Introduction

The present workshop was organized and sponsored jointly by ECMWF and SPARC[1]. Since 1999 the ECMWF (deterministic) operational forecast model and the 4D-Var data assimilation system have included a full coverage of the stratosphere, with the main aim of facilitating the assimilation of satellite radiance observations which have a significant contribution from the stratosphere. The number and quality of such radiance observations is expected to increase dramatically in the near future, making an accurate representation of the stratosphere in the assimilating model a necessity to be able to take full advantage of these measurements.

Significant progress has been achieved in the quality of the representation of the stratosphere in the ECMWF system, but some substantial problems remain.

Stratospheric processes play a significant role also in the earth's climate, and recognising the importance of these processes for the climate system was the reason for the setting-up of the SPARC programme. Both ECMWF and SPARC will benefit from a better understanding and a better representation of stratospheric processes in the models.

The workshop followed the usual format of invited lecturers followed by discussions in working groups and it concluded with a plenary session. Groups were set up to consider the subjects of: "Data assimilation", "Modelling issues", and "Processes". The discussions and recommendations of the three working groups are summarized in the following three reports. The contributions to the workshop have been posted on the ECMWF web site (http://www.ecmwf.int/publications/)

ECMWF and SPARC thank all the participants for contributing to a successful and stimulating workshop.

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[1] SPARC, the research project to study Stratospheric Processes and their Role in Climate was set up in 1992 by the World Climate Research Programme (WCRP)

1. Working Group 1: Data Assimilation

Participants:

A. O'Neill (chair), T.McNally (sec), A.Simmons, E. Andersson, A. Dudhia, N. Bormann, S.Pawson, A.Dethof, B.Kerridge, E.Holm, W.Lahoz, R.Menard, L.Thomason

General positive comments on the ECMWF system:

- A good representation of the stratosphere (in terms of resolution / domain / species)
- Good levels of diagnosis / data organization / tools / external provision
- Good forecast performance improvements
- Healthy analysis diagnostics (e.g. fit to assimilated and passive observations)
- Improved near-real-time observed data availability through collaboration with data producers
- Exploitation of novel datasets / interaction with data producers

1.1. Issues in need of attention

The group noted that there are significant biases (actually time / spatially varying systematic errors) in all fields of the forecast model that may hinder the quality of forecasts and the assimilation process. While a number of factors certainly contribute to these biases, it was considered that progress in the area of gravity wave drag parameterization to be very important (and suggested the use of extended range forecasts in such development)

The group noted the importance of capturing an accurate representation of the Brewer-Dobson circulation and mixing barriers and suggested the inclusion of longer-term tracer species (e.g. N2O/CH4, either as passive variables or explicitly assimilated) would assist this development. The key deficiency (from the viewpoint of this working-group) is the increments from the data assimilation system.

The group noted the important role of the Jb formulation within the assimilation system and discussed several aspects in detail. The very general point was made that development of the analysis system as a whole needs to be kept sufficiently flexible to allow for the particular characteristics of the stratosphere and future expansions of the scope of the assimilation system (e.g. environmental monitoring / applications).

The need to calibrate and retune the background error covariances for the stratosphere was stressed, considering the particular types of error encountered (e.g. a different mix of random and varying systematic errors compared to the troposphere). The group encouraged the use of non assimilated (independent) observations to validate and possibly contribute to the estimation of the error covariances. The specification of explicit correlations among tracers and between tracers and the dynamic variables in the error covariance was considered an important omission from the current system that should be rectified.

The issue of imposing additional constraints upon the assimilation system was discussed, such as balance and conservation. This area should be explored further.

Biases in the data and observation operators were considered to be a serious limiting factor and the group encouraged more progress in this area. In particular the approach of dealing with systematic errors within the analysis was suggested. However, the need for more use of existing independent data (from e.g. satellite and LIDAR, and in situ research data) was also identified. To this end it was thought that a greater level of external (e.g. WMO and the space agencies) organization and communication of such data to NWP centres should be encouraged.

The lack of knowledge of the accuracy of representation of tides in the ECMWF system was seen as a weakness.

1.2. Issues related to the observing system

The group noted that in general there is a significant volume of observational data relevant to the stratosphere from both operational and research missions. The AMSUA was identified as a particular example of a stable, well calibrated instrument with excellent time continuity that is having a significant positive impact upon the stratosphere. Good column values of ozone are available (from GOME/SBUV/TOMS), with ozone profile information from research satellites (and good prospects for expansion in the future ENVISAT /AURA).

ECMWF should continue to evaluate the need / value of LIMB data and the case for expanded operational deployment of such instruments.

A lack of organization and communication between the wide variety of research missions was seen as a problem. Also, while there are some good examples of research data being used in an operational environment (AIRS / scatterometers) there is no clear path from research to operations for many of the current / planned missions (factoring in NRT data availability for example).

The aircraft observations should be expanded, preferably by upgrading operational instruments to provide more comprehensive information (as MOZAIC).

ECMWF should investigate role of the R/S and satellite data in the current system and consider OSE / OSSE to evaluate the need for particular additional observing systems (e.g. stratospheric winds and high resolution water vapour). The current lack of stratospheric wind and humidity data is seen as a particular problem and the case could be strengthened with such experiments.

More comprehensive radiosonde time and location info should be provided and the group encouraged further improvements to humidity sensors (- communicated to WMO) Also, the NRT aspects of ozone sondes and ground based data should be improved.

Aerosols measurement (IR v VIS/UV with each having strengths / weaknesses) needs better integration of existing / future observation missions with a view towards providing useful NWP products (supporting RT modelling / parameterization / aerosol prediction)

1.3. Issues related to data assimilation methodology

The analysis formulation should continue to be developed in the direction of increased state dependence. The group stressed the importance choosing control variables and representations that facilitate the treatment of crucial regions such as the UT/LS and shear zones, and the wider issue of tropospheric / stratospheric exchange (e.g. humidity).

ECMWF should consider strategies for incorporating constituent modelling / assimilation for both NWP and environmental monitoring.

It should also keep open the options for the exact interface to the analysis used for the assimilation of remotely sensed data (i.e. retrievals and radiances).

Radiative transfer observation operators (i.e. RT models) should keep pace with the variety of measurement approaches (UV), but also keep pace in terms of adequate sophistication with new instrument developments.

1.4. Miscellaneous

Continue reanalysis activities (the group noting special interest in periods of the 1980s and 1990s that include significant volcanic events) and support for users (data access frequency / resolution of analyses / post-processed products and external availability to CTM users).

Investigate the location of the upper boundary and its impact on radiance assimilation and systematic errors in the assimilating model.

The group encouraged strong links between ECMWF and the wider stratospheric modelling community (e.g. SPARC).

2. Working Group 2: Modelling Issues

Participants:

J. Thuburn (chair), A. Untch (secretary), L. Bonaventura, M. Chipperfield, G. Roff, M. Miller, T. Shepherd, R. Swinbank

2.1. Dynamics

2.1.1. Mean meridional circulation and vertical transport

An accurate representation of the mean meridional circulation is crucial for accurately modelling the stratosphere: it directly affects temperature and constituents, and these in turn have further effects for example through chemistry and radiation. However, the mean meridional circulation is extremely difficult to observe directly and the data assimilation process does not constrain it well.

In the ECMWF model vertical transport, e.g. of ozone, appears to be excessively fast in the stratosphere. Some investigation is needed to determine the extent to which this is due to (a) excessive mean meridional circulation, and (b) vertical advection errors when the mean ascent is a small residual of a highly variable field. If the mean meridional circulation is excessive, some investigation is needed to determine the extent to which the problem is inherent in the free-running model, and the extent to which it is exacerbated by the data assimilation processes. (Excessive vertical transport of tracers, although not an excessive mean meridional circulation, is characteristic of chemistry-climate models). If vertical advection errors are significant then a higher order advection scheme, or possibly an alternative model vertical coordinate, should be considered (see below).

An important issue to understand is whether the addition of balanced wind and temperature increments in data assimilation, to compensate for incorrect or missing model gravity wave drag, will corrupt the vertical velocity field and in particular the mean meridional circulation. If so, then great care will be needed to infer anything about gravity wave drag from analysis increments (see below).

2.1.2. Lateral dispersion

Experience at NASA suggests excessive lateral dispersion of stratospheric tracers when using analysed winds for transport, but not when using winds from a free-running GCM. We recommend checking whether similar behaviour is seen with the ECMWF system. If so, the effect of data assimilation on horizontal winds, and any link to similar problems with vertical transport, could be investigated.

2.1.3. Model top, sponge layer and GWD

It is widely recognized in atmospheric modelling that a 3D model must have a "sponge layer" in the top portion of the model in order to absorb upward propagating waves and prevent spurious reflection at the upper boundary. This sponge layer should be considered as providing a reasonable numerical upper boundary condition, and located above the domain of geophysical interest. In order to properly absorb upward propagating waves, the sponge layer should extend over more than one vertical wavelength and should contain about 5-6 vertical levels per wavelength. Assuming a typical vertical wavelength of upward propagating stratospheric waves of order 10 km, this suggests, ideally, a sponge of approximately two scale heights (15 km), with a vertical resolution of about 2.5 km. The sponge drag coefficient should be ramped up slowly over a few layers, and held constant over the top several layers. Overly rapid variations in sponge-layer damping rates, or in layer thickness, can result in spurious reflection at the base of the sponge layer.

It is suggested that analysis information from the sponge layer should not be distributed to users. Rather, it should be understood that in order to provide a high quality analysis, a certain number of model levels need to be sacrificed in a sponge layer above the level of geophysical interest. Because the sponge layer is a numerical device, it is not necessary that the physics in it be particularly accurate. Thus, for example, it should not be necessary to include non-LTE radiation or chemical heating, even though these processes become important (though not dominant) for climate simulation above 65 km.

It was noted above that in order to resolve the stratospheric Brewer-Dobson circulation, the domain of interest must extend through the stratopause region. There is compelling evidence that this is required in order to obtain a reasonable simulation of stratospheric ozone and of wintertime stratospheric polar temperatures. This would suggest that the sponge layer should be located above 0.1 hPa. Moreover, the weighting functions of the nadir-sounding temperature instruments currently being assimilated at ECMWF extend up to 0.1 hPa. Assimilating data within a sponge layer would severely damp the model response to the data and could bias the impact of the data lower down. Hence, this also argues for placing the sponge layer above 0.1 hPa. In light of the arguments in the previous paragraph, this argues for a model lid at approximately 0.01 hPa, or 80 km, with the sponge turning on from 0.1 hPa (65 km).

However it is not enough to raise the sponge layer up above the domain of interest. If a sponge drag acts on the zonal mean zonal wind, then it introduces an unphysical external angular momentum source or sink, which will drive a spurious meridional circulation and lead to unphysical vertical influence well below the sponge layer - in practice, extending one or two scale heights below the sponge. To avoid this sponge-layer feedback, the sponge drag should be constructed to act only on the non-zonal-mean component of the flow.

Moreover, a zonal-mean sponge drag absorbs any momentum deposition applied within the sponge layer, whether it be from resolved or parameterized waves. Such momentum deposition should be driving a meridional circulation, and affecting temperatures and winds well below the forcing level. But if the drag is applied in the presence of a zonal-mean sponge, then its beneficial effects will not be realized. Thus also argues for removal of the zonal-mean component of the sponge drag.

With the sponge acting on only the non-zonal-mean component of the circulation, upward propagating resolved waves will be absorbed in the sponge layer and their angular momentum deposition will drive a meridional circulation. This is as it should be; those waves would have eventually dissipated, at some higher level, and so long as they did not undergo meridional propagation, would have driven exactly the same meridional circulation (in the steady limit) below the model sponge as is obtained when the waves are absorbed in the sponge.

But if the zonal-mean component of the sponge drag is removed, then the model zonal winds will tend to develop an excessive bias. In effect, the zonal-mean sponge drag used by ECMWF has been acting, up to now, as a surrogate for gravity-wave drag, which is believed to be responsible for the control of the zonal-wind speeds in the upper stratosphere and lower mesosphere. What is suggested is that in place of zonal-mean sponge drag, the model employ a non-stationary (non-orographic) gravity-wave drag scheme, which is constructed so as to be angular-momentum conserving. In this way, no spurious circulation feedbacks can arise.

A number of gravity-wave drag parameterization schemes exist, and stratospheric climate modelling groups have some experience in their implementation. The SPARC gravity-wave processes working group, and the SPARC GRIPS project, have important expertise in this area. While the configuration of these schemes remains poorly constrained by observations, there are some constraints and reasonable choices of parameters seem to be able to control the zonal wind speeds in the stratosphere within realistic limits. Useful constraints on the parameters may be obtainable from the increments produced in the assimilation. Serious attention should be paid to the specification of the gravity-wave source spectra for these parameterizations, which are likely to have a larger effect on the results than the choice of the parameterization scheme itself.

It is however important that the momentum fluxes simulated by these gravity-wave drag parameterization schemes be deposited within the model domain, because they must be deposited somewhere, and if they are "leaked" to space then they will not have the beneficial effect on meridional circulation and temperature that they ought to have. (In order to have this effect, the sponge drag must have no zonal-mean component, of course.) Thus, the vertical momentum flow through the model lid should be applied as momentum flux convergence immediately below the lid. As with resolved wave drag, the meridional circulation below the sponge layer induced by gravity-wave drag (in the steady limit) is independent of where the waves are actually dissipated.

Thus, the recommendation is to raise the model lid from 0.1 to 0.01 hPa, with the understanding that the levels between 0.1 and 0.01 hPa would act as a sponge layer and that information on these levels would not be released to the user community; that the zonal-mean component of the sponge layer be removed; and that a momentum-conserving gravity-wave drag scheme be introduced, with all drag applied within the model domain. These recommendations are all coupled to each other.

2.1.4. *Inertial instability*

It has become clear that inertial adjustment is a ubiquitous phenomenon in the tropical upper stratosphere and lower mesosphere during solstice, when the radiative equilibrium temperature has a non-zero gradient at the equator and thus cannot be achieved because it cannot be balanced by any zonal flow. It appears that the resulting thermally forced circulation (rising in the summer hemisphere and sinking in the winter hemisphere) is responsible for a considerable fraction of the annual mean tropical upwelling in the upper stratosphere. Since inertial instability has no natural scale selection and will tend to occur at the minimum vertical scale resolved by the model, models manifest inertial instability in a stack of meridional cells at the vertical grid scale. This could well lead to spurious vertical mixing. This is not numerical noise, but a physical instability which manifests itself at the grid scale.

Thus, the recommendation is to diagnose the presence of inertial adjustment in the model (and in the analyses), and to explore the possibility of parameterizing the effect (e.g. through the parameterization of Holton and Wehrbein). With a parameterization, vertical diffusion of tracer species should be reduced, which should have a positive effect on the modelling of trace species.

2.1.5. *Vertical resolution*

Several criteria for what might constitute sufficient vertical resolution were discussed. These included ability to resolve equatorial waves important in driving the QBO, and ability to resolve the temperature minimum and other Tropical Tropopause Layer processes such as thin cirrus that might be responsible for the final stage of dehydration. The importance of smoothly varying layer thickness was emphasized whenever simple finite difference approximations are used for vertical derivatives.

2.1.6. Vertical advection

The issue of vertical advection, including the trade-offs associated with quasi-monotone schemes, and the problems associated with spline interpolation near boundaries, should be revisited. The vertical velocity, especially in the "tape recorder" region should be looked at. If the mean ascent is a small residual of very large variations (as Gregory and West found with the Met Office UM) then a higher-order scheme should be considered.

2.1.7. Vertical coordinate

Despite some advantage for vertical transport, the difficulties of implementing a hybrid isentropic vertical coordinate make it unattractive at present. A quasi-lagrangian vertical coordinate (following Lin and Rood) might offer a similar advantage while being simpler to implement. These options should be considered if the problems with vertical transport cannot be resolved by simpler measures.

2.1.8. Mass conservation

The importance of conserving mass and tracer mass for certain problems was noted. However, the lack of exact mass conservation is not currently thought to be a serious problem for ECMWF (though it may become an issue for long seasonal forecasts). Conservative or not, it is important to ensure that the treatment of mass and tracers is consistent.

2.2. Chemistry

2.2.1. Prognostic Ozone

a) Investigate performance of current Cariolle-Déqué Scheme

There are clearly discrepancies between the forecast O3 field and observations. The Antarctic O3 hole appears seriously underestimated by the free-running model. The zonal mean O3 has a negative bias in the tropics and a positive bias in the mid-latitude extra-tropics.

The formulation of the Cariolle-Déqué scheme should be examined. (The method dates from the early 1980s when our knowledge of stratospheric O3 was much less complete). The results of the 2D model used to generate the 'climatology' should be compared to the observations to see how realistic it is. The coefficients of the scheme should be examined to see how important the different terms are in the bias. For example, comparison against a full chemistry scheme within a 3D CTM run could be useful.

The 'polar term' should be modified. The '195 K' threshold for PSC chemistry should be a function of altitude. The coefficients c4 should be checked against estimates based on observations (e.g. 3 ppmv O3 loss in 6 weeks at 20 km for 3.5 ppbv Cly). They can be recalculated as a function of height from observations. The dependence of the polar chemical loss on Cly under fully activated conditions is near-linear. The parameterisation should reflect this.

It would be useful to add a passive O3 tracer to the model. This can be used to separate dynamical and chemical change, e.g. diagnosing chemical O3 loss during Antarctic spring and in the lower stratosphere on seasonal timescales.

A surface sink should be included in the O3 scheme.

b) Explore better O3 parameterizations

The current parameterization is useful. However, it should be possible to improve it while still using just one tracer.

The current scheme is based on 2D model output which is likely not realistic (either in O3 amounts or tendencies). 3D CTMs produce much better O3 simulations and a scheme can be based on this.

The formulation of this new scheme could still follow the method of Cariolle-Déqué (see above) or be based on variations of linearised O3 scheme (e.g. LINOZ from Prather et al.) or other schemes.

c) Coupling prognostic O3 to radiation scheme

It will be important to couple the model prognostic O3 to the radiation schemes in the future. Given the current problems in O3 this should not be done now. This can be done when the scheme is improved and validated (as above).

2.3. CH4 Tracer

It would be useful to have a long-lived tracer in the model for diagnostics of the dynamics (e.g. BD circulation). The tracer could be any source gas (e.g. N2O) but if it was actually CH4 it would allow coupling with the stratospheric H2O scheme.

2.4. H2O

Extension of the model to the mesosphere may require inclusion of the chemical sink of H2O at high altitudes. Simple parameterizations exist (e.g. in current CH4/H2O GCM schemes).

3. Working Group 3: Processes

Participants:

H. Wernli (chair), M. Hortal (secr.), T. Peter, D. Fonteyn, J.J. Morcrette

3.1. Ozone

Ozone profile near the tropical tropopause. Verify with respect to ozonesondes whether the prognostic ECMWF ozone is more or less accurate than Fortuin & Langematz climatology (there exists a CD Rom dataset from project SHADOZ by Ann Thompson).

Cariolle & Deque parameterization: The threshold of 195K for heterogeneous chemistry activation should be made altitude-dependent and the memory of activated chlorine should be taken into account somehow (even after the temperature goes above the threshold). This parameterization is a very useful starting point but it will be useful to compare the ozone produced using it with results from chemical transport models (CTM's) and with MIPAS-like observations.

3.2. Vertical resolution and upward extension

In radiation, when the model top exceeds 60 Km we might have to include the effect of non-equilibrium radiative processes. It would be nice to have such a scheme available at ECMWF for testing and for assessing the magnitude of their influence.

High vertical resolution has a large influence on the accuracy of chemical models.

At about 85 Km altitude we might have to take into account the chemical heating.

3.3. Global circulation (in particular tape-recorder effect)

Is the too fast tape-recorder signal coming from too large mean vertical velocity at the equator, from variance in the vertical velocity or from excessive numerical diffusion either horizontal or vertical?.

There is concern in the user community about the quality of the vertical transport in the different datasets at ECMWF and at other modelling centres, as diagnosed by different methods. Data assimilation seems to make the problem worse rather than better.

Would it be possible to include N2O as a forecasted and analized quantity in the ECMWF model? (it is one of the best inert tracers, characterized by strong N-S gradient in the middle stratosphere). Would that improve the assimilation of wind in the stratosphere?.

We should aim to produce accurate winds in the tropopause region (3D).

3.4. Cloud parameterization:

Need to make the cirrus-cloud parameterization more physical. Cirrus clouds form at 150% RH due to homogeneous nucleation. They might cross the tropopause at the tropics with a supersaturation of about 20%, according to current microphysical studies.

The observed variability of cirrus clouds is very large, both in terms of particle size and optical properties.

3.5. Water vapour in the stratosphere

MIPAS is moist w.r.t. ECMWF analysis but dry w.r.t. HALOE.

Need for a systematic validation of ECMWF moisture analysis in the stratosphere compared with all available data sources (see SPARC assessment report on stratospheric water vapour).

Investigate whether the discrepancies come from methane oxidation or from cross-tropopause transport at the tropics.

Investigate the sensitivity of the forecast to the water vapour just above the tropopause.

3.6. Data availability:

Archive of diabatic processes (3D fields) from ERA40 is very useful.

It could be very useful to create user groups of a certain product.

It will be very useful to produce a short period (to be decided) of data assimilation with as many fields as possible archived every time step.

3.7. Recommendations

- Validate the prognostic ozone in the model by collocation (comparing it with individual vertical profiles) and by comparison with the results of CTM's.
- Validate the RT model, which assumes local thermodynamic equilibrium (LTE), by comparison with other (including non-LTE, perhaps more expensive) available models and through sensitivity studies.
- Parameterization upgrades recommended:
    - Change the Cariolle-Deque chlorine term to make it height-dependent and include memory of the activated chlorine.
    - Take into account the supersaturation in cirrus clouds.
- Assess whether tracer assimilation (such as N2O) will improve the quality of the analyzed stratospheric wind.
- Create user groups of people using a certain product from ECMWF.