fields fit radio-sounding observations before and after the minimization; results are presented over the northern hemisphere only, due to the small number of verifying observations over the other domains. The biases between the total-ozone observations and the total-ozone fields deduced from the 3D distribution of the tracer are sometimes important (for example, occasionally above 50 DU over domains with total-ozone fields of the order of 300 DU). The largest biases are located in some areas with pronounced structures of total ozone, that is where information on the wind field is expected to be derived from ozone observations (not shown). To see the impact of a better balance between ozone and wind fields at the beginning of the assimilation process, a second OSE was performed. It starts from the same background as previously, except for the ozone field initialized with the use of a 2D coordinate system (see section 3(b)). A negative impact of similar amplitude is found. The quality of the assimilated observations may also be questioned. In a third OSE, ozone columns were bias corrected, with a crude correction process far from a real instrumental-bias correction scheme; the negative impact is significantly reduced. For instance, the standard deviation between the zonal-wind analysed field and the radiosounding observations at 250 hPa is now equal to 6.62 m s⁻¹, while it was equal to 8.27 m s⁻¹ in the first OSE. The effect of a systematic bias in ozone observations is important as stressed by another experiment performed in the OSSE context of section 5:
In this extra run, ozone columns are taken to be equal to ‘true’ columns multiplied by only 1.01; though small, this error is sufficient to generate a negative impact upon wind analysis.

All these experiments show that the hypothesis of a perfect initial ozone field made in the context of an OSSE, becomes rather unpracticable when real ozone data are assimilated; ozone should be analysed in addition to usual variables. Moreover, a bias correction scheme is likely to be needed to be able to extract information from ozone data.

7. Conclusions

Some OSSEs have demonstrated that, as yet unexploited, ozone-column data have a potential use in the analysis of thermodynamic fields in NWP models and that 4D-Var algorithms may be useful tools for deriving information on wind and temperature fields from these data in areas with pronounced total-ozone gradients. The dynamical information provided by ozone observations may not be completely redundant in addition to information brought by currently assimilated data, especially over domains where conventional observations are sparse.

The accuracy of total-ozone measurements needs to be good enough to get any additional information from the ozone data. The accuracy of the NESDIS total-ozone retrieval algorithm seems not to be sufficient to extract this additional information. An improvement of the existing retrieval algorithms would be an advantage, if not at the expense of the data access time. It is also likely that ozone profiles provided for particular layers (as can be envisaged from future satellite sounders), and assimilated in the same way, would provide better information on the thermodynamic fields of NWP models. The objective of directly assimilating radiances measured by remote sensing, and sensitive to ozone, may also be aimed at by considering the adjoint of a radiative-transfer model in the 4D-Var system. Moreover, the monitoring of ozone observations and the development of a bias correction scheme seem to be unavoidable for good use of ozone data.

Assimilating actual ozone data is likely to require the analysis of the ozone field in addition to the usual variables. Ozone is to be introduced in the control variable of the 4D-Var minimization. In that way, the 3D ozone field and the assimilated ozone data should present a better agreement and a balance between ozone and wind fields should be obtained. With a full integration of the ozone variable in future NWP models and its assimilation, it is then possible that a definite benefit can be drawn in terms of forecast quality.

Acknowledgements

This work has benefited from several contributors and from the remarks and suggestions by the reviewers and Andrew Lorenc. We would like to thank colleagues of the assimilation team for their support, in particular Philippe Caille. Fernand Karcher, Franck Lefèvre and Vincent-Henri Peuch are also thanked for providing the REPROBUS fields and information on ozone. Some discussions with them and Daniel Carolle have been helpful. 3D-Var fields were kindly supplied by Thierry Bergot.

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A. PEUCH et al.


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