Some challenges in the assimilation of stratosphere / tropopause satellite data

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ABSTRACT

Recent developments, notably the wealth of data from research satellites, more sophisticated atmospheric models, and the availability of increasingly powerful computers, provide unprecedented opportunities to extend our knowledge and understanding of the atmosphere. These opportunities bring with them a series of challenges to be met. This paper provides several examples of these challenges, focusing on: (1) assimilation of water vapour data in the stratosphere / tropopause, (2) coupling of dynamics and chemistry components in assimilation schemes, and (3) assimilation of limb radiances. Future directions will be discussed.

1. Introduction

1.1. Importance of the stratosphere / tropopause regions

The stratosphere and tropopause are important for a number of reasons, including (1) the presence of important radiative-dynamics-chemistry feedbacks associated with stratospheric ozone and relevant to studies of climate change and attribution (WMO 1999, Fahey 2003), (2) quantitative evidence that knowledge of the stratospheric state may help predict the tropospheric state at time-scales of 10-45 days (Charlton et al. 2003), (3) the important role that UTLS water vapour plays in the radiative budget of the atmosphere (SPARC 2000), and (4) the need for a realistic representation of the transport between the troposphere and stratosphere, and between the tropics and extra-tropics in the stratosphere, as this plays a key role in the distribution of stratospheric ozone (WMO 1999).

The recognition of the key role of stratospheric ozone in determining the temperature distribution and circulation of the atmosphere has encouraged the incorporation of photochemical schemes of varying complexity into climate models (Lahoz 2003b). At the same time, the discovery of dramatic ozone losses during polar winter and spring (especially over the Antarctic) has led to many studies of the temporal and spatial evolution of ozone and other constituents that make use of sophisticated photochemical models such as CTMs (Khattatov et al. 2003). These activities are providing opportunities to develop climate/chemistry models (e.g. Austin 2002), and a hierarchy of coupled NWP/chemistry assimilation schemes, ranging from the Cariolle scheme (Cariolle and Déqué 1986) which parametrizes the photochemical sources and sinks of ozone, to a fully coupled NWP/CTM system (see, e.g., Lahoz 2003a, b).

1.2. Satellite data

During the past few years, the main space agencies (NASA, ESA, NASDA and CSA) have launched many research satellites, and also are involved in plans to continue launching satellites over the next 10-15 years (Lahoz 2003a). Examples of current and recent satellites include:

(1) *NASA EOS series:*

- EOS-Terra (launched December 1999) carries on board 5 instruments designed to provide information on land surface, water and ice (ASTER), radiation (CERES), radiation and biosphere parameters (MISR), biological and physical processes on land and the ocean (MODIS), and CO and CH_4 in the troposphere, where they are pollution markers (MOPITT).
- EOS-Aqua (launched May 2002) carries on board 6 instruments designed to provide information on clouds, radiation and precipitation (AMSR/E), clouds, radiation, aerosol and biosphere parameters (MODIS), temperature and humidity (AMSU, AIRS, HSB), and radiation (CERES).

(2) *ESA:*

- ERS-2 carries on board the GOME instrument. GOME is a nadir sounder that has been making measurements of total column ozone and NO_2 since 1995. Height-resolved ozone information from GOME is now being produced.
- Envisat (launched March 2002) carries on board 10 instruments designed to provide information on temperature, ozone water vapour and other atmospheric constituents using limb, nadir and occultation geometries (MIPAS, SCIAMACHY, GOMOS), aerosol (AATSR, MERIS), sea-surface temperatures (AATSR), sea colour (MERIS), land and ocean images (ASAR), land, ice and ocean monitoring (RA-2), water vapour column and land surface parameters (MWR), and cryosphere and land surface parameters (DORIS). The LRR instrument is used to calibrate RA-2.

(3) *NASDA ADEOS-1,-2 satellites:*

- ADEOS-1 (launched in 1996) carried several instruments on board, including ADEOS TOMS (which measured total column ozone) and ILAS (a limb instrument which measured temperature, ozone, water vapour and other atmospheric species). The ADEOS mission only lasted for 10 months.
- ADEOS-2 (launched in December 2002) carries on board 5 instruments designed to provide information on water column, precipitation, and ocean and ice parameters (AMSR), land, ice and biosphere parameters (GLI), winds over the ocean (SeaWinds), radiation parameters (POLDER), and temperature, ozone and other atmospheric species (ILAS-II).

(4) *CSA/ESA ODIN satellite:*

- ODIN (launched in February 2001) carries on board 2 instruments (OSIRIS, SMR), and is providing information on ozone and NO_2 (total columns and profiles).

Examples of future satellites include:

(1) *NASA:*

- EOS-Aura is due for launch in early 2004. It will carry on board 4 instruments designed to provide information on chemistry, upper tropospheric water, and the impact of volcanoes on global change (EOS MLS), temperature and species in the UT, stratosphere and mesosphere (HIRDLS), global maps of tropospheric ozone and its photochemical precursors (TES), and maps of total column ozone and UV-B radiation (OMI).

(2) *ESA:*

- CRYOSAT, GOCE, ADM, SMOS are part of ESA's Living Planet Programme, and are due to fly in the middle of the 2000's. CRYOSAT will measure cryosphere parameters, GOCE will measure the Earth's gravity field, ADM will measure winds in the troposphere and lower stratosphere, and SMOS will measure soil moisture and soil salinity.

(3) NASDA:

- GOSAT (new name for GCOM-A1) is due to be launched in the late 2000's. It also involves ESA and CSA. The latest information is that it will carry on board 2 instruments (SWIFT and SOFIS). It will provide information on winds, ozone and other atmospheric chemical species, and CO_2.

This wealth of satellite data is extending our knowledge of the atmosphere by: (1) measuring novel species (e.g. ozone and species involved in its photochemical destruction), (2) extending the range in space and time of observations (e.g. global measurements, higher resolution in the horizontal and vertical, measurements in the UTLS, long-term measurements), and (3) providing measurement synergies (e.g. limb / nadir which can be used to partition tropospheric and stratospheric information).

At the same time, there are many operational satellites (in orbit or planned) that provide data of interest to the NWP agencies, research groups and, potentially, end users of value-added data. Examples of future satellites include:

(1) METOP. These polar-orbiting satellites will carry instruments provided by ESA, EUMETSAT, NOAA and CNES. Instruments include IASI, AMSU-A and GOME-2. It will mainly make measurements of temperature, ozone, RH and clouds.

(2) MSG is a programme of geostationary satellites developed by ESA and EUMETSAT. Instruments include SEVIRI and GERB. It will make images of the Earth's disc, with cloud, land, ocean and ice information for day and night (SEVIRI), and make measurements of the Earth's output radiation (GERB).

Research and operational satellite data provides opportunities for synergy. Different viewing geometries (limb and nadir) can be used with techniques such as data assimilation to improve the representation of the atmosphere, and partition information between the stratosphere and troposphere. This approach is being used to estimate the global distribution of tropospheric ozone (which is very difficult to measure directly from space). A variety of geophysical parameters (dynamical quantities such as temperature, winds and water vapour, and photochemical species such as ozone) are also being used with data assimilation to improve the representation of the feedbacks between dynamics, radiation and chemistry.

Synergy between research and operational satellites, and the potential benefits to the NWP agencies accruing from this synergy, can make it attractive to use research satellites in an operational capability. This can happen in a number of ways: (1) one-off use of research satellite data (e.g. measurement of a key photochemical species such as ozone, or of a novel geophysical parameter such as stratospheric winds), (2) regular use of research satellite data (e.g. a satellite series that can extend the time record of key geophysical parameters such as ozone and water vapour), and (3) use of the research satellite instrument design in future operational missions.

1.3. Atmospheric models

Atmospheric models are being extended in many ways. Some of these developments are associated with increasingly powerful computers. The horizontal resolution is being increased (e.g. ECMWF currently produce analyses at T511 resolution). The vertical resolution is being increased in the UTLS region, which is recognised as a key region for the radiative balance of the atmosphere, and transport between the troposphere and stratosphere (SPARC 2000). The top of atmospheric models is being extended upward to include a comprehensive stratosphere.

These increases in resolution and extensions of the model domain help provide more accurate representations of the atmosphere. Together with appropriate data assimilation methods and adequate computer resources, these model developments can improve our forecasting and long-term capability in a number of ways: (1) extending the range of validity of forecasts, (2) allowing forecasts of novel geophysical parameters (e.g. tropospheric ozone, which is a marker of pollution and a health hazard), (3) making climate models more consistent and realistic, (4) using objective methods to confront and evaluate forecast and climate models with value-added observations.

1.4. Data assimilation

Allied to developments in satellites and models, data assimilation systems used by the NWP agencies to combine information from models ("understanding") and observations ("truth"), are increasingly being used by research groups outside the NWP agencies to study the atmosphere. Photochemical species (chiefly from research satellites) are routinely assimilated into sophisticated photochemical models driven by off-line winds and temperatures (e.g. Fisher and Lary 1995, Khattatov et al. 1999, Elbern et al. 1997, Eskes et al. 2003a, Errera and Fonteyn 2001, Štajner et al. 2001, Fonteyn et al. 2003). Ozone data (chiefly from research satellites) have been assimilated into NWP systems (e.g. Struthers et al. 2002). Research groups across the world are developing algorithms to couple NWP systems (focusing on dynamics-radiation feedbacks) with CTMs (focusing on chemistry-radiation feedbacks).

An example of the use of data assimilation techniques outside the NWP agencies involves ESA, which has recognized the value of data assimilation for a number of tasks, including: (1) evaluation of EO data, and (2) assessment of future EO missions. ESA has set up a team to evaluate Envisat atmospheric chemistry data (from the GOMOS, MIPAS and SCIAMACHY instruments) based on data assimilation techniques using CTMs (groups at KNMI and BIRA-IASB) and GCMs (groups at ECMWF and the DARC at the University of Reading). Preliminary results were presented at the ESRIN Envisat cal-val meeting held in December 2002 (http://envisat.esa.int/workshops/validation_12_02/presentations.html).

ESA is also recognizing the value of data assimilation to assess future satellite missions. ESA is funding Observing System Simulation Experiments (OSSEs; Atlas 1997) to assess the impact of future space missions (in an objective manner). Despite the shortcomings of OSSEs (e.g. use of the same model to create the "nature" run and perform the assimilation; model-dependent results; cost), it is worthwhile to use them to assess very expensive future missions. An example of a recent ESA-funded OSSE involves the SWIFT instrument, due to fly aboard the NASDA GOSAT platform in ~2007. SWIFT will measure stratospheric winds and ozone (important for studies of stratospheric dynamics and photochemistry, and for extending the global observing system). This study suggests that the assimilation of SWIFT stratospheric winds will have a beneficial impact on zonal wind analyses in the mid and upper stratospheric tropics, and in the upper stratosphere extra-tropics. This study also suggests that SWIFT ozone will have a beneficial impact on ozone analyses in regions where the vertical gradient of ozone is relatively high. Lahoz et al (2003) provides further details.

1.5. Computers

With increasingly powerful computers, it becomes feasible for atmospheric models to become more sophisticated, with developments such as: increased resolution, more components of the atmosphere (e.g. inclusion of photochemistry), and replacements of parametrizations by explicit representations of small-scale phenomena. Data assimilation techniques that are computer-intensive, but desirable on theoretical grounds (e.g. assimilation of limb radiances) now become feasible.

Currently, most EO data are accessed off-line and the service provided to the user community (which in Europe involves at least several thousand end-users) is far from being efficient, due to the complexity of product format, algorithms and processing required to meet the specific user needs (e.g. immediate access to integrated information in a form suitable to the end user). Meeting the user needs requires the effective cooperation of all members of the EO community: data providers, scientists, and end users. GRID technology (in terms of networks, distributed computing power, and an environment of collaboration) can and should help support these user needs.

Increased use of GRID technology is starting to make feasible the efficient use of data and models, and is encouraging collaboration and the development of web-based training tools. Examples include numerical experiments with remote access to the most appropriate models and databases, with unnecessary web traffic eliminated or minimized (e.g., http://www.esa.int/export/esaSA/SEMXUES1VED_earth_0.html -- the SpaceGRID project).

Many obstacles have to be removed to realize the efficient use of data and models:

- Access to large EO data archives, including metadata (today mainly available to NWP agencies).
- Common definition of metadata and data formats.
- Adequate network capacity across EO dedicated facilities.
- Access to adequate computing resources.
- Development of real time services.
- Development of effective tools for integrating different data sets.
- Common or compatible data policies for data access.

1.6. Challenges in data assimilation

The wealth of satellite data, developments in models and data assimilation techniques, and increasing computer power provide opportunities to the EO community (see Fig. 1). One notable success was the accurate forecasting of the split of the ozone hole during September 2002 by KNMI and ECMWF (Eskes et al. 2003b, Simmons et al. 2003). These opportunities, however, bring with them a series of challenges (the list is not exhaustive):

- Assimilation of water vapour in the stratosphere and tropopause region (this involves the estimation of the background errors, a challenge throughout data assimilation).
- Assimilation of novel geophysical parameters (e.g. ozone, stratospheric winds) into NWP systems.
- Synergy from measurement geometries (e.g. limb and nadir).
- Coupled dynamics and chemistry components in assimilation schemes.
- Limb radiance assimilation.
- Assimilation of novel photochemical species (e.g. CFC-11, CFC-12, $ClONO_2$).
- Aerosol assimilation (in stratosphere and troposphere).
- Tropospheric chemistry.
- Novel retrieval methods (e.g. tomography).
- Data management.

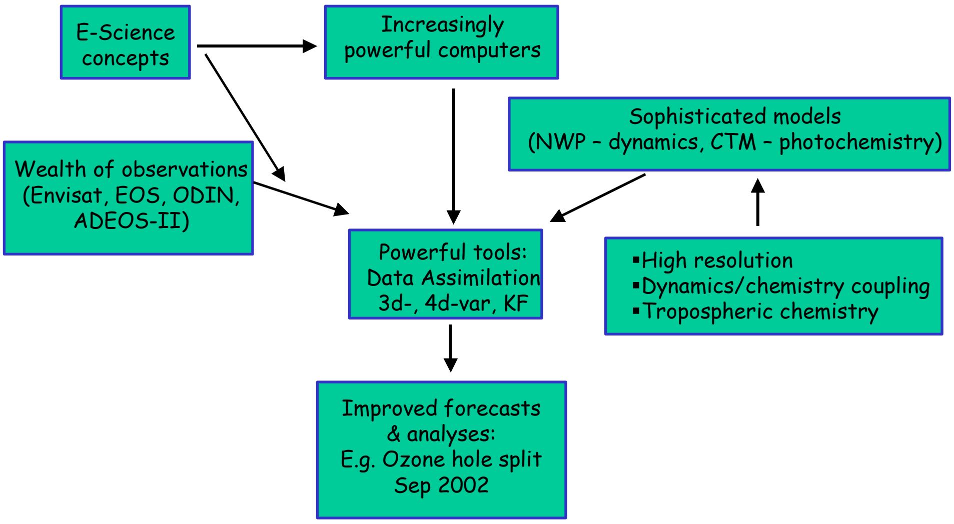

Fig. 1. Schematic of the opportunities offered by observations, models and computers to the data assimilation community.

1.7. The ASSET consortium

ASSET (http://darc.nerc.ac.uk/asset) is a major European initiative to exploit and develop EO data from Envisat using data assimilation. The project runs from January 1st 2003 until the end of 2005. ASSET will add value to the Envisat data by their assimilation into NWP systems and photochemical models, using data from AATSR, GOMOS, MERIS, MIPAS and SCIAMACHY. It aims to: (1) develop a European capability for chemical and UV forecasting, and (2) provide analyses for coupled climate/chemistry studies.

The scientific objectives of ASSET are: (1) to assess strategies for exploiting research satellite data by the NWP community, and (2) to investigate the distribution and variability of atmospheric chemical species by exploiting research satellite data

ASSET brings together experts from all aspects of the assimilation problem and builds on the Envisat calibration/validation effort. The project partners come from across Europe. Beneficiaries include NWP agencies, ESA, climate/chemistry researchers, government, industry and the public. The co-ordinator of ASSET is the DARC at the University of Reading.

The challenges listed in section 1.6 are being addressed by the ASSET partners (the list is not exhaustive):

- University of Reading (DARC) and Met Office (assistant contractor): Assimilation of water vapour in the stratosphere and tropopause region, assimilation of novel geophysical parameters (e.g. ozone, stratospheric winds) into NWP systems, synergy from measurement geometries.
- Météo-France and CERFACS (assistant contractor): Coupled dynamics and chemistry components in assimilation schemes, assimilation of novel geophysical parameters (e.g. ozone) into NWP systems.
- ECMWF: Limb radiance assimilation.
- KNMI: Synergy from measurement geometries, assimilation of novel photochemical species (e.g. NO_2).
- UPMC: Assimilation of novel photochemical species (e.g. NOy).

- BIRA-IASB: Assimilation of stratospheric aerosols, assimilation of novel photochemical species (e.g. CFC-11, CFC-12, $ClONO_2$).
- University of Köln and University of Karslruhe (assistant contractor): Tropospheric chemistry, assimilation of tropospheric aerosols, and assimilation of novel photochemical species (University of Köln). Novel retrieval methods to extend both the number of species measured by MIPAS and the vertical range of the measurements (University of Karslruhe).
- CNR.IFAC: novel retrieval methods (GEOFIT, based on tomographic ideas; Carlotti et al. 2001) to extend both the number of species measured by MIPAS and the vertical range of the measurements.
- NILU: Data management (e.g. standard formats, user flexibility, user-friendly interface, proper documentation).

2. Discussion

2.1. Assimilation of water vapour data in the stratosphere / tropopause

Knowledge of the distribution and temporal variability of water vapour in the UTLS is very important for a variety of current scientific problems. However, our knowledge shows some gaps, partly due to the paucity of long-term global observations of this region, and partly due to the difficulties of modelling some aspects of this region (e.g. convection).

The main impact of water vapour on the radiative balance of the Earth is through the long-wave, infrared part of the electromagnetic spectrum. Water vapour has an intense pure rotation band (50-400 cm^{-1}; 200-25 μm) and a strong ν_2 vibration-rotation band centred at about 1590 cm^{-1} (6.3 μm) (Goody and Yung 1989). In addition, water vapour exhibits “continuum” absorption across a wide range of the infrared spectrum, being most noticeable in the range 800-1250 cm^{-1} (12.5-8 μm; see, e.g., Burch 1981). Because of the strong absorption and emission by these bands, water vapour is the dominant greenhouse gas in the atmosphere.

Current radiative problems that require an accurate knowledge of water vapour distributions include (see SPARC 2000):

- Cooling to space in the UT in the presence of variations in water vapour. In this region there is competition between density and temperature. Emission takes place from a higher and colder layer if optical density increases, and from a lower and warmer layer if optical density decreases. This balance determines the radiative response of the UT to climate change.
- The sign of water vapour feedback in the UT.
- Whether the spectrum of outgoing long-wave radiation (reflecting the impact of water vapour variability), may contain signatures of climate change.
- The radiative impact of changes in stratospheric water vapour.

Water vapour distributions are strongly influenced by atmospheric dynamics, but also influence them in turn. Thus, observed water vapour distributions can serve as useful diagnostics of the atmospheric circulation, especially in the stratosphere where water vapour acts as a tracer on time-scales of about 3 months. Because water vapour condensation is a substantial source of heat in the atmosphere, knowledge of the water vapour distribution is needed for accurate predictions of the atmospheric circulation.

Despite the huge progress made in understanding the pathways of water vapour in the UTLS region and the stratosphere (see SPARC 2000), substantial uncertainties exist. The most prominent is what keeps the stratosphere so dry. Associated with this question is the difficulty that the large-scale phenomenon observed (the dry stratosphere) is likely due to the collective effect of one or more small-scale processes occurring in the tropopause region. The processes controlling the dryness of the stratosphere are very likely to be smaller than the scales represented in models, and also difficult to parametrize. They are also very difficult to observe, possibly because of this small-scale, or because of the difficulty of detection.

Water vapour is important for atmospheric chemistry in several ways. It is the source of OH (which plays a key role in many chemical cycles) in both the stratosphere and troposphere. HOx ($OH+HO_2$) plays an important role in the catalytic cycles that destroy ozone. OH also controls the oxidizing capacity of the atmosphere for short-lived gases and regulates the lifetimes of longer-lived species such as CO and CH_4. Thus it is important to understand the dynamics driving the distribution and variability of water vapour, as well as the photochemical reactions transforming water vapour into OH. Water vapour is also a constituent of PSCs (along with, e.g., HNO_3), and its distribution and variability can influence their presence and thus stratospheric ozone loss via heterogeneous chemical processes (see, e.g., Fonteyn et al. 2003).

The SPARC assessment on UT and stratospheric water vapour (SPARC 2000) made a number of recommendations:

- There is a need to quantify and understand differences between sensors. High resolution *in situ* data to study transport between the troposphere and stratosphere is also needed.
- There is a need for strong data evaluation programmes. Such programmes have been lacking in the UT.
- It is important to have continuity of measurements to determine long-term changes, especially in stratospheric water vapour.
- There is a need to monitor UT humidity to determine its long-term variability. Complementary observations (e.g. satellite, *in situ*) should be used.
- There should be more process studies of UT humidity and convection. To help these studies, there should be simultaneous measurements of water vapour, cloud microphysical properties and tracers with the signature of the "age of air".
- More observations (*in situ* and remote sensing) are needed in the tropical tropopause region (15-20 km) to understand stratosphere-troposphere exchange.
- There is a need to monitor stratospheric water vapour. CH_4 (a source of water vapour in the stratosphere) measurements are desirable. Future satellites should overlap with current instruments.
- Theoretical work is needed to understand the distribution and variability of observations.

Hitherto, there have been no major programmes to assimilate water vapour in the stratosphere and tropopause region. Previous analyses have either set the water vapour field to a fixed amount in the stratosphere (ERA-15; Gibson et al. 1997), or allowed the model to determine the amount of water vapour in the stratosphere (ERA-40).

The DARC, in collaboration with the Met Office, is assimilating stratospheric water vapour observations from Envisat (first MIPAS, subsequently GOMOS and SCIAMACHY) into the troposphere-stratosphere system of the Met Office (Swinbank et al. 2002). This uses the 3-d variational approach (Lorenc et al. 2000).

Assimilation of water vapour (and CH_4) from Envisat in the UT and stratosphere will help remedy the paucity of water vapour analyses in the stratosphere and tropopause region, and will address many of the recommendations in the SPARC report. The quality-controlled analyses produced by the assimilation will: (1) help evaluate water vapour observations (e.g. from Envisat), (2) help studies of climate change and attribution, (3) confront and evaluate forecast and climate models, (4) help studies of transport and dynamics in the UTLS and stratosphere, and (5) help constrain the hydrological budget (of benefit to the simulation and forecasting of precipitation).

The assimilation of water vapour data from Envisat is at a very early stage and results are being evaluated. The water vapour observations assimilated are: ATOVS (HIRS channels 10-12, AMSU-B channels 18-20) and radiosondes in the troposphere, MIPAS in the stratosphere. Currently the assimilation is being done with the so-called “old dynamics” scheme (an Eulerian scheme). The main features of the assimilation are: (1) RH is the control variable (i.e. used in the minimization), (2) the water vapour background error covariance matrix (the **B** matrix) is calculated with the so-called NMC method (Parrish and Derber 1992), (3) in the assimilation the information in the **B** matrix is turned off for levels above ~40 hPa, (4) the **B** matrix includes no flow dependence, and (5) there is no methane oxidation scheme. The so-called “new dynamics” scheme (a semi-Lagrangian scheme), will be available for assimilation of stratospheric variables around September 2003, and will remedy shortcomings in (3) and (5) above.

A number of problems with the existing stratospheric assimilation scheme will need to be overcome (these problems were originally found in the old dynamics formulation, but there is reason to believe they are present in the new dynamics). These include the ill-conditioned nature of the current vertical transform of the **B** matrix. This is currently weighted by the water vapour mass and the standard deviation of the error, and is maximum in the boundary layer. Another problem is that of excessive increments found in the lower stratosphere (e.g. at 50 hPa), suspected to be due to spurious correlations with lower levels in the troposphere, that are moister by several orders of magnitude. Because water vapour (as well as CH_4) is a marker of the stratospheric circulation, results are likely to be sensitive to the accuracy of the model’s advection scheme. Accurate advection schemes for the stratosphere tend to be expensive and are not necessarily the highest priority in NWP assimilation schemes.

To overcome these problems, the Met Office (in collaboration with DARC) is considering a number of possible solutions (in the context of the new dynamics). The **B** matrix will be recalculated: a new vertical weighting and rotation of the vertical modes will be implemented. A special treatment of the tropopause (where the vertical gradient in water vapour changes very rapidly) will be investigated. The performance of the advection scheme will be monitored and, if necessary, other candidates will be evaluated. It is hoped that many of these features will be ready during the last quarter of 2003, ready to be tested by assimilating Envisat water vapour data in the stratosphere and tropopause region.

Another issue that could be investigated includes the use of RH as the control variable (as opposed to specific humidity, used by ECMWF). Although this might make sense in the troposphere for the representation of clouds, it may not be the best approach for the stratosphere due to its extreme dryness. The dependence of RH on temperature could also cause problems (e.g. if the model and observed temperature differ substantially, and the latter is used to make the conversion to RH).

Finally, the explicit representation of flow dependence in the **B** matrix could also be investigated. For example, the ideas of Riishøjgaard (1998) could be applied.

Sample standard deviations for **B** (calculated using the new dynamics) are shown in Fig. 2a, and RH correlations with model level 29 (16 km) are shown in Fig. 2b. Note that this **B** matrix is not currently been used for the assimilation of MIPAS data (as this is done using the old dynamics).

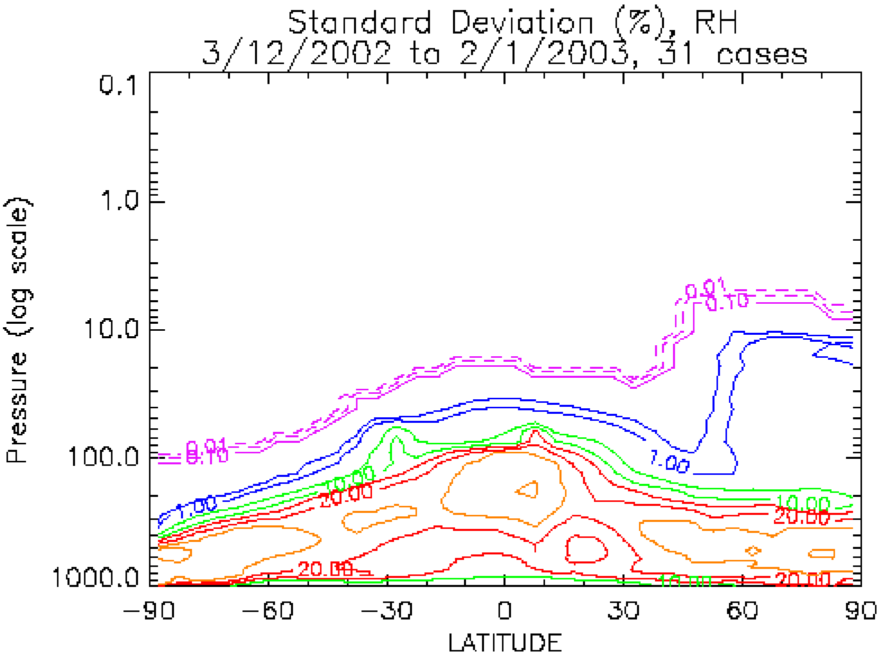

*Fig. 2a. Sample standard deviation for **B** for RH (units of %). Calculated using the NMC method and the new dynamics. Average for the period 3rd December 2002 to 2nd January 2003. Figure courtesy of David Jackson (Met Office).*

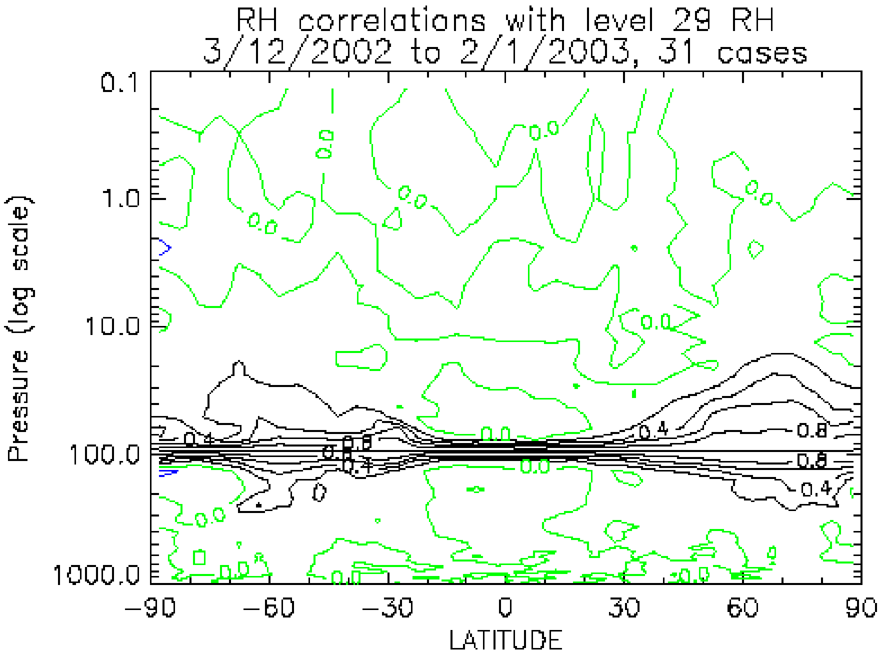

Fig. 2b. RH: Correlations with model level 29 (16km) in the B matrix. Calculated using the NMC method and the new dynamics. Average for the period 3rd December 2002 to 2nd January 2003. Figure courtesy of David Jackson (Met Office).

2.2. Coupling of dynamics and chemistry components in assimilation schemes

Increasing interest in chemical forecasting and climate/chemistry feedbacks, has made more attractive the inclusion of ozone and photochemistry into atmospheric models. Three approaches can be distinguished: (1) GCMs with a sophisticated dynamics formulation, incorporating relatively simple parametrizations of the photochemical sources and sinks of the species of interest (e.g. ozone), (2) CTMs with a sophisticated photochemical formulation, and which are forced by off-line winds, (3) coupled dynamics/chemistry models (e.g. a GCM coupled to a CTM), the coupling done at a number of time intervals (e.g. every time-step; every six hours).

ASSET partners are assimilating a number of Envisat parameters (e.g. temperature, ozone and water vapour. Three approaches are used: (1) NWP system with the Cariolle parametrization (DARC at the University of Reading and Met Office), (2) coupled NWP/CTM system (Météo-France and CERFACS), and (3) limb radiances (ECMWF). This will allow an assessment of different strategies for assimilating research satellite data into NWP systems (objective (1) of ASSET).

The main advantage of GCMs for data assimilation is that they tend to provide the most complete description of atmospheric dynamics, and incorporate feedbacks between dynamics and radiation. GCMs can also incorporate all available observations, including data from operational and research satellites. By incorporating into a GCM a hierarchy of photochemical models (ranging from simple parametrizations to sophisticated models incorporating heterogeneous photochemistry and aerosols), GCMs can take into account the feedbacks between dynamics, photochemistry and radiation.

The main disadvantage of GCMs for data assimilation is their complexity. This means that it can be expensive to incorporate sophisticated photochemical models into GCMs, and techniques such as the Kalman filter (requiring a very high level of computational effort) tend not to be used with GCMs. For large systems such as GCMs, the computational expense of the Kalman filter is in the analysis and the propagation of the covariance matrices. These are two expensive operations, involving the inverse of a large matrix for the former, and applying the tangent linear model/adjoint to elements of a large matrix for the latter. Partly for this reason, assimilation using GCMs tends to be implemented using variational techniques (3d-variational and 4d-variational).

GCMs are used routinely to produce weather forecasts by the NWP centres. Examples include the Met Office (Lorenc et al. 2000) and the European Centre for Medium-range Weather Forecasts (ECMWF) (Simmons et al. 2003). GCMs are also used for research, including the incorporation into operational systems of novel datasets such as ozone (Struthers et al. 2002), and to produce temperature and wind analyses for climate change studies (ERA-15; Gibson et al. 1997). In Struthers et al., the photochemical model used was the Cariolle scheme (Cariolle and Déqué 1986).

Recent developments in assimilation with GCMs include: (1) incorporation of novel atmospheric species, including data such as ozone, (2) extensions to the relatively simple photochemical parametrizations currently in use, (3) incorporation of novel observation geometries, such as limb sounders, (4) improvements in the error characterization of the assimilation model, and (5) radiance assimilation.

The dynamically consistent ozone, water vapour and dynamical fields produced by assimilation of data from several platforms into GCMs provide wind and temperature forcing fields of high quality for assimilation of photochemical species into models with a sophisticated representation of photochemistry (e.g. CTMs).

Assimilation of photochemical data into models with sophisticated photochemistry (CTMs) is increasingly taking place. The techniques used include simplified versions of the Kalman filter, and 4d-variational assimilation.

The main advantage of CTMs is their relatively simpler configuration compared to a GCM. This allows the inclusion of a large number of photochemical species. It also provides a tool for investigating the distribution and variability of atmospheric photochemical species, testing photochemical theories, and producing climatologies of observed and unobserved species (using the model photochemical relations). The main disadvantage of CTMs is that they do not allow feedbacks between the dynamics and photochemistry.

Recent developments in assimilation using CTMs include: (1) extension of models to include novel species, (2) improvements in heterogeneous chemistry, (3) incorporation of aerosols, (4) improvements in the error characterization of the assimilation scheme, and (5) radiance assimilation.

An alternative to GCMs incorporating a photochemical parametrization, is to couple a GCM to a CTM. This is the strategy followed by Météo-France (in collaboration with CERFACS) to assimilate Envisat data into a coupled NWP/CTM system. The coupling between the NWP system and the CTM will be intermittent and will use the PALM software developed by CERFACS. Dynamical variables are assimilated in the GCM (ARPEGE, which is the basis of the NWP system), and photochemical variables are assimilated in the CTM (MOCAGE). The GCM then provides the temperature, winds and humidity input to the CTM. After the assimilation of photochemical variables, the CTM passes the ozone analysis back to the GCM, where it is used in the GCM's radiation scheme. The cycle then repeats. This coupling allows feedbacks between the dynamics, radiation and photochemistry, and aims to combine the advantages of assimilation into a NWP system (assimilation of operational data, sophisticated representation of dynamics and radiation), with the advantages of a CTM (sophisticated representation of photochemistry).

Coupling the NWP and CTM in this way is expected to improve the assimilated winds and forecasts in the NWP model, and provide realistic ozone (and later aerosol) fields to the radiative transfer parametrization of the NWP model. The CTM is expected to provide improved distribution of photochemical species (observed and unobserved), and improved meteorological forcings and improved fluxes in the UV (in both cases via the NWP/CTM feedbacks). The main disadvantages of this approach are the complexity and cost of the assimilation system, although decreasing computing costs tend to make this approach more attractive. Figure 3 is a schematic of the procedure implemented by Météo-France in collaboration with CERFACS.

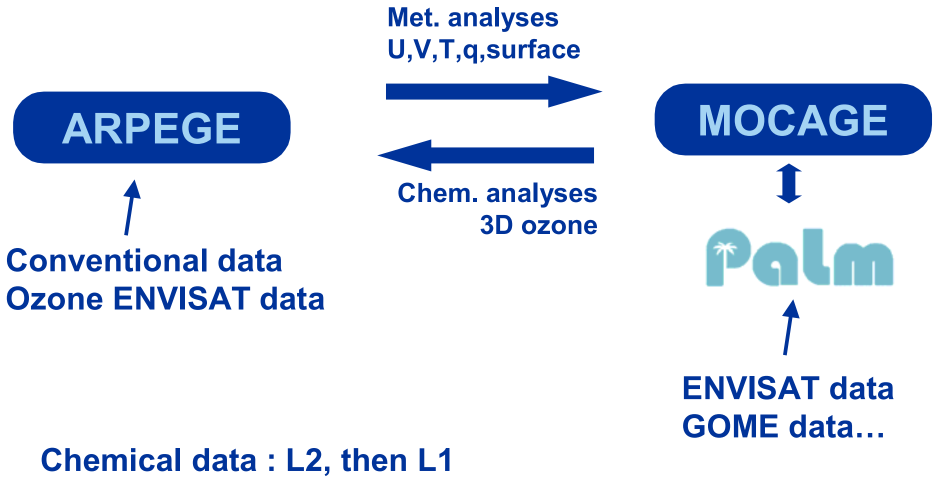

Fig. 3. Schematic of the coupling between the ARPEGE and MOCAGE models. Figure courtesy of Vincent-Henri Peuch (Météo-France).

2.3. Assimilation of limb radiances

The general view in the EO community is that it is preferable to assimilate information nearer in form to the actual data received by the observing instrument (i.e. radiances instead of retrieval profiles). This overcomes some of the shortcomings associated with the retrieval process: (1) the need to include climatological (*a priori*) information to make the problem well-posed and fill in data gaps – this approach tends to "contaminate" the solution, (2) the assumption that measurement errors are uncorrelated (commonly made in the assimilation process, and for reasons of expediency) is not strictly true in the case of retrieval profiles. (Note it is argued that these shortcomings can be overcome to a large extent by performing a SVD of the retrieval data; see, e.g., Rodgers and Connor (2003).) The assimilation of radiances overcomes both of these shortcomings to a large extent, although it has been argued that correlations between radiances can be important. Also, the estimation of observation errors and bias characteristics is generally easier for radiances than for retrievals.

Consistent with this perception, it is widely recognized and operationally established at several centres that direct variational assimilation of the radiances from the nadir-viewing infra-red instruments from the NOAA polar orbiters is a better approach than assimilating retrieval profiles of temperature and humidity (see, e.g., English et al. 2000). An example is also provided by the very successful assimilation of nadir sounder radiances by ECMWF (e.g. assimilation of clear-sky water vapour radiances from geostationary satellites). All these considerations are behind the current drive toward the assimilation of radiances (nadir and limb) in both the operational and research satellite communities.

To assimilate radiances, the observation operator must include a fast and accurate radiative transfer model that, given inputs of geophysical variables (e.g. temperature, water vapour, ozone), will compute a radiance which simulates that measured by the instrument, including antenna and filter effects if appropriate. Generally, institutions involved in the retrieval of data (e.g. KNMI for SCIAMACHY, UPMC for GOMOS, University of Karslruhe and CNR.IFAC for MIPAS) will have one or more versions of a radiative transfer model (needed to perform the retrieval). However, although the radiative transfer model may be accurate, it may not be fast enough for assimilation. Conversely, a fast radiative transfer model may not be accurate enough. This is a non-trivial problem that must be overcome by groups working on radiance assimilation regardless of whether they are assimilating nadir or limb radiances. This problem is well-understood for the direct assimilation of infrared nadir radiances, which is commonplace at the operational centres. For direct assimilation of limb infrared radiances (e.g. MIPAS at ECMWF), although good progress has been made recently, especially on understanding the technical issues involved, the state-of-the-art is not as advanced as for nadir infrared radiances. The direct assimilation of UV differential-absorption and backscatter measurements and stellar extinctions is much more difficult than for infrared radiances. Examples are SCIAMACHY nadir and limb radiances, and GOMOS absorptions.

ECMWF is involved in the pioneering and scientifically challenging development of a direct variational assimilation of data from a limb-sounding instrument, MIPAS. It will also compare the results of this assimilation approach with the results of assimilating the retrieved profiles provided by ESA. Radiative transfer models that are fast and accurate enough, at least for simplified atmospheric conditions, and carefully selected spectral regions (e.g. "micro-windows" for MIPAS), have been developed and will be evaluated during the MIPAS commissioning phase. Information such as that presented in Fig. 4, calculated with a line-by-line model, can be used to select the micro-windows.

ECMWF has a lot of experience in using parallel computers and has clear ideas on how to approach the technical issues for limb viewing and the handling of the errors implied by the MIPAS measurement technique. For example, one problem is that computer code at the NWP agencies tends to be designed for nadir geometries and not limb geometries. In this case, the development of the assimilation algorithm also requires substantial code changes to take account of information coming from different vertical columns in the atmosphere. ECMWF will liaise with CNR.IFAC and other members of the MIPAS instrument/science team to obtain the fullest possible understanding of the characteristics of MIPAS radiances

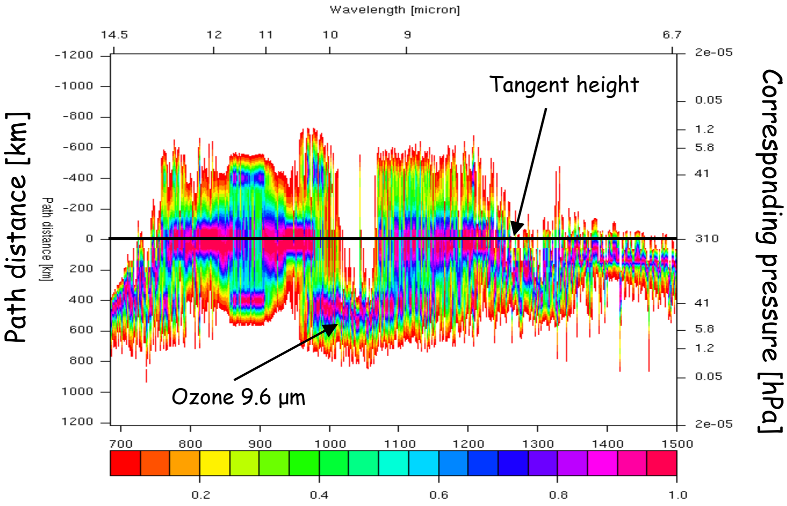

Fig. 4. Normalised weighting functions along a limb path for a 9km tangent height calculated with a line-by-line model. Figure courtesy of Niels Bormann (ECMWF).

Notwithstanding the progress made at ECMWF and elsewhere, a number of challenges must be met:

(1) *Limb geometry:*

- Infrared limb radiances have not been previously assimilated.

(2) *Computationally feasible forward model for infrared limb radiances:*

- Current fast radiative transfer models have to be extended.
- "Fast" means that the code is benchmarked to take ~3.4s for the simulation of 8,461 IASI channels on an IBM rs6000 workstation.

(3) *Data volumes:*

- MIPAS provides measurements of ~60,000 spectral points/"channels".
- It is necessary to select channels for the simultaneous assimilation of pressure, temperature, water vapour and ozone information, with the selection optimised within resource limitations.

(4) *Error characteristics:*

- Observations (error covariance matrix **O**): the inter-channel correlations for high-spectral resolution sounders must be investigated and incorporated if required.

- Background (error covariance matrix **B**): improved characterisation in the stratosphere and for ozone may be needed.

3. Future directions

The challenges identified in this paper point to a number of assimilation activities that are likely to become important in the future. These include:

- The operational use of research satellite data by NWP centres. Examples of data that could be used include ozone (already assimilated operationally by ECMWF) and stratospheric water vapour. An important part of this activity is the estimation of background error covariances. This is a challenge throughout data assimilation.
- The assimilation of limb radiances by research and operational groups. A lot of work is being done to develop fast and accurate radiative transfer models, and the interface between the radiative transfer model and the assimilation. Progress is more advanced in the case of infrared radiances than in the case of UV and visible radiances.
- Chemical forecasting, including tropospheric pollution forecasting.
- Coupled dynamics-photochemistry assimilation systems (e.g. a GCM coupled to a CTM).
- An Earth System approach to environmental and associated socio-economic issues. This would incorporate the biosphere and carbon cycle, and the coupling of all components of the Earth System (atmosphere, ocean, cryosphere, land and biosphere). These activities have hitherto not been as advanced as atmosphere and ocean modelling.

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Acronyms

AATSR: ....Advanced Along Track Scanning Radiometer

ADEOS: ....Advanced Earth Observing Satellite

ADM: ....Atmospheric Dynamics Mission

AIRS: ....Atmospheric InfraRed Sounder

AMSR: ....Advanced Microwave Scanning Radiometer

AMSU: ....Advanced Microwave Sounding Unit

ARPEGE: ....Action de Recherche Petite Echelle Grande Echelle

ASAR: ....Advanced Synthetic Aperture Radar

ASSET: ....ASSimilation of Envisat daTa

ASTER: ....Advanced Spaceborne Thermal Emission and reflection Radiometer

ATOVS: ....Advanced TIROS Operational Vertical Sounder

BIRA-IASB: ....Belgisch Instituut voor Ruimte-Aëronomie / Institute d'Aéronomie Spatiale de Belgique (Belgian Institute for Space Aeronomy)

CERES:	Clouds and Earth's Radiant Energy System
CERFACS:	Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique
CNES:	Centre National d'Études Spatiales
CNR.IFAC:	Consiglio Nazionale delle Richerche - Istituto di Fisica Applicata "Nello Carrara"
CTM:	Chemical Transport Model
CSA:	Canadian Space Agency
DARC:	Data Assimilation Research Centre
DORIS:	Doppler Orbitography and Radiopositioning Integrated by Satellite
ECMWF:	European Centre for Medium-range Weather Forecasts
EO:	Earth Observation
EOS:	Earth Observing System
EOS	MLS: EOS Microwave Limb Sounder
ERA:	ECMWF Re-Analysis
ERS:	European Research Satellite
ESA:	European Space Agency
ESRIN:	ESA Space Research INstitute
EUMETSAT:	EUropean organization for the exploitation of METeorological SATellites
GCM:	General Circulation Model
GCOM:	Global Change Observing Mission
GERB:	Geostationary Earth Radiation Budget experiment
GLI:	GLobal Imager
GOCE:	Gravity field and steady-state OCEan circulation
GOME:	Global Ozone Monitoring Experiment
GOMOS:	Global Ozone Monitoring by Occultation of Stars
GOSAT:	Greenhouse Observing SATellite
HIRDLS:	HIgh Resolution Dynamics Limb Sounder
HIRS:	High resolution Infrared Radiation Sounder
HSB:	Humidity Sounder for Brazil
IASI:	Infrared Atmospheric Sounding Interferometer
ILAS:	Improved Limb Atmospheric Spectrometer
KNMI:	Koninklijk Nederlands Meteorologicsh Instituut (The Royal Dutch Meteorological Institute)
LRR:	Laser RetroReflector

MERIS: ....MEdium Resolution Imaging Spectrometer

METOP: ....METeorological OPerational

MIPAS: ....Michelson Interferometer for Passive Atmospheric Sounding

MISR: ....Multi-angle Imaging SpectroRadiometer

MOCAGE: ....MOdèle de Chimie Atmosphérique à Grande Echelle

MODIS: ....MODerate Resolution Imaging Spectroradiometer

MOPITT: ....Measurements Of Pollution In The Troposphere

MSG: ....Meteosat Second Generation

MWR: ....MicroWave Radiometer

NASA: ....National Aeronautics and Space Administration

NASDA: ....NAtional Space Development Agency of Japan

NILU: ....Norsk Institutt for Luftforskning

NMC: ....National Meteorological Center

NOAA: ....National Oceanic and Atmospheric Administration

NWP: ....Numerical Weather Prediction

OMI: ....Ozone Monitoring Instrument

OSIRIS: ....Optical Spectrograph and InfraRed Imager System

OSSE: ....Observing System Simulation Experiment

PALM: ....Projet d'Asimilation par Logiciel Multiméthode

PSC: ....Polar Stratospheric Cloud

POLDER: ....POLarization and Directionality of the Earth's Reflectance

RA-2: ....Radar Altimeter 2

RH: ....Relative Humidity

SCIAMACHY: ....Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY

SEVIRI: ....Spinning Enhanced Visible and InfraRed Imager

SOFIS: ....Solar Occultation FourIer transform Spectrometer

SMOS: ....Soil Moisture and Ocean Salinity

SMR: ....Sub-Millimeter Radiometer

SPARC: ....Stratospheric Processes And their Role in Climate

SVD: ....Singular Value Decomposition

SWIFT: ....Stratospheric Wind Interferometer For Transport studies

TES: ....Tropospheric Emission Spectrometer

TIROS: ....Television and InfraRed Observations Satellite

TOMS:	Total Ozone Mapping Spectrometer
UPMC:	Université Pierre-et-Marie Curie
UT:	Upper Troposphere
UTLS:	Upper Troposphere / Lower Stratosphere
UV-B:	Ultra-violet B
WMO:	World Meteorological Organization