Chapter 15:

Sounding the Troposphere from Space: a New Era for Atmospheric Chemistry?

Overview of Subproject TROPOSAT

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15.1 Executive summary

The EUROTRAC-2 subproject, TROPOSAT (The Use and Usability of Satellite Data for Tropospheric Research) was established in the year 2000 to encourage the supply of, and develop the uses for, satellite data for the troposphere, which was then becoming available for the first time. With the work that has been done and the progress made, we can fairly claim that TROPOSAT has achieved its objectives.

The major satellite event during the period, which took place towards the end of the project, was the launch on February 28th/March 1st 2002 of ENVISAT carrying the instruments, SCIAMACHY, MIPAS, GOMOS and MERIS. SCIAMACHY is a powerful addition to the GOME instrument on the ERS-2, the data from which provided the impetus to form TROPOSAT and is the source of most of the scientific data in this report.

Among the many scientific highlights of the TROPOSAT work are the following:

- the development and improvement of algorithms to retrieve tropospheric data;
- the use of a neural network to yield tropospheric ozone profiles;
- a variety of case studies for model validation using satellite data;
- several studies of the intercontinental transport of pollutants, trace substances and aerosols from forest fires, volcanic eruptions and power plants;
- estimates of the production of NO_2 from lightning in tropical convective storms;
- comparing satellite and aircraft data to give upper tropospheric humidity;
- the production of global maps of water vapour; and
- the development of a variety of validation strategies for satellite data which draw upon a number of different conventional data sources.

Since its inception, TROPOSAT has had affiliated to it several investigators in the United States concerned with tropospheric observations. A brief account of some of their work is also included in this overview.

As well as looking forward to the new data being produced by GOME and SCIAMACHY, the community is also thinking about the long-term future, and a number of principal investigators are involved in a proposal for a new geostationary satellite system, GeoTROPE, which is essential if we are to study chemical weather and the daily development of photo-oxidants and other pollutants in the troposphere.

15.2 Introduction

The successful launch in early 2002 of the SCIAMACHY instrument (SCanning ImAging spectroMeter for Atmospheric CHartographY) on the ESA ENVISAT satellite opened the second phase of a substantial European effort to study trace substances and pollutants in the troposphere with measurements from space. It was also the culmination of an idea, first mooted fifteen years ago by two of the coordinators of TROPOSAT, *John Burrows and Ulrich Platt*, which found its first expression in 1995 with the launch of GOME (Global Ozone Monitoring Experiment) on the ESA ERS-2 (European Space Agency Earth Research Satellite 2).

The results already obtained from GOME, and the preliminary ones from SCIAMACHY and MIPAS (also launched on ENVISAT), more than justify the enormous effort made by so many people to bring the overall project to fruition. The results give a hitherto unobtainable picture of the chemical state of the atmosphere on global and regional scales. The continuing flow of results, and the hoped-for development of a geostationary platform for tropospheric chemical studies, are likely to change the way science is carried out in tropospheric chemistry and, in the long run, provide a reliable system for monitoring pollutants on regional scales, as well as monitoring the state of the atmosphere on a long-term basis.

The EUROTRAC-2 subproject, TROPOSAT, was set up in 2000 with the realisation that those engaged in developing the satellite data products and those using them required a common forum to ensure that the available data would be fully and correctly used. It was also evident that the results would directly affect the community engaged in tropospheric chemistry and that the community needed to be shown how to make best use of them. The coordination of TROPOSAT was supported by ESA/ESRIN.

The present overview outlines the scientific highlights of TROPOSAT and presents some lessons learned, together with some suggestions for the future. The whole shows how successful TROPOSAT has been, despite the short time it has been running. It also indicates the need for a follow-up project to ensure that full use is made of the plethora of data now becoming available on the concentration fields of chemical trace substances in the troposphere.

15.3 The aims of TROPOSAT

The aims of TROPOSAT were to explore and encourage the use of satellite data to determine two- and three-dimensional distributions and time series of trace gases and other parameters in the troposphere, and so facilitate future research and environmental monitoring on regional and global scales, in particular through:

- the development of algorithms for the retrieval of tropospheric species and parameters;
- the use of satellite data for understanding atmospheric processes;
- the synergistic use of different instrumentation and platforms for tropospheric measurements; and
- the development of validation strategies for tropospheric satellite data products.

Four task groups were set up to tackle these topics. In addition TROPOSAT decided to emphasise the following underpinning activities: the development of appropriate data assimilation techniques combining satellite measurements with modelling, and the specification of the requirements for future satellite instruments for tropospheric work.

As will be seen from the following sections, the aims have been amply fulfilled. However much work remains to be done and it will be necessary to continue the project so as to ensure that the increasing amount of data is fully utilised by the community for whom it is intended. Highlights of the work are given in the next sections with the name of the PI in parentheses.

15.4 Some TROPOSAT scientific highlights and activities

15.4.1 Data retrieval

The inherent difficulty with tropospheric satellite measurements to date is the retrieval of the tropospheric absorption from reflected earthshine, which is measured in a downward-looking (nadir) configuration from about 800 km through the stratosphere. Some trace gases of interest in the troposphere (e.g., O_3, NO_2) are also abundant in the stratosphere, and so interfere with the observation of the troposphere, while others (like SO_2 or HCHO) are not, so current retrieval methods tend to be species-specific.

The principal investigators in TROPOSAT task group 1 have largely devised, and extensively developed, all the present methods for retrieving tropospheric information from the satellite data stream. Among these are the Tropospheric Excess Method in which signals from known NO_2-free tropospheric regions are compared with those from polluted tropospheric regions to give the NO_2 in the boundary layer; the difference between “on-” and “off-cloud” signals can give concentrations at levels depending on the cloud height; and advantage can be taken of the differences in the spectroscopic features and temperature dependences to obtain profiles of ozone in the troposphere.

The task of retrieving the tropospheric contribution will be simplified by the new instruments on ENVISAT, which are capable of making measurements looking at the horizon (limb) as well as nadir observations. Comparison of these will yield tropospheric trace gas concentrations directly without resorting to any other assumptions or favourable conditions. However further retrieval algorithms are required to make the best use of the data.

The development of algorithms is a difficult task and, until now, most of data available is the product of detailed skilled work on individual data sets. But, as experience grows, automation can be expected. Algorithms have been developed or improved for NO_2, BrO, SO_2, O_3 and HCHO, with particular contributions to the problems posed by cloudy pixels. Several groups have concentrated on algorithms for determining aerosols in the troposphere, with specific work being done on the effects of volcanic eruptions on the aerosol load, the transport of Saharan dust and the effect of complex terrain on the aerosol distribution.

15.4.2 Neural networks

The most novel development concerned with determining tropospheric concentration profiles is that of Kaifel who is using a neural network ozone retrieval system, NNORSY, to determine profiles of O_3 from GOME data.

The network is trained with thousands of profiles obtained from sonde measurements and then, from the data for each pixel, yields the ozone profile in the atmosphere. These are still early days with much work to be done on both normal and neural retrieval; but here we appear to have a glimpse of the future, with trained neural networks rapidly yielding concentration profiles and free from many of the assumptions which are necessarily present in normal retrievals.

15.4.3 Validation of models

Task group 2 brought into TROPOSAT a number of modellers and other investigators interested in actually using the concentration fields and profiles produced from satellite data to compare and verify their model calculations, particularly on global scales. There was encouragingly free exchange of data and experience between the research groups who produced the data (mainly in group 1) and those in group 2 using it. The results are all heartening in the agreement between satellite and model although, necessarily, the differences highlight inadequacies, which may be in the models or perhaps in the data retrieval. One model under development concentrates on the details of the formation of aerosols and is looking forward to comparison with satellite data.

15.4.4 Environmental case studies

The use of data to explore both natural and anthropogenic phenomena, which show the potential of satellite data for studying the environment, include:

- studies of forest fires in Canada and Siberia together with the transport of the plumes between continents;
- the long-range transport of tropospheric NO_2 from power stations in the high veldt of South Africa to Australia;
- the estimation of NO_2 global source strengths using GOME data combined with other satellite information on lightning flashes and night-time surface light emissions;
- the source of NO_2 over the Indian subcontinent;
- the aerosol and SO_2 produced by volcanic eruptions;
- the transport of Saharan sand over the Atlantic Ocean and Mediterranean Sea; and
- the export of pollution from Europe into the northern hemisphere.

15.4.5 Synergism and global observation

Many of the studies mentioned use not only satellite concentration data but also data from ground stations, sondes, aircraft and other satellites. The “synergy” obtained by combining data from various sources will surely be the norm in the future and, for this reason, task group 3 was set up to encourage such work. It is not an easy task since the data from various sources is so different, in both temporal and spatial coverage.

Two major sources of data for the upper troposphere are the long-term programmes, CARIBIC and MOZAIC, in which instrument packages are flown regularly on long-distance passenger or freight aircraft. These provide concentrations along the popular intercontinental flight routes, and are to be used with data from SCIAMACHY to obtain information on water vapour and other trace species.

One long-standing problem that now can be tackled is how much NO_2 is produced by lightning. Data from two satellites has been combined to examine large tropical storms, and estimates can now be made which will improve NO_2 budgets as well as our understanding. Such estimates could only previously be guessed at.

Since TROPOSAT task group 3 started work, an international initiative has been taken by a number of global organisations to form IGOS, International Global Observation Strategy. The atmospheric part is IGACO, International Global Atmospheric Chemistry Observations. The IGACO planning group intends to foster the formation of an integrated system which will include satellites, ground-based stations, aircraft and ships, supported by comprehensive modelling to provide a continuous picture of the state of the atmosphere, the environmental situation of which can be assessed on a regular basis. IGACO is just what the principal investigators (PIs) of task group 3 had in mind at the start. Their brief assessment below gives an indication of the likely difficulties that will be encountered in setting up an observation system. The coordinators of

TROPOSAT together with Hennie Kelder now serve on the planning group for IGACO.

15.4.6 Data validation

Validation of satellite data is essential if the results are to have any meaning, so task group 4 was set up to bring together those involved. In fact validation activities are by definition synergistic so members of task group 3 are also involved. Comparison of data for ozone from several satellites, GOME, TOMS and TOVS, shows some systematic discrepancies between them.

A lot of effort has gone into setting up ground-based FTIR instruments to use for satellite validation. The instrument on the Jungfraujoch (Switzerland) has a long record of profile measurements in the upper troposphere which are used in climatology. To that is now added FTIR spectrometers and other instruments on the Zugspitze (Germany) and at Harestua (southern Norway). All will provide validation data for SCIAMACHY.

There are also validation activities using research aircraft such as the DLR Falcon and also, courageously, a micro-light aircraft. Aircraft allow measurements to be undertaken within a particular pixel, if this is desired.

15.4.7 Data assimilation

Data assimilation was designated as an underpinning activity at the start of TROPOSAT. Several of the modelling groups in TROPOSAT use data assimilation to integrate experimental results into the model framework in order to improve model performance. As is pointed out below, data assimilation offers perhaps the only way, in the long run, to bring together experimental observations from a variety of sources in order to generate a reliable comprehensive picture of the state of the atmosphere at any given time.

15.4.8 Geostationary satellites: the future?

The major activity in the underpinning activity, future instrumentation, was the formulation of a proposal for a geostationary satellite, GeoTROPE. The satellites used at the moment are sun-synchronous low earth orbit (LEO). They only provide a measurement of a particular area on the earth's surface every three days. The best environmental measurements require a better time resolution and this can be provided with a geosynchronous satellite orbiting at about 36000 km above a particular point on the earth. Despite the increased distance, the time integration advantage over an LEO satellite would provide a chemical picture of one third of the earth every half hour. A number of PIs prepared and submitted a proposal to ESA in 2001. Unfortunately, despite the overwhelming scientific case, and the potential of the satellite for environmental monitoring, the proposal has not yet been accepted. However discussions are continuing and it is to be hoped that the case for a geostationary satellite to study chemical weather will soon be accepted.

15.5 Policy-relevant results

The availability of satellite data for the troposphere will ultimately be the preferred method for those responsible for environmental policy development in Europe. Satellite data will be used by the authorities to monitor pollutant concentrations on a regional scale in order to verify the compliance with the control measures. Also, since the development of legislation to control pollutants must be based on sound science encapsulated in reliable chemical transport models, satellite-derived tropospheric data will be invaluable for the thorough validation of such models.

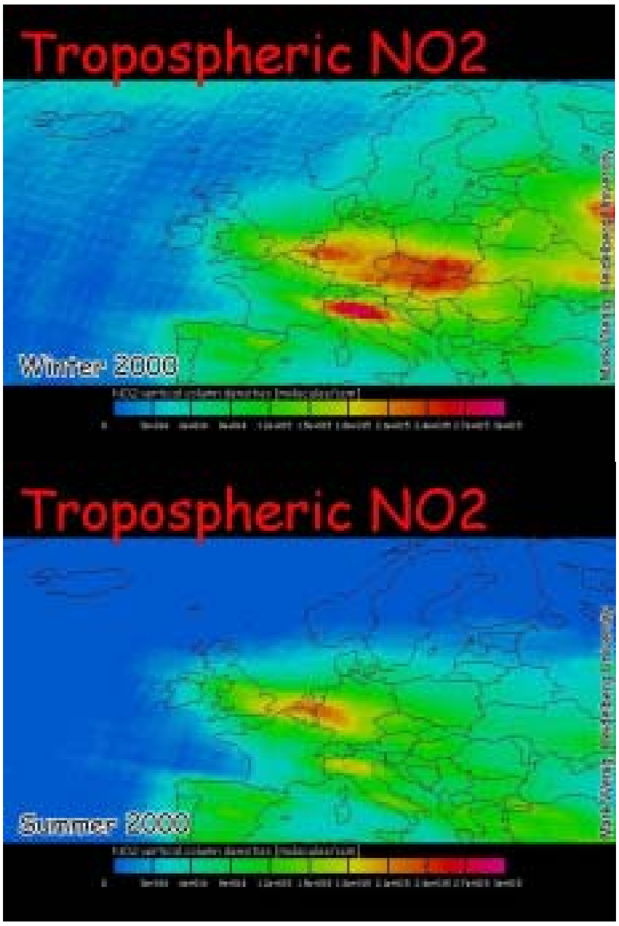


Figure 15.1. Seasonal variation of tropospheric NO_2 vertical column over Europe derived from GOME measurements. (Wenig, University of Heidelberg, 2001).

A nice example of the possibilities offered by satellite-derived data is provided by Figure 15.1, which shows the NO_2 concentrations over Europe in the summer and winter of 1999. The high concentrations generally seen over north-western Europe and in the Po valley are consistent with the model results and projections obtained by David Simpson from EMEP. These are just the regions where the NO_2 concentrations are high enough to titrate out much of the ozone formed in the boundary layer, and furthermore they are regions where a substantial *reduction* of NO_2 may actually lead to an *increase* in the photochemically produced ozone.

Several of the studies already mentioned also illustrate the potential of tropospheric satellite measurements for use in environmental management. These include the observation of intercontinental plumes containing NO_2, SO_2 and aerosol from forest fires, volcanoes and high-lying South African power plants; identification and quantification of sources of pollutant emissions on global and continental scales, the transport of sand from the Sahara over the neighbouring seas and lands, and the export of pollution from Europe into the northern hemisphere.

Here, a recent development involving members of TROPOSAT is the EC project EVERGREEN (EnVisat for Envirionmental Regulation of GREEN house gases) which is bringing together European expertise on calibration/validation, retrieval algorithm development, data assimilation and inverse modelling. In addition to the scientific members, the user community is represented by climate and environmental government organisations and a major coal industry.

The Kyoto agreement requires the long-term monitoring of the troposphere to try to identify changes which are due to human activities. Clearly satellites, once they have been launched and the instrumentation and data products validated, offer a definitive way to achieve reliable and long-term monitoring on global and regional scales. Finally, should the global observation system envisaged by IGACO be set up, satellite measurements of tropospheric constituents will be vital to its success.

15.6 New algorithms for obtaining tropospheric data from satellite measurements

Principal results from task group 1

15.6.1 Introduction

Task group 1 is aimed at the development and improvement of algorithms to derive information on tropospheric constituents from satellite measurements. The work performed in this task group is the basis of all the studies in the other task groups within TROPOSAT, and much progress has been made in this field within the last few years.

At the outset of TROPOSAT, there was only a very limited number of tropospheric products from satellite observations, mainly tropospheric ozone columns from TOMS, pioneered by Fishman, aerosol products over the ocean from ATSR, and the first results for tropospheric species from the GOME instrument. With the exception of TOMS ozone, little had been done in terms of validation and scientific exploitation of the data. To change this situation, scientists within task group 1 addressed a number of distinct topics, which can roughly be sorted into five groups.

- Improvements in the retrieval of minor trace species columns from UV/visible measurements, focussing on O_3, NO_2, BrO, and H_2O columns with some work on HCHO and SO_2.

- Improvements of algorithms to derive ozone profiles from UV/visible measurements to a point that can be retrieved from GOME or SCIAMACHY.
- Sensitivity studies and tests on IR measurements for the retrieval of tropospheric information, using data from CRISTA, MIPAS and MOPITT.
- The improvement of aerosol retrieval algorithms to allow measurements over land, and also to provide more detailed information such as aerosol type.
- Development of algorithms that derive more indirect products such as actinic flux or OH concentrations based on quantities measured by satellites.

A substantial part of the research in task group 1 was dedicated to developing software for the instruments on ENVISAT which will become operational as the data from the instruments is validated.

15.6.2 Main scientific results from task group 1

Tropospheric columns from UV/visible measurements

In the determination of tropospheric columns from UV/visible nadir measurements, the retrieval essentially consists of three steps: the derivation of the total slant column, the separation of tropospheric and stratospheric signals including treatment of clouds, and the conversion to a vertical column.

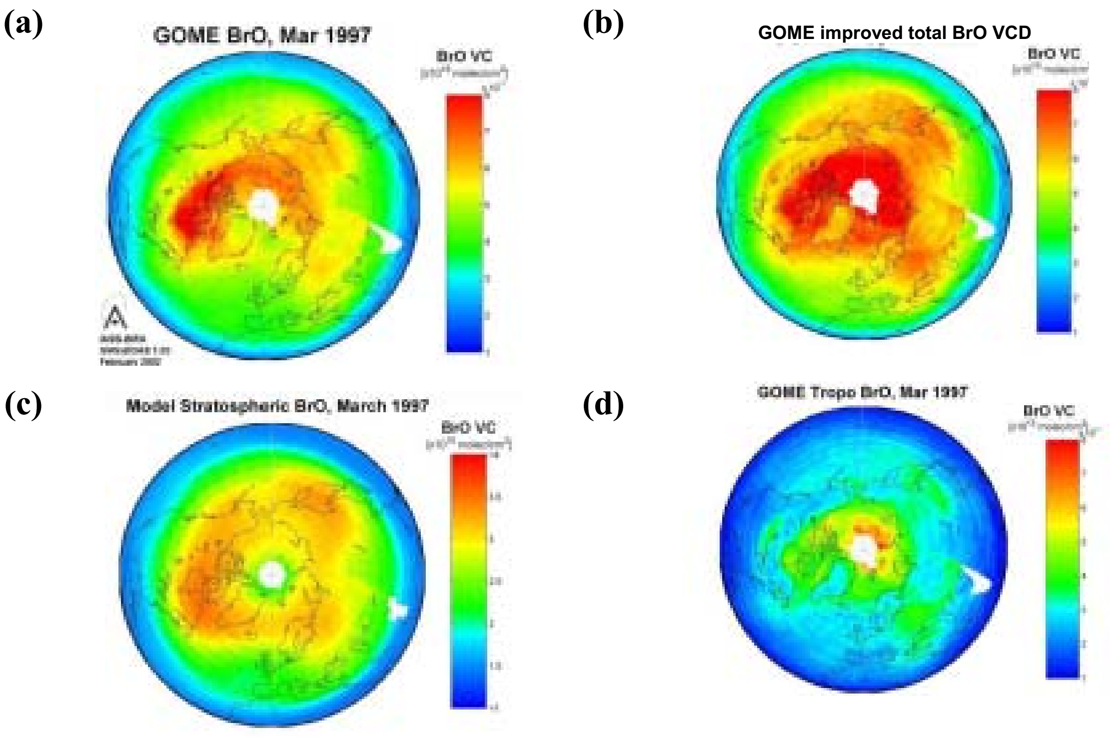


Figure 15.2. GOME BrO for March 1997; (a) compared to the improved prototype; (b) the stratospheric column from SLIMCAT 3-D-CTM data (c) the remaining tropospheric column; (d) using AMFs based on TOMS data.

One example of a tropospheric product from GOME is BrO, Figure 15.2, which is mainly located in the stratosphere, although in some situations also in the boundary layer and to some extent in the free troposphere. By using an estimate of the stratospheric column from the SLIMCAT 3-D CTM model and appropriate air-mass factors, the tropospheric BrO burden could be estimated (van Roozendaal).

In another example, tropospheric ozone was derived from GOME measurements using a Convective Cloud Differential (CCD) technique. While this method has already been successfully used for TOMS data, the challenge for GOME data is the much larger ground-pixel which makes selection for cloudy and clear pixels much more difficult. The resulting tropospheric ozone fields show good agreement with sonde measurements (Kelder).

Yet another method to separate tropospheric and stratospheric columns based on the wavelength dependence of the photon penetration depth was developed for NO_2. This approach allows a determination of the tropospheric content from a single measurement without the need to use measurements in a reference sector or data taken on days with cloud cover. It therefore is of particular interest for geostationary measurements such as the proposed GeoTROPE instrument (Richter).

One major problem for all UV/visible measurements of tropospheric constituents is the treatment of clouds. On the one hand, clouds shield the portion of the profile below cloud top from view; on the other hand, the sensitivity for absorptions directly above the cloud is increased. Therefore, reliable cloud fractions and cloud top pressures are needed for accurate tropospheric products on a global scale, and also over snow and ice. A study of a series of cloud sensitive parameters from the GOME instrument showed the potential that a combination of these parameters might provide a much improved cloud product, and thereby facilitate the derivation of more accurate tropospheric products (Wagner).

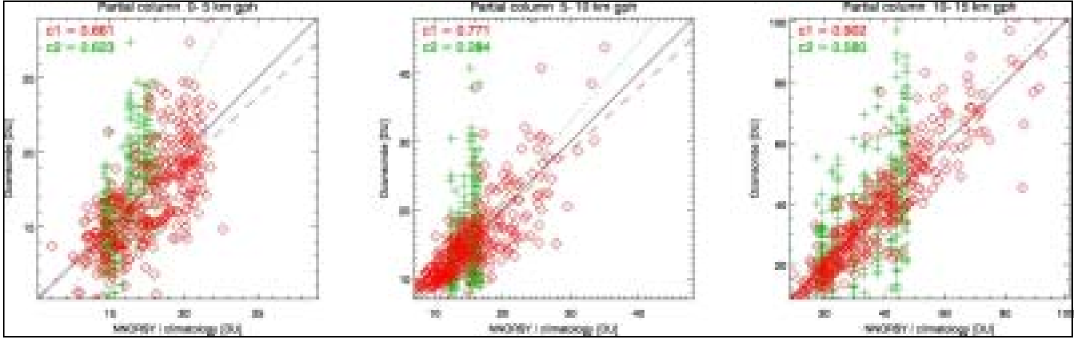
IR measurements for the retrieval of tropospheric information

Traditionally, IR limb measurements have been used for stratospheric applications, and extension to tropospheric species was not even considered. However, sensitivity studies for the MIPAS instrument show that, for the upper troposphere, a large number of species can be retrieved with differing accuracies. Total errors (systematic and random) for individual measurements are in the range of several percent for some species and on the order of several hundred percent for others. Accordingly, spatial and temporal averaging is necessary for most of the retrievals, but given the fact that many of the species have never before been measured on a global scale, even monthly zonal averages would represent a big step forward (Stiller).

Ozone profiles from UV/visible measurements

For the retrieval of ozone profiles, two different approaches have been used. A physical approach, in which the measurements are simulated by radiative transfer calculations and iterated until convergence is reached, and a neural network approach. While the classical physical approach has the advantage of conceptual clarity and direct control of the various variables of importance, the neural network offers much higher computational speed and automatic adaptation to complex phenomena such as instrument degradation. As Figure 15.3 shows, extensive studies with the neural network retrieval NNORSY show, that not only the tropospheric columns compare well with ozone sondes, but that up to three independent layers can be retrieved in the lowest 15 km (Kaifel).

Hohenpeißenberg, (47.8°N, 11.0°E)



Syowa, (69.0°S, 39.6°E)

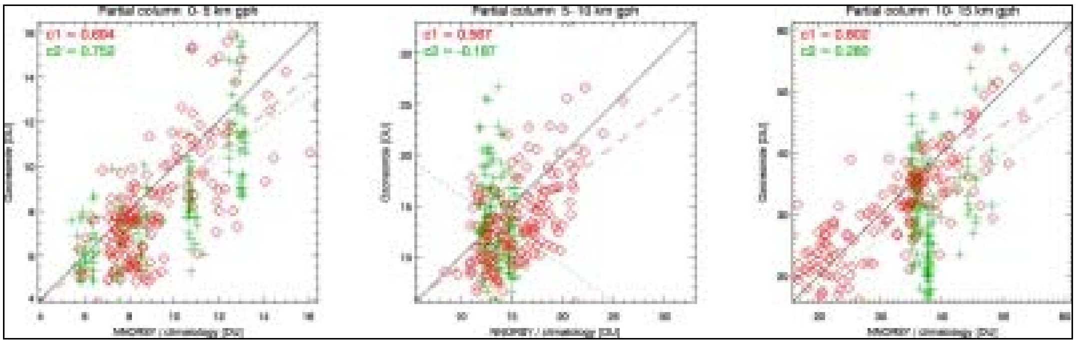


Figure 15.3. Scatterplots of NNORSY versus. ozone sondes (◊) and the F and K climatology versus sondes (+). c1 is the Pearson correlation for NNORSY, c2 for F and K. Regression curves are printed dashed and dotted, respectively (Kaifel).

The main problem in tropospheric ozone profiles from UV/visible sensors is the lack of sensitivity in the lowest layers. This could be improved by adding the relative Stokes parameter as polarisation information to the measurements, as will be the case with the GOME-2 instrument. Using this information in the retrieval not only reduces the errors introduced by scalar radiative transfer models but also improves the vertical resolution (Landgraf).

Improvement of aerosol retrieval algorithms

Aerosol products were derived from two different types of instruments and algorithms. From imaging sensors, spatially highly-resolved maps of aerosol properties can be generated. These types of observations can only yield limited information on the type and vertical distribution of the aerosols. Within

TROPOSAT several aerosol products from imaging sensors have been developed, in particular over land surfaces.

When retrieving aerosol properties over land, the main problem is to correct for the influence of the surface reflectance, that varies not only with wavelength and viewing geometry, but also with location and season. In a novel approach, the bi-directional reflectance distribution function (BRDF) for a given location is determined empirically by comparing ground-based AERONET measurements with satellite retrievals using data from VEGETATION. After a limited data set has been analysed, the ground-based measurements are no longer needed, and satellite data can be used to derive AOT for this location with excellent accuracy, assuming that the BRDF is not changing with time (Verdebout).

An aerosol algorithm for GOME observations was improved which yields data on different kinds of aerosols over water such as Sahara desert dust or volcanic aerosol. The algorithm has been applied to selected volcanic eruptions and also (Figure 15.4) to export of sand from the Sahara (Guzzi).

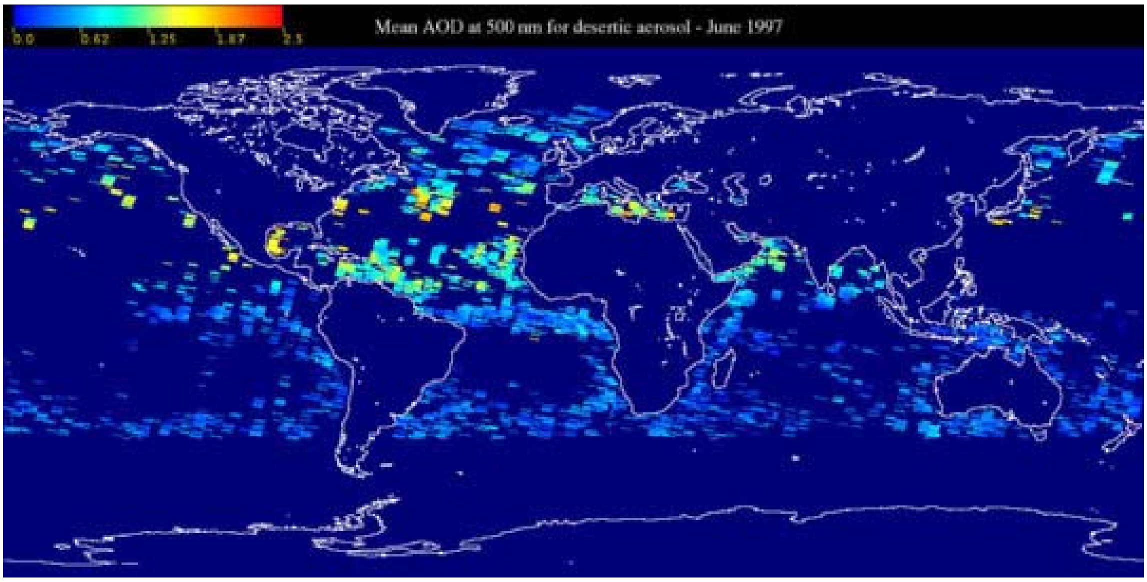


Figure 15.4. Aerosol climatology of Sahara desert dust from GOME data. Here the average value of desert dust is reported for June 1997. The yellow-red range indicates the presence of desert dust events embedded into a maritime aerosol and residual clouds (light blue) (Guzzi).

A different approach to retrieve aerosols over land has been developed for the ATSR-2 instrument that makes use of the dual view measurements. Using look-up tables for the impact of different aerosol types on the radiation observed by ATSR-2 not only gives AOT over land and ocean (the latter using the nadir viewing mode), but also gives information on the aerosol type. This algorithm has been successfully applied to measurements over the Indian Ocean during the INDOEX campaign, Figure 15.5 (de Leeuw).

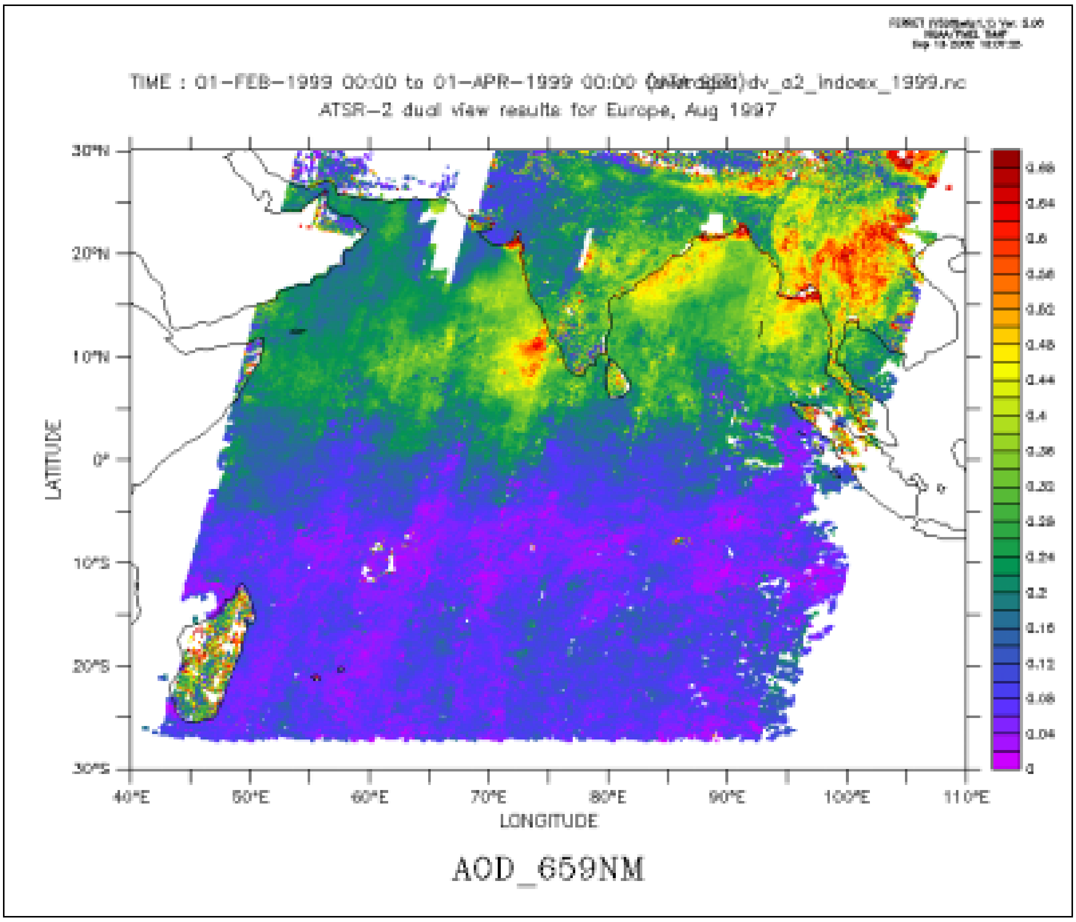


Figure 15.5. Composite map of the mean AOT at 0.659 µm retrieved using ATSR-2 data for February and March, 1999 over the INDOEX area. No data is available for the white areas (de Leeuw).

Indirect products

Several indirect tropospheric products have been developed: in particular vertical profiles of the actinic flux and the OH concentration have been derived from a combination of different sensors. While to date the uncertainty of these data products is still large, these prototype algorithms are promising for future applications when satellite data with increased accuracy should become available (Verdebout, Tuinder).

15.6.3 Conclusions from task group 1

A large step forward has been made with respect to algorithms for the retrieval of tropospheric information from satellite measurements. This progress has a direct impact on several key requirements for future applications.

- Algorithms have been developed and improved to quantitatively retrieve tropospheric columns of species such as O_3, NO_2, BrO, HCHO, SO_2, and H_2O.
- Algorithms have been developed that use different approaches to derive height-resolved tropospheric ozone columns from UV/visible nadir measurements.

- Algorithms have been developed to retrieve information on upper tropospheric concentrations of a large number of species from IR measurements.
- Algorithms have been developed to derive aerosol optical depth over land and in some cases also aerosol type
- Much data has been made available to, and used by, the scientific community. An overview of what is available can be found on the TROPOSAT web page *http://troposat.iup.uni-heidelberg.de.*

With the data that will become available from the instruments on ENVISAT in the near future, the algorithms developed over the last few years will prove useful for a large number of tropospheric products, and satellite data will provide input for many studies on tropospheric chemistry.

15.7 Applications of satellite data in tropospheric research

Principal results from task group 2

15.7.1 Summary of task group 2 objectives

Task group 2 has aimed to demonstrate how tropospheric data products derived from satellite measurements can be evaluated and employed for scientific applications. The synergistic usage with model results and with data from aircraft and ground measurements has been carried out, in order to improve the qualitative and quantitative interpretation and the understanding of dynamical, physical and chemical processes in the troposphere and the tropopause region. Satellite data are ideally suited to supply initialisation, boundary conditions, and test data for chemistry transport models (CTMs) on regional and global scales, and coupled global chemistry-climate models (CCMs). In this sense, the activities of this TROPOSAT task group has included:

- case studies with CTMs including inversion of transport processes, e.g., with Lagrangian tracer models;
- validation of CTMs and CCMs; and
- comparison and interpretation of model results and individual observations with satellite data.

15.7.2 The aim of task group 2 research

The studies have addressed the following scientific points:

- identification of sources and sinks of pollutants;
- export of pollutants from Europe into the free troposphere and to the East;
- assessment of the role of tropospheric-stratospheric exchange in the tropospheric ozone budget;

- study of the NO_x emissions, e.g., from the surface (natural and anthropogenic), from aircraft (in the upper troposphere/lower stratosphere), and from lightning; and
- accurate characterisation of the atmosphere and its change in composition with time, employing data assimilation analysis.

15.7.3 Recent activities in task group 2

A pleasing and important aspect of task group 2 has been the intensive co-operation between the scientific groups, not only of those within the group, but also with those of other task groups. Data were exchanged, interpretations were carried out jointly, and common scientific articles have been published in peer-reviewed journals.

A cornerstone for the activities of this task group was the preparation of tropospheric NO_2 columns from the GOME instrument onboard the satellite ERS-2 (Lawrence; Richter). The data employed in the TROPOSAT project mostly concentrate on the time series from 1996 to 2000.

In the first independent validation by comparison of tropospheric NO_2 columns derived from satellite instrumentation, two subgroups were involved in the intercomparison of tropospheric NO_2 columns from GOME. Column densities were derived (a) from aircraft NO_2 profile measurements, and (b) from ground-based observations, covering the profile with stations situated at different heights. The *in situ* aircraft NO_2 profiles were measured with the DLR Falcon in May 2001 (Schlager) under cloud-free conditions favourable for the satellite instrument. The NO and NO_2 mixing ratios on the aircraft were measured with two independent chemiluminescence detectors, sampling the same air mass as observed by GOME. The tropospheric NO_2 column of $(4.2 \pm 1.7) \times 10^{15}$ molec. cm^{-2} derived from the *in situ* measurements agrees well with the near real time results of $(3.5 \pm 0.9) \times 10^{15}$ molec. cm^{-2} from GOME. If the shape of the vertical NO_2 distribution from the *in situ* measurements is used, the GOME value increases to $(4.1 \pm 1.0) \times 10^{15}$ molec. cm^{-2} which leads to an even better agreement with the DLR Falcon results.

NO_2 measurements by the GOME instrument have been checked with night-time light emissions observed from space. Interestingly, these light emissions correlate much better with tropospheric NO_2 columns than with estimated anthropogenic emission data, as provided by the EDGAR data base. NO_2 column densities together with satellite-derived information of global lightning frequencies (LIS/OTD) and accounts of fires due to biomass burning (ATSR) should help to get a better knowledge of the relative contributions and the geographic distribution of nitrogen oxide emissions (Rohrer).

A number of models were employed to explore atmospheric processes: (a) a Lagrangian particle dispersion model, (b) chemistry transport models (CTMs), and (c) a fully coupled chemistry-climate model (CCM). In general, models are needed to assess processes related to policy (whether regions are NO_x or VOC-limited for example), but there are virtually no observations in regions such as Asia so satellite data assumes a crucial role.

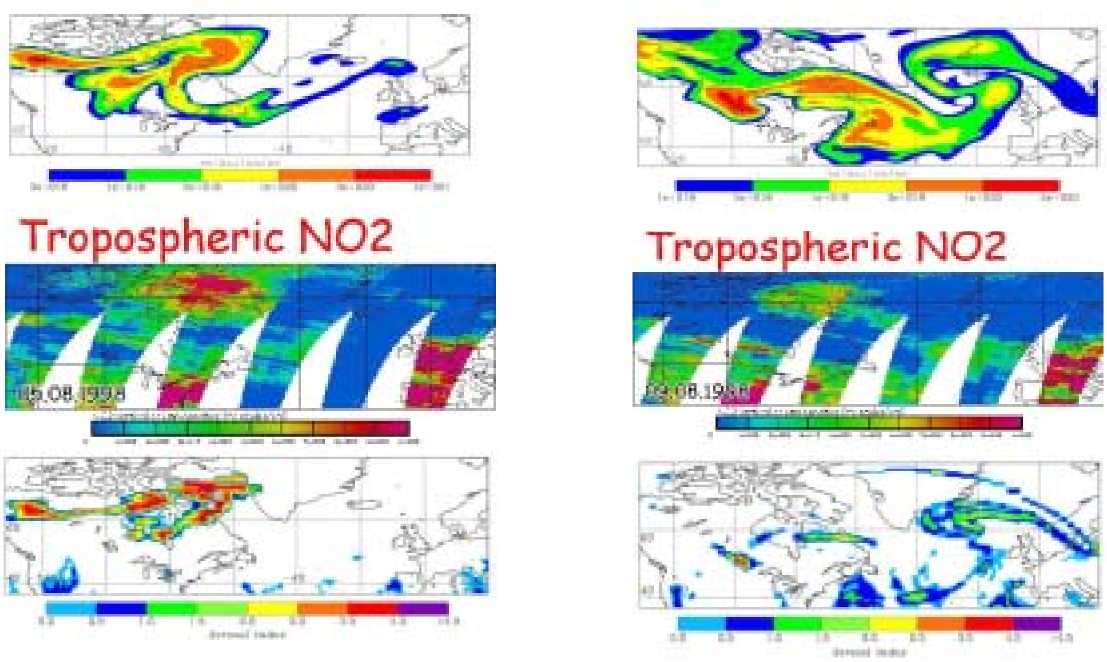


Figure 15.6. August 5th , 1998 (left), August 9th, 1998 (right); FLEXPART NO_x (top), GOME NO_2 (middle), TOMS aerosol index (bottom).

An interesting application of satellite-derived information of tropospheric values is the combination with transport modelling to determine the sources and sinks of specific chemical compounds. For example, simulations with the Lagrangian particle dispersion model FLEXPART were taken to determine tropospheric NO_x sources from, for example, biomass burning, combustion and lightning. The analysis in combination with satellite-derived information indicated that NO_x can be transported over long distances (Figure 15.6), if the emissions are injected or quickly transported in the free troposphere, above the tropospheric boundary layer (Stohl).

A similar study was carried out with the fully coupled chemistry-climate model E39/C (Dameris), which also aimed at checking the abilities and deficiencies of the model system, in order to calculate the distribution and seasonal cycle of the tropospheric NO_2 column correctly. The general pattern of GOME and model data are qualitatively in good agreement, but the model values are significantly higher, especially over industrial areas, i.e., regions with high surface concentrations (Figure 15.7). This may indicate that either the prescribed surface emissions by industry and traffic are overestimated in the model, or the GOME retrieval has some problems regarding the measurements of higher concentrations near the earth’s surface.

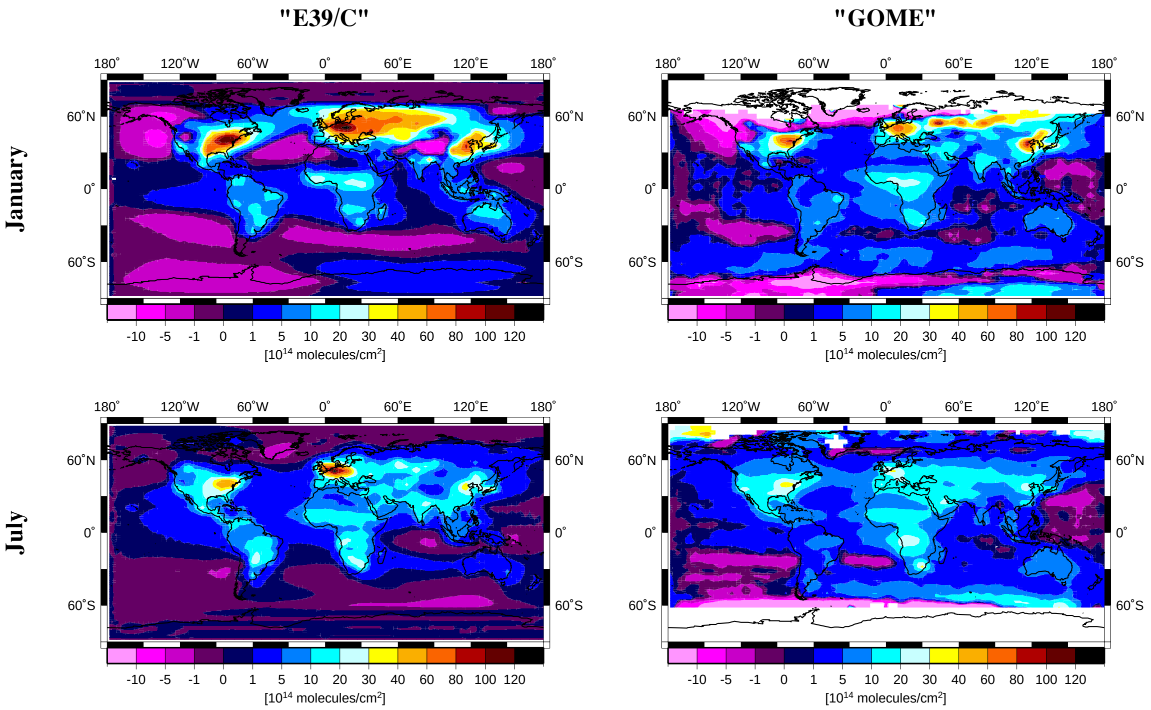


Figure 15.7. Climatological monthly means of the tropospheric column amounts calculated by E39/C ("TEM") and derived from GOME measurements for January and July, respectively. White coloured areas are data gaps. (Dameris).

The studies carried out with the CTM MATCH-MPIC (Lawrence) aimed at improving the understanding of NO_x in the troposphere over Asia. It was shown that the model simulates the mean NO_2 amount in this region fairly well, in agreement with the assessments provided by GOME observations, with the conclusion that the adopted total magnitude of NO_x in the model is reasonable. The results of the CTM TOMCAT have been used to discover how far it is possible for this model system to get output which can be directly compared to results derived from GOME. TOMCAT tropospheric NO_2 columns compared well with respective GOME data, i.e., the highest concentrations of NO_2 were identified in the same regions and were of the same order of magnitude. Additionally, the TOMCAT CO and HCHO data have been compared to MOPITT CO data and GOME HCHO data. (Savage)

The potential for using satellite data for studying and monitoring pollution has been amply demonstrated with results on forest fires in Canada and Siberia and on power plant emissions from the High Veldt stations in South Africa. It is clear from all these that NO_2 has a longer life time in the free troposphere than in the boundary layer and that if injected high up, it can be transported intercontinentally (Stohl). Results for air pollution over Switzerland were obtained by comparing results from ground stations with those from GOME and using trajectory analysis to identify the sources. Better results were obtained with the satellite data than from the ground stations (Weiss).

Using results from various satellite sources (GOME NO_2; DMSP, night-time light emission; ASTR, surface temperatures; LIS/OTD, lighting flashes) the global emission estimates for NO_2 have been examined. It appears that the standard data base values, used to initialise most global model calculations, may be substantially in error (Rohrer).

15.8 Synergistic use of different instrumentation and platforms for tropospheric measurements

Principal results from task group 3

15.8.1 The perspective of task group 3

An integrated observational strategy building on the synergism of observations made from different platforms is a pre-requisite to explore physico-chemical processes in the atmosphere and their impact on the earth's climate and its future changes. An urgent need for such data is also identified in the recently issued IPCC-2001 report. The aim of this task group is, through selected process studies, to develop strategies for the integrated use of satellite and non-satellite (ground based, aircraft and balloon) observations. The integration process of data sets of different origin, each with their own specific characteristics with regard to detection, resolution in time/space, continuity and precision/accuracy, is a careful process of data quality control, considerations of spatial and temporal resolution/overlap, developing and using advanced interpolation techniques and retrieval methods. In this task group the different contributions are subject to different approaches of integrated use of data sets of multiple satellites, satellite and aircraft, satellite and ground-based or a combination of each.

15.8.2 Scientific activities of task group 3

The Bremen group (Burrows) has used multiple satellite data to study NO_2 produced by lightning using NO_2-column data from GOME in combination with the lightning flash detection by the Tropical Rainfall Measuring Mission (TRRM) satellite. The study showed enhanced NO_2 concentrations produced by lightning and transported by convective uplifting. Although GOME is insensitive to NO_2 below the cloud, the largest sensitivity is obtained in the upper region of the cloud, as 70% of the lightning discharges are above the cloud. NO_X production by lightning has been estimated to be in a range of $1–4 \times 10^{25}$molecules per flash for a thunderstorm. The work will be continued in order to attempt to estimate and quantify the annual and seasonal budgets of lightning produced NO_2 in both hemispheres.

Using GOME, TOVS and TOMS satellite data sets, the group at the University of Leicester (Monks) identified significant and systematic differences between the tropospheric ozone columns derived from the different satellites. Influence of clouds on residuals seemed to be of minor importance; however, it was found that topographic features and albedo are significant factors in determining multi-platform residuals. Other platforms like SAGE and MLS are intended to be incorporated, particularly to investigate the differences between UV/visible and IR retrieval techniques.

In the process of developing and validating the CRISTA-2 satellite observations of water vapour in the tropopause region the Wüppertal group (Riese) used aircraft data of *Geophysica* and MOZAIC. Through this synergistic use of satellite and aircraft data together with the assimilation with meteorological data, global maps of retrieved water vapour fields of CRISTA-2 could be constructed which enables us to resolve important dynamical structures in the tropopause region. Figure 15.8 shows an assimilated H_2O map at the 215 hPa pressure level for August 12th, 1997 which exhibits a variety of interesting dynamical features. The study shows clearly that quantitative process studies in the tropopause region require a synergetic approach to use instrument data (satellite, aircraft) and atmospheric models (global, regional).

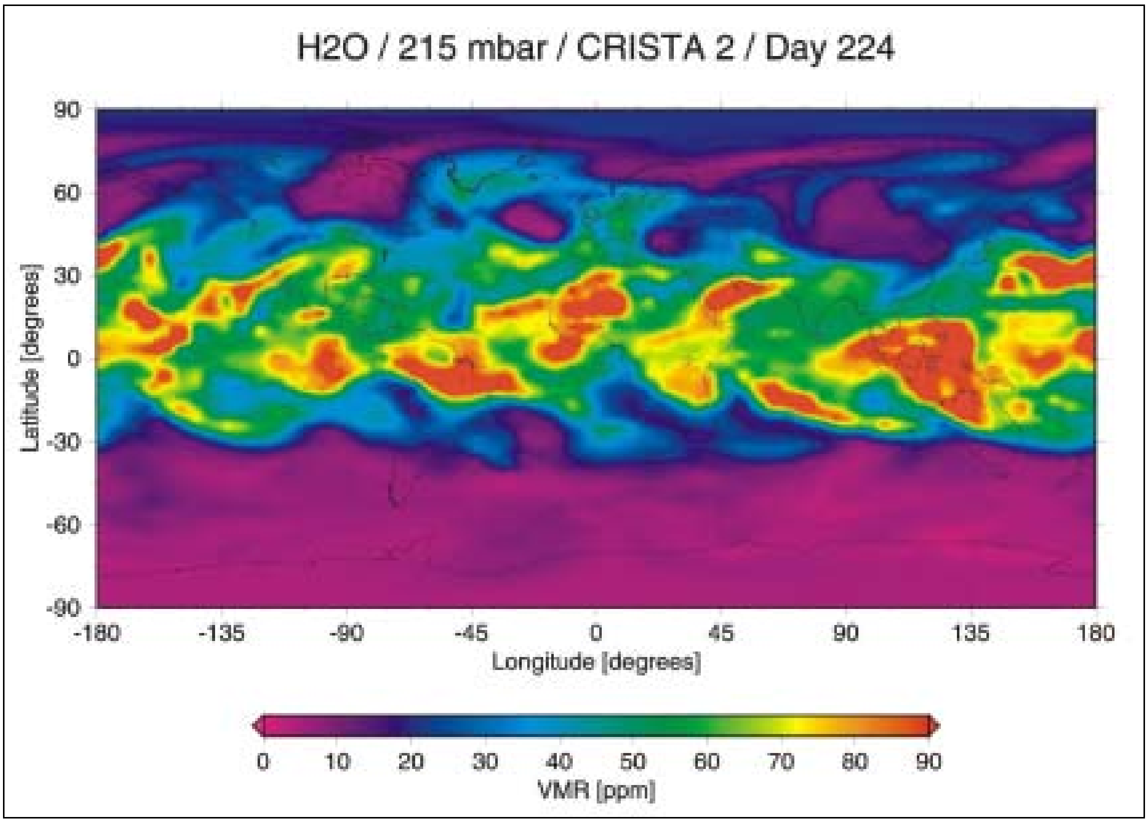


Figure 15.8. Assimilated water vapour field at 215 hPa on August 12th, 1997. The assimilation procedure combines CRISTA trace gas observations with meteorological data. It does not account for micro-physical processes.

The Jülich group (Smit) used upper tropospheric humidity (UTH) observations obtained from MOZAIC aircraft in conjunction with METEOSAT-7 satellite data to investigate the control mechanisms of UTH. Their investigations have been focused on the fate of humidity in the outflow regions of tropical cumulonimbus (Cb) convection. Their analysis shows that the relative humidity in the outflow decreases in time much more slowly than subsidence under cloud-free conditions would predict. The most plausible explanations are either an unknown humidity or energy source originating from the radiative interaction of sub-visible cirrus clouds.

From the MOZAIC aircraft data, the Laboratoire d'Aerologie/CNRS (Thouret) has developed enhanced products such as the tropospheric ozone columns and the horizontal ozone climatology at different altitudes ($z = 9–12$ km) in reference to the tropopause altitude at different seasons. These derived data products will be used for comparisons, for example, with the SCIAMACHY instrument. The tropospheric columns derived from MOZAIC have been compared with the corresponding columns derived from TOMS data.

The APE (Airborne Platform for Earth observation) community (McKenzie), which coordinates the geophysical research using the *Geophysica* aircraft, reports results obtained during the THESOE mission over the Indian Ocean in 1999. The satellite (METEOSAT-5) and aircraft data were used to distinguish non-convective tropopause cirrus from underlying convective anvils. In conjunction with the extremely cold tropopause, the data indicated a region of active dehydration in the lower stratosphere.

Two studies by the groups from BIRA-IASB (De Mazière) and IFU (Sussmann) combined satellite and ground-based FTIR observations of tropospheric trace gases. Advanced retrievals are being developed to investigate their complementarities with respect to satellite derived vertical concentration profiles. The BIRA-IASB group have used successfully the techniques of vertical inversion to derive vertical ozone distribution from the ground-based FTIR at the Jungfraujoch. The capabilities of the method have been demonstrated for ozone and CO; for CO a good sensitivity has also been demonstrated at surface level. The results will be used for validation of MOPITT and SCIAMACHY satellite data. It is planned to extend the analysis to other species like CH_4, N_2O and possibly HNO_3.

In preparation for the SCIAMACHY validation the IFU group have developed retrievals for inverting vertical profile information of several chemical parameters (e.g., O_3, CO, CH_4 etc.) from their ground-based FTIR spectrometer. The group has also set up a site on the Zugspitze, Germany, 47°N, 11°E, 2964 m a.s.l., equipped with FTIR, LIDAR, GPS and radio soundings to validate water vapour data from the AIRS and SCIAMACHY satellites. In summer 2002 two successful validation campaigns were conducted.

Weber (Bremen group) has derived ozone profile retrievals from broadband nadir UV/visible satellite spectra and investigated the accuracy by comparison with ground-based Dobson total ozone column observations and detailed vertical profiles from the worldwide ozone balloon sonde network.

The results in task group 2 show the power of the synergy between satellites and models. For example, the work from the Cambridge group (Savage) is investigating the application of model/satellite observation synergy in determining, not only model validation, but also the ability to constrain global emission inventories. This point is further exemplified by the work of Rohrer looking at the ability to match EDGAR emission inventories through the MOZART model with the GOME NO_2 data. This form of synergy should not be forgotten when considering the output of this task.

15.8.3 Evaluation and recommendations from task group 3

The results from task group 3 demonstrate that an integrated approach of using observations from different platforms can increase the scientific content appreciably compared to that from the individual measurements/platforms themselves.

Further, the different scientific contributions have demonstrated that each study requires its own scientific and operational specifications, such that generalisation of integration is often not possible.

An important lesson we have learned is that it is almost imperative to explore appropriate strategies to establish and document the different methodologies to synthesise data sets based on the experience from the different contributors, not only from this task group, but also from the other TROPOSAT task groups. The process of synergistic use of different data sets is a continuous process of developing retrievals, validation and integration. Particularly the development of such a strategy of synergistic use would really be a significant step towards the establishment of an “Integrated Observation System” as part of an integrated research approach to explore the troposphere and its future changes. The crucial importance of such an approach has been recently pointed out by the IPCC-2001 report, whereby an integrated observation network is a pre-requisite. Initiatives in this field are pioneering work and a large challenge for the scientific community in the coming years.

15.9 Validation and Data Assimilation for Tropospheric Satellite Data Products

Principal Results from task group 4

15.9.1 Summary and aims

The objectives of task group 4 are to develop strategies for the geophysical validation of tropospheric satellite data products and apply them, and data assimilation models, on satellite data. Data assimilation is used for validation purposes and to augment the value of satellite measurements.

Validation of satellite products independently establishes the precision and accuracy of the data product, which is to be compared with the error estimates resulting from the retrieval and included the product. Validation results are an essential source of information for the use of the satellite data. Identified users of validated satellite data are: (i) protocol monitoring (Montreal, Kyoto, UNECE CLRTAP), (ii) support of environmental policy development for the troposphere, and (iii) mapping and interpreting air pollution on global and regional scales.

Validation typically involves the collection of experimental or model data with the similar characteristics to the satellite product, but gathered by independent means: i.e., *correlative data*. The correlative data is gathered by ground-based, airborne, or (other) satellite instruments, or by model runs. The correlative data is compared to the respective satellite product and differences are quantified.

Validation requires correlated data for a large range of representative locations, times and conditions.

The quality of satellite products often varies during its lifetime; this may be due to possible degradation of the instrument, or to updates of the retrieval algorithm. Therefore, validation activities need to be carried out throughout the full lifetime of the satellite.

A different type of validation is the use of data assimilation. Data assimilation is an important tool for the validation and quality control of satellite measurements. Exploiting data assimilation models fully makes it possible to determine random and systematic errors in the measurements and perform quality control of the instruments. Assimilating measurements (ground-based or other validated satellite measurements) into an atmospheric model enables continuous, co-located comparison with assimilated satellite measurements.

TROPOSAT task group 4 validation activities take place in each of the following categories:

- collection of comparative **measurements** (ground-based, aircraft, and other satellite measurements) and intercomparison of these measurements with the satellite data,
- comparison of the satellite data with **model** results,
- analysis of different **retrieval** methods,
- the use of **data assimilation** models for validation, and
- the **coordination** of validation.

This diversity of the TROPOSAT validation activities helps to achieve an optimal validation result. Coordination of validation is essential to identify and remedy any possible deficiencies, for example, products not considered or complementary methods not used. In addition, general activities in the field of data assimilation of satellite data are included.

15.9.2 Activities and results of task group 4

Below, the activities of the principal investigators are summarised.

Collection of comparative measurements and intercomparison

Ground-based measurements

Arlander discusses the use of the long-term NO_2, ozone, SO_2, VOC and aerosol measurements available in the EMEP data base for case study validation of GOME, SCIAMACHY and MIPAS data products. The ozone sonde results available in the NILU/NADIR database are important for case study validation of ozone in the free troposphere over Europe. NILU has assisted several TROPOSAT partners in obtaining data from EMEP and NADIR for use in various TROPOSAT studies.

Galle has performed ground-based FTIR measurements at Harestue (60°N, 11°E) of HCl, HF, O_3, CH_4 and CO. These measurements are used within the validation projects for the CRISTA, MOPITT, ACE, Odin and ENVISAT satellite instruments. Formaldehyde measurements will be used for the ENVISAT validation programme; the instrument was used to probe urban air pollution in the Po valley in summer 2002.

Aircraft measurements

Junkermann describes air-borne measurements on UV, aerosols, clouds and formaldehyde performed in winter 2001/2002 and July/August 2002. The spatial variability within ENVISAT pixels has been probed. Comparisons with satellite-derived formaldehyde columns should take the free tropospheric mixing ratios into account. Complex vertical aerosols structures have been found for polluted conditions.

Meister has performed test measurements of an air-borne ozone DIAL. The instrument allows measurement of two-dimensional along-flight sections of ozone with high spatial and temporal resolution. It is not yet intended to use this instrument for satellite validation.

Satellite measurements

Aben is investigating SCIAMACHY CO and CH_4 products by comparison with MOPITT measurements. Only the CO measurements by the MOPITT instrument have been extensively validated so far. They will be compared to SCIAMACHY CO data.

Comparison with model results

The SCIAMACHY CO and CH_4 tropospheric columns will be compared with model calculations of the 3-D chemistry transport model TM3 by Aben and co-workers. A zoom version of TM3, TM5, has been applied to simulate CO concentrations at Mace Head in Ireland and on the island of Crete. The comparisons show a good agreement.

Preliminary results from the SRON CH_4 retrievals are available. Comparison with TM3 runs shows that the SCIAMACHY columns are 15% lower than the model columns. Improvements of the retrieval are underway.

Analysis of different retrieval methods

Aben plans to validate SCIAMACHY CO and CH_4 total columns by direct comparison of the operationally retrieved CO and CH_4 columns with the values obtained with two retrieval algorithms developed at SRON: an iterative maximum likelihood algorithm and a non-linear least-squares algorithm using the Phillips-Tikhonov regularisation.

Use of data assimilation models

Aben proposes to use data assimilation to enable the comparison of non co-located satellite measurements for the global validation of SCIAMACHY CO and CH_4 products with MOPITT and ground-based measurements. A high-resolution single tracer version of TM3 has been developed for the assimilation of CH_4: TM3-TMSCIA. The assimilation system has been tested using synthetic satellite observations.

Eskes is developing data assimilation methods to validate O_3 and NO_2 measurements of GOME and SCIAMACHY. A webpage *http://www.knmi.nl/gome_fd/tm3/lvl4.html* has been constructed to aid the validation community and contains data and tools for the validation of GOME and SCIAMACHY ozone data.

Elbern provides an overview of all data assimilation activities within TROPOSAT and discusses the advantages and challenges of assimilation of tropospheric satellite products.

Validation co-ordination

Kelder co-ordinates the validation of all SCIAMACHY products (near-real time and off-line) as chair of the SCIAMACHY Validation and Interpretation Group (SCIAVALIG). Special attention is being paid to the validation of the new tropospheric products, such as the tropospheric trace-gas distributions derived from combined nadir-limb observations. The main validation phase of SCIAMACHY will last until the end of 2003. Detailed information can be found on the SCIAVALIG web site *http://www.sciamachy-validation.org/.*

15.10 Tropospheric data from the United States

15.10.1 Introduction

There are several tropospheric data fields available from the U.S.A. Tropospheric constituent species are limited primarily to ozone and water vapour abundance. Global satellite fields such as cloud optical thickness/fraction, aerosols, surface UV, etc., are important for the analysis of the troposphere which includes climate change applications and the effects on the photochemistry of constituents in models. The first section gives a summary of the data fields most used, together with some current developments at NASA in deriving tropospheric ozone profiles. The upcoming EOS Aura tropospheric constituent measurements are then discussed.

15.10.2 Data currently available

The tropospheric data associated currently available in the U.S.A. are tropospheric column ozone (TCO), tropospheric cloud cover, surface UV, and absorbing/non-absorbing aerosols derived from the TOMS instrument. Since late 1978 the TOMS instrument has provided nearly global coverage of these parameters with an average surface resolution down to approximately 100 km by 100 km (Fishman *et al.*, 1990). Absorbing and non-absorbing aerosols are detected from TOMS using a defined Aerosol Index (Torres and Bhartia, 1999). Cloud cover is measured as an effective surface reflectivity and represents combined effects from cloud fraction and cloud optical depth. Surface UV (erythemally weighted and for selected wavelengths) is determined from TOMS total column ozone and reflectivity measurements. TCO is provided in monthly averages for low tropical latitudes (15°S to 15°N) for January 1979 to the present (Ziemke *et al.*, 1998). A number of other similar data sets are also available.

Since 1991 the instruments onboard the Upper Atmosphere Research Satellite (UARS) have produced measurements of many atmospheric parameters including upper-tropospheric H_2O from the Microwave Limb Sounder (MLS) instrument. These data extend nearly pole to pole. (Read *et al.*, 2001).

There is now a large and growing database of additional tropospheric data from the Earth Observing System (EOS) series of satellite platforms and instruments. In 1999 the EOS TERRA platform was launched with several instruments on board including a CERES instrument, having the capability of measuring. aerosols and cloud properties, and the Moderate Resolution Imaging Spectro radiometer (MODIS) for measuring aerosol and cloud properties. Onboard TERRA is also the MOPITT instrument which measures carbon monoxide and methane in the troposphere. In May 2002 EOS Aqua was launched. Onboard EOS Aqua were additional CERES, MODIS, and other instruments to monitor global clouds, aerosols, and ocean parameters over the globe.

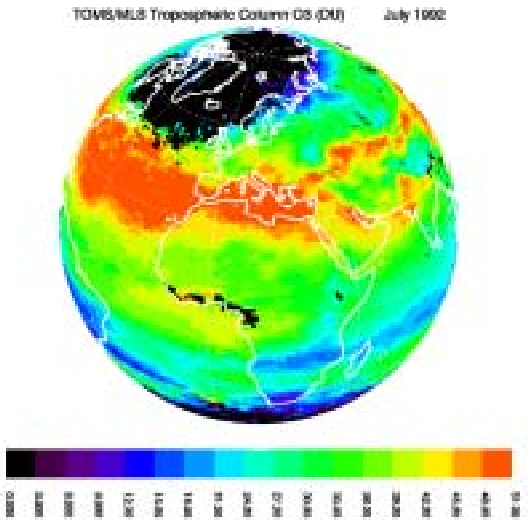


Figure 15.9 (a)

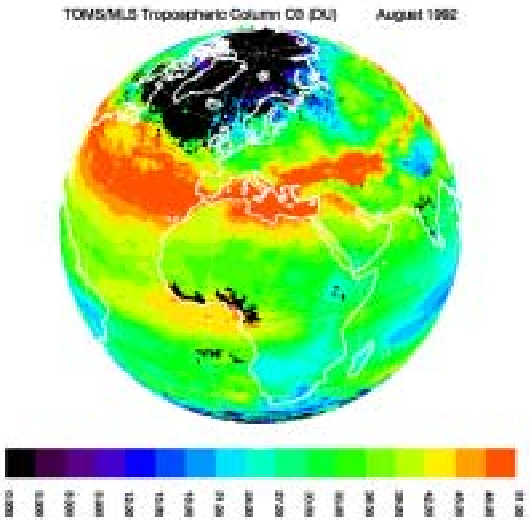


Figure 15.9 (b)

Another development (NASA Code 916) has been to produce a more extensive tropospheric ozone data product than that is currently available. The work involves combining TOMS data with that from the MLS instrument aboard UARS, and will extend the global coverage of the TOMS data. Figures 15.9 (a) and (b) show examples of the final data product of TCO from TOMS/MLS for data averaged over a month time period. Dark pixels in these figures are regions with persistent clouds and/or snow and ice. Figure 15.9(a) indicates large TCO over the broad Mediterranean and northern African region compared to middle and northern Europe. Figure 15.9(b) shows that most of these features were still present during August 1992.

15.10.3 Future perspectives

The new data treatment will be used to derive high-resolution daily TCO maps from the upcoming EOS Aura satellite which is planned to be launched in 2004. Onboard Aura will be four instruments: the High Resolution Dynamics Limb Sounder (HIRDLS), the Microwave Limb Sounder (MLS), the Ozone Mapping Spectrometer (OMI), and the Tropospheric Emission Spectrometer (TES). Total ozone from OMI at resolution 13 km by 24 km will be combined with cross-calibrated SCO measurements from either HIRDLS or MLS. It is also anticipated that both HIRDLS and MLS will make measurements in the upper troposphere of O_3, CH_4, N_2O, H_2O, and other constituents. The TES instrument will produce retrievals of tropospheric NO_y, CO, O_3, H_2O and several other constituents.

15.10.4 Further information

Information on obtaining US data can be obtained from the following web sites

TOMS ozone data:	*http://hyperion.gsfc.nasa.gov/Data_services/*
H_2O data:	*http://mls.jpl.nasa.gov/*
Aura Mission:	*http://eos-chem.gsfc.nasa.gov/instruments/*

15.11 Future space infrastructure

15.11.1 Introduction

TROPOSAT relies for its data on space missions presently in operation, mainly the ESA ERS-2 with GOME and ATSR on board. Recently, the ESA ENVISAT (March 2002) with SCIAMACHY and AATSR on board and the Meteosat Second Generation (August 2002) with SEVERI on board have become available. The NASA operational missions EOS TERRA (MOPITT) and EOS Aqua (AIRS) provide complementary information on methane and CO. In future, space missions already approved will provide continuity of data from the EUMETSAT MetOp 1, 2 and 3 series (2005–2015) with GOME-2 and IASI on board, as well as the NASA EOS Aura (2004–2007 with OMI, TES, HRDLS and MLS) providing new data in addition. The NASDA ADEOS-II (end 2003) with TES and ILAS-2 on board and GCOM-A1 (2007, Greenhouse Gas Monitoring Satellite) missions represent the Japanese contribution to troposphere observation from space.

With the very long lead times required to launch a satellite, it is important to define now the requirements for space missions that will be needed in the 2015–2020 time frame.

15.11.2 GeoTROPE

In the troposphere the variability induced by the daily dynamic transport coupled with chemical reactions produce short-term (sub-hourly) variations and substantial spatial variability of constituents and parameters. The observational limitations encountered with low earth orbit (LEO) satellites (at most, a daily revisit time, sometimes corrupted by cloud cover) dictate that the troposphere is significantly under sampled. Measurements from geostationary orbits offer a practical approach to the observation of the diurnal variation from space with adequate horizontal and vertical resolution, while still maintaining the global synoptic view. In combination with LEO satellites in polar orbit and ground-based measurements, geostationary satellites would link diurnal with seasonal to annual time scales, and local with regional, continental and global spatial scales. The short response time could form the basis for early pollution warning system.

The targeted geophysical parameters for GeoTROPE, derived from a quantitative assessment of the scientific requirements, are:

- total and tropospheric column amounts (including the planetary boundary layer) of O_3, CO, CH_4, NO_2, SO_2, HCHO, C_2H_6, PAN, BrO, H_2O, OCS, CO_2 and N_2O;
- tropospheric height resolved information (including the planetary boundary layer) of O_3, CO, CH_4 and N_2O;
- vertical profiles of H_2O and temperature;
- the radiation field at top of the atmosphere;
- aerosol optical thickness, aerosol layer height;
- cloud top height and cloud cover.

The chosen geographic area covers the Europe, Africa, and surrounding oceans. The area will be covered every 30 to 60 min. with a horizontal sampling of 11.5 km× 23 km to 23 km × 23 km (at sub-satellite point), depending on the measurement mode of the instruments.

In their evaluation of the GeoTROPE proposal (May 2002) the Earth Science Advisory Committee of ESA recognised “the urgent need of such atmospheric composition measurements”. GeoTROPE is now included in the ongoing definition process of future European geostationary satellites (Post-MSG, 2015–2025). EUMETSAT is also strongly interested in geostationary satellite observations for operational chemical applications and air quality monitoring.

15.11.3 TROC, a non sun-synchronous LEO satellite

The TROC proposal (TROpospheric Chemistry and climate), submitted in response to the ESA call (2002) for Earth Explorer Opportunity Missions, is also directed at diurnal variation of the troposphere, albeit in more explorative sense rather than monitoring as is GeoTROPE. It is intended to measure vertical profiles of O_3, CO and CH_4 as well as total and tropospheric columns for NO_2, HCHO, SO_2, BrO, C_2H_6, and height resolved information on tropospheric aerosol. Information on other species (H_2O, CO_2, N_2O, CFCs, OCS) of importance for climate studies will also be measured.

While still being an LEO satellite, TROC differs from the present sun-synchronous vehicles. Its orbital characteristics are: (a) non-sun synchronous polar orbit optimised to sample the diurnal/nocturnal cycle; (b) 3-day revisiting period for any 100 km × 100 km area between 68°S and 68°N.

The TROC proposal has been favourably reviewed by the ESA Earth Science Advisory Committee (ESAC). It seems likely that the TROC mission will be selected for Phase A studies in one of the later rounds of ESA Earth Explorer calls.

15.12 The use of data assimilation to augment the utility of satellite data

15.12.1 Introduction

The assimilation of tropospheric satellite data into chemistry transport models was envisaged by TROPOSAT from the outset. Data assimilation combines both direct and indirect information about the state of the chemical system, whatever the source of information: satellite data, other remote sensing data, and *in situ* observations with models and climatologies. The measurement data are generally scattered in time and space and have various error characteristics as well as spatial and temporal representativity. The cost associated with this flexibility is the highly demanding mathematical and computational requirements.

Despite its potential, assimilation of chemistry satellite data is still in its infancy. This is because traditional two or three-dimensional assimilation mono-variate methods are lacking, as they are incapable of accounting for chemical dynamics. In many cases, though, their use might be sufficient; for example, it might be adequate to analyse only ozone concentration fields for use in the radiative transfer equation of meteorological forecast models by intermittent ingestion into the model. This nudging approach might also be helpful in improving chemical weather forecasts, if success is verifiable.

However, it is only with state of the art CTMs, that the full benefits can be achieved from theoretical knowledge about the system, using models, which are introduced as an integral part of the data assimilation algorithm. In addition, for the reason of scientific rigour, it is mandatory to apply data assimilation algorithms which act as best linear unbiased estimators (BLUE). Algorithms which include models that have the BLUE property are work and computer intensive. Adherence to this standard will enable us to provide information about the accuracy of products via the analysis error covariance matrix.

15.12.2 Data assimilation activities within TROPOSAT

The data assimilation projects active during the lifetime of TROPOSAT implemented a variety of different methods. Strictly only four projects are dedicated to this field.

Assimilation activities at KNMI include both ozone and nitrogen dioxide assimilation (Kelder). In the former case GOME ozone profiles are assimilated into the TM3 chemistry transport model by an adapted Kalman filter technique. For NO_2 a combined retrieval and assimilation tool has been developed and implemented, which accounts for the effects of aerosols, surface albedo, fractional cloud cover and the height-dependent sensitivity of the UV/visible spectrometers.

The assimilation of aerosol data is developed by the TNO-LOTOS group (Builtjes). The underlying algorithm is a Kalman filter with reduced complexity. The assimilation quantity is the aerosol optical density as retrieved from ATSR-2 (de Leeuw), from which information about SO_2, NO_3, and NH_4 concentration levels is inferred.

A four-dimensional variational data assimilation method from the University of Cologne EURAD chemistry-transport model has been developed and set up to assimilate monthly mean NO_2 tropospheric columns retrieved from GOME. The adjoint calculus implemented here is applied, to combine emission rate and initial value optimisation.

By exploiting multi-channel GOME image sequences, Wagner introduced a non-legacy concept to construct sequences of tropospheric NO_2 column maps. Special care is taken to account for the irregularities introduced by the cloud cover variation.

15.12.3 The future

With systematic application of advanced data assimilation algorithms it will be possible to quantify the skill of our models, or, in recompense, identify systematic model faults. With the complexity of today's models the latter is rather beyond the intuition of even experienced modellers. In addition, the fixing of the deficiencies, in order to introduce targeted model ameliorations, is not a mere technical issue. It also serves to verify our understanding of the observed system as a whole. Within given predefined error margins, there are algorithmic means to decide whether the system, as observed, is in compliance with our coded knowledge or not, or whether the data base is too poor to decide.

The discussion about the proper optimisation quantity, namely the emission rates, motivates the use of satellite data which is not directly related to atmospheric chemistry. The land cover and vegetation type figure most prominently in this respect, as they represent key factors for the surface-atmosphere interaction. Suspension of mineral dust and the release of precursors of biogenic secondary aerosols is controlled by processes for which the crucial conditions can be observed from space. With the aid of this data, biogenic emission rates and deposition velocities, as two of the prime forcing quantities of tropospheric chemistry, can be constrained to attain unprecedented inversion results. Augmented by surface observations and by emission inventories, satellite data and advanced data assimilation can reach far beyond the scope of a single information source. This is of utmost importance for air quality information, and it is these data assimilation techniques, prominently based on Bayesian reasoning, which will guide us through all the heterogeneous information sources to form consistent pictures for scientific and operational use in the future.

15.13 Future perspectives and opportunities

15.13.1 Atmospheric chemistry

What opportunities do these still newly available satellite data offer to atmospheric chemists? A simple scrutiny of the concentration maps on global and regional scales should provide confirmation of, or provoke questions about, what was hitherto not observable. The data will provide a direct comparison with the output from CTMs on global and regional scales and will be used for realistic validation and sensitivity work to improve substantially the accuracy and reliability of CTMs. Satellite measurements should also be useful in providing real boundary conditions for operational models. In addition source strengths of trace gases can be derived. For field campaigns, a knowledge of the actual concentrations of appropriate species in the vicinity of the campaign area will be available. In short, satellite data will soon be an essential adjunct to the major activities in atmospheric chemistry in the future.

15.13.2 Environmental policy development

For those engaged in environmental policy development, satellites used together with CTMs will provide a method to monitor pollutant concentrations on a continuous basis, allow the firm identification of pollutant sources, and trace the transport of pollutants in the atmosphere both globally and regionally. In addition, satellite data will be an essential component for any global observation system such as that envisaged by IGACO.

15.13.3 Integrated use of data from several satellite instruments

Probably the biggest challenge within the field is to integrate the data from several sensors, such as aerosol and cloud data from MERIS and trace gas information from SCIAMACHY and MIPAS, to obtain more useful data products. If such a synergistic use is to be implemented at the retrieval level, and not only in the final products, it will necessitate new approaches and much interaction between the algorithm communities. TROPOSAT task group 1 is already at work on starting this process, and much progress is expected in the future.

15.13.4 Synthesis and integration of data from many sources

An important lesson learned by task group 3 is that the synergistic use of different data sets is a continuous process of developing retrievals, validation and integration. It is imperative to explore the required strategies to bring together data produced with different techniques to obtain an overall picture of the atmosphere. Such strategies will be an essential step in the construction of an "Integrated Observation System" for the observation and monitoring of the troposphere and its future changes. The crucial importance of such an approach has been recently pointed out by the IPCC 2001 report. Initiatives in this field are pioneering work and a large challenge for the scientific community in the coming years.

15.13.5 The necessity for a geostationary satellite

The most pressing requirement for the future is the early acceptance of a project to launch a geostationary satellite capable of measuring tropospheric concentrations of pollutants and trace species. The integrated observation system desired by the international community and required for environmental policy development, needs the daily time-resolved data from such a satellite to combine with the information from low earth orbit satellites, ground-based and *in situ* sensors, in order to obtain a continuous picture of the atmosphere. Considering the lead time required to launch such a satellite, such a project should be initiated now.

15.13.6 Conclusions

It is evident from this report that, though much has been achieved, even more remains to be done to realise the full potential for the data becoming available. The formation of TROPOSAT and its clear success has shown that a group devoted to producing and exploiting the data, and to bringing together "producers" and "users" is necessary, and every effort will be made to continue the project, if not under the good auspices of EUROTRAC-2, then perhaps with the help of the EU, or ESA itself.

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