SPARC
STRATOSPHERIC PROCESSES AND THEIR ROLE IN CLIMATE
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# Report on the 13th Session of the SPARC Scientific Steering Group

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### Introduction

The 13th session of the SPARC Scientific Steering Group (SSG) was held at Lady Margaret Hall, University of Oxford, at the invitation of **A. O'Neill**, Co-Chair of SPARC. In opening remarks **A. Ravishankara**, Co-Chair of SPARC, noted that SPARC is at an important stage in its lifecycle, taking on new issues in the framework of the three-theme project structure. The development of COPES presents new challenges and opportunities for the WCRP, necessitating even stronger interactions with IGBP and other agencies. The next IPCC and WMO/UNEP Ozone Assessments are in full swing so that the next 2-3 years will provide the opportunity to shape the science for future assessments and to position SPARC to make key contributions.

### COPES and SPARC

**P. Lemke**, Chair of the WCRP JSC, presented an overview of WCRP achievements and its future activities in the context of the COPES strategic framework. The WCRP has worked towards understanding and predicting the Earth system through international coordination of global observation, process studies and modelling. These activities have been carried out within the WCRP projects and various working groups. Through such interaction, the WCRP has helped to enhance the understanding of the climate system, make significant improvements in observing systems, improve coupled climate models, and make advances in assimilation techniques and forecast models.

Future activities within the WCRP must address a number of outstanding science questions relating to climate variablity and change, including causes of potential abrupt climate change (mechanisms and thresholds), simulation of ice age cycles, prediction of sea level rise, studies on the role of chemistry and its interaction with climate, and interaction of water vapour, clouds, radiation, precipitation and aerosols. Development of ensemble methods will enable the prediction of extreme events, and understanding, quantifying and reducing uncertainties of future predictions and projections. Society will benefit from decision making based on regional climate prediction and early warning systems.

Several task forces and coordinating bodies have been established by the WCRP to facilitate implementation of COPES initiatives. The new WCRP Modelling Panel and Observations and Assimilation Panel

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(WMP and WOAP) have a coordinating role. The Task Force on Seasonal Prediction (TF-SP) determines the seasonal predictive skill achievable with today's models and observations. The goal is to identify sources for as yet untapped additional predictive potential. More task forces will be established in the near future to address studies of monsoons, atmospheric chemistry and climate and, possibly other topics. P. Lemke noted that SPARC will continue to address and provide leadership for a number of issues that overlap with other WCRP projects, working groups, and partner organizations, especially in the area of chemistry and climate.

**V. Ryabinin** informed the meeting about the new COPES project office in Paris. It has been in operation since March 2005 and has already supported several important WCRP events. Jean Jouzel is the Administrative Director and Hervé Le Treut is the Scientific Director. The office may be reached by email at copes@ipsl.jussieu.fr. More information may be obtained on the website at http://copes.ipsl.jussieu.fr. The office is supporting the organization of the ESSP Open Science Conference on Global Environmental Change (9-12 November 2006, see www.essp.org/essp2006).



**A. O'Neill** discussed overarching issues for SPARC, and developments since the last SSG meeting. He noted that a wider range of questions will be considered in future SPARC activities, and that the SPARC themes and activities emphasising prediction, predictability and observations map directly onto COPES. The questions put to the JSC in regard to the chemistry and climate issue, and the JSC response, were summarized in SPARC Newsletter No. 25. In regard to this issue, the JSC re-affirmed the need to develop a road map for chemistry-climate models (CCMs), observations and process studies. The establishment of a joint WCRP-IGBP Task Force was proposed, and planning is now under way for a small group to meet in Boulder later this year to discuss the way forward. The need for inter-calibration of stratospheric data from various satellites was drawn to the attention of GCOS, and a "reprocessing" project has been proposed under WOAP to increase the accuracy of climate data sets obtained from remote sensing. The concept of this project is being developed. Several workshops joint with other WCRP and IGBP projects are in the planning stages for 2006/2007. In addition, SPARC will work with WGCM to update top-of-atmosphere solar forcing data, and will continue to pursue activities and interests in solar effects on composition and atmospheric variability.

The JSC strongly encouraged SPARC working with CLIVAR. This was explored further at the joint SPARC-CLIVAR session at the AMS meeting in June 2005, which served to highlight a number of overlapping SPARC and CLIVAR interests:

- Stratosphere-troposphere coupling and the North Atlantic Oscillation (NAO)
- Detection, attribution and prediction of stratospheric changes and the CLIVAR themes of climate change detection, attribution and prediction
- Chemistry-Climate Interactions (IGBP/IGAC)

A joint CLIVAR/SPARC Workshop on the NAO in the "Fully" Coupled System was proposed, probably for 2007. This workshop will focus on mechanisms, and NAO predictability and timescale. A goal of the workshop is production of reader-friendly review article on the state of knowledge and where we go next.

## SPARC THEMES: PROGRESS and ISSUES

### *Stratosphere – Troposphere Dynamical Coupling*

**S. Yoden** discussed recent and ongoing work in regard to this theme, with relevance to the TF-SP. The timescales considered are intraseasonal to seasonal (*e.g.* wave dynamics, 10 days to several months), interannual (*e.g.* internal variations, responses to 'external' forcings such as the QBO and ENSO), and interdecadal and longer (*e.g.* changes in the Brewer-Dobson circulation and polar vortex). Processes that involve ST-coupling include ST exchange and transport processes, changes in the Brewer Dobson circulation, processes involving the polar vortex, extreme weather events, *etc.* Evidence was presented of an internal intraseasonal variation that showed persistent circulation anomalies in the lowermost stratosphere, and allowed for extended-range forecasts of the monthly-mean Arctic Oscillation (AO), especially during boreal winter. The TF-SP held a workshop on Seasonal Prediction in Trieste, Italy, August 22-24, 2005 (http://users.ictp.trieste.it/~h093/) with a focus on 'seamless' weather to climate prediction, and the importance of the stratosphere in forecasting models. In addition, a joint CLIVAR/SPARC workshop on the NAO and the stratosphere has also been proposed (noted above), as well as a SPARC stratosphere-climate workshop. The next ST Coupling Workshop will also be a Chapman conference in Santorini, Greece, in June 2007. This will be a natural fit after the experience with the Chapman Conference on Jets held in Savannah, USA, January 2006.

P. Kushner and W. Robinson have proposed a SPARC project to explain the dynamics of the most robust results among current climate models using dynamical analysis and simple dynamical models. The questions to address are: (a) Why would we expect the Brewer-Dobson Circulation (BDC) to strengthen? (b) Which parts of the BDC response to climatic change are attributable to the greenhouse gas warming and which to ozone depletion? (c) To what extent are the models sensitive to their treatment of unresolved (*e.g.* gravity) waves and other dissipative processes? A subproject will systematically examine the dynamics of the BDC response to climate change, using a variety of tools including stationary wave modelling, diagnosis of reflective surfaces, zonally symmetric model calculations, and simplified GCMs. Still needed are: (a) a better characterization of PWD variability and its chemical consequences; (b) a distinction in model diagnostics between the pure radiative response to a forcing and the PWD feedback; (c) understanding of tropospheric *vs.* stratospheric effects on PWD; (d) reduction in uncertainty of PWD predictions; (e) ensembles of model integrations; (e) PDFs of short-term behaviour.

### *Detection/Attribution/Prediction*

**W. Randel** noted that the main thrust of this theme at the moment is the updated trend assessment. The scope is to provide an update of the observed stratospheric temperature record (through 2004), and improve the understanding of past changes and predictions of future stratospheric temperature changes, especially by reducing uncertainties in the predictions. The first meeting occurred in March 2005 in Reading to plan the scope of the project and to take an initial look at the updated observations. It was decided that the group would first write a paper on the updated observations, with focus on satellites, radiosondes and lidar data. A draft should be completed before the second meeting planned for October 20-21 in Boulder.

The initial results show a flattening of trends at the stratopause, and a small long-term cooling in the middle stratosphere. However, biases in the data are as large as the signal and these biases extend into the upper and middle troposphere. Some key points to consider are that the stratospheric temperature record is highly dependent on SSU data (currently, only one analysis of combined SSU record), and that there are small trends in the tropical lower stratosphere in MSU4 and SSU15x data and that these trends are very different from ones obtained using radiosonde data. This is probably a result of artificial cooling biases in the radiosonde ascent observations, causing jumps in the timeseries at some stations. The strong upper stratospheric cooling ends after 1995, in reasonable agreement with the HALOE data, and there are small global trends in the middle stratosphere in the SSU data. A small cooling trend is also seen in the tropics when the less biased sondes are used.

Two questions that arise are: a) Why are the middle atmosphere trends so small? and b) Why does the Boulder data not agree with the HALOE data, which shows a sharp drop in water vapour after 2001? Of all the data, the Boulder data is the only data that are not fully understood. In addition, it has been shown that using reanalysis or operational analyses/reanalyses data sets is problematic for studying trends.

**T. Shepherd** continued discussion of the Detection, Attribution and Prediction theme by highlighting questions concerning understanding of the natural variability. In 1997, there was considerable concern about the rapid decrease seen in both temperature and ozone in Arctic spring. Today, that behaviour looks more like a fluctuation. In addition, changes in total ozone over the last 25 years in both hemispheres seem roughly consistent with $Cl_y$ loading, but there are also shorter term fluctuations that we would like to understand. This may be possible using imposed "forcings" (volcanic aerosols, solar, SSTs, QBO), however, some of these forcings are actually internal variability, and so imposing these in models gives only partial understanding of the climate system. One key question for the attribution, detection and prediction theme is quantifying the natural variability, which appears to possess long time-scales that are comparable to the perturbations themselves. It cannot be assumed that every decadal fluctuation is a trend.

## *Chemistry-Climate*

**A. Ravishankara** opened the discussion on the Chemistry-Climate Interactions theme. This is becoming of major importance for SPARC because of the CCMVal activity, now the umbrella for chemistry-climate modelling, and interactions with other agencies such as IGAC, which force us to consider including the 'lower' atmosphere in our work. Clearly, the SPARC mandate now includes the upper troposphere. Key questions for this theme are to determine if we are on the right track and to identify the needs for future assessments and the community.

There have also been collaborations with IGAC on some activities (usually reviews, reports, workshops, "priming" participants for assessments, *etc.*). Issues for discussion now are how to manage the activities of CCMVal, how to collaborate with other WCRP and IGBP projects, in anticipating the key needs for the future, and the SPARC contribution to IPY.

**V. Eyring** discussed the current structure and ongoing activities of CCMVal. In consultation with the CCM community, CCMVal has proposed reference simulations for ensemble predictions to support upcoming ozone and climate assessments (published in SPARC Newsletter No. 25). In order to serve the CCM community, and to facilitate the set-up and encourage the use of the reference simulations, a website where the forcings for the simulations can be downloaded has been established at http://www.pa.op.dlr.de/CCMVal/Forcings/CCMVal_Forcings.html.

The proposed scenarios were developed to address the following key questions outlined by the WMO/UNEP Steering Committee to be of significance to the upcoming assessment:

1. How well do we understand the observed changes in stratospheric ozone (polar and extra-polar) over the past few decades during which time stratospheric climate and constituents (including halogens, nitrogen oxides, water, and methane) were changing?
2. What does our best understanding of the climate and halogens, as well as the changing stratospheric composition, portend for the future?
3. Given this understanding, what options do we have for influencing the future state of the stratospheric ozone layer?

In order to address questions (1) and (2), two reference simulations and two sensitivity simulations have been proposed and the forcings have been made available on the website. Ftp sites are currently available to store CCM data at the UK MetOffice, the British Atmospheric Data Centre (BADC), and the SPARC Data Center.

A comprehensive intercomparison of CCM results and observations has successfully started. The CCMVal 2005 workshop in Boulder will assess progress in the validation of current CCMs and assess how CCM model results can support the 2006 UNEP/WMO Scientific Assessment of Ozone Depletion. (See the workshop report in this issue).

**C. Granier** discussed two other international chemistry-climate projects using a multi-model approach similar to CCMVal — the SANTAFE project coordinated by NCAR, and the ACCENT European network, funded by the EC (2004-2009). The focus of the SANTAFE project is to produce simulations for the 1850-2000 and 2000-2100 periods with no specification of emissions except for 2100 (scenario A2). A paper analysing nitrogen deposition has been accepted for publication. ACCENT/IPCC had a larger number of models involved and a central goal of providing information for the IPCC assessment.

These exercises have made clear that fully coupled CCMs, some including oceans and biospheres, are becoming more available for such experiments. However, these models require large computer (and human) resources. A coordination effort in defining the intercomparisons and runs for assessments is needed so that both tropospheric and stratospheric studies may be done with as much overlap in the computer experiments as possible, with similar boundary/initial conditions, and overlapping archives. To this end, SPARC would need to establish formal contacts with other WCRP/IGBP groups. It is noteworthy that the AIMES Project (Analysis, Integration and Modelling of the Earth System) of the IGBP is now under way and will hold its first steering committee meeting in November 2005.

**T. Shepherd** described the proposal to support Canadian contributions to SPARC for the 2006-2011 period, which has been submitted to Canadian funding agencies (CFCAS and NSERC). The Canadian proposal follows the main SPARC themes and includes a component on stratospheric and mesospheric data assimilation. The issue of understanding natural variability and long-term memory enters the proposal plans in various ways: (a) statistical analysis of coupled (A-O) transient simulations, (b) separating direct and indirect response to forcings, (c) analysis of the statistics of extreme events and short-term trends (and their sensitivity to SST variability and the QBO).

On behalf of S. Pawson, **N. McFarlane** presented a plan to do AMIP-style evaluations for GCMs with well-resolved stratospheres. The participating models would preferably have the capability of running with chemistry, but would not run with chemistry for these runs. The study focuses on the abilities of the models to represent the basic dynamical features of the middle atmospheric circulation, as well as their links with the troposphere. There is an emerging realization that statistical uncertainty limits confidence in comparisons, and that model simulations of only a decade or so may be inadequate to properly characterize variability in the stratosphere. The AMIP-style experiments, like GRIPS, would focus on the stratosphere, but would have more constraints.

The proposed activity should complement CCMVal, in which the main focus is chemistry-climate, and processes-oriented validation. There remain a number of first-order questions about GCM performance such as the ability to represent polar vortices, sudden warmings and final breakdowns, stratosphere-troposphere relationships, tropical dynamics, and stratosphere-troposphere exchange. These issues are unlikely to be impacted by the inclusion of chemistry, and multi-annual simulations are needed to study them, making runs with full chemistry expensive. While there was general support among the SSG for this proposed activity, the matter of organizing it and determining when it may take place was left for further discussion at the CCMVal workshop, or following it.

**A. Ravishankara** led a brief discussion on the WMO/UNEP 2006 Ozone Assessment and SPARC's possible contributions to it. The assessment is well under way and the first draft is due at the beginning of November. A large number of SPARC members are the lead authors for the assessment and T. Shepherd, M.-L. Chanin and A. Ravishankara are on the scientific steering committee. CCMVal runs will be a major input, and many of the SPARC assessments (ASAP, temperature trends, PSC report) will provide direct input. The joint SPARC/IGAC UTLS workshop in May 2005 also provided some key legwork on bromine.

**G. Braathen** gave a short presentation on WMO matters. In regard to ozone bulletins, he identified some outstanding issues and posed several questions to SPARC:

1. Is there a better way to characterize the polar vortex dynamics?
2. Can the SPARC community assist ECMWF in fixing the problem of spurious oscillations in analysis data?
3. Ozone Recovery: How can we measure it? Where can we measure it? What are the criteria? How can we be sure that a change in ozone is due to reduced EESC?
4. Can the SPARC community help GAW/NDSC to look out for recovery?

**L. Thomason** summarized key features of the Aerosol Assessment Report (ASAP), which is near completion and will be printed in November 2005. Key results from the report are summarized later in this issue of the newsletter. Briefly, it was found that no long-term trends in stratospheric aerosol have been observed, the dominant precursor gases are OCS and $SO_2$, and that disagreements between the various data sets and models indicate that substantial questions remain regarding the nature of stratospheric aerosol during volcanically quiescent periods particularly in the lower stratosphere. In addition, it was found that in the last three decades only the last several years can be confidently referred to as 'background'.

**T. Peter** presented an update on the SPARC PSC Assessment (SPA) report and the kick-off meeting for the lead authors, on behalf of K. Carslaw. The SPA Kick-Off meeting was held at the Coolfont Resort in West Virginia, USA in March 2005. An update report on the main progress at the KO meeting was included in SPARC Newsletter No. 25 (July, 2005). Agreement on the organisation of the chapters and writing tasks was achieved at this meeting, including the possibility of adding a chapter aimed at the broader atmospheric science community entitled "Twenty Questions About PSCs". A further SPA Science meeting (for review and discussion of preliminary chapters) will be held in April 2006. The target date for completion is the end of 2006.

## The Role of SPARC in IPY

**N. McFarlane** presented progress in developing a proposal for IPY. On behalf of SPARC, an Expression of Intent (EoI) was submitted to the IPY International Programme Office with the title "The structure and evolution of the stratospheric polar vortices during IPY and links to the troposphere" (SPARC-IPY, EoI #807). This EoI proposed to (a) coordinate the IPY related activities of the SPARC community, (b) promote initiatives to increase understanding of the polar middle atmosphere during the IPY period in the context of the SPARC thematic programmes, (c) make available the services of the SPARC Data Center to facilitate acquisition and archiving of key data that will be used for projects or generated by them during the IPY period.

Preliminary recognition was awarded by IPY Joint Committee (JC) in mid-April with an invitation to submit a full IPY Activity proposal by one of the three posted deadlines dates. The IPY JC assigned proposals to "clusters" with certain EoIs as "lead" proposals. SPARC-IPY was selected as a lead EoI for Cluster 7.1 (IPY SPARC) and requested to prepare a full proposal, which includes other EoIs in the cluster and links to other full proposals that have relevant/related activities. At the time of the SSG meeting an activity proposal was in preparation with the tentative title: "The Structure and Evolution of the Polar Stratosphere and Mesosphere and links to the troposphere during IPY". In addition to the EoIs that are clustered with IPY SPARC there are a number of other IPY Activity proposals that are closely related and of interest to SPARC. Among these are the POLARCAT proposal and the ORACLE-O3 proposal.

**K. Law** presented a summary of the POLARCAT (Polar Study using Aircraft, Remote Sensing, Surface Measurements and Models, of Climate, Chemistry, Aerosols, and Transport) proposal. The overall goal of POLARCAT is to study the role of long-range poleward transport of aerosols and trace gases for climate change in the Arctic. It will include two multi-aircraft campaigns - a winter/spring 2007/8 campaign, and a summer 2008 campaign, as well as several smaller field studies. The summer campaign will focus on the transport of pollution from boreal forest fires to the Arctic troposphere and stratosphere. The winter/spring campaign will target transport of anthropogenic pollution, in particular from Eurasia, to the Arctic. There will be extensive use of satellite data, ground-based lidars, Lagrangian balloons, surface station measurements, and models, to support the campaigns.

**G. Braathen** presented a summary of the ORACLE-O3 (Ozone layer and UV radiation in a changing climate evaluated during IPY) proposal. The main foci of this proposal are (a) Ozone loss (detection and impact on UV radiation), (b) PSC (polar stratospheric clouds) and cirrus, (c) Atmospheric chemistry, (d) UV radiation, (e) Ozone and climate change and feedback, (f) Data management, (g) Education, outreach and communication.

In discussion it was noted that IPY presents an opportunity to do new science and to leave a legacy of research and data. The SSG supported the overall structure and aims of the SPARC-IPY proposal and encouraged completion and submission to meet the 30 September 2005 deadline. *(Postscript: The SPARC-IPY Activity Proposal was submitted and is listed as IPY Activity 217 on the IPY website. It has been awarded recognition by the IPY JC).*

## Cross-Cutting Issues

**M. Geller** discussed issues and activities of joint interest to SPARC and SCOSTEP/CAWSES. There are four themes under CAWSES: (a) Solar Influence on Climate; (b) Space Weather (Science and Applications); (c) Atmospheric Coupling Processes; (d) Climatology of the Sun-Earth System. The first of these themes was the focus of the ISSI workshop on Solar Variability and Planetary Climates held in Bern, Switzerland, June 6-10, 2005. Some conclusions from this workshop which are relevant to the WCRP are: (a) there is considerable uncertainty in the reconstructions of past variations in solar irradiance (total and spectral); (b) this, together with predictability issues, makes attribution of cooling in the mid-20th century to variations in solar output very uncertain; (c) significant progress is taking place on modelling solar UV effects of the troposphere-stratosphere system (good agreement with Labitzke and van Loon, and Kodera results); (d) IPCC models are likely not including solar effects properly at the present time.

Future CAWSES efforts include holding a small meeting (20-30 people) at ISSI, April 19-21, 2006, to move forward plans to write review papers covering (1) observational evidence for solar influences on climate; (2) our ability to make reliable reconstructions of solar outputs that influence climate; and (3) what the isotopic record tells us about solar influences on past climates.

**K. Kodera** discussed the SOLARIS Project (Solar Influence Study for SPARC), a follow-on project from the GRIPS solar influences activity. Its objective is to model and understand the solar influence on climate through stratospheric chemical and dynamical processes. There are currently 13 participating modelling groups, and there are new aspects which go beyond the original GRIPS comparisons. These include modelling solar influences using fully coupled models with oceanic components, chemistry, resolved mesospheres and, for some groups, extensions into the thermosphere.

A SOLARIS planning meeting was held in Toulouse in July, 2005. A number of questions were addressed including time-varying *vs.* perpetual solar max/min runs, multiple forcing *vs.* solar only forcing, spatial structure of solar signals, solar cycle modulation of the QBO period, and influence of energetic particles in the stratosphere. Several coordinated studies are under way: (i) TMST-model (Thermospheric and mesospheric response - coordinated by V. Fomichev); (ii) CCM Ozone and temperature response (continuation from GRIPS coordinated by U. Langematz); (iii) AGCM Dynamical response and the role of the QBO (coordinated by L. Gray).

**N. McFarlane** and **S. Woolnough** (representing the GEWEX Global Cloud System Study) discussed plans and motivation for a joint SPARC-GEWEX/GCSS-IGAC workshop on modelling of deep convection and its role in the tropical tropopause layer (TTL). The purpose of this workshop is to bring together expertise from the SPARC, GEWEX, and IGAC communities to initiate collaborative activities to study key processes within the TTL. The goals of the workshop are to discuss key scientific questions and recent results, develop research strategies, and evaluate modelling and observational capabilities and constraints. This workshop will be held in Victoria, BC in the period of June 12-15, 2006.

**M. Geller** discussed a possible new SPARC initiative on QBO influences on tropical convection. He noted previous work identifying apparent correlations between the phase of the QBO and tropical systems such as the incidence of hurricanes (Gray *et al.* 1984), and modulation of outgoing longwave radiation, highly reflective cloud index, tropopause pressure, and 50-200 hPa zonal wind shear (Collimore *et al.* 2003). Possible lines of research on this topic include studies using ISCCP data, and using cloud resolving models (CRMs) to examine individual effects. It was suggested to hold a SPARC workshop on "QBO Influences on Tropical Convection" in late 2006. This workshop would include papers on observational analyses, GCM modelling and analyses, CRMs, and lead to discussion of future actions.



**S. Polavarapu** discussed recent activities of the SPARC Data Assimilation Working Group (SPARC DA WG). The activities of the SPARC-DA group focus on physical aspects of middle atmosphere data assimilation and on science issues that drive the need to improve assimilation techniques and draw on experts in SPARC themes. Middle atmosphere DA has to deal with problems that are not so critical in NWP focused DA (bias, accumulation of errors over long time scales, large mesospheric variability, vertical coupling). The goals of the SPARC-DA group are achieved through holding thematic workshops, preparation of reports and review articles, and intercomparison/collaborative projects. The recent Joint SPARC Workshop on DA and Stratospheric Winds was held in Banff, Alberta, Canada in September, 2005 and was very successful (see the workshop report in this newsletter). The next SPARC-DA workshop will be held in Noordwijk, The Netherlands in conjunction with ADM workshop 26-28 September, 2006.

**S. Liess** reported on the current status of the SPARC Data Center (DC) and plans for the near future. The SPARC DC has been operational since July 1999 at Stony Brook University, NY, supported by NASA, with M. Geller as the principal investigator. However, present funding is exhausted. Interim funding has been requested but none had been received as of the reporting date. Currently the SPARC DC has a total of approximately 40 Gb of data holdings. Proposed upgrades would increase this capacity to 1.1 Tb. This upgrade in hardware is critical for expected future needs of the CCMVal project and the data archiving anticipated for SPARC-IPY. Additional features, which the SPARC DC hopes to provide in the future, include an online plotting capability and enhanced security. Last year, the SPARC scientific steering group requested that the SPARC scientist become a full-time position. Thus, the position for the research scientist is proposed to be 50% Data Center administrator and 50% research scientist within SPARC. However, the SPARC DC funding crisis must be solved as soon as possible for the Data Center to continue its operation.



**S. Yoden** discussed plans to mirror all or a subset of the SPARC DC data holdings at Kyoto University in Kyoto, Japan. Data accessibility will be enhanced and downloading times will be shortened, since the bandwidth will be shared between SPARC DC and its mirror. The security of a remote backup will protect from data loss.

## Co-ordination with other Agencies/Programmes

**S. Doherty** discussed IGAC/SPARC interactions. IGAC activities address two important questions: (a) What is the role of atmospheric chemistry in amplifying or damping climate change? (b) Within the Earth System, what effects do changing regional emissions and depositions, long-range transport, and chemical transformations have on air quality and the chemical composition of the planetary boundary layer? The science involved in dealing with these questions has much in common with SPARC themes, particularly that of Chemistry-Climate. SPARC-IGAC interactions that have taken place and are in progress include: (a) the SPARC/IGAC Chemistry-Climate Workshop (Giens, 2003); (b) the SPARC/IGAC Workshop: Processes controlling mid-latitude UTLS chemical composition (Mainz, 2005), (c) the POLARCAT (IPY) Project, (d) parts of the IGAC AICI project – i.e. ice phase chemistry, and (e) discussions on next steps at both SPARC/IGAC and WCRP/IGBP levels.

**V. Ryabinin** reported on the SOLAS and OASIS programmes. Although these programmes deal primarily with processes at the surface and in the lower troposphere, their focus on surface fluxes and emissions of key constituents are of interest to SPARC in that they provide critical information for a comprehensive understanding and modelling of the transport and transformation of these constituents in the troposphere and stratosphere. The goal of SOLAS (Surface Ocean Lower Atmosphere Study) is to achieve quantitative understanding of the key biogeochemical-physical interactions and feedbacks between the ocean and the atmosphere, and how this coupled system affects and is affected by climate and environmental change. The goal of OASIS (Ocean-Atmosphere-Sea Ice-Snowpack) is to determine the importance of chemical, physical and biological exchange processes on tropospheric chemistry, the cryosphere, and the marine environment, and their feedback mechanisms in the context of a changing climate.

**V. Yushkov** summarized the second expert meeting on the LAUTLOS campaign (Helsinki, 29-31 August 2005). A paper on the vertical distribution of water vapour in the Arctic stratosphere in January-February 2004 from data of the LAUTLOS field campaign is now available (Yushkov *et al.* 2005). Some preliminary results were also summarized in the SPARC Newsletter 25. The campaign provided vertical profiles of water vapour between 0 to 70 km, and the database is now open for users.

**M. Kurylo** gave a presentation on the NDSC (http://www.ndsc.ws), which is a set of more than 70 high-quality, remote-sensing research sites for observing and understanding the state of the stratosphere and upper troposphere, and assessing the impact of stratospheric changes on the underlying troposphere and global climate. The goals of the NDSC are to study the temporal and spatial variability of atmospheric composition and structure, to provide early detection and subsequent long-term monitoring of changes in the chemical and physical state of the stratosphere and upper troposphere, and to provide the means to discern and understand the causes of such changes. The NDSC also provides independent validations, calibrations and complementary data for space-based sensors, supports field campaigns, and provides verified data for testing and improving chemistry and transport models. The NDSC has participation by more than 20 countries and is still expanding.

One of NDSC operating principles is that investigators subscribe to a protocol designed to ensure that archived data are of as high a quality as possible within the constraints of measurement technology and retrieval theory. Instruments and data analysis methods are evaluated prior to NDSC acceptance and are continuously monitored throughout their use. Data must be submitted to the central archive within one year of the measurement, and are made available within two years of measurement. In some cases, this timescale is much shorter.

NDSC measurement contributions to GAW and IGACO include stratospheric temperatures, total ozone, ozone profiles, compounds related to ozone loss, greenhouse gases and water vapour, stratospheric aerosols and PSCs, and UV radiation. The ground–based measurements are consistent with satellite observations and indicate that the upper stratosphere ozone decline is not continuing. Whether this indicates recovery of the ozone layer will be clearer after the next solar minimum. In addition, it appears that the increase in water vapour is not continuing. Future developments include water vapour in the UTLS from raman lidar and balloon soundings, closer collaboration with other networks such as SHADOZ, establishment of more stations in the tropics, and provision of data in near real time.

Following this presentation, M. Kurylo discussed the NASA programme in considerable detail, first summarizing the current Climate Science and Technology Management structure within the US Federal Government and noting that the new Presidential initiatives on space exploration includes National Objective 5: “To Study the Earth system from space and develop new space-based and related capabilities for this purpose.” The new Science Mission Directorate includes Space Science and Earth Science components.

The Aura mission, designed to answer questions about changes in our life-sustaining atmosphere, was successfully launched. The observatory is in a nominal and stable operating condition. MLS, TES and OMI instruments are operating and returning exciting observations, and while HIRDLS has experienced an anomaly, it is likely to achieve much of its science payoff. The validation and operations phase of Aura is now under way with several validation campaigns to be carried out. The Aura satellite is a component of the Earth Observation System A-Train (Aerosol/Clouds/Radiation), which relies on the "formation flying" concept to sample the same air parcel over approximately 20 minutes. More details on the Aura mission can be found in the article by M. Schoeberl *et al.* in this newsletter.

**T. Wehr** described the current and future ESA missions. ESA's current operational satellite missions for Earth observation include ERS-2 (with GOME) launched April 1995, ENVISAT (including MIPAS, GOMOS, SCIAMACHY) launched March 2002, METEOSAT and MSG, a meteorological mission in cooperation with EUMETSAT consisting of at least three geostationary weather satellites, and PROBA, a micro-satellite with an high-resolution imaging spectrometer, high-resolution camera, wide-angle camera, Space Radiation Environment Monitor (SREM), and Debris In-orbit Evaluator (DEBIE), launched 2001. ESA missions are organized within the framework of the Earth Observation Envelope Programme (EOEP). This programme has two major components: (i) the Earth Explorer Programme, which has as subcomponents Earth Explorer Core Missions and Earth Explorer Opportunity Missions; (ii) the Earth Watch Programme which has as subcomponents Cooperative Missions with EUMETSAT and GMES (Global Monitoring of Environment and Security). ADM-Aeolus and EarthCARE have been selected for Phase A studies as future Earth Explorer missions, and will focus on atmospheric measurements. The SWIFT mission to measure stratospheric winds was not selected for Phase A but remains a Canadian national project.

ADM-Aeolus, to be launched in 2006, is a Doppler Wind LIDAR Mission. Winds are derived from back-scattered laser light, Doppler-shifted by aerosols and molecules along the lidar line-of-sight. In addition to wind profiles, variability, and clear air turbulence it will provide cloud profile and cover (cloud heights, extinction, optical thickness), and tropospheric aerosol extinction, optical thickness and stratification. The Earth Clouds, Aerosols and Radiation Explorer (EarthCARE) mission will be launched in 2012. Its scientific objective is to quantify aerosol-cloud-radiation interactions so they may be included correctly in climate and numerical weather forecasting models. It includes a lidar which will provide vertical profiles of aerosols and clouds (but is attenuated by thick clouds), and a Doppler Cloud Radar, a Multi-Spectral Imager (MSI) to provide high resolution data to supply the horizontal context of the vertical column observations, and a Broad Band Radiometer (BBR) which measures the SW and LW radiances at the top-of-the-atmosphere.

In addition to providing a comprehensive description of the above missions and an overview of ESA future missions, T. Wehr also summarized other climate and atmospheric chemistry preparatory activities within ESA. These include activities in atmospheric chemistry research and monitoring, stratospheric dynamics and ozone transport, and data assimilation, which includes support for SPARC-DA workshops (see the report on the Banff workshop in this issue).

**S. Hayashida** reported on progress in research on Polar Stratospheric Clouds (PSCs) within the ILAS/ILAS-II projects, which operated onboard the AEOS/ADEOS-II satellites in the periods November, 1996 – June, 1997 and April – October, 2003 respectively. To understand the interaction of PSCs and gas species, simultaneous measurements of PSCs and gas species are highly needed. However, optical remote sensing cannot achieve this easily because of interference of light scattering by particles with gas absorption spectra. A new retrieval algorithm was developed for the ILAS instrument to derive aerosol/PSCs and gas species simultaneously (Oschepkov *et al.* 2005). The data quality of methane, $NO_2$, and water vapour is remarkably better with the new (Version 7) algorithm, the data set includes both PSC and non-PSC cases, and seems to be promising for investigating microphysical and chemical processes related to PSCs. In addition to development and validation of the new algorithm, ongoing activities include PSC analysis, ongoing analysis of temperature history and denitrification/dehydration with improved $N_2O$ and $CH_4$, and analysis (Ver. 6: Hayashida *et al.*) and reanalysis (Ver. 7) of $ClONO_2$ activation/deactivation.

***Location of the Next General Assembly:*** **E. Manzini** offered to form a local organizing committee to facilitate hosting of the next SPARC General Assembly (GA) in Italy in 2008. Two possible locations have been considered. The SSG expressed its appreciation to E. Manzini for her offer and efforts and encouraged her to continue to interact with the SPARC IPO to finalize the decision as to the location of the next GA and form a local organizing committee.

***Location of the next SSG meeting:*** Offers to host the next SSG meeting were received from P. Canziani and A. Ravishankara. The SSG expressed its appreciation for these offers. After some discussion it was unanimously decided to hold the next SSG meeting in Boulder, CO, USA during October 16-19, 2006.

## Closure of the Session

The 13th Session of the SPARC SSG was closed at noon on Thursday, 29 September 2005. The SSG unanimously thanked A. O'Neill and J. Fillingham for organizing the excellent local arrangements for the session in the very congenial setting of Lady Margaret Hall in Oxford.



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# Processes governing the chemical composition of the extratropical UTLS A report from the joint SPARC-IGAC Workshop

## 18-20 May 2005
## Max Planck Institut für Chemie, Mainz, Germany

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## Introduction and Background

The links between atmospheric chemistry and climate are receiving increasing attention on several fronts. One region where the two are tightly coupled is the Upper Troposphere/Lower Stratosphere (UTLS), which spans the altitude range from ~8-16 km (depending on latitude). Transport in this region and, in particular, exchange between the troposphere and stratosphere occurs through a combination of processes including, in the tropics, cumulus convection, and in the extratropics, synoptic-scale weather systems, together with the large-scale Brewer-Dobson circulation. It is recognized that net exchange from troposphere to stratosphere in the tropics and from stratosphere to troposphere in the extratropics is under large-scale dynamical control (Holton *et al.* 1995). However, the net exchange alone does not determine many important aspects of chemical distributions in the UTLS region. Recent observational and modelling studies have further revealed important complexities in UTLS dynamical processes and chemistry, the interplay between the two, and consequences for chemical distributions in the UTLS. In particular these studies have raised questions about the best definition of the boundary between the troposphere and stratosphere, *i.e.* the tropopause. This applies both to the tropics and to the extratropics. The processes and scientific questions in the two regions are rather different and confining attention to one or the other has some advantages. The subject of this report is the extratropical UTLS, *i.e.* poleward of the subtropical jets. Many important aspects of the tropical UTLS are discussed in recent papers by Folkins (2005), Folkins and Martin (2005), Gettelman *et al.* (2004) and Küpper *et al.* (2004) and references therein.



Based on this new information, a more sophisticated picture is being put together of the factors controlling UTLS chemistry and climate feedbacks. Perturbations to the distributions of trace gases such as $O_3$, $H_2O$, and aerosols in this region can lead to direct forcing of climate. Indirect effects through, for example, changing cirrus following new particle production or contrail formation from aircraft emissions can also impact the radiative balance in this region. In turn, climate change, through changing temperatures and transport patterns, has the potential to effect the chemical composition of the extratropical UTLS and thus the composition of the troposphere and stratosphere. Transport of ozone from the stratosphere to the troposphere may change in response to ozone recovery and greenhouse gas impacts in the stratosphere. Also, as noted in the WMO 2003 Ozone Assessment, transport in the extratropics from the troposphere to the stratosphere of very short-lived halogenated species (VSLS; in particular bromine-containing compounds) and pollutants may be important for understanding current and future stratospheric ozone change.

In an effort to integrate and synthesize new findings and their implications, the IGAC Project (International Global Atmospheric Chemistry; under IGBP and CACGP) and the SPARC Project (Stratospheric Processes and their Role in Climate; under WCRP) held a joint workshop at the Max Plank Institut für Chemie, Mainz in May 2005 to discuss processes governing the chemical composition of the Upper Troposphere and Lower Stratosphere (UTLS) in the extratropics. One aim of the workshop was to update our current state of knowledge following previous workshops discussing the tropopause (*i.e.* in Bad Tölz, Germany, 2001; Haynes and Shepherd, 2001) and chemistry-climate interactions (Giens, France, 2003; Ravishankara *et al.* 2004) which both included some discussion about extratropical UTLS composition. It was also felt that it is timely to review these issues given the upcoming WMO assessment in 2006 and given the issues raised in the previous ozone assessment (WMO, 2003). It was also noted that it is nearly 10 years since the publication of the very influential review by Holton *et al.* (1995), which summarized the state of knowledge at that time related primarily to dynamical drivers of stratosphere-troposphere exchange (STE). Recent observations and modelling studies allow for refinement of these concepts, especially with respect to small(er)-scale dynamics and coupling to chemical composition.

*This article also appears in the IGAC newsletter.*

## Workshop Design & Discussion Topics

The workshop discussions were designed around four major scientific questions (outlined below) pertinent to improving our understanding about UTLS extratropical chemical composition. Invited overview presentations were given on sub-themes identified within each topic and these were followed by lively discussions in plenary. Discussions were also held in breakout sessions where it was decided to combine the first two topics and discuss the roles of dynamical and chemical processes together. Rapporteurs summarized the discussions on the last day of the meeting. This report summarizes these discussions, focusing on the main highlights from the workshop.

The four framing questions for the workshop were:

***1) Which dynamical and meteorological processes govern the chemical composition, especially ozone and water vapour, of the extratropical UTLS on seasonal and interannual timescales?*** On a large scale, both temporally and spatially, the chemical composition of the extratropical UTLS is influenced by the downward transport of trace gases *via* the large-scale stratospheric circulation and the upward transport of trace constituents from the troposphere by dynamical processes such as frontal uplift and deep convection. Coupling of air masses between the subtropical UT and the extratropical LS may also be important. Many important details of these transport processes still need to be understood. Analyses of various data sets are now providing insights into the causes of large-scale seasonal and possibly interannual variability in transport processes and chemical composition. The extent to which small-scale processes (*e.g.* gravity wave breaking near the tropopause, turbulence in the vicinity of jet-streams, radiative processes associated with upper level clouds and condensation) play a role in governing the composition and exchange within the extratropical UTLS is also not well known. In addition, there is increasing evidence that deep convection or convection embedded in frontal systems could be important.

***2) What is the relative importance of chemical versus dynamical processes in governing the chemical composition of the extratropical UTLS?*** Analysis of observational data sets has shown that an extratropical tropopause layer (ExTL) exists in chemical composition between the stratosphere and troposphere which exhibits characteristics of both regions. The extent to which dynamical and/or chemical processes are influencing the composition of this region still remains to be quantified. A better characterization of how strongly the 3-D spatial (latitudinal, longitudinal, altitudinal) and seasonal chemical fields in this region are perturbed by exchange processes between the stratosphere and troposphere is needed in order to identify the relative importance of the chemical and dynamical processes. The impact of different processes such as (pyro-) convection and small-scale mixing on chemical composition are very uncertain and require better quantification.

***3) Which chemical/physical processes are important in governing UTLS composition?*** The physical conditions of the UTLS region (low T, decreasing pressure) give rise to particular conditions such that chemical reactions proceed at different rates than in the lower troposphere or the main bulk of the stratosphere. Large uncertainties still surround our knowledge about many reaction rates and pathways (*e.g.* VOC degradation, VSLS degradation) which could be important for the chemical composition of this region and which influence the distributions and budgets of $HO_x$, $NO_x$, $BrO_x$ and $O_3$, for example. Very little is known about the aerosol budget in this region. In addition, heterogeneous reactions on ice/aerosols are also very uncertain, as are the processes governing aerosol formation/ageing, ice super-saturation and cirrus properties. Scaling up from the process scale to realistic parameterizations in global models is also an issue.

***4) How do we better quantify the net exchange of ozone and other trace constituents between the stratosphere and the troposphere?*** The flux of ozone from the stratosphere is an important term in the tropospheric ozone budget but global model estimates of net flux still vary by more than a factor of two (EU Chemistry-Climate report, 2004). In addition to the climate impacts, intrusions of ozone-rich stratospheric air into the troposphere can occasionally have significant implications for local regulation of allowable ground-level ozone concentrations and the achievability of established limits. Given that the flux may already have changed or may change in a future climate, it is important to quantify this flux more accurately using new, better metrics. Variations in the methods used to determine the flux together with the paucity of independent estimates based on observations is contributing to these uncertainties. In particular, there is a need to define more meaningful parameters by which to quantify STE; *i.e.* ones which can be derived from observations and calculated in models. The concept of a chemical tropopause or exchange boundary between the stratosphere and troposphere is an important issue for defining the exchange, and the choice made for this boundary often influences the conclusions of STE studies. Advances in our knowledge about the processes governing the chemical composition of the UTLS region, refined methods to diagnose fluxes from meteorological data sets and the use of new observational data sets could lead to improved quantification of fluxes. There is also a more basic need to continue the evaluation of global model performance in the UTLS region given that these are the tools being used to integrate our current knowledge and provide predictions of future composition and climate to policy makers.



## Discussion Summaries

Summaries of the plenary talks and breakout sessions follow. Reference is made in some cases to talks given by specific speakers, but we note that this does not preclude the valuable contributions on the topic made by other participants. A full list of workshop participants and talks can be viewed on the workshop web page: http://www.atmosp.physics.utoronto.ca/SPARC/UTLS%20IGAC/Index.htm. As many acronyms (for field projects, satellites, *etc.*) are used herein, an acronym list with translations is also provided at the end of the paper.

## Chemistry and Dynamics: Indicators and Controlling Factors of UTLS Chemistry

### *The Extratropical Tropopause Layer (ExTL)*

While the boundary between the troposphere and stratosphere is generally considered to be defined by the thermal tropopause, this definition is not necessarily appropriate or meaningful when discussing chemical composition. The chemical and thermal tropopause are not generally coincident and

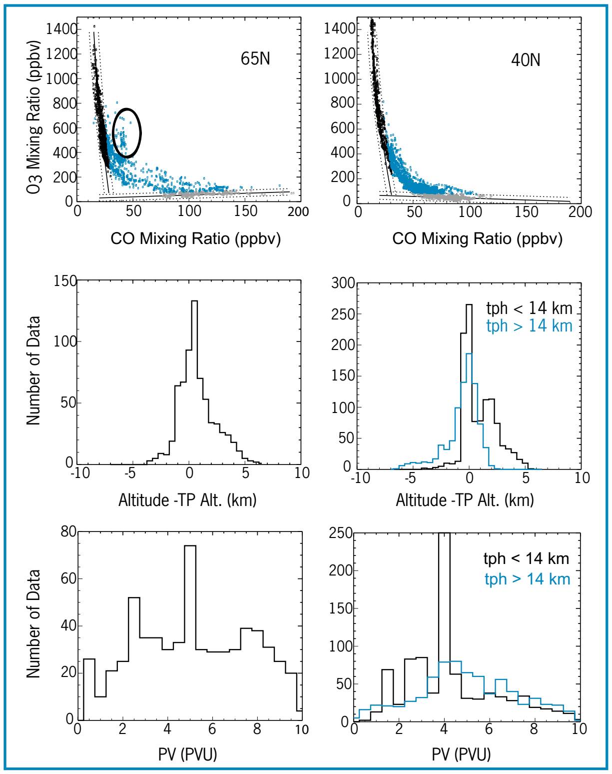


***Figure 1**. CO-$O_3$ correlation has been used to identify the location and thickness of the extratropical transition layer (ExTL). The top panels display the relationship of stratospheric tracer $O_3$ and tropospheric tracer CO for the two extratropical locations sampled by the in situ measurements on board NASA research aircraft ER-2 during STRAT and POLARIS field campaigns (1995-1997). The solid lines represent the empirical stratospheric and tropospheric O3-CO relationships, determined imperically from the data. The dash lines mark the 3σ of the respective distribution. The identified stratospheric, tropospheric, and transitional points are represented by black, gray and blue. The centre panels show the altitude distribution of transition points (blue) relative to the thermal tropopause. In the case of 40° N, the distributions are given as two populations, depending on whether the respective thermal tropopause height is below or above 14 km. The bottom panels show the potential vorticity distribution of the transition points. The 40°N distributions aregiven as two populations, similar to the center panels. (Adapted from Pan et al. 2004)*



further, the chemical transition from UT to LS is not as abrupt or well-defined as the temperature transition. The workshop discussions followed the progress made in the last five years to identify and characterize the ExTL from various *in situ* and satellite observations of chemical tracers. Trace gas profiles of $O_3$, CO, $CO_2$, $N_2O$ and $H_2O$, as well as scatter plots among these species, obtained from recent observations made as part of the airborne MOZAIC, CARIBIC, SPURT, STRAT/POLARIS and AIRS satellite projects, clearly reflect the existence of a transition layer in the upper troposphere/lowermost stratosphere (UT/LMS) where the chemical composition gradually changes from tropospheric (*e.g.* high CO, low $O_3$) to stratospheric (low CO, high $O_3$). Figure 1 shows an example of a CO-$O_3$ correlation in the tropopause region where mixing lines (light blue) in the ExTL connect a tropospheric (gray) and a stratospheric (black) trace gas reservoir. Number density distributions relative to the thermal tropopause show that the lower bound of the ExTL extends into the UT. The exact position is hard to determine, since it is neither associated with the thermal tropopause nor with a fixed value of potential vorticity (PV). The upper bound of the ExTL (or the depth of the layer) depends to some extent on the residence time of the tracer under investigation. It is generally higher for species that have a long photochemical lifetime in the LMS (*e.g.* $H_2O$) than it is for short-lived species like CO, whose tropospheric signature is erased on a time-scale of a few months due to net oxidation by OH in the LMS.

As outlined in a talk by **K. Rosenlof**, the chemical composition of the LMS is a function of the relative strength of several processes, such as episodic diabatic upwelling, in particular in NH summer, quasi-isentropic cross-tropopause transport, and diabatic downwelling from the overworld in the Brewer Dobson circulation. The first process is associated with deep overshooting convection and pyro-convection, and its bulk impact is largely unknown. In contrast, the upwelling is relatively easy to quantify *via* the calculation of EP fluxes[1], however there is still considerable uncertainty about the main forcing that drives the upwelling and about the observed trend of increased tropical upwelling during the last 7 years.

Analysis of seasonal variations of trace gas measurements, presented by **P. Hoor** for the SPURT project, reveals the importance of three reservoirs for the understanding of the chemical composition of the ExTL (Figure 2). The seasonal cycle of $CO_2$ in the UT (Figure 2, black) and the ExTL (light blue) is in phase, demonstrating the strong coupling between the ExTL and the UT due to frequent cross-tropopause exchange. Above the ExTL in the LMS (gray) the $CO_2$ maximum is shifted by approximately 3-4 months indicating transport from the tropical LMS. This transport to extratropical latitudes occurs within 2-4 months and leads to mixing with photochemically aged air diabatically descending from the overworld (Rosenlof *et al.* 1997).

## *Meteorological processes*

Several key meteorological processes in the troposphere contribute to the aforementioned episodic diabatic upwelling into the LMS. These processes include synoptic-scale transport events referred to as conveyor belts as well as smaller-scale deep convective systems. Both conveyor belts and deep convective events are associated with significant latent heat release due to condensation of water vapour and therefore they are distinct from isentropic transport. The role of these non-isentropic transport events for stratosphere-troposphere exchange (STE) has gained increased attention during the last years and hence constituted the main items of the presentations by **A. Stohl** and **M. Lawrence**.

The discussion of meteorological processes that are associated with significant transport events from the stratosphere to the troposphere (STT) or *vice versa* (TST) started on the synoptic scale. In his presentation on this topic, A. Stohl focused on the Lagrangian perspective and first suggested the terminology introduced during the STACCATO project, whereby STE is regarded as the overall STT plus TST processes, and deep exchange refers to rapid transport on synoptic time scales between the boundary layer and the LS. Deep exchange defined in this way is regarded as particularly important because it brings together stratospheric and boundary layer air masses, with strongly differing chemical compositions, and does so on a short timescale (≤ 1 day, *e.g.* Stohl *et al.* 2003). The concomitant occurrence of deep STT and deep TST can lead to a vertically inverted

[1] *Eliassen-Palm flux (EP flux) is a measure of atmospheric wave propagation in the meridional plane.*

pattern with air of stratospheric origin close to the ground and polluted boundary layer air at the tropopause (Stohl and Trickl, 1999). Particular attention was given to the role of warm conveyor belts (WCBs) that occur ahead of intense cold fronts and which transport warm and moist air from the subtropical boundary layer to the northern extratropical UT within 1-2 days. According to the recent WCB climatology of Eckhardt *et al.* (2004), boundary layer starting points frequently occur near very polluted areas (east coasts of North America and Asia). About 5% of the WCBs eventually enter the LMS. The processes associated with the diagnosed increase in potential vorticity of the WCB air parcels entering the stratosphere is not yet well understood. One hypothesis is that diabatic potential vorticity changes occur due to radiative processes in the WCB outflow regions, characterized by strong vertical humidity gradients and clouds. **V. Wirth** showed results from idealized studies on this issue which indicated that significant PV changes can occur due to radiative processes near the interface of humid upper tropospheric and dry stratospheric layers. Other synoptic-scale processes that are relevant for STE in the mid-latitudes (*e.g.* the formation of tropopause folds, Rossby wave breaking) were not discussed in detail.

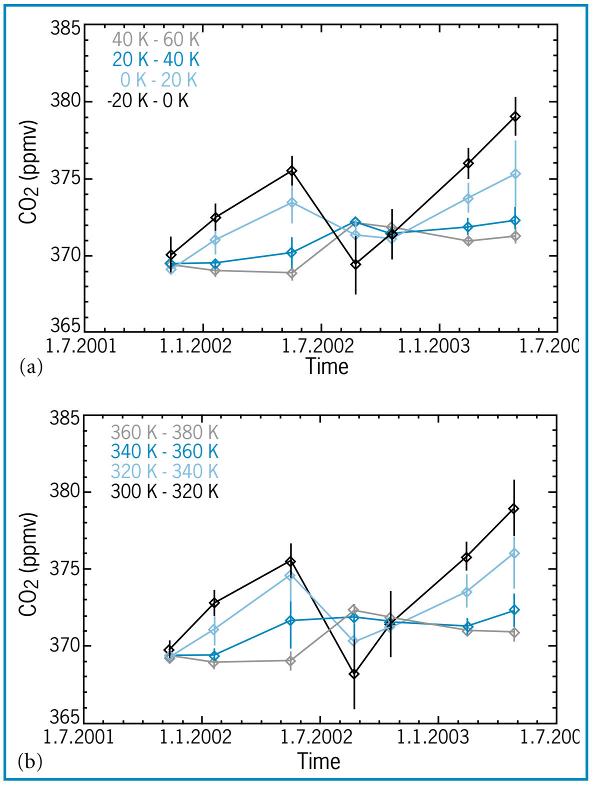


***Figure 2**. Seasonal variation of $CO_2$ concentrations as a function of distance in potential temperature relative to the tropopause (2 PVU surface) (a) and the potential temperature (b) (Hoor et al. 2004).*

**M. Lawrence** presented a concise overview on the role of deep convection for STE. He showed that observations, parameterizations and cloud resolving models (CRMs) have been used to study this process. Almost no direct observations exist for STT due to convection, but idealized model simulations – for instance with the WRF model – show that convection can trigger STT. For upward transport across the extratropical tropopause (TST) associated with convection, there are several observational and model studies that provide clear evidence for the existence of this process, in particular during the summer months. However, the net quantitative impact of this process is still largely unknown and requires further investigation.

Analysis of observations (*e.g.* STERAO, EULINOX, TRACE-P) has shown that transport of pollutants by this mechanism is important at extratropical latitudes, especially over Asia and central North America, leading to perturbations in upper tropospheric trace constituent budgets (*e.g.* $O_3$, HOx). Interestingly, data collected by the MOZAIC programme over the last three years shows significant enhancements in $NO_y$ and $O_3$ in the upper troposphere over North America, and these are often not correlated with CO (Petzoldt *et al.* 2005; Figure 3; see colour plate I). This indicates that lightning or possibly aircraft emissions may be a principal source of $NO_x$ in the UT over continental regions, something that was also suggested by analyses of previous aircraft campaign data (NOXAR, SONEX; *e.g.* Jeker *et al.* 2000). This is in contrast to regions downwind of continents, where frontal uplift of surface pollutants may be more important. More recent campaigns have shown that trace gases, including short-lived VOCs or OVOCs, can also be transported into the lower stratosphere (*e.g.* MINOS, **H. Fischer**). However, further study is needed on the significance of these measurements and processes for lower stratospheric composition (*e.g.* transport of short-lived bromine containing species). Continued analysis of data collected during previous campaigns has also led to reductions in the range of estimates for the global amount of $NO_x$ from lighting emissions to 2-9 Tg N per year. The combination of cloud-resolved modelling of convection/chemistry (DeCaria *et al.* 2005) and anvil $NO_x$ observations suggests that on average an intra-cloud flash produces nearly as much NO as a cloud-to-ground (CG) flash (**K. Pickering**, Figure 4). This is very different from previous estimates which assumed that an intra-cloud flash produced only one tenth of that of a CG flash (Price *et al.* 1997). Also, the newer estimates of the number of moles of NO per flash in CG lightning are significantly lower than previous estimates.

Recent evidence indicates that convection associated with forest fires, so-called pyro-convection, may also have a significant impact on mid-latitude UTLS composition. New modelling work presented by **G. Luderer** using the ATHAM model showed that the initiation of a deep pyro-convection event is very dependent on background meteorological conditions (*e.g.* cold frontal passage) as well as the sensible and latent heat budgets of the storm, the fire and the environment. There is a wealth

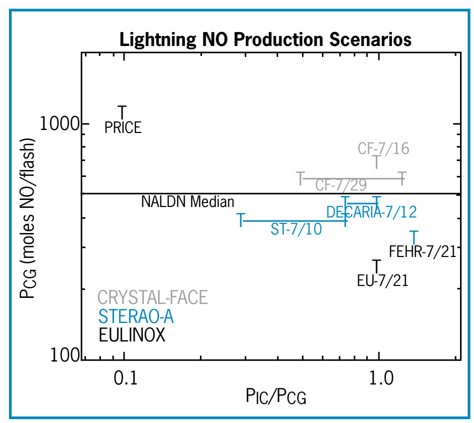


***Figure 4.** From the presentation by K. Pickering, this figure shows recent estimates of the ratio of NO production via intra-cloud (IC) versus cloud-ground (CG) lightning for different data sets in the northern hemisphere extratropics. These ratios are much higher (mean: 0.86) than previously assumed by, for example, Price and Rind (1997) who used a ratio of 0.1 in their lightning parameterization in global chemical models. Also shown as a black line is the NO production rate per flash for cloud-to-ground flashes ($P_{CG}$) for the median peak current for North America. This value of just over 500 moles NO/flash is much lower than was assumed by Price et al. (1997; >1000 moles/flash).*

of new evidence from airborne instruments (*e.g.* recent ICARTT campaign over North Atlantic in 2004; MOZAIC data over Siberia in 2003; MOPITT CO satellite data – 2003/2004) of significant enhancements to the levels of trace gases such as CO during summertime periods of boreal forest burning. Whilst mainly confined to the free troposphere, certain very large pyro-convective storms can also penetrate above the tropopause, injecting material into the LMS. **M. Fromm** showed examples of enhanced values of aerosol (as viewed in terms of aerosol index by the POAM II satellite) several kilometers above the local tropopause in the LS. Enhanced CO and acetonitrile concentrations have also been observed in the LS and are attributed to forest fire emissions (*e.g.* Crystal-FACE, Jost *et al.* 2004; Livesey *et al.* 2004; MOZAIC, **J.-P. Cammas**; Ray *et al.* 2004). The significance of these events – which may be occurring several times per year – is the topic of ongoing research, as is their impact on stratospheric composition (aerosols, $O_3$) and the radiative budget. It is possible that even one large event per year may cause significant perturbations to background aerosol levels (M. Fromm) Figure 5.

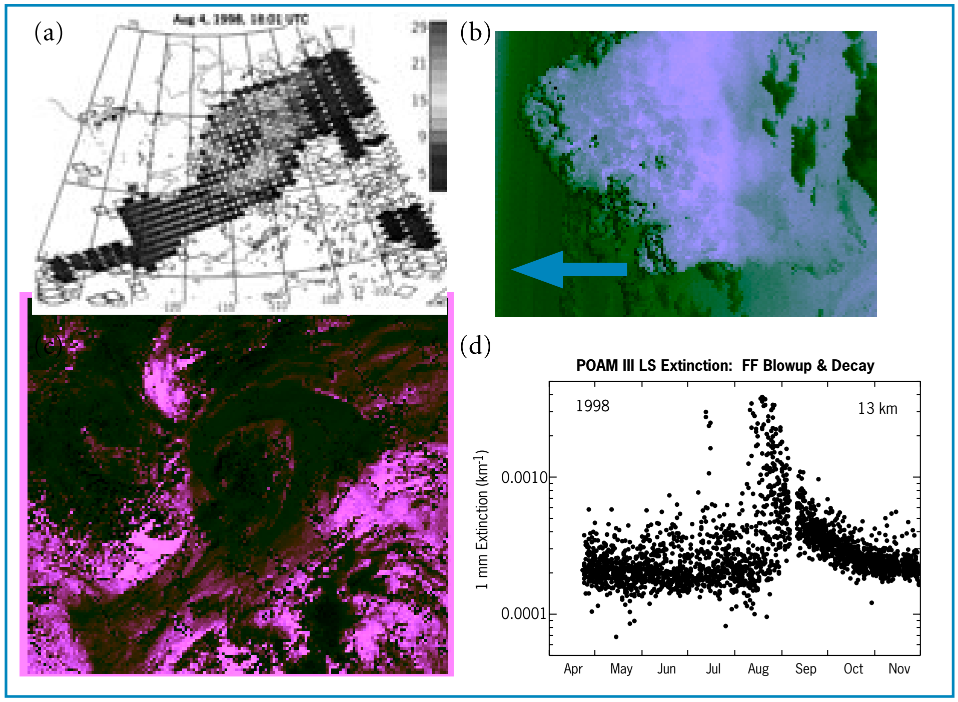


***Figure 5**. Panels showing the impact of pyro-convective events (Fromm et al. 2005). (a) Earth Probe TOMS aerosol index (AI) over far northern Northwest Territories, 4 Aug 1998, a day after a pyro-convective eruption at Norman Wells (blue asterisk). The very high AI values suggest a high-altitude plume. (b) A photograph of a pyro-convective cloud (Courtesy: Mr. Noriyuki Todo of Japan Airlines International Corporation). Details of the circumstances are: Flight data ID : JAL009 B747-400; Cruising Flight Level: FL340 ( 34,000 feet); location: N57 42.1 W125 00.0; time: 20hr 48min 27sec UTC on 27 June 2004. (c) Defense Meteorological Satellite Program (DMSP) Operational Linescan system (OLS) visible-channel reflectance image, 4 Aug 1998 at 1820 UTC, just minutes from TOMS AI map shown in (a). The croissant-shaped cloud is significantly less reflective than water-ice clouds. Infrared imagery (not shown) shows a gray plume which is opaque at the UTLS level. (d) POAM III 1-micron extinction at 13 km altitude, for latitudes that vary gradually between 55 and 70N. Brief enhancement in mid-July was caused by a pyroCb described by Fromm et al. (2000). The large extinction enhancement in August followed the Norman Wells pyroCb of 3 August. Decay of the extinction can be seen over the successive three months.*

In addition to the new information emerging from field campaigns and satellites there have also been significant developments in the complexity of processes included in Cloud Resolving Models (CRMs) and mesoscale models, such as the inclusion of detailed chemical schemes including soluble species as well as aerosol and microphysical processes. However, many discrepancies still exist between different models, as shown by recent comparisons (**M. Barth**). In particular, further validation is required of trace gas transport by convective systems into the LS and for this purpose new data is needed, particularly on short-lived species above convective systems. In addition, many of the mechanisms being studied/evaluated using CRMs or mesoscale models are not included in global models. For example, downdrafts and gravity wave breaking at the tropopause, associated with deep convection, may be leading to STT in the extratropics. Embedded convection in frontal systems can be important for transporting trace gases such as CO into the UT and possibly the LS, although the overall role of this mechanism still needs to be quantified and validated in models. There is also a need to compare results from CRMs with those from global models using the single column modelling approach and to continue with improvements to parameterizations of deep convective transport of tracers in global models, and in particular treatments of soluble species and lightning emissions.

## *Mixing processes*

During the workshop discussions it was evident that there is a need to clarify the terminology around small-scale mixing phenomena. "Mixing" is sometimes used to mean "molecular mixing" and sometimes used to mean "stirring", *i.e.* deformation of material surfaces (and hence concentration fields of chemical species) by differential advection so that molecular diffusion is potentially enhanced, but without that diffusion necessarily acting to homogenize chemical concentrations. Stirring is a route to molecular mixing, but does not itself imply molecular mixing. This distinction is important because it is only molecular mixing that leads to chemical reactions (*e.g.* between species in previously chemically distinct airmasses).

The distinction between stirring and mixing is particularly important in the context of models. Lagrangian models can predict large gradients in chemical concentrations as a result of stirring but cannot (without significant modification from their usual form) describe the final step of molecular mixing. Eulerian models, on the other hand, assume that chemical concentration fields are constant – in other words well-mixed – within a grid box (typically 100 km x 100 km x 1 km for a global model). On the other hand, *in situ* atmospheric data shows that chemical concentrations vary significantly in space – essentially down to the resolved scale of the observations (~1 km for horizontal sections and a few tens of meters for vertical sections).

Two different types of stirring may be important to molecular-level mixing. The first is stirring *via* the large-scale flow, which can be resolved by global climate models and in global meteorological data sets. Here the distinction between stirring and mixing is important because the time-scale for molecular mixing may be significantly larger than the time-scale for stirring, as estimated by stretching rates. The second is stirring by three-dimensional turbulence arising in convective clouds, through breaking of gravity waves, and other such processes. The nature of three-dimensional turbulence, where stretching is dominated by the smallest eddies, is such that the time-scale for molecular mixing (again for chemical species whose molecular diffusivity is similar to the viscous diffusivity) is similar to the time-scale for stirring. In this case, distinguishing between stirring and mixing is not as critical.

**J. Whiteway**, **G. Vaughan** and others noted that inertia-gravity waves are likely to play a significant role in mixing in the tropopause region and above since their breaking gives rise to intermittent layers of three-dimensional turbulence (Figure 6; see colour plate I). These waves may be generated by topography, by convection, or by synoptic-scale processes. However, the importance of convection for gravity-wave generation in the extratropics is not clear, and furthermore the generation of inertia-gravity wave breaking by synoptic-scale systems is still poorly understood, though the fact of the generation is not in dispute. The tropopause level and above is a preferential region for breaking because of the change in static stability when going from the troposphere to the stratosphere. Wave breaking is regularly observed, such as over relatively weak topography in the U.K. mountains, and sometimes results from interactions between short wavelength gravity waves (perhaps directly generated by topography) and longer wavelength inertia-gravity waves (generated by synoptic scale processes). The resulting turbulent layers may be greater than 1 km in depth and hence imply substantial vertical transport.

One way of assessing the quantitative aspects of mixing is direct observations of the mixing processes themselves (**J. Whiteway**). Another is to try to infer the characteristics of mixing from the observed structure of chemical concentrations fields, and determining which model representation of mixing gives the best fit to observations (**B. Legras**). An interesting conclusion that comes out of this approach is that the strength of mixing processes is highly variable, as might be expected from the intermittency of three-dimensional turbulence and the likely association with particular geographic features such as topography. A related approach was used in the incorporation of mixing into the CLAMS model (a Lagrangian model with adaptive generation/destruction of parcels) where it is possible to optimize the mixing formulation to give best agreement with chemical observations (**P. Konopka**).

We know that global models with horizontal resolution of 100 km or greater and satellite observations with resolutions of tens of kilometers cannot represent observed chemical concentration variations on scales of 1 km or less. However, a more important question is whether the neglect of these variations leads to systematic large-scale errors in chemical predictions. This has been investigated in three different ways: (i) the implications of changing model resolution have been explored (Esler *et al.* 2004); (ii) the chemical implications of smoothing *in situ* observations to give spatial resolutions typical of global models have been investigated (Crowther *et al.* 2002, Esler *et al.* 2004); (iii) the effect of mixing between different boxes in Lagrangian calculations has been explored (Esler *et al.* 2001). Here the strongest effects are seen when the different boxes have very different initial chemical concentrations. In the UTLS context, this occurs when mixing air that originated in the boundary layer with air with the characteristics of the lower stratosphere. The extent to which this actually happens is not clear (G. Vaughan). Approach (i) is the most straightforward to interpret with respect to implications for global-scale models and suggests that at current resolutions models may be making errors of up to 15% in key chemical quantities such as ozone production efficiency.

At present there are, as noted above, clearly several limitations to the representation of mixing in models. With Lagrangian models the difficulty is how to represent mixing effects without losing the essential simplicity of the Lagrangian approach. With Eulerian models the difficulty is how to reduce mixing to avoid unrealistic smoothing of important chemical contrasts (such as the tropopause itself). It is clear that mixing is, in reality, intermittent, but whether or not the details of that intermittency are important for large-scale chemical distributions or whether they must simply be taken into account to interpret individual observations remains to be determined.

## In situ Chemical and Microphysical Processes

The large- and small-scale dynamical processes discussed in the previous section alter the extratropical UTLS chemical composition by moving and mixing air masses between the troposphere and stratosphere. *In situ* chemical and microphysical processes in this thermodynamically and chemically unique region further alter its composition. Here we discuss several key species of particular importance to chemistry/climate interactions, controlling processes, and what steps are needed to better constrain them. Discussions below are based on presentations given by **K. Carslaw**, **J. Crowley**, **M. Dorf**, **A. Gettelman**, **D. Murphy**, **T. Peter**, **A. Ravishankara**, **H. Singh**, **B. Thornton**, and **R. von Glasow**.

### *Photochemistry*

*Upper tropospheric $HO_x$ and $NO_x$*: An accurate knowledge of the abundances of $HO_x$ and $NO_x$ in the upper troposphere is critical, since photochemical production of $O_3$ is controlled by the reactions of NO with $HO_2$ and $RO_2$. Recent observations in the field and laboratory have yielded insights to some important controlling processes. Observations from many tropospheric aircraft flights indicate that models tend to overestimate $HO_x$. These data were generally obtained at lower altitudes and at a higher ambient humidity than earlier observations that exhibited a discrepancy in the opposite direction. Observations also indicate that models tend to underestimate the $HO_2$/OH ratio at high levels of NO by large amounts (Figure 7). Recent laboratory observations show that, at high NO concentrations, the production of a few percent yield of $HNO_3$ by the NO+$HO_2$ reaction may alter the $HO_2$/OH ratio to be more consistent with observations (Butkovskaya *et al.* 2005). Finally, laboratory data have shown that acetone photolysis may be a less efficient source of $HO_x$ than was previously believed (Blitz *et al.* 2004). Future approaches for constraining controlling processes on UT $HO_x$ and $NO_x$ include: i) efforts to validate measurements of $HO_x$ precursors *via* simultaneous observations by different instruments as

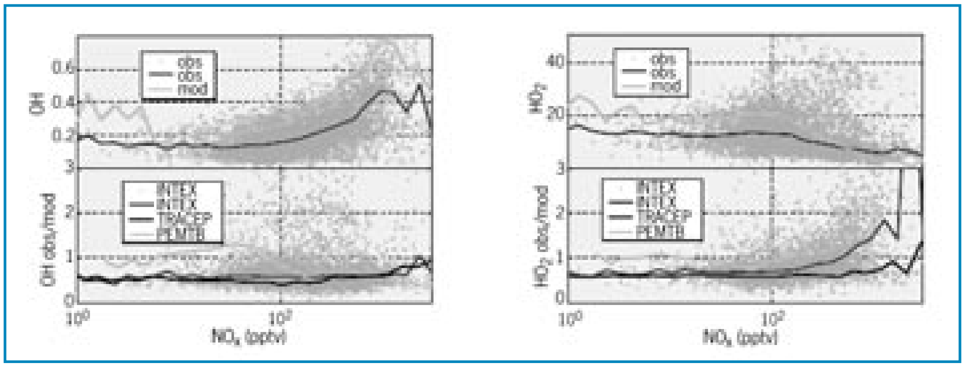


***Figure 7**. Comparison of measured and modelled $HO_x$, as a function of $NO_x$, for data collected during INTEX, TRACE-P, and PEM Tropics B. (Presented by H. Singh; Courtesy Bill Brune, private communication).*

well as budget studies; ii) determining the level of agreement between modelled and measured OH and $HO_2$ if, in the models, only sources from $O(^1D)+H_2O$ and $CH_4$ oxidation as a function of NO or $NO_x$ are considered (*e.g.* how important are non-water and non-methane sources of $HO_x$?), such as is done by Olson *et al.* 2004; and iii) comparing observations of NO, $HNO_3$, and CO with CCM and CTM output in order to better quantify the efficiency of production of NO by lightning (H. Singh, **R. Salawitch**, breakout discussions).

*Chlorine Activation*: Recent aircraft data show that levels of ClO between 30 and 40 pptv are quite commonly observed at high latitudes in the northern hemisphere for stratospheric air masses within several kilometres of the tropopause (Thornton *et al.* 2003). Levels of ClO between 20 and 30 pptv are also observed in the extra-tropical, UTLS region (Figure 8). These observations suggest that Cl activation on sub-visible cirrus, or on cold sulphate aerosols, might be responsible for a significant component of observed depletion of lower stratospheric ozone (Solomon *et al.* 1997; Bregman *et al.* 2002), in contrast to earlier studies in dry, particle-poor regions of the extratropical UTLS (Smith *et al.* 2001). The global significance of these regions of activated ClO is unclear. The observations of high ClO tend to occur in a spatially non-homogeneous manner. This could be due to variations in available chlorine along the flight track, which is difficult to assess without accurate, precise, high-temporal resolution measurements of HCl, a surrogate for $Cl_y$. On the other hand, the patchiness could be related to the sporadic character of Cl activation, such as could be induced by mixing that combines particle or water-rich air with air that has high levels of $Cl_y$. It remains unclear whether formulations for Cl activation by PSCs (polar stratospheric clouds) can be applied to the heterogeneous activation of ClO on extratropical cirrus, given the nature of the water-rich aerosols and particles that form in the UTLS. Efforts needed to resolve these issues include simultaneous measurements of ClO and HCl in the UTLS, analysis of ice frost point temperature and cloud data from satellite data to assess global significance, and the modelling of existing ClO measurements to evaluate the heterogeneous chemistry schemes used in CTMs and CCMs (B. Thornton, plenary and breakout discussions).

*Bromine and Iodine*: Measurements of total column BrO by the GOME instrument reveal abundances that are more than a factor of two higher than found in typical models (Figure 9). The first issue raised by these observations is the need to define the relative contribution of tropospheric BrO and stratospheric BrO to this discrepancy. Results to date are not consistent. Ground-based measurements of the variation with solar zenith angle of differential slant column BrO suggest most of the discrepancy is caused by a global, ubiquitous, 2 to 3 pptv level of background BrO in the free troposphere (*e.g.* Müller *et al.* 2002). On the other hand, ground-based measurements of diffuse and direct solar radiation indicate an upper limit for tropospheric BrO of 0.9 pptv at 45°S, with mean values of ~0.2 pptv (Schofield *et al.* 2004). This suggests the discrepancy between measured and modelled column BrO might be the result of significantly higher levels of bromine in the LS than are commonly found in models. If BrO really is ~2-3pptv throughout the troposphere as suggested by the former study, then the $BrO+HO_2$ cycle could represent an important sink for $O_3$ (von Glasow *et al.* 2004), the hydrolysis of $BrONO_2$ could be an efficient route for production of $HNO_3$ (Lary, 2004), and BrO could be a significant oxidant for DMS (and perhaps other species) in the marine boundary layer (Boucher *et al.* 2003). If the “excess” bromine is in fact in the LS, this bromine could be supplied by the decomposition products of very short lived (VSL) bromocarbons and could have important consequences for our understanding of ozone trends (WMO, 2003). The substantial organic content of many aerosol particles just above the tropopause suggests there is injection of tropospheric particles into the stratosphere, and the presence of Br on these particles provides the possibility of cross-tropopause transport of bromine, in both directions, by aerosols (Murphy and Thomson, 2000). Also, the presence of iodine on aerosols may explain the lack of stratospheric IO (*e.g. via* aerosol uptake of $I_y$ species). Resolution of these issues requires accurate and precise measurements of BrO in the UTLS region (*i.e.* that have sensitivity as low as 0.5 pptv), the simultaneous measurement of a suite of organics and inorganic decomposition products, and laboratory measurements of heterogeneous chemical reactions of inorganic bromine species and the kinetics of the organic decomposition products of VSL bromocarbons (R. Salawitch, M. Dorf, R. von Glasow, D. Murphy, and plenary and breakout discussions).

## *Humidity and Microphysics*

*Water abundance and supersaturation*: An accurate knowledge of the abundance of $H_2O$ and ambient temperature is crucial for understanding cirrus cloud formation, estimating radiative forcing, and accurately retrieving aerosols and trace chemical spe-

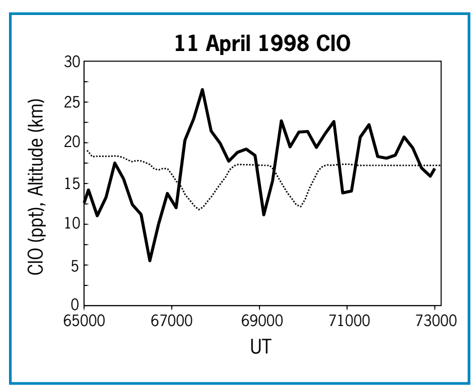


***Figure 8**: ClO (solid) and altitude (dotted) for portion of 11 April 1998 WB-57F flight over central United States. Time is UT seconds. ClO is averaged for 120 sec (Courtesy Brett Thornton).*

cies from satellites. Ice super-saturation has been frequently detected in clear air and inside cirrus clouds, predominantly in the UT (Jensen *et al.* 2001; Haag *et al.* 2003). Satellite observations point to a high variability of relative humidity in the ExTL in regions of major storm tracks (Figure 10; see colour plate II). These are regions of significant dynamical perturbations, likely coinciding with enhanced mixing of tropospheric $H_2O$ across the tropopause. This picture is corroborated by a few case studies of cross-tropopause tracer transport. Mixing ratios of $H_2O$ well above stratospheric background levels are observed, reaching far into the LMS, especially in summer (**C. Schiller**, break-out discussions). Supersaturation and the nucleation of the ice phase appears to be confined to a vertically narrow layer (up to 1 km thick at mid-latitudes and more extended polewards) above the tropopause (Pan *et al.* 2000). *In situ* processes affecting $H_2O$ amount and cloud formation/frequency near the ExTL do not seem to influence the observed trends in mid-latitude stratospheric $H_2O$ (A. Gettleman, breakout discussions). The quantification of the different microphysical and dynamical sinks and sources of $H_2O$ is still very uncertain. It remains to be determined how often cirrus formation takes place in ice-supersaturated regions.

*Aerosol transport and composition*: Aerosol precursor gases and primary aerosol particles are injected into the UTLS by rapid vertical transport processes such as WCBs and deep convection (including pyro-convection), thereby influencing the aerosol budget and high cloud occurrence around the ExTL (K. Carslaw). Besides organics, many UT particles contain both sulfate and carbon and a large fraction contain insoluble inclusions such as mineral dust and soot (Murphy *et al.* 1998; Kojima *et al.* 2004). A small number of such particles may act as efficient heterogeneous ice nuclei, affecting cirrus formation by freezing at lower supersaturations than for liquid particles. The influence of aerosols originating in the troposphere on the highly variable and non-uniform UTLS particle composition is seen in measurements at up to 5 km above the tropopause (D. Murphy). This challenges the conventional wisdom that those aerosol particles in this region are entirely composed of $H_2SO_4$ and $H_2O$. It remains unclear to what degree vertical transport affects the UTLS aerosol, how lofted aerosols are modified by interacting with gases and hydrometeors in convective clouds, and how these aerosols in turn modify the evolution of deep convective clouds and the formation of cirrus. A global, speciated mass budget of the UTLS aerosols including sources and sinks is lacking, and therefore it is currently not possible to accurately validate recently developed global aerosol models.

*Ice formation from aerosols*: Ice cloud formation and characteristics may be changing due to two influences: a change in the abundance and properties of ice-nucleating aerosols (*i.e.* the aerosol indirect effect), and changes in the small-scale dynamical forcing patterns (Kärcher and Ström, 2003). The relative importance of these two is not well known. The dependence of the number of ice crystals on the updraft speed in a rising air parcel is much stronger than in liquid clouds, making cloud formation processes more susceptible to small dynamical changes than in the mid- to lower-troposphere. Frequent observations of high ice supersaturation in conjunction with high ice crystal number densities suggest a global-scale predominance of homogeneous freezing in the UTLS (DeMott *et al.* 2003; Gayet *et al.* 2004; Hoyle *et al.* 2005). Homogeneous freezing is sensitive to changes in the variability of vertical air motion on spatial and temporal scales unresolved by global models (Figure 11; see colour plate II). The organic aerosol fraction does not seem to contribute significantly to ice formation (Cziczo *et al.* 2004; T. Peter), but a few heterogeneous ice nuclei could modify cirrus development and high cloud cover if they cause ice formation at lower supersaturations than required for homogeneous freezing (Figure 12; see colour plate III). Changes in dynamical forcing could easily mask changes in cloud properties induced by ice nuclei, and these two influences are difficult to separate in measurements. Discriminating between natural and anthropogenic causes of cirrus changes in a future climate requires that mesoscale temperature fluctuations to be understood and that their sources (typically gravity waves) be accurately parameterized in global models. It is furthermore important to know to what extent ice nuclei modify radiatively important cirrus cloud properties.

*Gas uptake in cirrus clouds*: Uptake of chemically active trace gases by cirrus ice crystals could possibly lead to vertical redistribution or even irreversible removal of the gas from UT air masses, potentially altering the ozone budget there (J. Crowley). Molecules residing at the surfaces of ice crystals might alter ice particle growth rates by modifying the super-saturation over individual crystal facets (Gao e*t al.* 2004). Cubic ice may alter ice crystal nucleation and growth, possibly over a wider range of temperatures than previously thought (Murray *et al.* 2005). A number of field measurements indicate there is substantial uptake of $HNO_3$ in low temperature cirrus clouds, in one case even in concert with enhanced in-cloud super-saturation. According to recent laboratory measurements, equilibrium uptake models frequently used in the past to calculate the uptake of $HNO_3$ on ice are inapplicable at the low $HNO_3$ partial pressures typical for the ExTL (Ullerstam *et al.* 2005). Perhaps more important, atmospheric ice is not in equilibrium. Both laboratory studies examining $HNO_3$ and HCl uptake and theoreti-

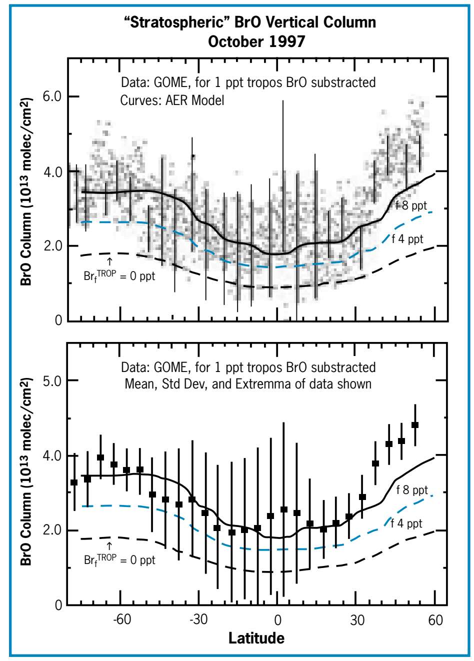


***Figure 9****. Comparison of estimated stratospheric column BrO from GOME, October 1997, assuming a uniform 1 ppt distribution of BrO in the troposphere (close to the upper limit of 0.9 reported by Schofield et al. JGR, 2004) compared to stratospheric column BrO from the AER 2D model, for the WMO 2003 baseline* $Br_y$ *scenario (labeled* $Br_y^{TROP}=0$*) and for model simulations assuming non-zero levels of* $Br_y$ *at the tropopause (*$Br_y^{TROP}$*) equal to 4 ppt and 8 ppt, respectively.* Top panel*: raw GOME data.* Bottom panel*: mean, standard deviation (thick error bars), and extremma (thin error bars) of GOME data in 5o wide latitude bins. After Salawitch et al., 2005.*

cal work suggest that growth and evaporation of ice may strongly affect the amount of species taken up (Kärcher and Basko, 2004). Growth models for small ice crystals that are valid for UTLS conditions and which are capable of accounting for habit changes and surface pollution are not available. It is unclear to what extent non-equilibrium processes connected to ice growth in cirrus conditions affect trace gas uptake and heterogeneous reaction rates.

## Quantifying Net Exchange of Trace Constituents

Quantifying the global stratosphere-troposphere exchange (STE) of atmospheric species is a prerequisite for identifying the roles of different dynamical and photochemical processes in controlling this flux. In particular, the net flux of ozone (from stratosphere to troposphere) and of water, as well as aerosols (from troposphere to stratosphere) are critical elements in the stratosphere-troposphere coupling and thus in the overall chemistry-climate coupling. As has been discussed, the area of transition from the troposphere to stratosphere is a region of partial mixing, small-scale dynamical processes, and unusual chemistry since it combines the characteristics of both the stratosphere and the troposphere. Key questions now being asked include:

(1) How important is $O_3$ STE to the tropospheric $O_3$ budget and the overall tropospheric oxidative capacity (*i.e.* OH)?
(2) How will climate change alter the flux of $H_2O$ into the stratosphere?
(3) Do chemical processes in the tropopause transition region alter the STE of key species like $O_3$ and aerosols?
(4) How important are the large-scale, planetary disturbances *vs.* the small-scale dynamical processes in controlling this STE?
(5) What dynamical-chemical measurements would be needed to detect a significant change in STE?

Answers to the above questions form the knowledge base required for estimating the chemical feedback in a changing climate.

Over the last decade, significant progress has been made in quantifying STE flux on both global and regional scales, and over both annual and synoptic times. Studies have ranged from high-resolution process studies to global integrations. In terms of the global pattern and magnitude of STE there is increasing convergence from the knowledge base of a decade ago, but complete agreement has not yet been reached. An example is given in Figure 13 (see colour plate III), where mass flux calculations using two different models (one Eulerian and one Lagrangian) show similarity in the preferred location of the net diabatic flux (Figure 13a; Olsen *et al.* 2004) and the downward flux (STT, Figure 13b; Sprenger and Wernli 2003). These two quantities are comparable since STT is the dominant component of the net flux in the extratropics. The knowledge base is such that it is possible to generate maps of the $O_3$ STE on regional and monthly scales and to produce the now classic latitude-by-month plot of zonal mean $O_3$ STE to match the similar $O_3$ vertical column plots, as shown in Figure 14 (Hsu *et al.* 2005). With increasing model resolution and the use of analyzed meteorological fields, global CTMs are beginning to be able to reproduce the spatial and temporal variability observed in trace gas distributions, and they have become a useful tool for case studies of STE events. Examples from several field campaigns and intensive modelling studies have shown that in some cases we can model the fine, filamentary structure of ozone folds at the tropopause. Nonetheless, this remains a difficult task, as shown in Figure 15 (see colour plate III) (Wild *et al.* 2003), due to the fact that current CTMs still lack the full resolution of the observed structures. (**M. Prather**, **M. Olsen**, **L. Pan**, **A. Gettelman**, **A. Stohl**, **K. Law**).

Ten years ago, an important observational constraint to the calculated stratospheric ozone flux was given by the relationship of ozone with $N_2O$ (Murphy and Fahey, 1994). Tracer correlations in the LMS have proven useful in deriving global, annual mean fluxes of many constituents between the stratosphere and troposphere and in understanding the age of stratospheric air (*i.e.* time since it last was in the troposphere). Recently, a new observational study has shown the potential of $O_3$-HCl correlations to be a more accurate tracer relationship for constraining the amount of UT ozone that is of stratospheric origin (Marcy *et al.* 2004). (**D. Fahey**)

Troposphere-to-stratosphere transport of water vapour and aerosols across the extratropical tropopause is an important yet not fully investigated aspect of STE. While evidence of "fresh" tropospheric air can be readily seen in the tropopause region

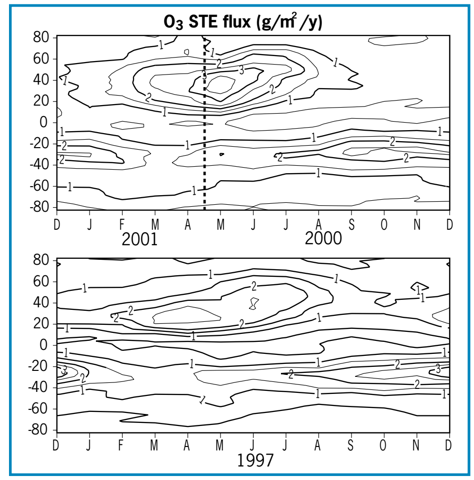


***Figure 14**. STE flux in units of g-$O_3$ $m^{-2}$ $y^{-1}$ as a function of latitude and month for (top) year 2000/2001 and (bottom) year 1997 as calculated using ECMWF pieced forecast met fields and the UCI CTM. (Adapted from Hsu et al. 2005).*

where tracer correlations identify a mixed stratosphere-troposphere chemical regime, it is not clear from models or measurements how large the flux of this fresh material is and whether it influences the middle stratosphere. Volcanic eruptions provide a test of our ability to model the reverse flux in this region, such as for simulations of Mt. Pinatubo aerosols mixing across the extratropical tropopause from the LS and thus contributing to the UT aerosol burden. (**J. Penner**)

Despite recent progress, the community has yet to digest and incorporate this new knowledge into current applications. For example, the STE terms in the tropospheric ozone budgets among major models still differ by a factor of 2 to 3. This raises the important question: How can our improved knowledge of the extratropical UTLS actually be implemented to improve the models? (**M. Prather**)

One key issue is what metric to use to calibrate the performance of global models in calculating STE flux. The use of newly-established tracer-tracer correlations across the tropopause is one option, although the theory of tracer relationships within the troposphere is incomplete. Many intensive field studies (*e.g.* from TRACE-P to MOZAIC) clearly demonstrate that $O_3$-$H_2O$, CO-$O_3$, or HCl-$O_3$ correlations can be used to define purely stratospheric, purely tropospheric, and mixed air masses. What is uncertain is whether a CTM simulation that reproduces these correlations necessarily implies the correct STE. New generations of satellite data provide the opportunity of using tracer-tracer correlations on a global scale and with spatial resolutions comparable with that of global models. AIRS (on the Aqua satellite) $O_3$- $H_2O$ correlations and MLS (on the Aura satellite) $O_3$-CO correlations are two examples of such data sets. These data sets, however, often represent spatial averages over small-scale features. It is important to compare the satellite data with *in situ* data sets like MOZAIC to understand the limitations of the data due to spatial averaging. (K. Law, M. Prather, L. Pan)

A confounding factor in determining STE in models is that observations of chemical discontinuities show that transport barriers appear to exist across the tropopause (Figure 16) and the choice of the precise transport boundary may make a significant difference in the calculated flux. Models, on the other hand, often produce much smoother chemical transitions, in part due to numerical diffusion within the models. A key question is whether the calculated flux depends on the choice of boundary, which would imply that chemical transformations in the transition zone are important. (L. Pan, M. Prather, A. Gettelman)

Further, defining a correct location for the "boundary" between the stratosphere and troposphere can be ambiguous because of the presence of ExTL, which has a mix of stratospheric and tropospheric chemical characteristics. Should we determine a new way of defining STE flux with consideration of this transitional layer? Would accurate simulation of the ExTL change the STE flux? This is only important if there are chemical sources/sinks in this layer, because in the absence of chemical processes, the ozone flux is conserved across the ExTL. (K. Law, M. Prather)

Over the past 25 years, there have been significant long-term declines in mid-latitude LS ozone levels, and this is an important factor in changing the STT flux of ozone. Both dynamics and chemistry likely contribute to this long-term ozone depletion. The possible importance of VSLS to enhancing the chemical loss of $O_3$ due to $Cl_y$ and $Br_y$ species was discussed. More observations are needed to quantify the significance of VSLS-related long-term ozone depletion, as well as the relative contribution of chemical and dynamical forcings to the observed long-term changes in ozone. (J. Logan, R.Salawitch)

New satellite data provide an exciting opportunity for validating and constraining models in the UTLS region. In particular, the AIRS instrument on Aqua and TES, MLS instruments on Aura all provide global ozone field in the UTLS region (see Figure 17, colour plate IV). To date we have only begun to explore the use of these data sets for characterizing and quantifying the integrated effect of STE. (L. Pan, A. Gettelman)

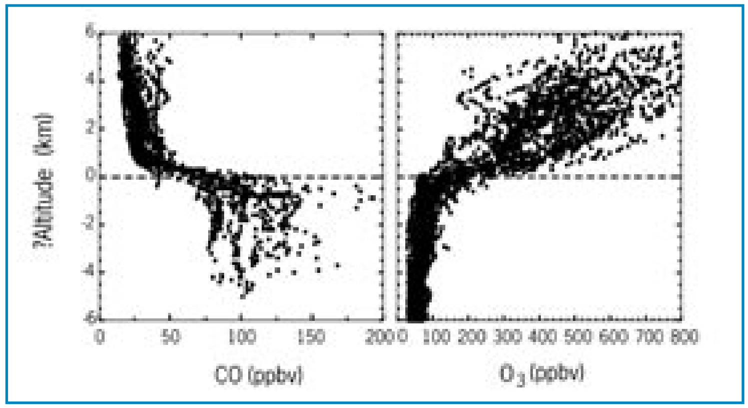


***Figure 16****. Chemical discontinuity across the tropopause. The CO and* $O_3$ *data are from ER-2 measurements during POLARIS campaign near Fairbanks, Alaska, April-August 1997. When altitude relative to the thermal tropopause is used as the vertical coordinate, the tracer profiles show abrupt change near the tropopause. (Adapted from Pan* et al.*, 2004).*

## Concluding Remarks

While perhaps more questions than answers emerge from the above discussions, the convergence of knowledge at the workshop was very useful in helping better define what is known regarding processes controlling the composition of the extratropical UTLS. Just as important, the workshop helped to identify the remaining outstanding questions.

It is clear that consistent use of well-defined terminology (*c.f.* STE=STT+TST) is imperative, so that disparate studies can be integrated for a larger-scale picture. In this regard there is especially a need to better understand the newly-identified ExTL. Given the complex thermodynamic and chemical state in this region, what metrics should be used to define the ExTL? What is its special role in the chemical, physical and dynamical state of the extratropical UTLS?

In some cases, focused measurement campaigns would allow us to clarify which processes are significant to the extratropical UTLS region and therefore warrant more extensive study. For example, targeted measurements of aerosol composition in the northern hemisphere UTLS, in conjunction with satellite data analysis, could help determine how pyro-convection is influencing the chemical and optical properties of particles in this region. *In situ* measurements could also be used to investigate, for example, the effects of short-lived bromine containing species transported to the UTLS.

Laboratory studies of reaction rates and heterogeneous ice cloud formation processes under conditions appropriate for the mid-latitude UTLS region are needed for more accurate model representation. Focused studies are also needed to understand how the coupling of dynamical processes over a range of scales control the chemical mixing and microphysical cloud formations in the extratropical UTLS (*i.e.* How "mixed" is the air in this region?) and to improve our modelling capability in this region (*i.e.* What processes are essential to include in order to represent the chemical and microphysical state of this region?). While the importance of deep convection in this region is now recognized, the measurements needed to quantify its effect on a global scale remain to be identified.

Finally, there is a need to incorporate existing knowledge into models in order to assess regional and global-scale impacts on, for example, cirrus cloud formation. In particular, while some key species and processes are starting to be included in CTMs and CRMs there is still the need to determine appropriate parameterizations for GCMs and CCMs. While models' predictions of STE across the extratropical tropopause have recently improved, large uncertainties in flux calculations still exist. New metrics must be found for validating these models against observations.

## *Acknowledgements:*

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*Acronyms:*

AIRS – the Atmospheric Infrared Sounder on the Aqua satellite (http://www-airs.jpl.nasa.gov/)
Aura – One of NASA's EOS (Earth Observation System) satellites (http://eosdatainfo.gsfc.nasa.gov/eosdata/aura/mls/mls.html)
CARIBIC – Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container (http://www.caribic-atmospheric.com/)
CCM – chemistry-climate model
CLAMS – Chemical Lagrangian Model of the Stratosphere
Crystal-FACE – The cirrus Regional Study of Tropical Anvils and Cirrus Layers – Florida Area Cirrus Experiment (http://cloud1.arc.nasa.gov/crystalface/)
EULINOX – The European Lightning Nitrogen Oxides Project (http://www.pa.op.dlr.de/eulinox/)
GOME – instrument on the ERS-2 satellite for global monitoring of ozone (http://earth.esa.int/ers/gome/)
ICARTT – International Consortium for Atmospheric Research on Transport and Transformation (http://www.al.noaa.gov/ICARTT/)
MINOS – Mediterranean Intensive Oxidant Study
MLS – Microwave Limb Sounder on the Aura satellite (http://mls.jpl.nasa.gov/)
MOPITT – Measurements of Pollution in the Troposphere (http://terra.nasa.gov/About/MOPITT/about_mopitt.html) instrument on the TERRA satellite (http://terra.nasa.gov/About/)
MOZAIC – Measurement of Ozone and Water vapour by Airbus In-service Aircraft (http://www.aero.obs-mip.fr/mozaic/)
NOXAR – Measurements of Nitrogen Oxides and Ozone Along Air Routes (http://www.iac.ethz.ch/en/research/chemie/tpeter/Noxar.html)
POAM II – Polar Ozone and Aerosol Measurements (http://wvms.nrl.navy.mil/POAM/poam.html)
POLARIS – field study; Photochemistry of Ozone Loss in the Arctic Region in Summer
SONEX – SASS Ozone and Nitrogen Oxide Experiment
STRAT – Stratospheric Tracers of Atmospheric Transport (http://cloud1.arc.nasa.gov/strat/strat.html)
SPURT – SPURenstofftransport in der Tropopausenregion (Tracegas transport in the tropopause region; http://www.meteor.uni-frankfurt.de/spurt/)
STACCATO - Stratosphere-Troposphere exchange in a Changing Climate on Atmospheric Transport and Oxidation Capacity
STE – stratosphere/troposphere exchange
STERAO – Stratosphere-Troposphere Experiment - Radiation, Aerosols and Ozone (http://chill.colostate.edu/sterao.html)
STT – stratosphere-to-troposphere transport
TES – Tropospheric Emission Spectrometer instrument on the (http://tes.jpl.nasa.gov/), on the Aura satellite
TRACE-P –TRAnsport & Chemical Evolution over the Pacific field campaign (http://code916.gsfc.nasa.gov/Missions/TRACEP/)
TST – troposphere-to-stratosphere transport
(O)VOCs – (oxygenated) volatile organic compounds
VSLS – very short-lived species: *e.g.* lifetime with respect to photochemical removal <~0.5 year

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# Report on the Joint SPARC Workshop on Data Assimilation and Stratospheric Winds

## 12-15 September 2005, Banff, Canada

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## Background

Data assimilation is the process whereby observations are combined with model forecasts to produce an optimal estimation of the state of the atmosphere, known as an *analysis*. While the primary motivation for data assimilation is to provide an initial condition for weather forecasts, analyses also provide a record of the global state of the atmosphere that includes all relevant variables. Thus analyses can be used for process studies and, in some cases, to examine long-term changes. At the same time, data assimilation can help to identify observation biases or sudden changes in observation quality.

For these reasons, data assimilation contributes significantly to SPARC science. Yet there are many issues with the quality of assimilation products in the stratosphere (Rood 2005). SPARC Report No. 3 (2002) documented many of these. Especially in the tropics, differences between analyses can sometimes exceed the seasonal or interannual variability, making them of little value for studies of atmospheric variability (Figure 1). There are also significant polar temperature biases, which give uncertainty to studies of polar stratospheric clouds — this will be the subject of a future SPARC Report. Many studies (*e.g.* Schoeberl *et al.* 2003) have highlighted the severe errors that can arise when using assimilated winds in off-line transport models.

These problems arise because of the special challenges of data assimilation in the stratosphere. In the troposphere, the models are mature and the availability of plentiful observations from numerous independent observation types helps to separate model and observation bias. In the stratosphere, in contrast, models are known to exhibit severe biases (Pawson *et al.* 2000) such as the "cold pole problem" and the lack of a quasi-biennial oscillation (QBO), while at the same time there are relatively few observations, especially of winds, and little redundancy between those that do exist. In addition, the interest in stratospheric chemical transport has exercised the analyses in ways they were not intended for. In particular, stratospheric applications are often limited by errors that involve long time scales, which are not adequately reflected in the error covariances that underlie operational data assimilation.

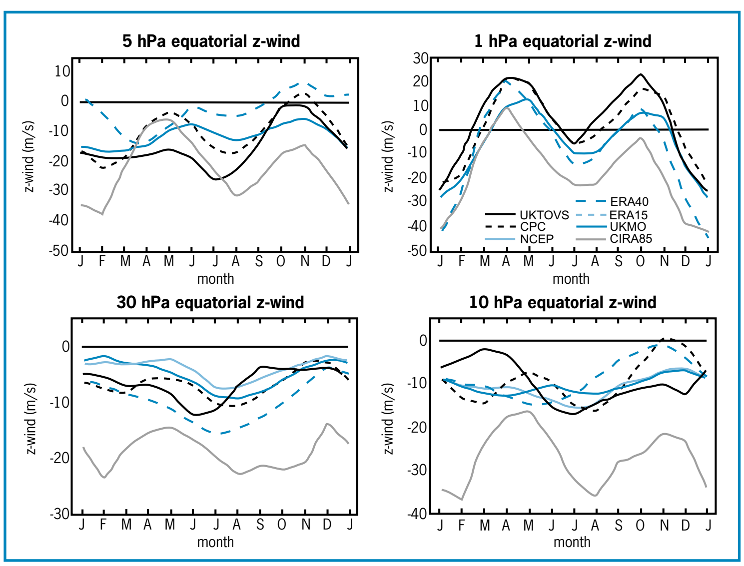



***Figure 1:*** Climatological seasonal cycle of zonal mean zonal wind at the equator from various analyses at 30 hPa (bottom left), 10 hPa (bottom right), 5 hPa (top left), and 1 hPa (top right). (*From SPARC (2002).*)

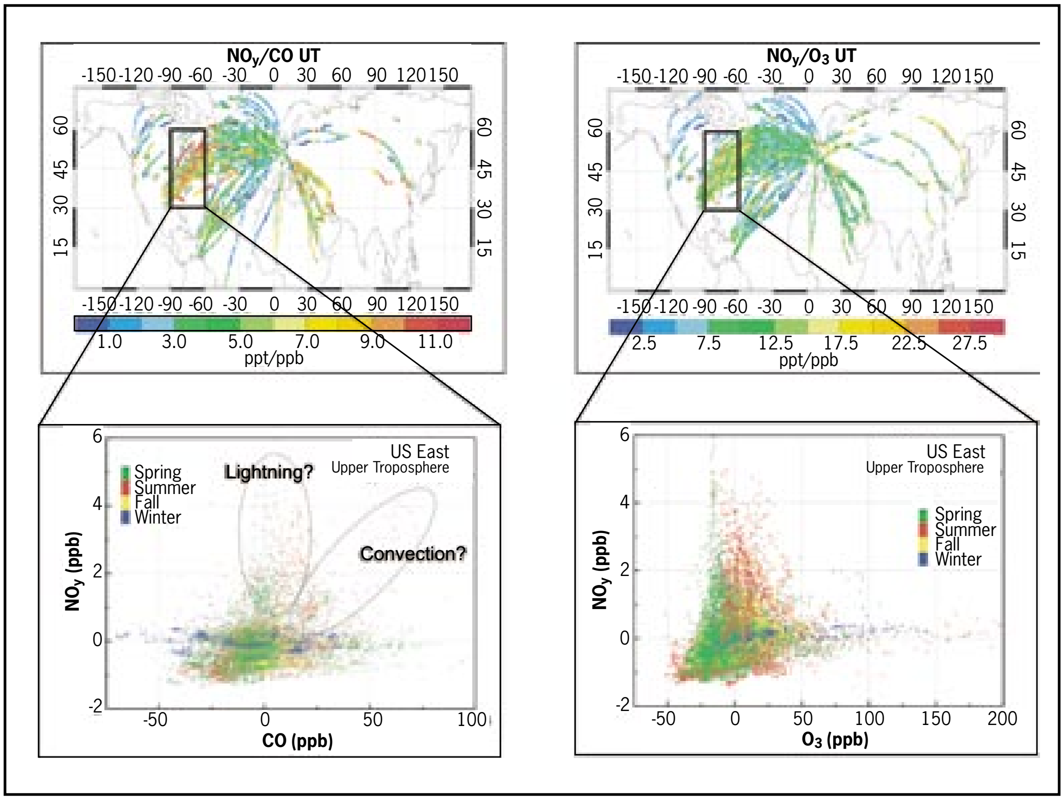
Because the process of data assimilation requires as inputs not only measurements and model forecasts, but also estimates of their accuracy (the mean and covariance of their errors), knowledge of the underlying physics of each measurement type, and of a model's numerical discretization and physical parameterizations, is required. In addition, data assimilation itself requires expertise in statistics and estimation theory. Finally, the outputs of assimilation must be assessed not only statistically, but also in terms of physical realism. Thus, data assimilation is a multi-disciplinary activity that requires the involvement of many different research communities to be effective: the measurement community, modellers, assimilators and theoreticians who understand the physics and chemistry of the real atmosphere.

## The SPARC Data Assimilation Working Group

The goal of the SPARC Data Assimilation Working Group (DAWG) is to advance data assimilation science in areas relevant to SPARC science. While other coordinated assimilation activities certainly exist (*e.g.* WGNE, THORPEX), the middle atmosphere context provides a rather different perspective on the process of data assimilation. For example, the interest in long time scales and the ubiquitous presence of gravity waves in the mesosphere challenges assimilation schemes designed for the troposphere (*e.g.* Polavarapu *et al.* 2006). The SPARC community already contains the wide variety of expertise needed to advance the science of middle atmosphere assimilation, and the SPARC organization provides the means to achieve the goals of the Working Group.

The goals of the SPARC DAWG are many. Firstly, the group will collect and document information on data assimilation systems. This is important information for the SPARC community members who use assimilation products for diagnostic studies. At the same time, the Working Group will encourage users of assimilation products to include multiple analyses in studies of processes or long-term changes, to

# Processes governing the chemical composition of the extratropical UTLS
# A report from the joint SPARC-IGAC Workshop




**< Figure 3**

*Correlation of $NO_y$ against CO (left) and $O_3$ (right) over North America as a function of season (3 years of data, seasonal cycle removed). High $NO_y$ with low CO in summer suggests lightning influence and possibly aircraft emissions, whereas high $NO_y$ with high CO indicates the influence of convective transport of boundary layer pollution (anthropogenic emissions) into the UTLS over this region. In contrast, high $O_3$:CO correlations exists in UT over Asia/Siberia in certain years such as 2003. (Petzoldt et al. 2005).*

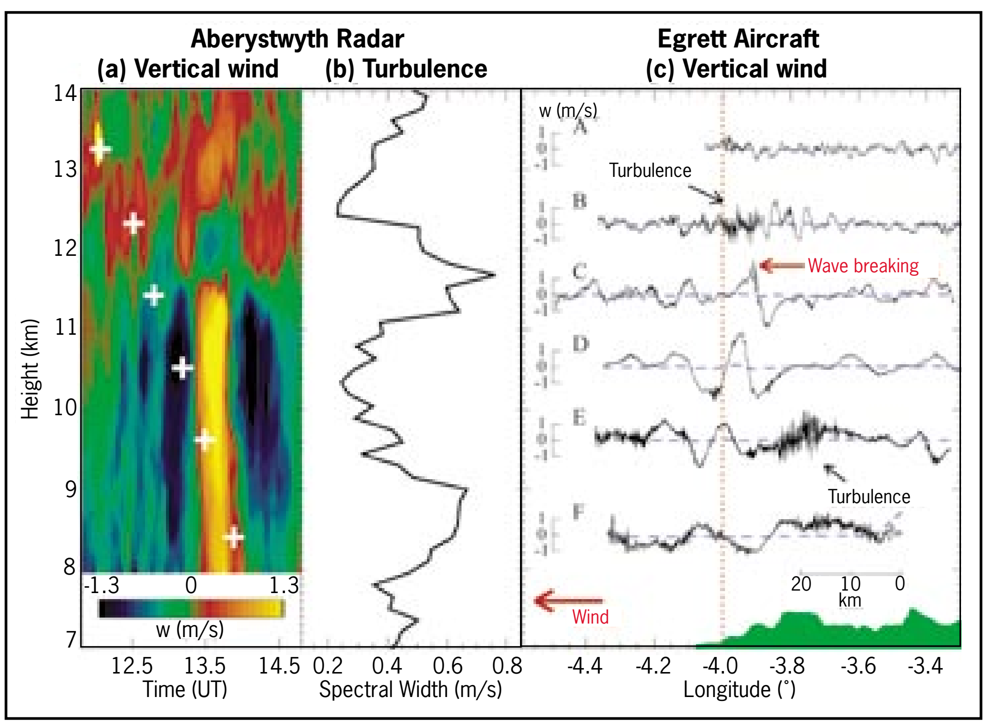



**Figure 6 >**

*(a) Measurements of vertical wind by the Aberystwyth VHF radar. (b) The spectral width of the radar signal averaged between 12:30 and 01:00 UTC. (c) Vertical wind measured on the Egrett. Each flight leg is placed at its height relative to the vertical scale in (a). The topographic height below the Egrett track is shown in green at the bottom with the same relative vertical scale as in (a). The coast of Wales is at 4.1° longitude; the position of the Aberystwyth radar is indicated by the vertical dotted line at 4.0° longitude. Crosses in (a) indicate the time and height when the Egrett passed directly above the radar. The turbulent layer between 11-12 km is estimated to have an internal turbulent diffusivity of about 2 m²/s (*Whiteway, 2003*).*

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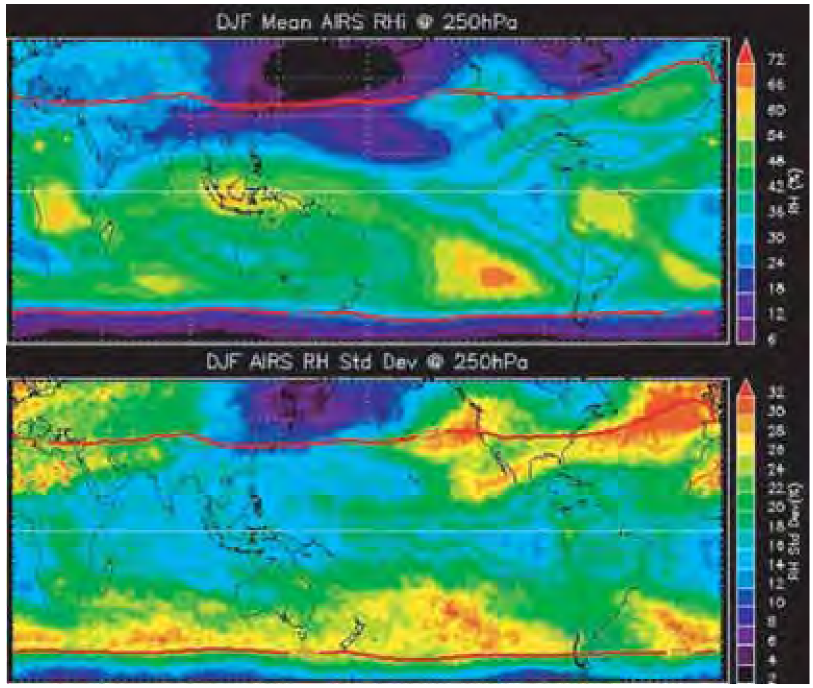
**Figure 10 >**

*From the presentation by A. Gettelman. Relative humidity over ice (RHI) from the Atmospheric Infrared Sounder (AIRS) at 250hPa averaged for December-February (top) and standard deviation of daily RHI from AIRS at 250hPa for an average of December-February 2002-2005 (bottom). The thick red line marks the thermal tropopause at 225hPa, showing that the extratropical stratosphere poleward of the tropopause is very dry and that the tropopause marks the boundary of high humidity regions. In contrast, the upper troposphere has high RHI, particularly in convective regions. The daily variance of RHI maximizes around the tropopause at this level, and is highest in the North Atlantic and North East Pacific, mostly equatorward of the thermal tropopause. High variance is also found along the tropopause in the southern hemisphere. Variations do not imply transport, but fluctuations between tropospheric and stratospheric air at this level.*

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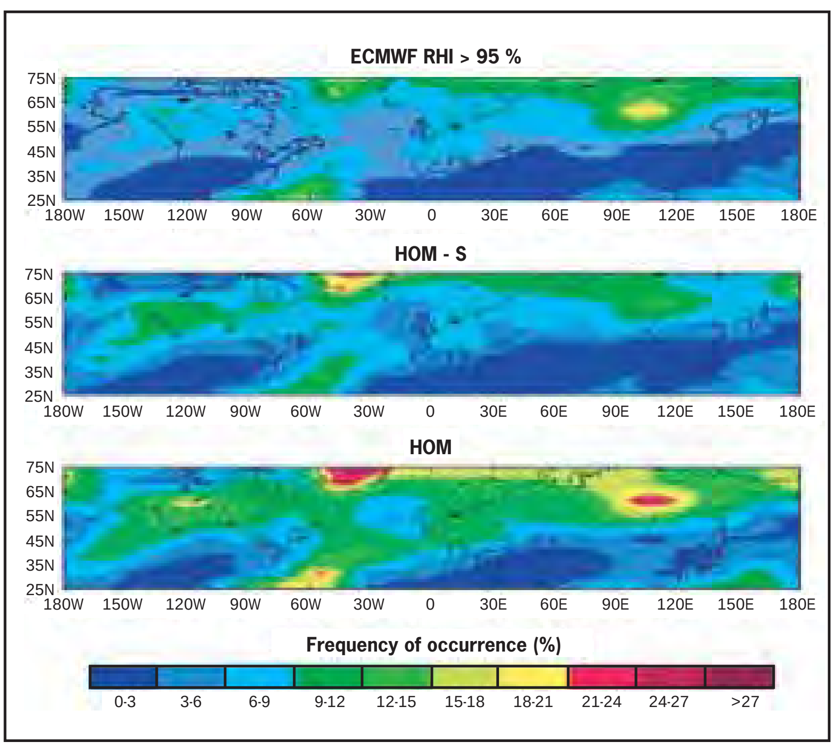


**< Figure 11**

*Calculated frequencies of cirrus cloud occurrence during fall 2000 based on meteorological fields taken from the ECMWF model in T511/L60 resolution (Haag and Kärcher, 2004). The regions in which the relative humidity over ice (RHI) exceeds 95% are evaluated along synoptic trajectories driven by the ECMWF winds and are used as a measure for cirrus cloud cover (top, ECMWF). The forecast model uses a thermodynamically-based cloud scheme and forms cirrus at ice saturation. The other panels show results from explicit calculations of aerosol and cirrus cloud microphysics along the trajectories. This approach takes into account that cirrus form at significant supersaturations via homogeneous freezing and consider kinetic effects during growth and evaporation of ice crystals. The microphysical simulations use the synoptic temperatures (middle, HOM-S) and synoptic temperatures with superimposed small-scale temperature oscillations (bottom, HOM) caused by parameterized gravity waves. The occurrence frequency is lower in case HOM-S than in HOM, because average sizes of ice crystals are larger and their sedimentation speeds are faster in HOM-S, decreasing average cloud lifetimes.*

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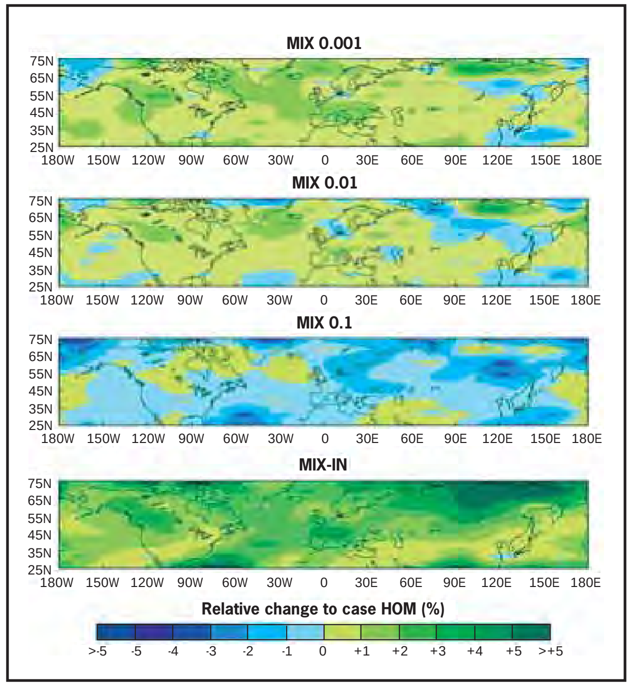
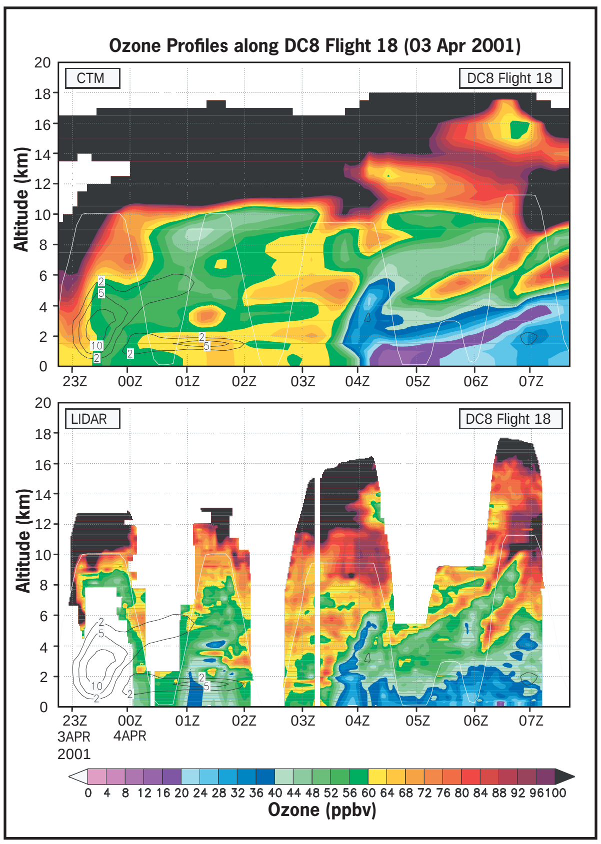
**Figure 12 >**

*Changes of the frequency of cirrus cloud occurrence relative to case HOM shown in Figure 11 caused by additions of heterogeneous ice nuclei (IN) forming ice at 130% RHI. Total IN concentrations are x $cm^{-3}$ in the cases MIX x (first 3 panels). The case MIX-IN (bottom) assumes 0.01 $cm^{-3}$ with extremely efficient IN that nucleate ice at 105% RHI. Field measurements suggest that background IN concentrations do not exceed 0.01 $cm^{-3}$, but higher values may occur locally. The cloud occurrence is a nonlinear function of ice nucleation thresholds and IN concentrations (for details see Haag and Kärcher, 2004). Changes in gravity wave properties also strongly modify the cloud occurrence (not shown).*





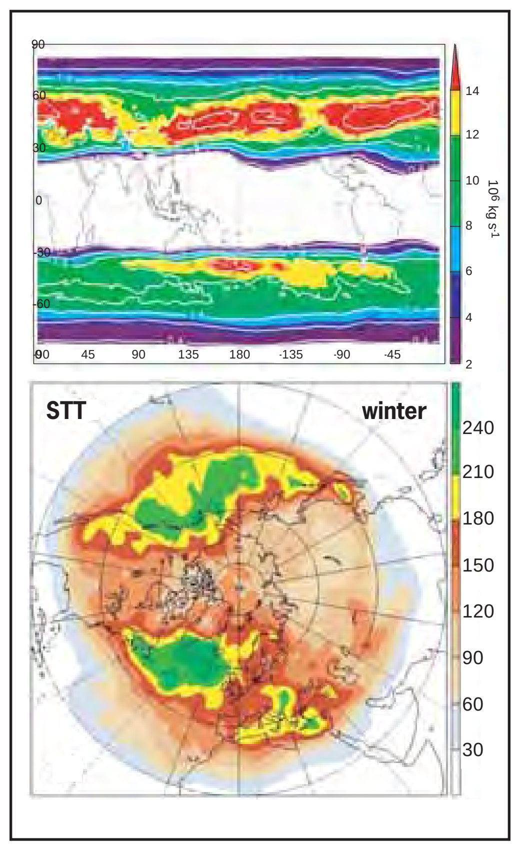




**^ Figure 15**

*Comparison of FRSGC/UCI chemistry-transport model and DC-8 LIDAR ozone profiles for Flight 18 from Hong Kong to Hawaii on 3 Apr 2001 showing stratospheric $O_3$ intrusions. The colour scale highlights $O_3$ abundances less than 100 ppb, with 100-500 ppb shown as black, and greater than 500 ppb masked (white). The flight track of the DC-8 is shown in white, and black contours indicate approximate cloud optical extinction (per km) specified from the met fields. (Adapted from Wild et al. 2003).*

**Figure 13 >**

*Examples of stratosphere flux by Eulerian and Lagrangian models. (a) Five-year mean extratropical diabatic flux of mass (colour shading) and ozone (white contours) from the Goddard model. The ozone flux contour interval is 0.5 kg/s beginning at 0.4 kg/s (adapted from Olsen et al. 2004). (b) 15 year climatology of STT mass flux for the Northern Hemisphere based on Lagrangian calculation using ECMWF meteorological fields. (Adapted from Sprenger and Wernli, 2003)*



# Processes governing the chemical composition of the extratropical UTLS
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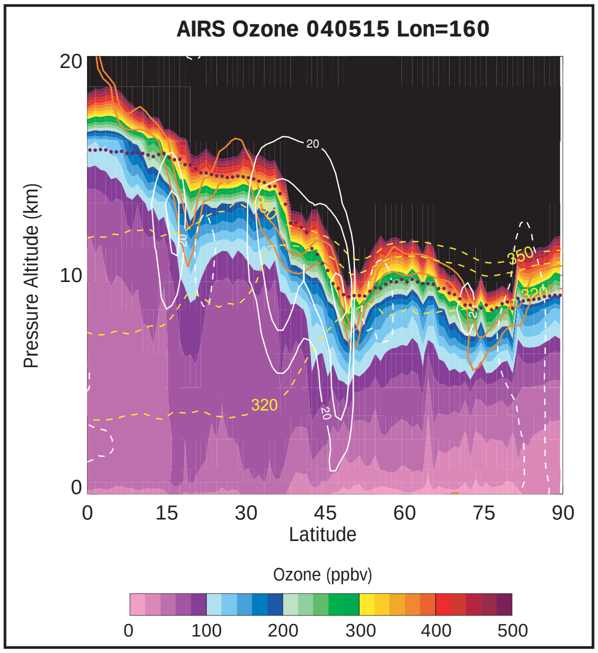
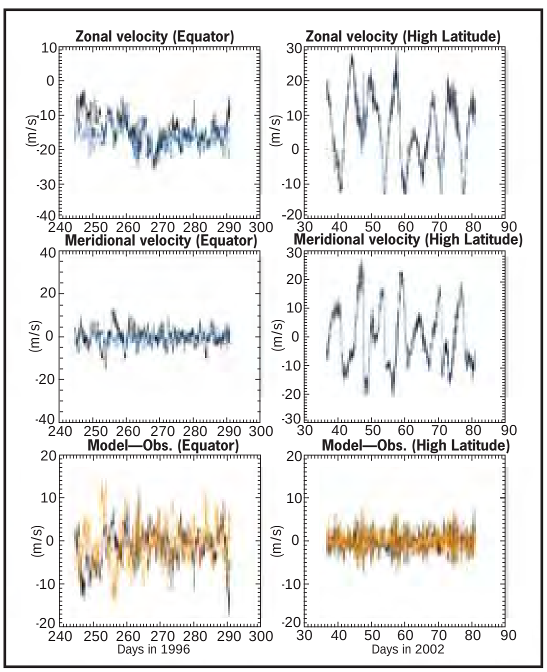



**< Figure 17**

*The colour image shows a cross section of ozone data from satellite instrument AIRS. The data shown are 1°x1° binned averages. The white contours represent the zonal wind, highlighting the subtropical jet and polar jet locations. The light yellow dash contours are potential temperature. Orange contours are 2 and 4 PVU potential vorticity. These meteorological fields are from 1°x1° degree and 26 level NCEP GFA data.*

# Report on the Joint SPARC Workshop on Data Assimilation and Stratospheric Winds





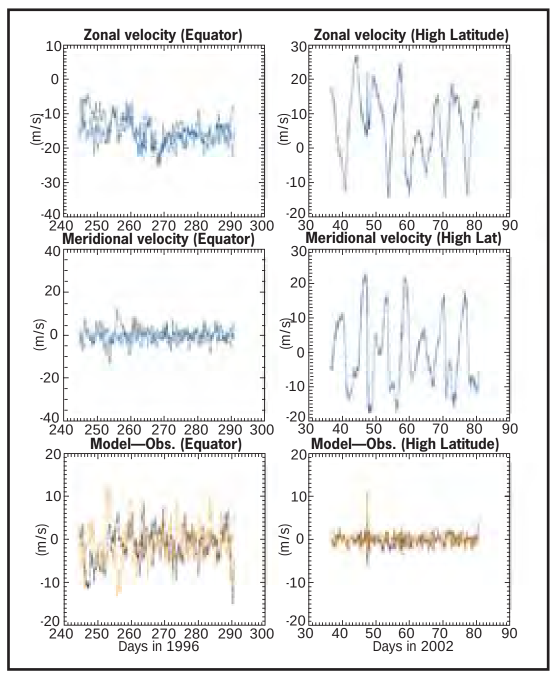



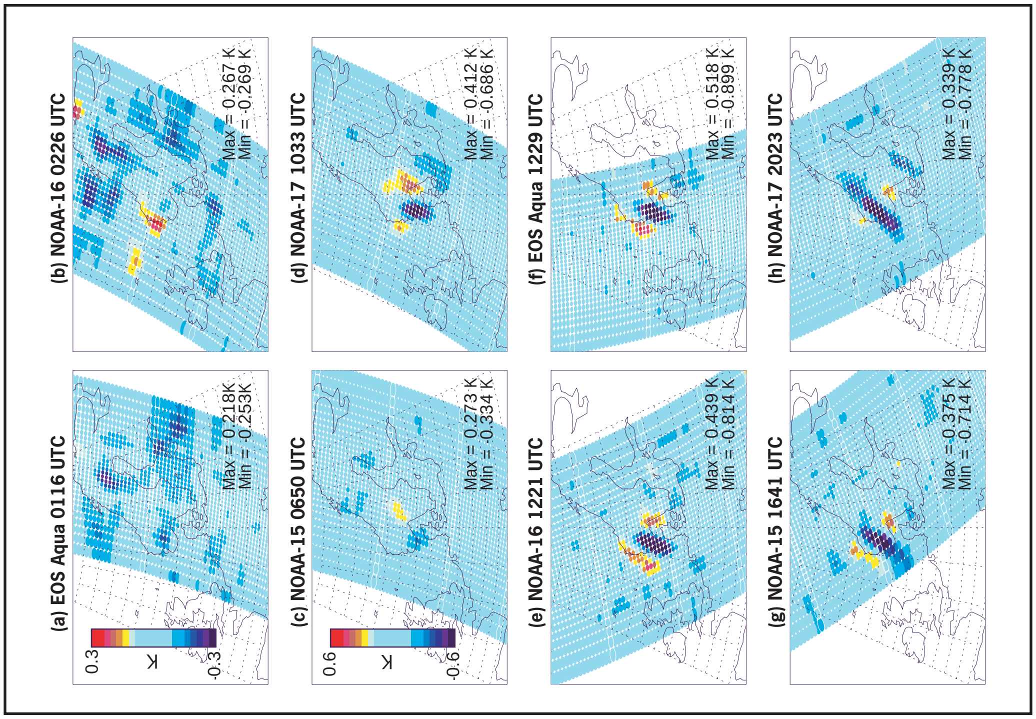

**Figure 3 >**

*Comparison of direct wind measurements from long-duration balloon flights at 60 hPa (Vial et al. 2001) with ECMWF analyses at the same point in the flight path. Left column shows equatorial measurements (taken in 1998), right column shows high-latitude measurements (taken in 2002). The top row shows zonal wind velocity and the middle row, meridional wind velocity; in both cases black denotes the balloon measurements and blue the ECMWF analyses. The bottom row shows the differences: black for zonal wind, and orange for meridional wind. Figure courtesy of Albert Hertzog, LMD.*

**^ Figure 4**

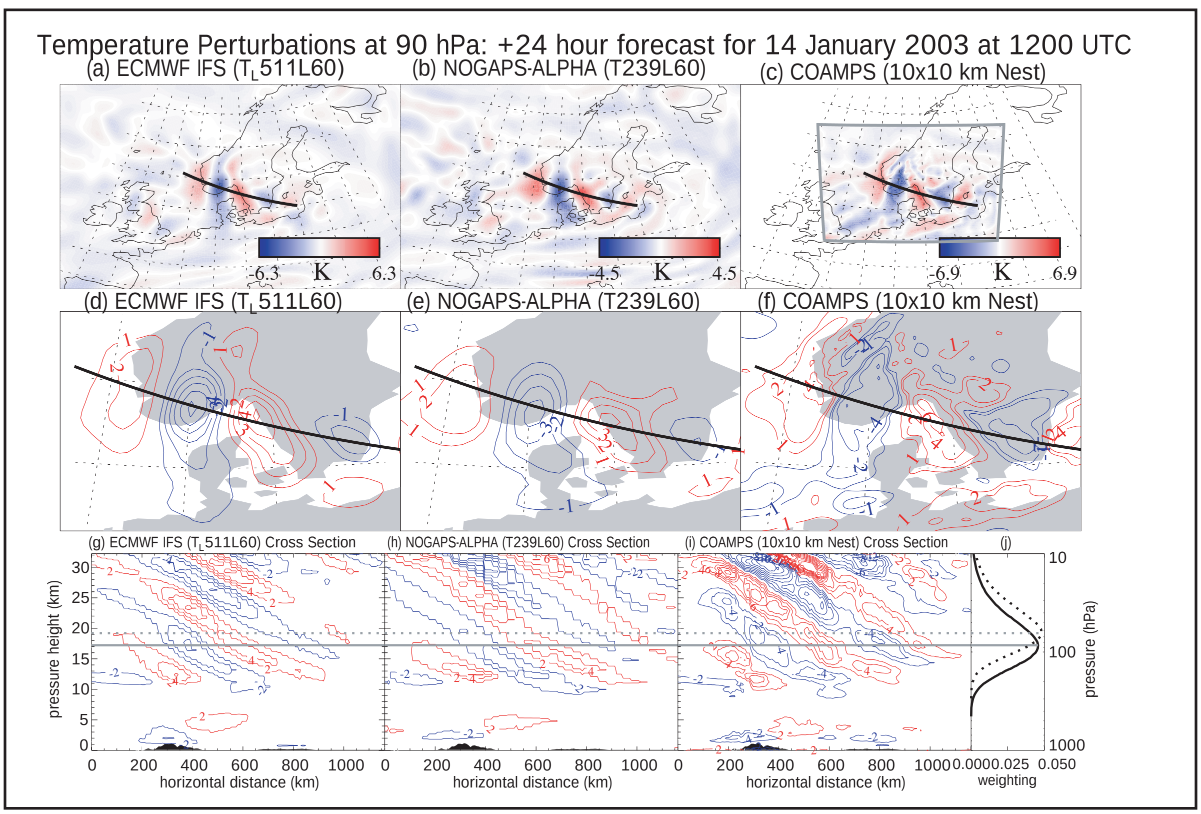
*The same, but with the directly measured winds filtered to exclude periods shorter than 12 hours. The difference with Figure 3 is attributed to inertia-gravity waves.*

# Imaging Gravity Waves in Lower Stratospheric AMSU-A Radiances




**^ Figure 4**

*AMSU-A Channel 9 brightness temperature perturbations $T_B(\hat{\lambda}_j, \hat{\phi}_j)$ in Kelvin: for panels (a) and (b), the colour bar range is ±0.3 K, and for panels (c)–(h) the range is ±0.6 K. The panels are arranged in chronological order: the universal time and platform of each overpass is given in each plot title. Data are plotted as colour-coded footprint ellipses at the measurement location, and white curves outline these measurement footprints for every tenth scan. Maximum and minimum values for each map are shown in the lower-right portion of each panel. We applied 3x3 point smoothing to suppress gridpoint noise.*

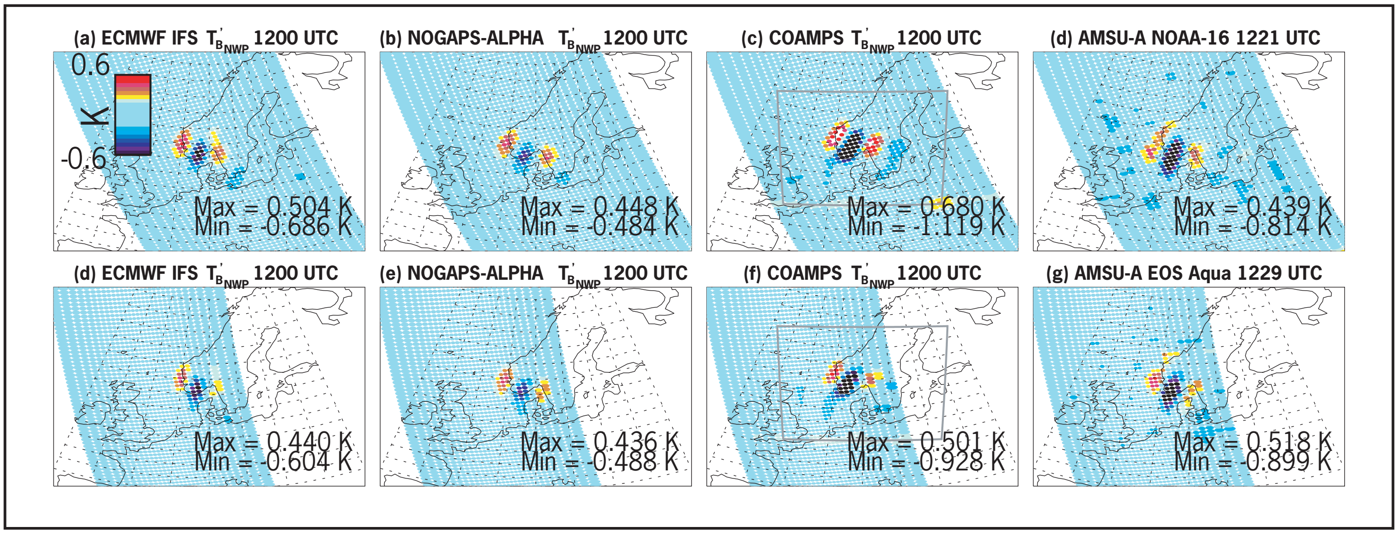



V

**Figure 5 ^**

*Top row plots temperature perturbations $T'(\hat{\lambda}, \hat{\phi}, p)$ at $p$ = 90 hPa extracted from +24 hour forecasts from ECMWF IFS (left column), NOGAPS-ALPHA (middle column) and COAMPS (right column) runs. See colour bar in the lower-right corner of each panel for temperature range. The middle row plots the same fields, but now focused over southern Scandinavia. The contour interval is 1 K. The bottom row of plots shows altitude contours of $T'(\lambda,\phi,p)$ along the horizontal cross-section indicated by the black curve in the panels above. Negative (cold) temperature anomalies are blue, positive (warm) temperature anomalies are red, and the contour interval is 2 K (zero contour is omitted). Cross-sections of topographic surface elevations are shaded in gray. Panel j shows AMSU-A Channel 9 1-D vertical weighting functions at the near-nadir position (solid) and far off-nadir position (dotted).*

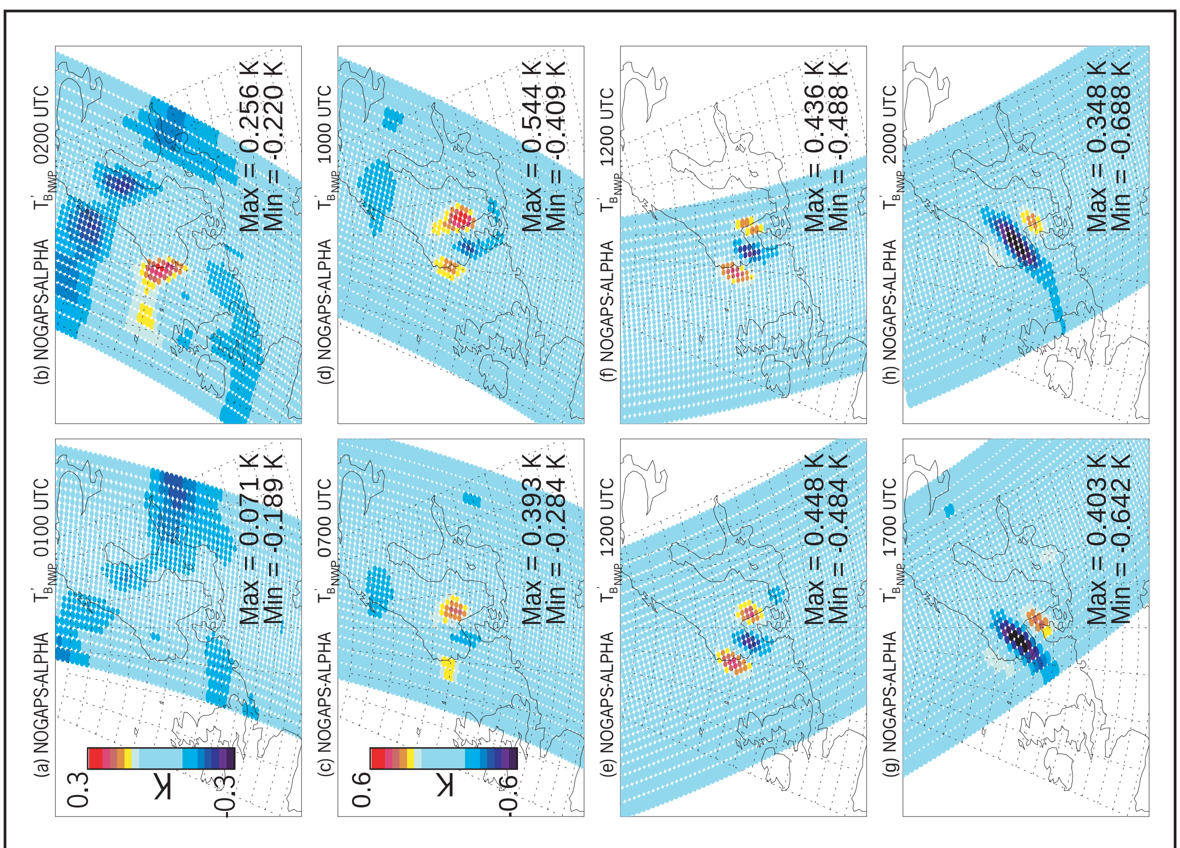
# Imaging Gravity Waves in Lower Stratospheric AMSU-A Radiances




**^ Figure 6**

*Top row: brightness temperature perturbations $T'_{B_{NWP}}(\hat{\lambda}_j, \hat{\phi}_j)$ extracted from 1200 UTC (+24 hour) NWP temperature fields $T(\hat{\lambda}, \hat{\phi}, p)$ from (a) ECMWF IFS, (b) NOGAPS-ALPHA, and (c) COAMPS runs, using the AMSU-A scan pattern from the NOAA-16 1221 UTC overpass. The data from Figure 4e are replotted in panel d. The bottom row shows the same sequence of plots for the 1229 UTC EOS Aqua overpass. Gray squares in (c) and (f) show the regional COAMPS domain. The colour bar scale (±0.6 K) is given at the top-left of panel a. Maximum and minimum values for each map are shown in the lower-right portion of each panel.*

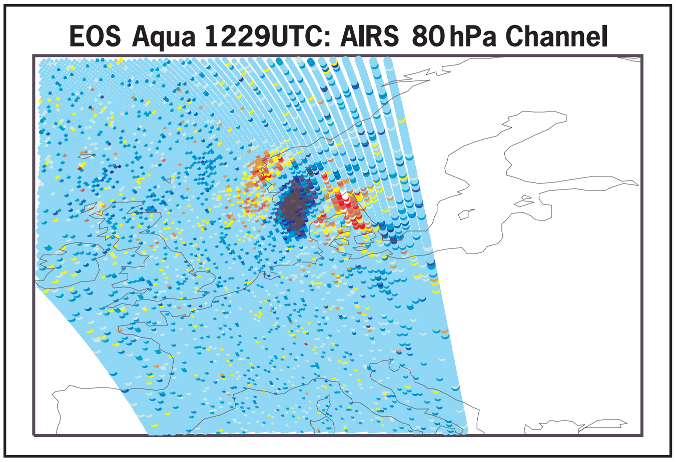
VI




**^ Figure 7**

*Similar presentation to Figure 4, but showing brightness temperature perturbations $T'_{B_{NWP}}(\hat{\lambda}_j, \hat{\phi}_j)$ derived from hourly NOGAPS-ALPHA temperature fields closest to the satellite overpass in question. Values are in Kelvin (see colour bars): for panels (a) and (b) the range is ±0.3 K, whereas for panels (c)–(h) the colour bar range is ±0.6 K. Maximum and minimum values for each map are shown in the lower-right portion of each panel.*

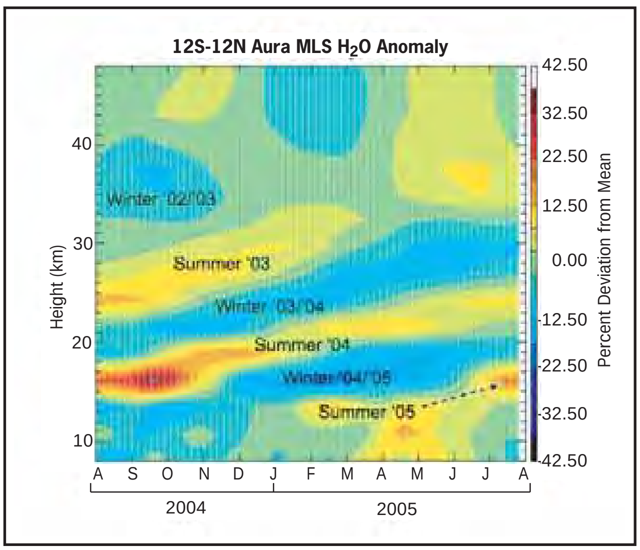
# Imaging Gravity Waves in Lower Stratospheric AMSU-A Radiances




**< Figure 8**

*Perturbations extracted from AIRS infrared radiances for a channel peaking near 80 hPa, during the EOS Aqua overpass of 1229 UTC on 14 January 2003.*

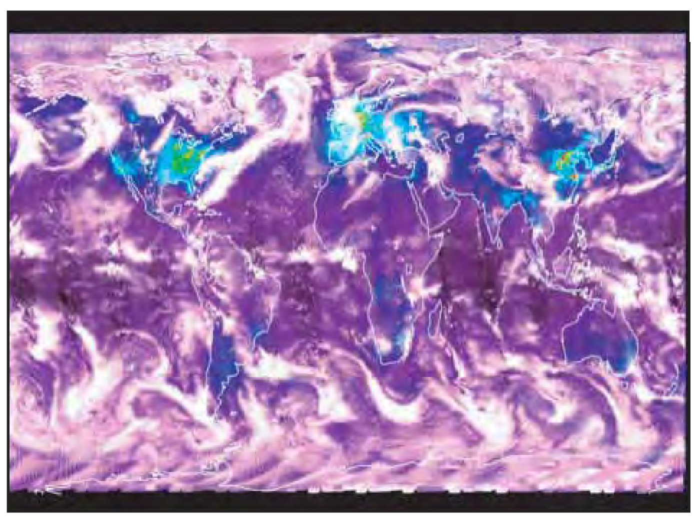
# EOS Aura Mission - One Year of Operations




**< Figure 4**

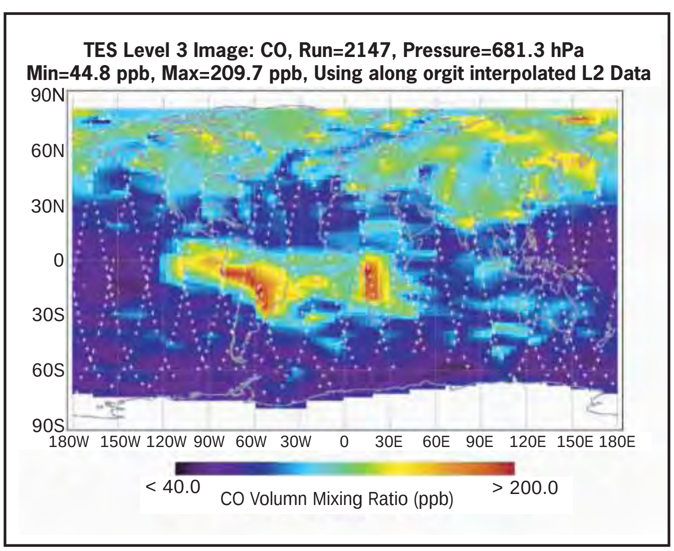
*Zonal mean tropical water vapour anomalies recorded by MLS showing the upward propagating dry and wet regions associated with the annual modulation of the tropical tropopause temperature. Date labels show when the bands were formed. (W. Read, JPL)*





**^ Figure 5**

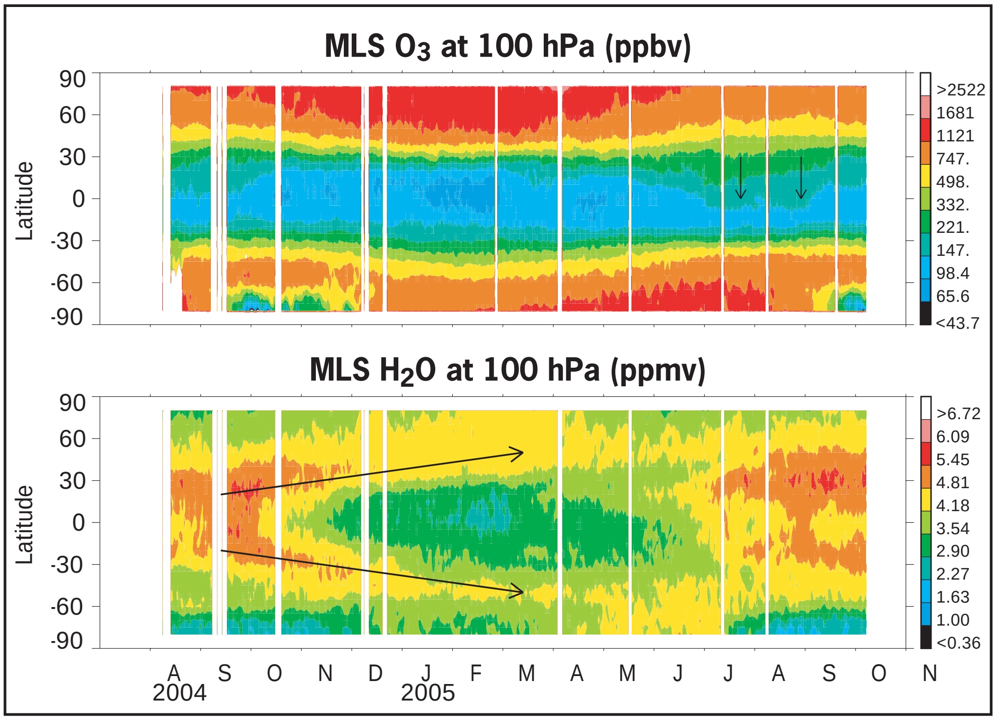
*$NO_2$ measured by the OMI instrument on April 15, 2005. Red indicates high values, blue low values, and clouds are indicated in white. (E. Bucsela, GSFC).*




**< Figure 6**

*TES CO at lower tropospheric pressure levels from the global survey mode. Measurements are made at the white crosses and interpolated to form a map. Northern Hemispheric fossil fuel combustion sources and tropical biomass burning are evident sources of CO.*

# A Highlight of the First-Year Aura MLS Observations



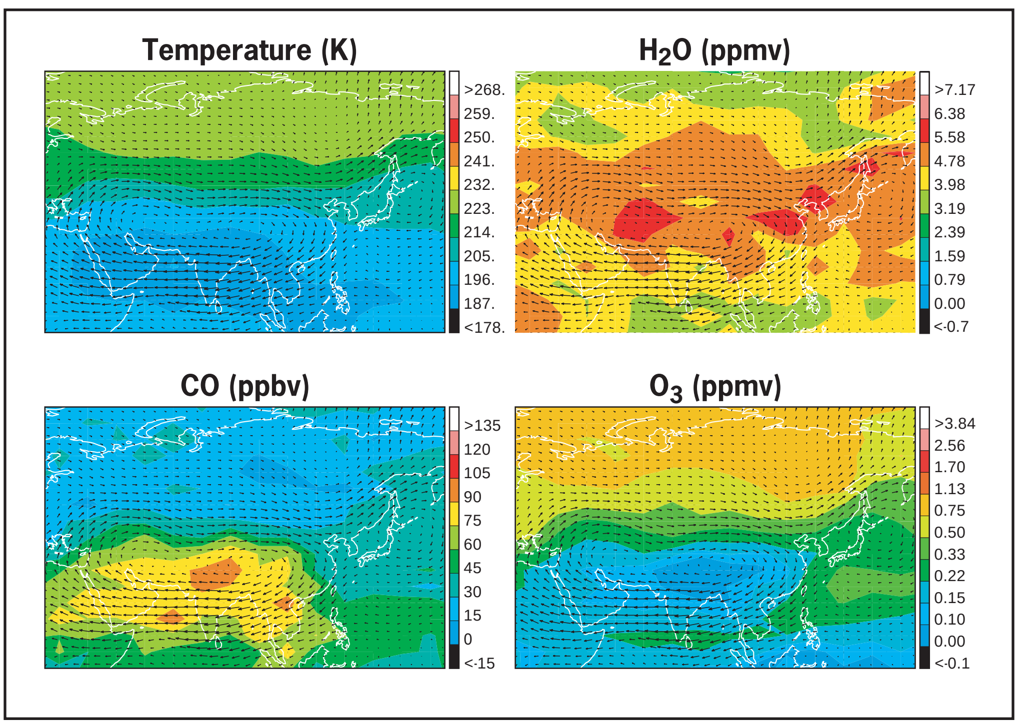

**< Figure 1**

*The first year of Aura MLS $H_2O$ and $O_3$ data at 100 hPa. A large amount of $H_2O$ is transported to the high-latitude LS (indicated by the arrows in the bottom panel) after the summer monsoon. More $H_2O$ is transported to the high-latitude Northern Hemisphere than to the Southern Hemisphere, partly because of a more abundant $H_2O$ supply, due to stronger anticyclones associated with the Asian monsoon in the UT/LS region. During the early monsoon season, the significant amount of $O_3$, extending from the mid-latitudes to the tropics (indicated by the arrow in the top panel), is related to UT anticyclones over Asia.*



**Figure 2 >**

*Maps of MLS temperature, $H_2O$, CO and $O_3$ at 100 hPa during 16-19 August 2005 when a strong anticyclone was anchored above Asia. Superimposed are the 100 hPa wind vectors from UK Met Office. High CO and $H_2O$ concentrations are lifted up and maintained inside the anticyclone where the tropopause is pushed higher. Conversely, the $O_3$ concentration is lower at the centre as a result of the lifted tropopause. A strip of high $O_3$ is spun off following the anticyclone, from mid-latitudes to the subtropics. The northern jet of the anticyclone provides a transport barrier separating air between the LS and the UT, producing anti-correlated CO and $O_3$ distributions around the anticyclone. However, the high concentration of $H_2O$ along and north of the jet is indicative of transport of UT air across the barrier into the middle world.*



emphasize the differences between analyses from different systems. The data assimilation community requires information on measurement data sets (meteorological and chemical) such as quality, availability, and the software needed to access it. The Working Group intends to gather such information and make it accessible on the SPARC Data Center website. An important feedback to data assimilators is obtained from process-oriented assessments. One obvious example of such feedback is the identification of errors in assimilated winds on long time scales obtained from examining age of air and trajectory calculations. Since assimilated products have particular difficulties in polar regions and in the tropics, physically based diagnostics of these regions will be the starting point. Because the SPARC community contains many users of reanalyses, the Working Group can provide guidance for reanalysis efforts. Finally, the Working Group will liaise with space and other agencies (*e.g.* IGACO, GCOS) on SPARC data needs through the SPARC SSG.

How will all these goals be achieved? At the very minimum, an annual workshop will be held. This will serve to gather assimilators interested in the middle atmosphere, and from which information on the various systems can be documented. By inviting experts in the dynamics and chemistry of the true system (the middle atmosphere), a more physically based assessment or criticism of assimilation products can take place. A specific theme can be identified to help select a few experts for a given workshop. The workshops can also serve to connect assimilators with the users of assimilation products. Thus attendance at these workshops should include assimilators, dynamicists and chemists with an interest in atmospheric processes, and users of assimilation products. Besides specialized workshops, periodic special sessions at large conferences will be organized to facilitate interaction with other research communities.

Reports such as this one will be written to disseminate information on the Working Group's activities, or to provide an overview of current or new ideas in assimilation to the wider SPARC community. In addition, the value of an article on the issues in middle atmosphere data assimilation for a general audience (*e.g.* Bulletin of the American Meteorological Society) is being considered.

The workshops will include more than scientific presentations. The workshops will also serve to identify the need for collaborative work, such as intercomparison projects. Such projects will advance the science of assimilation through the assessment of many different schemes with standard, physically-oriented diagnostics. The themes of intercomparison projects, or of the workshops themselves, will identify outstanding issues in the field. Proposed themes for upcoming workshops include: transport, water vapour, the tropical tropopause layer, and gravity wave drag. The latter topic refers to the goal of using the assimilation process to help identify the missing gravity wave drag force that parameterizations try to account for. An outcome of such research could be the estimation of parameters needed by gravity wave drag parameterizations. Finally, an ozone analysis intercomparison project has been proposed to continue the coordination started by the ASSET project.

## The 2005 Joint SPARC Workshop

As noted above, observations of stratospheric winds are very limited. There are some historical observations from rocketsondes and from the HRDI instrument on UARS. Rocketsondes are extremely sparse and geographically biased, while HRDI's stratospheric measurements had poor signal-to-noise and thus were heavily smoothed. Above 10 km, operational measurements come only from radiosondes, which have an inherent geographical bias and leave enormous data gaps; even then, only 20-30% reach 10 hPa (~35 km). While some information on winds can be obtained from satellite-derived temperatures, this relies on a balance between the mass and wind fields, which is a powerful constraint in the extratropics but a far weaker constraint in the tropics. The unbalanced component of the flow also is believed to increase strongly with altitude (Koshyk *et al.* 1999; Shepherd *et al.* 2000). Furthermore, operational temperature observations come from nadir sounders, which have poor vertical resolution and significant bias problems in the upper stratosphere.

The poor quality of stratospheric wind analyses in the tropical lower stratosphere is illustrated by comparisons with direct wind measurements, where those exist. In Figure 2, NCEP reanalyses are compared with winds measured from the ER-2 aircraft, flying at around 20 km altitude. In the extratropics, the agreement is excellent over a wide dynamic range. In the tropics, in contrast, the agreement is seen to be very poor. In Figure 3 (colour plate IV), ECMWF analyses are compared with winds measured from long-duration balloon flights at around 60 hPa. Again, the agreement is found to be much better in the extratropics than in the tropics. In Figure 4 (colour plate IV), the directly measured winds are filtered to exclude periods shorter than 12 hours, thus filtering the inertia-gravity waves which are not represented in the analysis (Hertzog *et al.* 2002). Now the agreement in the extratropics is remarkable, but the filtering has little impact on the discrepancies in the tropics.

Yet analysed winds are highly important for SPARC science. Many important problems of stratospheric variability, including the QBO and solar effects on climate, involve tropical winds which are poorly characterized at present. This makes it difficult to validate stratospheric climate models, whose representation of the QBO and Semi-Annual Oscillation (SAO) tends to be very model-dependent. Also, present



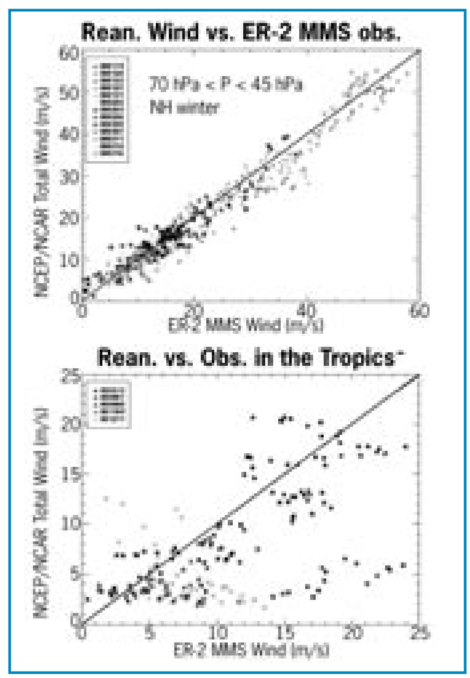



***Figure 2:*** *Scatter plot comparing total horizontal winds in the lower stratosphere around 20 km altitude from in situ aircraft measurements (horizontal axis) with NCEP/NCAR reanalyses (vertical axis) in the wintertime (a) extratropics and (b) tropics. Note the different scale in the two plots. (Figure courtesy of Paul Newman, NASA GSFC.)*

analyses appear to be of inadequate quality for long-term transport studies. This compromises our attribution of ozone changes, and also introduces biases in chemical data assimilation. Although better assimilation methods may improve the situation, there remain fundamental limitations that are ultimately tied to the quality of the wind observations.

While there is some prospect of inferring winds from observations of chemical species using four-dimensional assimilation methods, such observations are only sensitive to the component of the wind parallel to the tracer gradient. Unfortunately, tracer gradients tend to align *perpendicular* to the wind (the "stirring" effect). Moreover most tracer gradients tend to be quite slack in the tropics, where wind observations are most needed. In any case, any such derived wind products would require validation.

Thus, it seemed timely to assess the current knowledge of stratospheric winds, the science questions that require such knowledge, and the prospects for improved knowledge in the future. This led to the 2005 Joint SPARC Workshop on Data Assimilation and Stratospheric Winds. There were a total of 37 participants: 14 from Europe, 13 from Canada, 8 from the USA, 1 from India and 1 from Japan. Of this number, only 16 were from the data assimilation community; the others represented climate modelling, diagnostics, measurements, theory, and process studies. This sort of cross-fertilization between the data assimilation and the more 'physically oriented' communities is an exciting development, and as noted above is key to the success of the SPARC DAWG. The results of the Joint Workshop are now summarized, organized by theme.



## *Transport errors*

One of the most important issues concerning middle atmosphere data assimilation is the inability of analysed winds to adequately represent the Brewer-Dobson circulation. Such a failing limits their use in chemistry-transport models (CTMs) when the scientific interest lies in processes spanning more than a few weeks. Recent work at the ECMWF suggests that there is some hope for improving analysed winds in this respect. **S. Polavarapu**, in an overview presentation on issues in middle atmosphere data assimilation, showed a slide of recent age-of-air calculations by B. Monge-Sanz and M. Chipperfield (University of Leeds) (Figure 5). The ages of air computed from operational analyses (using 4D-Var) were far older (and more realistic) than those computed from ERA-40 analyses (using 3D-Var). Since 4D-Var analyses tend to be in better balance than 3D-Var analyses (*e.g.* Gauthier and Thépaut 2001), the former are less noisy and therefore produce less spurious mixing of tracers. Furthermore, using an even more recent version of the ECMWF system (also 4D-Var) resulted in ages of air which are approaching observed values in the northern extratropics. This latter result is likely due to the improved bias correction of ATOVS data, and the introduction of an improved balance in the initial forecast error covariance matrix (based on the nonlinear balance and omega equations) (A. Simmons, personal communication).

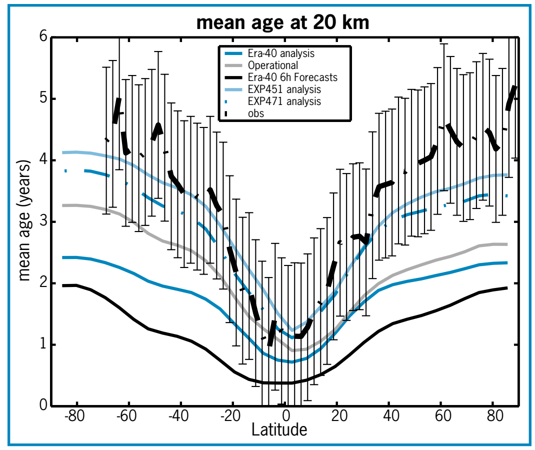



***Figure 5****: Mean age of air at 20 km altitude from simulations of the TOMCAT CTM (solid coloured lines) using different ECMWF meteorological analyses to drive the model, compared with the mean age of air derived from ER-2 aircraft observations of $CO_2$ and $SF_6$ (dashed lines). 2σ error bars have been included for the observations. (Figure courtesy of Beatriz Monge Sanz, University of Leeds.)*

Because of the transport errors associated with assimilated winds, **K. Miyazaki** and colleagues developed a system which first nudges ECMWF winds into a GCM, which then drives a CTM. The idea is that the GCM will be kept close to analyses, while model dynamics will reduce imbalance. Miyazaki found that nudging of wind fields created imbalances between the nudged fields and the GCM fields, while nudging of both temperature and wind fields was slightly better in this regard, although biases in the GCM remain despite the nudging. This system will be used for an extensive (1957-2002) ozone reanalysis using ERA-40 fields to clarify the roles of mean and eddy transports on the interannual and decadal variability of constituent distributions.

## *Dynamical variable assimilation*

The assimilation of satellite data remains both a major motivation and a major challenge for middle atmosphere data assimilation. One challenge arises from the fact that satellite measurements are generally related to atmospheric variables integrated over some path, whether vertical (nadir) or slant (limb). **Y. Rochon** noted that background error correlations can introduce small-scale structure into the analyses that is not necessarily physical. The specification of variances can also cause problems; *e.g.* the assimilation of total column ozone can result in the displacement of the climatological ozone maximum from the lower stratosphere to the upper troposphere, if background error variances reflect the variability of the upper tropospheric jets. While *ad hoc* procedures such as the removal or modification of covariances can reduce undesirable effects, Rochon developed a more general mathematical framework for choosing how to spread analysis increments along a path of integration.

Since analyses may not be in balance, as far as the forecast model is concerned, gravity waves may be generated in a geostrophic adjustment-like process when a model integration is started from an analysis. In the past, with 3D assimilation schemes, a separate filtering (or initialization) scheme was implemented. **D. Sankey** investigated the impact of several schemes on the middle atmosphere and found that a digital filtering of the full fields reduced vertical dispersion of parcels in trajectory analyses, but also eliminated the diurnal tide. An incremental analysis updating scheme was found to preserve the model's tide but to enhance vertical dispersion of parcels.

Since air irreversibly enters the stratosphere through the tropical tropopause, it is important to correctly capture upwelling in the tropical troposphere in order to simulate stratospheric moisture. However, moisture is an exceedingly difficult variable to assimilate. **H. Thornton** showed that unrealistic analysis increments are produced in the upper stratosphere as a result of improper background error covariance specification. Modification of covariances can reduce the problem. The choice of moisture variable for assimilation can also be important. Using relative humidity results in more Gaussian forecast errors than, say, the logarithm of specific humidity, because relative humidity will be adjusted even in the absence of moisture data if temperature data is assimilated. The Dee and da Silva (2003) approach was found to improve the assimilation up to about 5 hPa but did little to help above this level. The non-Gaussianity of errors in the moisture variable was addressed using the Holm (2002) variable, but preliminary results showed that the impact on stratospheric analyses was minimal.

Background error covariance specification is important not only for moisture, but for all variables. Thus proper covariance specification remains an area of active research. **D. Jackson** showed results from assimilation experiments with the Met Office's research stratospheric model (60 levels up to 84 km) comparing background error statistics derived using (i) the NMC-method and (ii) Yves Rochon's method which is based on model climatology (with the diurnal tide removed). Rochon's method provided better verification against analyses, but work is still ongoing. **S. Pawson** showed that by using inhomogeneous and anisotropic covariances (longer correlation lengths in the zonal direction in the tropics), the GEOS-4 system was better able to capture the easterly to westerly transition of the QBO by allowing the equatorial radiosonde wind observations to have more weight. The rationale is that these sparse radiosonde observations are believed to be representative of the zonal mean wind. (Moreover, there are reasons to expect zonally elongated error correlations in the tropics.) Without this modification, analyses would lag several months behind the Singapore wind observations in switching from easterly to westerly winds. With the modification, the analyses appear to be much better, based on comparison with Strateole balloons and with the QBO signal in ozone seen at Nairobi.

**Y. Jaya Rao** noted that cirrus clouds and aerosols are both observable with lidar measurements. Vertical velocity measurements with a VHF radar over a tropical station show vertical wind reversal within the clouds suggesting enhanced mixing. Such measurements may be very useful for determining the radiative impact of cirrus clouds on climate. **M. Salby** discussed the impact of convection on the temperature structure of the tropical tropopause. Representation of this process is a challenge for data assimilation, because of the small length scales involved both in convection and in the mean state response.

## *Chemical data assimilation*

Chemical data assimilation remains an important activity at major weather centres around the world. As **D. Jackson** noted, the main motivations for assimilating ozone include the improved assimilation of radiance measurements, improved radiative heating rates, the ability to exploit new satellite measurements, and the capability to assess proposed new satellite instruments. At the Met Office, a 3D-Var system based on an N48L50 version of the model is used for ozone assimilation with a Cariolle-based chemistry parameterization. The University of Cambridge is also developing a coupled chemistry model approach within a version of the Met Office Unified Model, and some preliminary results of UARS MLS ozone assimilation were shown by **M. Parrington**.

NCEP has been assimilating SBUV ozone data operationally since 1997 with a 3D-Var scheme. Now ozone data from EOS-Aura, consisting of OMI total column and profile measurements, are being assimilated in test mode and will later be assimilated operationally. **S. Zhou** showed some results that indicated that OMI data is dominant due to its high density. Assimilation of high resolution profile data from MLS is in progress and assimilation of HIRDLS data is also planned.

**R. Ménard** described the operational assimilation of surface ozone data at the Canadian Meteorological Centre, as well as plans for on-line chemistry assimilation and transport with the operational forecast model and complex chemistry models for both the troposphere and stratosphere. **B. Bregman** presented examples of current work at KNMI involving the assimilation of SCIAMACHY total column measurements of ozone. This has been running operationally since January 2004. KNMI uses an off-line CTM with a sequential (Kalman filter-type) assimilation scheme. **H. Elbern** described an ambitious new assimilation scheme SACADA (Synoptic Analyses of Chemical constituents by Advanced Data Assimilation) in development at a consortium led at the University of Cologne and designed to run operationally at the German Space Agency (DLR-DFD). The system employs the German Weather Centre's (DWD) global forecast model GME online, based on an icosahedral grid and including a complex chemistry module. A 4D-Var approach was taken to ensure a-temporal consistency of chemical constituents. Sample results from the assimilation of ten species from MIPAS were shown.

Middle atmosphere measurements from the recent ENVISAT, EOS-Aura and Odin satellites have motivated work outside of operational centres as well. **A. O'Neill** showed that MIPAS ozone improved analyses between 100 and 10 hPa when assimilated using 3D-Var with the ECMWF model at T159L60. **J. Rösevall** used an off-line isentropic transport model with a Kalman filter-type algorithm to assimilate Odin SMR data and estimate descent rates and ozone loss rates within the polar vortex.

Because data assimilation is a very expensive operation, the additional cost of chemistry models remains an important issue. **M. Bourqui** presented a new chemistry solver which uses pre-computed nonlinear transfer functions that represent average diurnal chemistry. This new approach could be very useful in a data assimilation context. The issue of the level of complexity of chemistry needed in the assimilation context was a topic of considerable discussion. **R. Ménard** presented results of a surface ozone assimilation which showed better analyses (in terms of standard deviation and bias against observations) without chemistry than with it. However, the forecast biases were greatly reduced with chemistry. In addition, **W. Lahoz** showed results from an intercomparison study (under the auspices of the EU-funded ASSET project) of five ozone assimilation models and found that having complex chemistry did not necessarily improve the ability to capture ozone depletion in the polar vortex. The same study also found that variants of the Cariolle parameterization gave rather different instantaneous rates of change of ozone and led to different ozone distributions. The discussion led to a proposal of a theme for a future SPARC-DAWG workshop: *the minimum level of complexity of chemistry needed for data assimilation.*

## *Quality of current analyses*

**G. Manney** assessed the impact of differences between analyses for the study of transport in the 2002 Antarctic Stratospheric Sudden Warming (Manney *et al.* 2005). While the different analyses exhibited overall qualitative agreement in a coarse sense, there were very significant differences in detail, as revealed in sensitive diagnostics such as effective diffusivity. These differences are also reflected in the sensitivity to the choice of analysed data sets of other diagnostic studies such as Match-estimated ozone loss, age of air, and stratosphere-troposphere mass fluxes — all of major importance for SPARC science. In terms of dynamical fields, while the zonal-mean zonal wind at 60N and 10 hPa agrees between all analyses, the NCEP/NCAR reanalysis is clearly unreliable for stratospheric temperature, while ERA-40 temperatures are unreliable for PSC studies because of spurious vertical oscillations.

**M. Giorgetta** addressed the question of whether a model needs to be able to simulate a self-generated QBO in order to properly represent a QBO through assimilation. This is not so clear; once the zonal mean winds are reasonably close to the observations, the wave fluxes in the model, both resolved and parameterized, will presumably respond to the shear layers. On the other hand, the model will certainly have a bias that will depend on the state of the real atmosphere, and if these wave fluxes are poorly represented then the model response to QBO winds will be incorrect.



**E. Manzini** focused on variability in the Arctic wintertime vortex associated with ENSO, contrasting its representation in ERA-40 and in the NCEP/CPC analysis. Above 10 hPa, there are substantial differences in amplitude (though not in structure). In general, ERA-40 has a stronger planetary wave 1 signature in the upper stratosphere — though much less so before 1980.

In a **discussion session**, the following consensus was reached for our knowledge of stratospheric winds. In the extratropics, up to 10 hPa there is a reasonable overall agreement between analyses, and between analyses and radiosondes. Whether the extent of agreement is suitable for long-term transport or mixing is not clear. Vortex mixing appears to be reasonably well represented, however. But overall the quantification of the quality of analyses is process dependent. As a general rule, we would like the differences between different analyses to be less than the interannual variability. For vertical wind, the only validation data is from tracers, which can be difficult to interpret because of mixing. It is recommended that analyses should use and provide, diabatic heating rates. Above 10 hPa, analyses differ more substantially. In this region, there are no direct wind measurements, and no other data constraints on the TOVS radiances. Furthermore, the model impact on the analysis, either from parameterized gravity-wave drag or from the location of the model lid, is stronger. Thus, in this region there are likely to be significant biases in both models and observations, leading to unreliable analyses.

In the tropics, the situation is much worse. With respect to the zonal wind, the SAO is not well characterized (models may force their own SAO quite strongly), and the observations are of temperature, not winds. The QBO is reasonably well characterized below 10 hPa qualitatively, but not quantitatively. Above 10 hPa, better characterization is needed. Since models don't always simulate a self-generated QBO, periodic biases are present. There is also no validation of the longitudinal structure of the QBO. With respect to the meridional or vertical wind, we do not know much about the quality of the analyses, but they are likely to be quite poor. For these fields, tracer observations may provide the only validation opportunity. On the other hand, a better knowledge of the zonal wind should help constrain the meridional wind, as the horizontal flow can perhaps be expected to be non-divergent to a first approximation (even in the tropics).

## *Unbalanced dynamics and mesospheric assimilation*

**E. Källén** described work addressing the assimilation of equatorial waves — Kelvin waves, mixed Rossby-gravity waves, equatorial Rossby waves and inertia-gravity waves — exploiting knowledge of the spatio-temporal structure of the waves. For ECMWF, 60-70% of the forecast error variance in the tropics is associated with equatorial waves, so it is important to attempt to represent them in analyses. The study was motivated by the ADM-Aeolus instrument (see below), which will only measure line-of-sight wind and so requires assimilation in order to obtain the vector wind. Rather surprisingly, 4D-Var does not do much better than 3D-Var, and observing the height field is not so helpful in getting the wind components.

While the middle atmosphere includes the mesosphere, most assimilation work is concentrated on the stratosphere. However, interest in estimation of the mesosphere and lower thermosphere has been increasing as operational centres raise their lids. (The U.S. Navy has model versions with lids at 85 and 100 km. ECMWF will raise their lid to 0.01 hPa and the Met Office will have a version of their model with a lid at 110 km.) With mesospheric data assimilation it becomes possible to couple the neutral atmosphere to "space weather." Since the mesosphere is dominated by wave disturbances generated from below (*i.e.* tides, planetary, gravity and Kelvin waves), an assimilating model should ideally include the wave source region.

**R. Lieberman** and **D. Ortland** both addressed the subject of data assimilation in the mesosphere and lower thermosphere (MLT), where unbalanced motions are strong. In this respect there may be parallels with the ocean, where inertial oscillations are the dominant signal of current-metre measurements. The subject is timely because of the launch of the TIMED spacecraft in December 2001. A dominant feature of MLT variability is thermal tides, which cause strong aliasing problems for most satellite observations (which are slowly precessing in local time) and can lead to a misrepresentation of tides and transient planetary waves. While ground-based observations can resolve the diurnal variability, they need to be optimally combined with satellite observations to produce a complete picture (Figure 6). Thus, for TIMED, ground-based measurements were an integral part of the science plan and represented a "fifth instrument". For this strategy to work as part of assimilation, however, the underlying model must have a realistic representation of thermal tides.

**T. Matsuo** found that one challenge of using an ensemble Kalman filter for assimilation in the mesosphere-lower thermosphere region was the collapse of the ensemble spread due to insufficient model variability compared to observed variability. This may be related to the use of a mechanistic

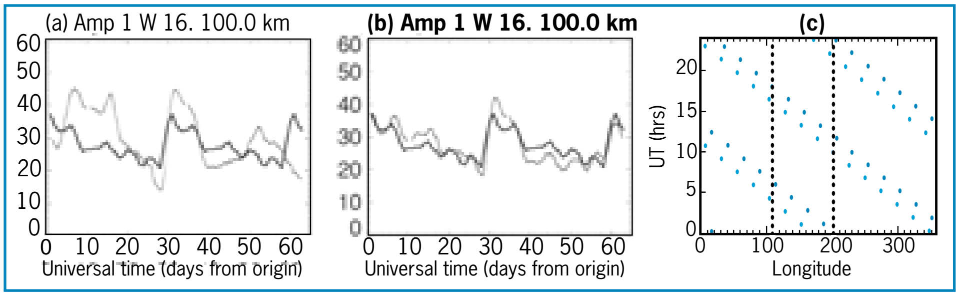



*Figure 6: (a) Retrieval of the migrating diurnal tide at 100 km modelled in NCAR-WACCM (black curve) by a sequential estimator based upon TIDI sampling alone (gray curve). The retrieval is hampered due to TIDI undersampling in local time. (b) As in (a), including sampling by 7 ground-based radar wind profilers. The retrieval is subtantially improved due to the higher sampling rate of the ground-based stations, located at a sufficient number of sites (> 4) so as to resolve the migrating semidiurnal tide. (c) Longitude versus universal time sampling of satellite (negatively sloped curves) and ground-based observations (vertical curves). (Figure courtesy of Ruth Lieberman, Colorado Research Associates.)*

model, which forces planetary waves at the tropopause. A covariance inflation factor, estimated from observations, was a proposed solution.

## *Problems requiring improved wind measurements*

**T. Dunkerton** highlighted the upper stratosphere/lower mesosphere as a region of particular interest. This is where variances tend to maximize and much interesting dynamics occurs: planetary waves break down violently, barotropic and inertial instabilities occur, and mean flows evolve rapidly, *e.g.* during the spring and autumn transitions. Thus, it is an exciting frontier for middle atmosphere data assimilation. There is some evidence that in polar regions, stratospheric disturbances are associated with mesospheric precursors (*e.g.* stratospheric warmings with mesospheric coolings). In order to understand the dynamics of such connections, and whether there is any causal element, it is necessary to separate upward and downward components of planetary wave fluxes. This will require accurate measurements of winds in this region. In the tropics, there is a medley of interesting dynamical phenomena involving winds, which will be a challenge to properly characterize from observations. Inertial instability is clearly occurring, but is difficult to observe because of its rapid timescale and small (as yet unknown) vertical scale. (In models, it tends to occur on the smallest resolved vertical scale.) Equatorial waves, both of intermediate frequency (1-3 day period) and intermediate scale (zonal wavenumber 10), play a crucial role in the QBO. Observing the properties of inertia-gravity waves requires high vertical resolution in the lower stratosphere, and high temporal resolution in the upper mesosphere.

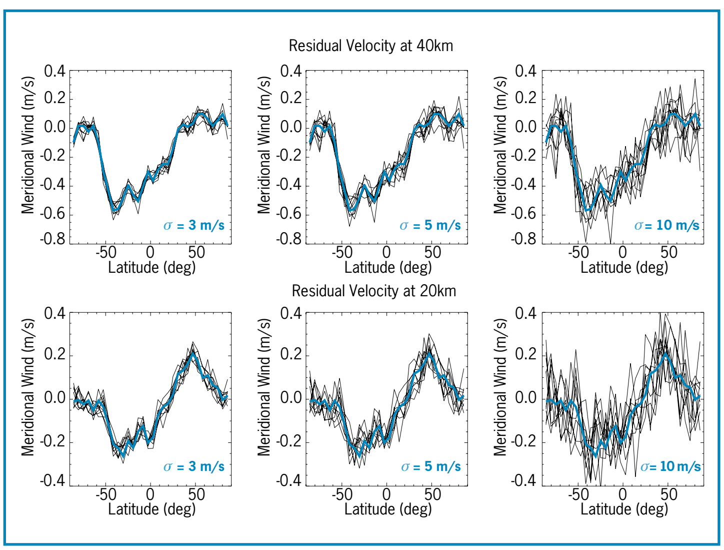



*Figure 7: Estimation of SWIFT measurement requirements for the meridional residual circulation $\bar{v}^*$, using pseudo-observations computed from the Canadian Middle Atmosphere Model for July: upper stratosphere (top panels) and lower stratosphere (bottom panels). The blue curve denotes the 'truth'; the black lines show results of ten different estimations, for one month of simulated SWIFT measurements, with Gaussian random noise added to both the meridional and zonal wind components before computing $\bar{v}^*$. The noise standard deviation is given in the lower right-hand corner of each panel. (Figure courtesy of Charles McLandress, University of Toronto.)*

In related comments, **T. Shepherd** emphasized the increasing dominance of inertia-gravity waves (IGWs) with increasing altitude, leading to drastically shortened auto-correlation times for winds, for example. This represents a challenge for data assimilation in the upper stratosphere and mesosphere. IGWs are present even in relatively coarse resolution global models, although only represent the tip of the iceberg with respect to the real atmosphere. By the same token, any measurement technique will only observe part of the IGW spectrum, a constraint that needs to be borne in mind when interpreting the measurements (Alexander, 1998). Considerable thought will need to go into understanding forecast and observation "errors" under these conditions. In the tropical stratosphere, while conditions for a "semi-geostrophic" balance (which would include Kelvin waves) appear to exist, it seems likely that the flow is nevertheless highly imbalanced because of direct forcing of unbalanced motions.

## *New wind instruments*

There are two new wind instruments that promise to increase our knowledge of stratospheric winds in the near future. **P. Ingmann** discussed **ADM-Aeolus** (Stoffelen *et al.* 2005), which will be launched by the European Space Agency in 2008 to address the most important measurement need identified by WMO (2001): namely a global coverage of direct wind measurements. ADM-Aeolus will measure line-of-sight winds using an active optical system (lidar), and is focused on the troposphere. However, it now appears that it will be possible to obtain measurements up to 30 km, making these measurements of great interest for SPARC. As noted earlier, the use of ADM-Aeolus measurements will require the use of data assimilation to get information on the two horizontal wind components, a concept that was built into the instrument design from the outset.

The other stratospheric wind instrument is **SWIFT**, which has been approved for launch by the Canadian Space Agency in the 2010 time frame. SWIFT is a passive imager that will measure vector winds in the 20-50 km altitude range, and will thus not be dependent on data assimilation — although there is certainly great interest in the prospect of using SWIFT winds for assimilation, or at least validation. **A. Scott** presented the SWIFT instrument concept and its implementation on the proposed Chinook satellite, while **Y. Rochon** discussed its expected error characteristics. Assessing the potential value of measurements from a new satellite instrument is always a challenge. **C. McLandress** presented the results of simple calculations, using the Canadian Middle Atmosphere Model to provide a surrogate atmosphere, in order to determine the required measurement errors for SWIFT in order to meet its science goals (*e.g.* meridional residual circulation, zonal mean wind, amplitude and phase of equatorial planetary waves). An example is shown in Figure 7. The results show the expected dominant winter hemisphere branch of the poleward Brewer-Dobson circulation in the upper stratosphere, and the two-cell structure in the lower stratosphere. If the goal is to capture the dominant structure of the meridional transport, then at 20 km $\sigma$ = 3 m/s is optimal, $\sigma$ = 5 m/s is acceptable, and $\sigma$ = 10 m/s is unacceptable, while at 40 km $\sigma$ = 5 m/s is optimal and $\sigma$ = 10 m/s is acceptable. **W. Lahoz** described the results of a more sophisticated Observation System Simulation Experiment (OSSE) performed for ESA to assess the impact of SWIFT winds relative to the current operational suite of observations. Not surprisingly, the greatest impact was found to be in the tropics. Finally, **S. Pawson** briefly described some lessons learned from an OSSE performed by Ricky Rood's group at the NASA DAO for the SWIRLS instrument, which was proposed for EOS-B (eventually EOS-Aura) in the early 1990's, but then never flown (in part because of this OSSE). However, the problems in interpreting OSSE's were noted, because OSSE's are so dependent on the assimilation system used for the study and therefore may not be relevant to the real data when the instrument is actually flown.



There are also some prospects of observing winds in the mesosphere. This is of interest for data assimilation, now that several assimilation models include the mesosphere within their model domain. **W. Ward** discussed plans for a potential Canadian instrument called WaMI, and the possibility of an Atmospheric Dynamics Mission.

In a **discussion session**, the measurement requirements developed for SWIFT while it was being considered by ESA as a Stratospheric Dynamics mission were discussed (Table 1). Those requirements were developed on the basis of certain science goals. Other potential science goals for

| Target/threshold | Science goal |
|---|---|
| 3/5 (20-30 km)<br>5/10 (30-50 km) | Meridional wind |
| 5/10 | Zonal wind |
| 3/5 | Equatorial planetary wave amplitude |
| 5/10 | Equatorial planetary wave phase |
| 3/5 (20-30 km) | Ozone flux |
| 3/5 (20-30 km)<br>5/10 (30-50 km) | Residual circulation |

***Table 1****: Required horizontal wind component accuracies (1σ total error) for SWIFT (in m/s), as developed in the ESA Stratospheric Dynamics Mission Requirements Document.*

SWIFT were raised in the discussion. One was the possibility of assessing whether current analyses are adequate to reproduce the tracer distributions that are arising with new measurements during periods of rapid evolution in the polar vortex (*e.g.* sudden warmings). Another was characterization of the subtropical mesospheric jet, the bottom part of which would be seen by SWIFT. A third was the potential for providing a constraint on extratropical upper stratospheric temperature, which would help with the known AMSU bias problems. Finally, the question was raised (but not answered) as to whether there would be any value in complementary ground-based measurements.

## International Polar Year

The International Polar Year (IPY) refers to an extensive, multi-national, interdisciplinary period of observations covering the 2007 and 2008 calendar years. SPARC has prepared a proposal for participation in the IPY which was described in the Newsletter No. 25 (July 2005). SPARC's contribution is entitled "The structure and evolution of the stratospheric polar vortices during IPY and their links to the troposphere." The main idea is to document the dynamics, chemistry, transport and microphysical processes of polar vortices, highlighting the themes of ozone depletion, and the links between the stratosphere and troposphere and between the stratosphere and mesosphere. This is a step toward the ultimate goal of understanding the connection between the polar climate and the stratosphere. The proposal involves the coordination of satellite and ground-based campaigns, as well as specific initiatives to increase understanding of major features and processes. The SPARC Data Center will play an essential role in this effort by archiving key data.

Because the SPARC IPY proposal aims to document the current state of the stratosphere in the Arctic and Antarctic, data assimilation can play an important role in this effort. The IPY effort was discussed during the workshop and a number of recommendations were made. Firstly, the SPARC-DAWG will contribute to the overall SPARC proposal by archiving assimilation products from many centres and research groups for the 2007-8 period. The SPARC Data Center would be used as a repository for the collected products. The precise products and the participating centres and research groups will be identified in the coming months. In order to attract many participants, the products requested will have to be as flexible as possible. Thus they will likely be entirely at the discretion of the data provider. Other details such as data formats will be determined in collaboration with the SPARC Data Center. Such a repository of analyses and forecasts over the IPY year can serve as a resource for process-oriented studies of the polar regions. A second way that SPARC-DAWG proposes to assist the overall SPARC IPY activities is to consider how to combine multi-model assimilations into a probability density function. Just as an ensemble of model forecasts can be used to indicate forecast uncertainty, an ensemble of analyses may be able to indicate analysis uncertainty. At the very least, a range of possible states can be provided. The question is then whether value can be added by combining products in an objective way.

Besides the two activities outlined above, the discussion led to some recommendations for SPARC. Firstly, the group recommends gathering and archiving special purpose data sets for validation of assimilation products. This would be very helpful for participants who will provide assimilation products to be archived by SPARC. The DAWG also requests an attempt to define observation requirements for surface measurements relevant to data assimilation. Similarly, it would also be useful for assimilation if gaps in measurements (*e.g.* during the polar night) were identified, and then filled. What is the potential for *in situ* observations in this respect? Finally, the group would like to use IPY activities to argue for the extension of existing satellite measurements such as Odin, TIMED and SCISAT-1.

It will be important to link to other IPY activities related to this one. SPARC has endorsed the POLARCAT IPY proposal which deals with the impact of long range aerosol transport on climate through an examination of pollutant transport into and out of the Arctic. Another related activity is ORACLE-O3 which focuses on stratospheric ozone measurement and the processes leading to ozone loss. Because ORACLE-O3 does not include an assimilation activity thus far, the repository of analysis products created by SPARC IPY work could be of interest. Finally, WGNE has a polar vortex forecasting activity which may already have coordinated groups willing to contribute to the SPARC data repository.

## Other SPARC-DAWG activities

In the short term, the IPY will be the main focus for the DAWG. Nevertheless, a few other activities are planned for the coming year.

What has become very clear from analysis intercomparison exercises in the past (*e.g.* SPARC 2002) is that analyses differ from each other, especially in the middle atmosphere. Therefore, considerable caution must be taken when comparing modelling results or measurements to a single analysis. What is preferable is to plot several different analyses, to indicate the level of uncertainty in the analyses. Because many intercomparison studies have already been done, it would be useful for the climate research community to be able to easily access the results. Therefore, the DAWG plans to create a "clearing house" for intercomparison studies located on the SPARC Data Center website.

While the "clearing house" just described can serve the climate research community, what is needed for the middle atmosphere data assimilation community is the identification of a standard set of physically oriented diagnostics that can be used to validate assimilation products. **G. Manney** has agreed to help coordinate this activity, by providing appropriate diagnostics for polar processes. The Tropical Tropopause Layer (TTL) is another region where assimilation products can be improved. Relevant diagnostics for this region should assess water vapour, temperature, clouds, and diabatic heating rates. SPARC's CCMVal activity (see report this issue) has already identified many diagnostics for their model intercomparison exercise. Some of these diagnostics may also be useful for assimilated fields, and therefore the CCMVal diagnostics can serve as a starting point. At the same time, the DAWG can contribute to CCMVal by helping to assess the analyses used for some of the CCMVal diagnostics.

The presentations of Matsuo, Lieberman and Ortland reflect a growing interest in the estimation of the mesosphere and lower thermosphere. The SPARC Data Center will be used to add links to mesospheric measurements (pre-existing websites for the TIMED satellite mission and ground-based measurements, to start with). Similarly, the SPARC Data Center will provide a link to the website for the ASSET ozone intercomparison project described by Lahoz.

## Next meeting

The next SPARC-DA working group meeting will be held during the week of 18-22 September 2006 in Noordwijk, the Netherlands. As with this meeting, the goal is to focus on process-oriented evaluation of middle atmospheric (and upper tropospheric) analyses. For this, experts from outside the assimilation field are necessary, and will be invited to participate. The planned themes for the next meeting include transport errors on long time scales, and the tropical tropopause region. Both themes will highlight problems with assimilated fields in the tropics.


### *Acknowledgement*

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# Summary of the CCMVal 2005 Workshop on "Process-Oriented Validation of Coupled Chemistry-Climate Models"

## 17-20 October 2005, Boulder, USA

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### Introduction

The CCM Validation Activity for SPARC (CCMVal) is a response to the need for consistent evaluation and validation of coupled chemistry-climate models (CCMs) with detailed descriptions of the stratosphere, which have been developed over the last 5-10 years. These CCMs provide valuable indications of how stratospheric ozone will evolve in the future as halogen concentrations decline in an atmosphere with a changing climate (*e.g.* WMO, 2003). The high complexity of CCMs requires a systematic evaluation process in order to demonstrate that the models are representative of the atmosphere and to quantify the uncertainty of the model results.



The first CCMVal workshop was held in November 2003 in Grainau, Germany, to develop a more comprehensive approach to CCM validation. The concept was based on model intercomparisons of the dynamical-radiative state such as those within the GCM-Reality Intercomparison Project for SPARC (GRIPS) (Pawson *et al.*, 2000) and on an assessment of chemistry-climate models of the stratosphere (Austin *et al.*, 2003). The strategy developed was to identify the core processes that determine the stratospheric state and to select a number of diagnostics for each process within four main categories: dynamics, stratospheric transport, radiation, and stratospheric chemistry and microphysics. Processes associated with the Upper Troposphere/Lower Stratosphere (UTLS) were also included in these categories. A full description of the approach can be found in Eyring *et al.* (2005). An essential part of the strategy is that the diagnostics would evolve over time, *e.g.* as new data sets or approaches become available.

A second CCMVal workshop was held at the National Center for Atmospheric Research (NCAR), Boulder, USA, on 17 – 19 October 2005. The goals of the workshop were to assess the progress in the validation of CCMs following the guidelines developed in the first CCMVal workshop, and to assess how CCMs can support upcoming UNEP/WMO and IPCC Assessments. Approximately 90 members of the atmospheric and climate communities from Europe, the United States, Canada, Japan, and New Zealand attended the workshop to take stock of the progress and to identify near-term and long-term goals within the validation framework. The attendees included representatives from nearly all the major stratospheric CCM groups in the world. The agenda and a list of participants can be found at the workshop's website at http://www.pa.op.dlr.de/workshops/CCMVal2005/.

### Main points of discussion

The introductory session reviewed the context for the CCMVal activity, including WMO/UNEP and IPCC assessments, discussed related activities in the tropospheric climate modelling community, and emphasized the importance of understanding uncertainties in corroborative measurements.

The central part of the workshop consisted of oral and poster sessions on the progress made in the four main areas of CCMVal. The presentations and the accompanying discussions showed that (a) good progress was being made in the evaluation of CCMs since the first CCMVal workshop; (b) the evaluation needs to be more quantitative in the future; and (c) a more detailed description of the individual diagnostics is necessary in order to make the table of validation processes more practical, and to allow individual groups to perform the diagnostics themselves.

Some analyses compared the results of several models with observed quantities based on model data submitted to the CCMVal/SCOUT-O3 database at the British Atmospheric Data Centre (BADC), others were 'ad hoc' intercomparisons, while still other studies described evaluations of single models, often based on new diagnostics that they had developed. While all approaches have their merits, the advantages and need for a central data archive to allow consistent analyses between models was clearly identified during the meeting.

It is important to maximize the resources available to CCM groups. Most of the meeting was spent discussing how to ensure that CCMs can be evaluated better and more consistently in the future, given the finite resources available to the stratospheric CCM groups. Each diagnostic was considered in turn and most were refined considerably. This was done in a number of ways. In some cases precise descriptions of each diagnostic will be produced, specifying the method of calculation, the measurement set to be used for comparison, providing central software tools for more complicated diagnostics, *etc*. In others, particularly for the chemistry assessment, individuals volunteered to analyze data placed in the database.

The diagnostics were prioritized again according to whether they were considered to be: 1) *core*, 2) *important*, or 3) *useful*. A *core diagnostic* is considered to be proven, straightforward to calculate, and important for illuminating the model processes. An *important diagnostic* is important, but somewhat difficult to calculate or not well defined and requiring additional research. Finally, a *useful diagnostic* is well defined and of importance, but only complementary to the core diagnostics.

The *core*, *important*, and *useful* categorization of the diagnostics will be updated. This will allow for future diagnostics to be added to our current tables, and new diagnostics will be added that illuminate key model processes. In addition, current *important* and *useful* diagnostics will be re-evaluated in response to modelling and research results. In particular, considerable discussion was devoted at the workshop to two areas of great importance where further research is needed to define suitable core diagnostics: UTLS transport, and polar chemical ozone loss. These diagnostics are currently listed as *important* but it is expected that they will evolve into *core* diagnostics in the future. The up-to-date version of the CCMVal process table will be maintained on the CCMVal website (http://www.pa.op.dlr.de/CCMVal/).

## Future plans

Several aspects of future plans related to CCMVal activities were actively discussed. The plans relate to maintaining progress and awareness with CCMVal tasks, interacting with the broader atmospheric sciences and climate communities, and documenting the progress of CCMVal. The following were considered of high priority:

- *Presentations at international scientific meetings*. Presenting the results of model intercomparison activities is considered valuable for documenting the skill of CCMs and their improvements, for creating awareness of CCMVal activities and thereby entraining new participants, and for addressing the scientific understanding issues that have arisen in the model intercomparisons. Suggested meetings are those of the European Geophysical Union and the American Geophysical Union.

- *Documenting the progress of CCMVal*. Progress matrices will be set up to document the state of the evaluation of the listed diagnostics and the participation of individual CCM groups. Again, the up-to-date version of the progress matrices can be found at the CCMVal website.

- *Creating an Ensemble and Central Archive of CCM runs*. A central archive of CCM model runs for the 20th and 21st centuries which can be used to assess model performance and to support upcoming WMO/UNEP and IPCC assessments has been created as part of CCMVal and the European Integrated Project SCOUT-O3. In the future this archive will be made available to the community as an 'ensemble of opportunity'.

- *CCMVal 2007 Workshop*. A third CCMVal workshop is tentatively planned for 2007. The workshops have been very effective at bringing together climate modellers to discuss and plan evaluation and validation activities. The workshop goals at this early stage are: (i) show analysis of recent model results using CCMVal diagnostics, (ii) update CCMVal model diagnostics, (iii) review scientific results from the 2006 UNEP/WMO Scientific Assessment of Ozone Depletion, (iv) form an outline and a team to write a model evaluation report for SPARC, and (v) make recommendations for forcing scenarios that could support the expected 2010 UNEP/WMO assessment.

- *SPARC Report in 2008/2009*. A SPARC Report on CCMVal results was proposed for the 2008/2009 time period. The Report would be a comprehensive summary of the progress and results obtained from CCM intercomparisons and the use of CCMs in the ozone and climate assessment activities. The Report would document the CCMVal approach and discuss the table of processes and diagnostics that has been developed and used over a period of years since the inception of CCMVal. The Report would be peer-reviewed by the atmospheric sciences community.

In addition, the possibility of using some of the approaches developed for assessing climate models at PCMDI will be considered in order to make the evaluation more quantitative and to have a better understanding of the overall stratospheric CCM ensemble.

In summary, good progress was made during the second CCMVal workshop. Several people agreed to take the lead for specific diagnostics and analyses, and it is hoped that all CCM groups will have joined in the intercomparison by the next CCMVal workshop in 2007 so that a more quantitative evaluation will be reached. Participation in and comments on CCMVal are requested from the international community. For full details on CCMVal activities and contacts see http://www.pa.op.dlr.de/CCMVal/.


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# Imaging Gravity Waves in Lower Stratospheric AMSU-A Radiances

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## Introduction

Gravity waves drive important aspects of the global stratospheric circulation, climate and chemical state (*e.g.*, Fritts and Alexander, 2003; Alexander and Rosenlof, 2003; Mann *et al.* 2005), and thus are a focus area for SPARC. The satellite remote sensors and global models so crucial to increased understanding of larger-scale stratospheric dynamics have (until recently) lacked the necessary horizontal and vertical resolutions to resolve gravity waves and gravity wave breaking. As a result, the observational record on stratospheric gravity waves has relied mostly on suborbital observations at scattered locations around the globe. This has motivated several SPARC activities: *e.g.*, an initiative to record radiosonde data at higher resolution to resolve gravity wave motions better (Vincent, 2003; Wang and Geller, 2003), and field programmes to observe and understand gravity wave generation from deep convection (Hamilton *et al.* 2004). The inability of global models to fully resolve gravity wave dynamics has also led to SPARC-sponsored workshops aimed at improving sub-gridscale gravity wave parameterizations for these models (Hamilton, 2004), and GRIPS studies of the energy spectra of resolved dynamics in global models (Koshyk *et al.* 1999).



Advances in both computing power and remote-sensing technology are now yielding higher resolution global model fields and satellite data from the stratosphere that can explicitly resolve some of the long wavelength "outer scales" of the gravity wave spectrum (*e.g.* Hamilton *et al.* 1999; Wu *et al.* 2005). Here we provide a preliminary report on the gravity wave detection and imaging capabilities of the Advanced Microwave Sounding Unit's (AMSU-A) lower stratospheric temperature channels.

## Background and Motivation

The stratosphere contains a spectrum of many gravity waves which span a wide range of propagation directions and wavelengths. Those few remote-sensing instruments that have resolved gravity waves to date do so only at the very longest wavelength portions of this spectrum, and thus measure only a small fraction of the total wave variance. Furthermore, the "visibility" of waves to each instrument is generally a complex three-dimensional function of channel, orbit position, viewing direction and atmospheric location. To complicate matters further, the wavelengths of individual gravity waves also vary significantly *via* refraction by the background flow. Thus, different waves are constantly moving into and out of the narrow visibility windows of the instrument. Such effects have made these new gravity wave observations challenging to analyze and to compare with model predictions (Alexander, 1998; Jiang *et al.* 2004; Wu *et al.* 2005).

Furthermore, satellite gravity wave data acquired to date often resemble a global distribution of sub-orbital measurements, in the sense that they provide only a one-dimensional cross-section through three-dimensional wave fields. For example, some limb instruments yield vertical temperature profiles with superimposed wave oscillations that resemble a sequence of radiosonde profiles (Eckermann and Preusse, 1999; Tsuda *et al.* 2000). Others yield high-resolution measurements at a given altitude along the orbital track that contain wave fluctuations, similar to *in situ* aircraft data (Wu and Waters, 1996; Jiang *et al.* 2004).

We need new generations of satellite instruments that can improve upon these initial observations. Specifically, we seek data with well-defined visibility characteristics that permit meaningful physical interpretation of the wave signals, and that provide two-dimensional or even three-dimensional views of the wave fields.

## Advanced Microwave Sounding Unit-A

The Advanced Microwave Sounding Unit (AMSU) is a passive microwave scanner currently deployed on five different satellites: the NOAA 15 through 18 meteorological satellites (Kidder *et al.* 2000), and NASA's Earth Observation System (EOS) Aqua satellite (Lambrigtsen,

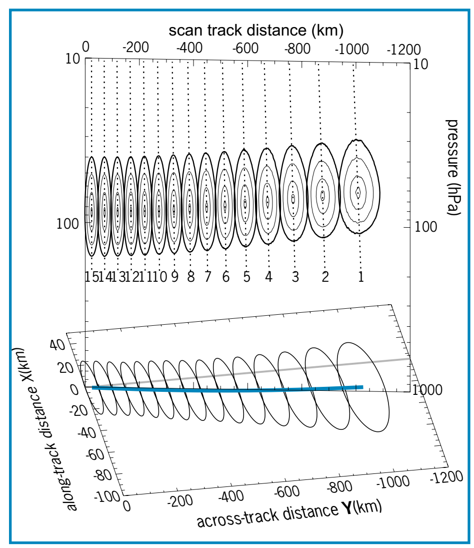


***Figure 1**: Two-dimensional cross-sections of modelled Channel 9 weighting functions, plotted versus pressure, cross-track distance Y and along-track distance X for beam positions j=1...15. Thick contours show half-power levels, which are projected to the surface to depict horizontal footprints. Other contours show the 70%, 90% and 99% levels. Dotted lines show line-of-sight ray paths from the peaks in each weighting function to the satellite.*

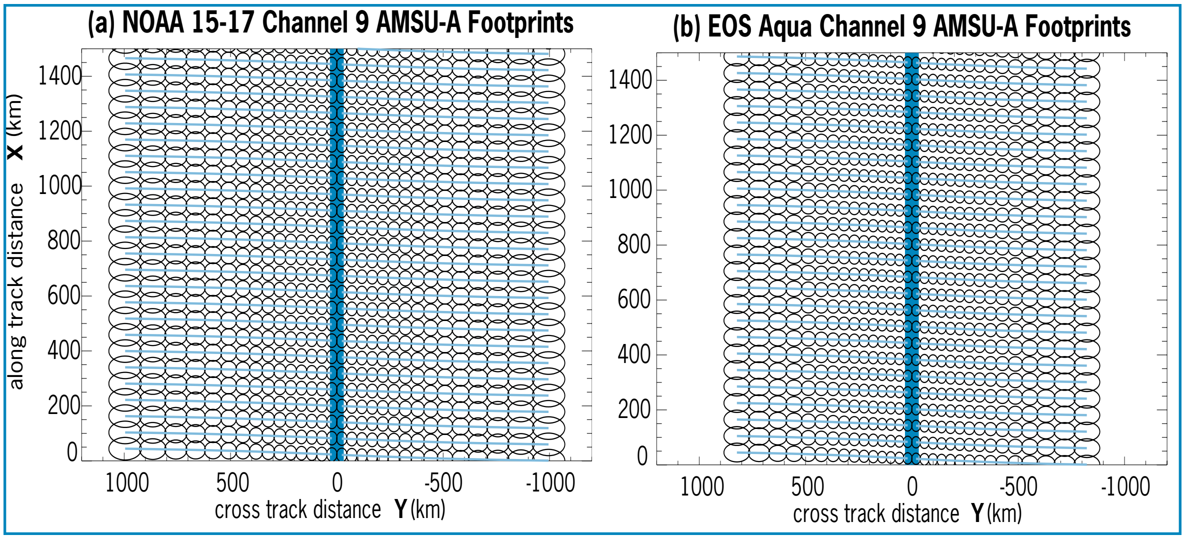


***Figure 2**: AMSU-A Channel 9 horizontal footprints traced out as a function of along-track and cross-track distances by the AMSU-A scanning measurements from (a) NOAA-15 through NOAA-18 satellites and (b) EOS Aqua. The dark blue line shows the satellite ground track, and the light blue lines show the scanning pattern from right-to-left across Y as the satellite moves along X, with footprints at each beam position j overlayed.*

2003). The instrument scans across the satellite track in 30 sequential step-and-stare measurements at equi-spaced, off-nadir scan angles between ±48.33°. The AMSU-A module has 15 measurement channels, 6 of which (Channels 9–14) are stratospheric temperature channels measuring $O_2$ wing line emissions centred at 57.29 GHz.

To model how gravity waves might appear in AMSU-A radiances, we've developed a simplified model of the AMSU-A radiance acquisition that yields three-dimensional temperature weighting functions, which we've validated against more detailed modelling results (see Wu (2004) and Eckermann and Wu (2005) for complete details). Figure 1 shows cross-sections of the derived Channel 9 weighting functions at 15 adjacent scan angles for the AMSU-A on the NOAA satellites. They show radiances from the near-nadir beams peaking at 80-90 hPa, while those at the largest scan angles peak higher at 60-70 hPa due to the limb effect (Goldberg *et al.* 2001). Figure 1 also shows the horizontal measurement footprints, specified by half-maximum contours of the weighting functions at the altitude of peak response. Figure 2a shows how the scanning pattern and the 7.4 km $s^{-1}$ velocity of the NOAA satellites maps these footprints into a pixelated two-dimensional radiance map with a cross-track width of 2100 km. The lower altitude orbit of EOS Aqua yields smaller footprints and cross-track swath widths (Figure 2b).

## Simple Forward Modelling

Each AMSU-A measurement yields a brightness temperature

$$T_B(X_j, Y_j) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{Z_{SAT}} W_j(X - X_j, Y - Y_j, Z) \, T(X, Y, Z) \, dX \, dY \, dZ \quad (1)$$

that characterizes the radiance *via* the Rayleigh-Jeans approximation to the Planck function. $T(X,Y,Z)$ is the atmospheric temperature field, $W(X,Y,Z)$ is the 3-D AMSU-A temperature weighting function, $Z$ is pressure height, $X$ and $Y$ are along-track and cross-track distances. To assess the instrument's ability to detect gravity waves, we specified infinite three-dimensional monochromatic gravity wave temperature oscillations

$$T'(X, Y, Z) = T_{PEAK} \cos(k_X X + k_Y Y + k_Z Z), \quad (2)$$

where $T_{PEAK}$ is the peak temperature amplitude. We varied the vertical wavelength $\lambda_Z = 2\pi/|k_Z|$, horizontal wavelength $\lambda_h = 2\pi/k_h$, and horizontal propagation angle $\phi$ with respect to the AMSU-A scan axes $(X,Y,Z)$, where $k_X = \pm 2 /\lambda_X = k_h \cos\phi$, $k_Y = \pm 2/\lambda_Y = k_h \sin\phi$, and $k_Z<0$. We then used (2) as the temperature field in (1) and evaluated this integral numerically at each measurement location $(X_j, Y_j)$ using realistic scanning patterns.

Figure 3 plots the resulting NOAA AMSU-A perturbation brightness temperatures $T'_B(X_j, Y_j)$ for a wave of $\lambda_h$ = 400 km and $\lambda_Z$=12 km, propagating in three different directions. The results are plotted as a normalized "visibility" $T'_B(X_j, Y_j)/T_{PEAK}$, and show peak values of ~13%. Thus, a gravity wave of this type with a peak temperature amplitude $T_{PEAK}$=5 K would yield oscillations in Channel 9 brightness temperatures of 0.65 K in amplitude, according to the model. Since nominal Channel 9 noise floors are 0.16 K (Lambrigtsen, 2003; Wu, 2004), this wave signal is (theoretically) large enough to appear in the measurements. Though the response is not always uniform across the swath and some distortion of wave phase lines is produced by limb effects (Eckermann and Wu, 2005), Figure 3 predicts that this wave is imaged horizontally by the radiance maps swept out by the AMSU-A scanning pattern.

## AMSU-A Measurements on 14 January 2003



Figure 4 (see colour plate V) plots perturbations in Channel 9 brightness temperatures, $T'_B(\hat{\lambda}_j, \hat{\phi}_j)$, acquired by AMSU-A during overpasses of Scandinavia by Aqua, NOAA-15, NOAA-16 and NOAA-17 on 14 January 2003. Here $(\hat{\lambda}_j, \hat{\phi}_j)$ are the longitudes and latitudes of the various measurement footprints. The perturbations were extracted from raw radiances by computing and then subtracting a large-scale radiance field (see Eckermann *et al.* 2005, for details).

At 0116 UTC and 0226 UTC, the perturbation maps are essentially featureless, with values near nominal noise floors. During the 0650 UTC NOAA-15 overpass, Figure 4c shows the first suggestions of a wave-like oscillation over southern Scandinavia (note the change in colour scale from ±0.3 K to ±0.6 K in the maps at this time). In subsequent AMSU-A overpasses at 1033 UTC, 1221 UTC and 1229 UTC, this oscillation grows in amplitude to a maximum of 0.9 K. In the final two measurements at 1641 UTC and 2023 UTC the amplitude weakens slightly, but also changes it's horizontal structure, acquiring a longer wavelength that is aligned differently and has a packet width that is noticeably more elongated in the along-phase direction.

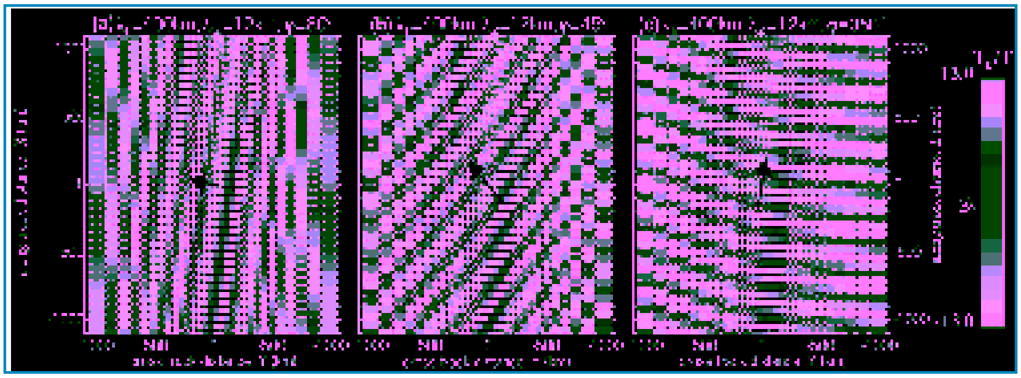

***Figure 3**: Relative brightness temperature perturbations (visibilities) $T'_B(X_j,Y_j)/T_{PEAK}$ resulting from model NOAA AMSU-A Channel 9 sampling of (2) with $\lambda_h$= 400 km, $\lambda_Z$= 12 km, and $\phi$ values of (a) 80°, (b) 45°, and (c) 350°. The white vector at the centre of each plot shows the direction of horizontal wave propagation $\phi$. The colour scale is visibility expressed as a percentage.*

## NWP Model Simulations

A three-dimensional description of the wave temperature field is needed to model the AMSU-A radiance signal. Thus we analyzed output from high-resolution numerical weather prediction (NWP) models that might resolve any wave induced temperature perturbations in the stratosphere over Scandinavia at this time. We used:

(a) archived 6 hourly operational forecast fields from the European Centre for Medium-Range Weather Forecasts (ECMWF) Integrated Forecast System (IFS) $T_L$511L60 global spectral model (Untch and Hortal, 2004).

(b) hourly hindcast fields from a developmental T239L60 version of the Navy Operational Global Atmospheric Prediction System (NOGAPS) global spectral forecast model with Advanced Level Physics and High Altitude (NOGAPS-ALPHA: Eckermann *et al.* 2004).

(c) hourly hindcast fields from a nested 10x10 $km^2$ hindcast run using the Naval Research Laboratory Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS®: Hodur, 1997).



All the model runs were initialized on 13 January 2003 at 1200 UTC. Further details are given in Eckermann *et al.* (2005). Each model run brought something unique to this study. For example, the high spatial resolution of the COAMPS fields was expected to be sufficient to model any waves AMSU-A might resolve, whereas the lower resolution NOGAPS-ALPHA and ECMWF IFS global fields were expected to resolve waves but underestimate their amplitudes (Skamarock, 2004). Yet unlike the global models, COAMPS could not produce output over the full geographical range of AMSU-A data plotted in Figure 4, nor does it extend to the middle and upper stratospheric altitudes.

The upper two rows of Figure 5 (see colour plate V) plot temperature perturbations $T'(\hat{\lambda},\hat{\phi}, p)$ at $p$ = 90 hPa extracted from the three NWP models' +24 hour forecast fields, valid at 1200 UTC on 14 January. They show a mountain wave oscillation over southern Scandinavia with a geographical extent and phase structure that resembles the 1200 UTC AMSU-A data in Figures 4e and 4f.

The bottom panels of Figure 5 show altitude cross-sections of the temperature fields along the horizontal black line plotted in the panels above. Each model produces a similar-looking mountain wave oscillation that grows in amplitude up to 10 hPa and beyond. The horizontal wavelength $\lambda_h$ is ~400 km and vertical wavelength $\lambda_Z$ is ~12 km.

## Conversion to Brightness Temperatures

We convert the NWP temperature fields into synthetic Channel 9 brightness temperatures $T_{B_{NWP}}(\hat{\lambda}_j, \hat{\phi}_j)$ by numerically evaluating equation (1) on the sphere using the actual AMSU-A scan patterns over Scandinavia, using the methods outlined by Eckermann *et al.* (2005). We then isolate brightness temperature perturbations $T'_{B_{NWP}}(\hat{\lambda}_j,\hat{\phi}_j)$ using exactly the same data reduction algorithms that we applied to the radiance data to produce Figure 4.

Figure 6 (see colour plate VI) plots the resulting $T'_{B_{NWP}}(\hat{\lambda}_j, \hat{\phi}_j)$ fields using the 1200 UTC NWP fields profiled in Figure 5, based on the 1221 UTC NOAA-16 and 1229 UTC EOS Aqua overpass scans, whose data are reproduced in the far right panels. All three NWP models reproduce a wave oscillation over southern Scandinavia with similar amplitude, phase and wave packet structures to those measured by AMSU-A. Figure 7 (see colour plate VI) plots $T'_{B_{NWP}}(\hat{\lambda}_j, \hat{\phi}_j)$ maps based on the closest hourly NOGAPS-ALPHA fields to each corresponding measurement in Figure 4. The structure in each panel of Figure 7 resembles that seen in the AMSU-A data in Figure 4, especially the evolution of the resolved wave pattern from 0700 UTC to 2000 UTC, though amplitudes in Figure 7 are somewhat weaker. Corresponding maps using COAMPS temperatures (not shown) yield larger amplitudes that are closer to the observations.

## Summary and Outlook

These comparisons prove that the radiance perturbations extracted from the AMSU-A Channel 9 measurements in Figure 4 are stratospheric gravity waves, and they validate our model predictions of the anticipated radiance signals based on our derived weighting functions. This work supports preliminary experimental studies by Wu (2004) and Wu and Zhang (2004) who found apparent gravity wave oscillations in radiances from AMSU-A's stratospheric channels.

The comparisons also show that the global ECMWF IFS and NOGAPS-ALPHA NWP models explicitly resolve the gravity wave observed over Scandinavia on 14 January 2003, though they underpredict its amplitude. Based on each global model's horizontal resolution, this $\lambda_h$~400 km wave is expected to suffer some amplitude attenuation from the effects of scale-dependent numerical dissipation operating on the smallest resolved scales (Skamarock, 2004). Further comparisons like these, among gravity wave fields explicitly resolved by models and satellite instruments should help to improve our understanding and description of stratospheric gravity wave dynamics.

The modelling results also suggest that other current and future cross-track scanners that have resolutions comparable to or better than AMSU-A should be able to resolve and image stratospheric gravity waves too. Examples on the microwave side are the Special Sensor Microwave Imager/Sounder

(SSMIS) on the Defense Meteorological Satellite Program (DMSP) satellite, and the Advanced Technology Microwave Sounder (ATMS) and Conical Scanning Microwave Imager/Sounder (CMIS) slated to fly on the National Polar-orbiting Operational Environmental Satellite System (NPOESS). Another interesting example is the Advanced Infrared Sounder (AIRS), which operates in co-manifested form with AMSU-A on EOS Aqua with a scan pattern of 90 sequential step-and-stare measurements and horizontal footprint diameters three times smaller than AMSU-A. These properties should allow AIRS to image smaller horizontal wavelength gravity waves than AMSU-A. As preliminary proof of its gravity wave detection capabilites, Figure 8 (see colour plate VII) plots perturbations in AIRS infrared radiances near 80 hPa from the EOS Aqua 1229 UTC overpass, showing a very similar wave structure to that imaged by AMSU-A in Figure 4f.

### *Acknowledgements*

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# EOS Aura Mission - One Year of Operations

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## Introduction

Aura (Latin for breeze, formerly EOS CHEM), the last of the large EOS observatories, was launched on July 15, 2004 and has now been operating for over a year. Aura is designed to make comprehensive stratospheric and tropospheric composition measurements from its four instruments, HIRDLS, MLS, OMI and TES. All of the instruments are performing well, although HIRDLS will only deliver data products along one scan position. Aura flies in formation about 15 minutes behind Aqua. The Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) and Cloudsat, to be launched together, hopefully in late fall 2005, (Stephens *et al.*, 2002) will fly a few minutes behind Aqua. The "A-train" includes this group of satellites, the CNES PARASOL satellite which was launched in December 2004, and the ESSP Orbiting Carbon Observatory (OCO), scheduled for launch in 2008. The measurements from Aura will be within 30 minutes of these other platforms. The A-Train can be thought of as an extended satellite system focusing on climate change.



Figure 1 shows the Aura spacecraft and its four instruments (Table 1): the High Resolution Dynamics Limb Sounder (HIRDLS), the Microwave Limb Sounder (MLS), the Ozone Monitoring Instrument (OMI) and the Tropospheric Emission Spectrometer (TES). These instruments were selected because of their complementary measurements, their technological heritage, and the new capabilities they bring to measuring the Earth's atmosphere. Figure 2 graphically shows the vertical range of the various Aura measurements and the instrument that provides them.

## Science Objectives of the Aura Mission

The objective of the Aura mission is to address three principal science questions:

1) Is the ozone layer changing as expected?
2) What are the processes that control tropospheric pollutants?
3) What are the roles of upper tropospheric aerosols, water vapour and ozone in climate change?

The strategy Aura will employ in answering these questions is to obtain a comprehensive set of chemical observations at high vertical and horizontal resolution throughout the atmosphere (see Table 1 for details). These measurements, when combined with measurements from field campaigns, other satellite measurements (*e.g.* Aqua measurements that are made 15 minutes ahead of Aura on roughly the same ground track), and ground-based instrument data, should provide unprecedented insights into the chemical and dynamical processes associated with our atmosphere.

## Spacecraft and Instrument descriptions

The Aura spacecraft is designed for a life of five years with an operational goal of six years. The spacecraft is in an ascending sun-synchronous orbit (98° inclination) at 705 km with an equator-crossing time of 13:45 ±15 minutes. Aura limb instruments were designed to observe roughly along the orbit plane, however, due to an anomaly (discussed below) HIRDLS observations will be off to the side of the Aura ground track. MLS is on the front of the spacecraft (the forward velocity direction) while HIRDLS, TES and OMI are mounted on the nadir side. HIRDLS and TES make limb soundings observing backward while MLS will make limb soundings observing forward. OMI and TES make nadir soundings as shown in Figure 3. The advantage of this instrument configuration is that MLS, OMI and TES would observe the same air mass within minutes.

### *HIRDLS*

HIRDLS is a 21 channel infrared limb-scanning filter radiometer designed to make the measurements listed in Table 1 (Gille *et al.*, 2003). HIRDLS can also determine the altitude of polar stratospheric clouds and tropospheric cloud tops.

The HIRDLS instrument has a long heritage extending back to Nimbus-6, and was designed to obtain profiles over the entire globe, including the poles, both day and night. Complete Earth coverage (including polar night) could be obtained in 12 hours. HIRDLS was designed to achieve high horizontal resolution using commandable azimuth scans which, in conjunction with a rapid elevation scan, would provide

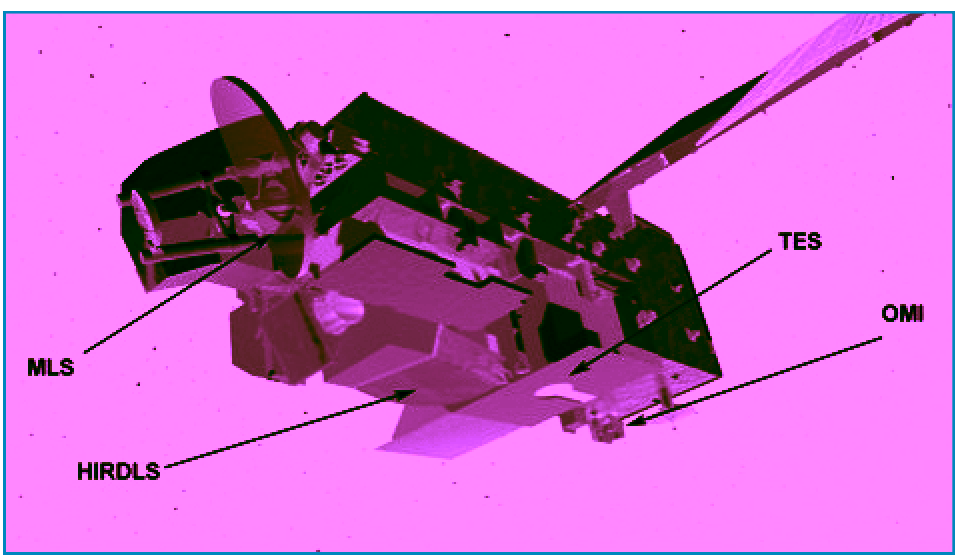


***Figure 1**: A model of the Aura spacecraft showing the location of the four instruments, HIRDLS, MLS, OMI and TES.*

*__Table 1__: Aura Instruments and Measurements.*

| Acronym | Name | Instrument PI | Constituent | Instrument Description |
|---|---|---|---|---|
| HIRDLS | High Resolution Dynamics Limb Sounder | John Gille, National Center for Atmospheric Research & U. of Colorado;<br>John Barnett, Oxford University | Profiles of T , $O_3$, $H_2O$, $CH_4$, $N_2O$, $NO_2$, $HNO_3$, $N_2O_5$, $CF_3Cl$, $CF_2Cl_2$, $ClONO_2$,<br>Aerosols | Limb IR filter radiometer from 6.2μ to 17.76μ<br>1.2 km vertical resolution up to 50 km. |
| MLS | Microwave Limb Sounder | Joe Waters, Jet Propulsion Laboratory | Profiles of T, $H_2O$, $O_3$, ClO, BrO, HCl, OH, $HO_2$, $HNO_3$, HCN, $N_2O$, CO, cloud ice. | Microwave limb sounder<br>118 GHz to 2.5 THz<br>1.5-3 km vertical resolution |
| OMI | Ozone Monitoring Instrument | Pieternel Levelt, KNMI, Netherlands | Column $O_3$, $SO_2$, aerosols, $NO_2$, BrO, OClO, HCHO, cloud top pressure, $O_3$ profiles, UV-B. | Hyperspectral nadir imager, 114° FOV, 270-500 nm, 13x24 km footprint for ozone and aerosols |
| TES | Tropospheric Emission Spectrometer | Reinhard Beer, Mike Gunson, Jet Propulsion Laboratory | Profiles of T, $O_3$, $NO_2$, CO, $HNO_3$, $CH_4$, $H_2O$. | Limb (to 34 km) and nadir IR Fourier transform spectrometer 3.2-15.4μ<br>Nadir footprint 5.3x8.5 km, limb 2.3 km |

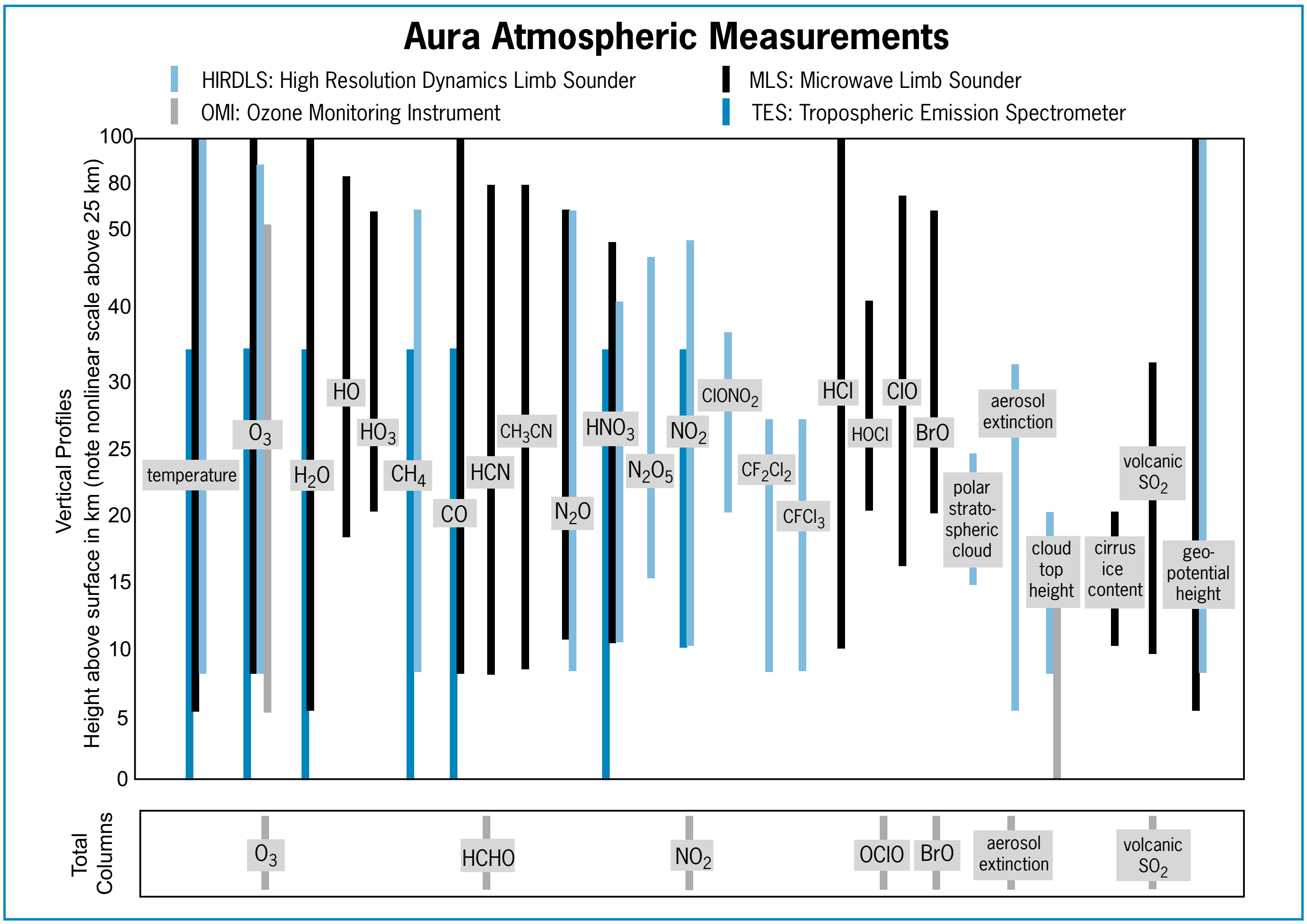


*__Figure 2:__ A graphical representation of the various Aura instrument measurements and their height range based on pre-launch design. For HIRDLS, post launch capability is being demonstrated, and 50 km is expected to be the upper limit of the measurements. Column measurements are indicated in the lower part of the figure.*

profiles up to 3,000 km apart in an across-track swath. The primary design advantage of HIRDLS over previous infrared limb instruments (LIMS, SAMS, ISAMS, CLAES) was its high vertical and horizontal resolution that extends from the upper troposphere throughout the stratosphere.

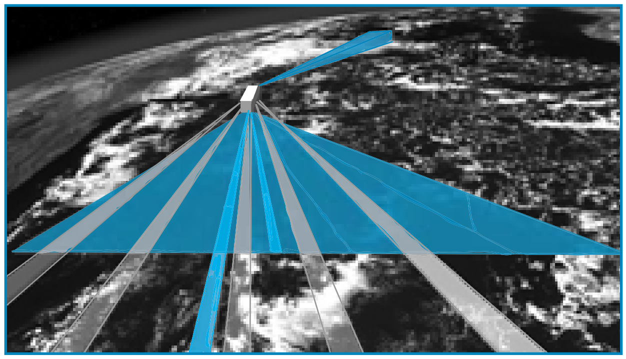

***Figure 3**: Aura instrument fields of view are shown as coloured beams. The viewer is looking at the back of the spacecraft. MLS performs forward limb sounding dark blue). OMI nadir measurements are indicated with the blue swath. TES limb and nadir measurements are shown in cyan. HIRDLS originally planned measurements (5 scan positions) are shown in gray. TES and HIRDLS measurements are made in the anti-velocity direction. Because of the Kapton® blocking the HIRDLS optical system, HIRDLS will only be able to make measurements in the lighter gray scan position on the far right.*

*Current status*: After launch, activation of the HIRDLS instrument immediately revealed that something was blocking the optical path so that only a small portion of the aperture could view the Earth's atmosphere. Studies of the engineering model suggested that a piece of thermal blanketing material ruptured from the back of the instrument during the explosive decompression of launch. This material covers most of the scan mirror. Attempts to remove this material by moving the scan mirror failed. However, even with the 80% blockage, measurements at high vertical resolution can still be made at one scan angle. As of this writing, the HIRDLS principal investigators have demonstrated high vertical resolution retrievals of temperature and ozone and they believe that they can retrieve most of the other constituents as planned. HIRDLS will no longer have its designed horizontal coverage, and with only one side of the aperture available, HIRDLS will not be able to make measurements over the Antarctic.

## *MLS*

MLS uses microwave emission to measure stratospheric temperature and constituents, and upper tropospheric constituents (Table 1) (Waters *et al.*, 1999, Waters *et al.*, 2006). MLS also has a unique capability to measure upper tropospheric water vapour in the presence of tropical cirrus, and the cirrus ice content. Aura MLS continues the successful effort of UARS MLS (Waters *et al.*, 1993) using advanced technology to provide new measurements. These measurements will be especially valuable for diagnosing the potential for severe loss of Arctic ozone during the critical period when abundances of stratospheric chlorine will still be high, and slight cooling of the stratosphere could exacerbate ozone loss due to chlorine chemistry. MLS is making the first global stratospheric measurements of OH and $HO_2$, constituents that play an important role in stratospheric chemistry. The MLS instrument observes in spectral bands centred near five frequencies: 118 GHz (temperature and pressure); 190 GHz ($H_2O$, $HNO_3$); 240 GHz ($O_3$ and CO); 640 GHz, ($N_2O$, HCl, ClO, HOCl, BrO, $HO_2$, and $SO_2$); and 2.5 THz (primarily for OH).

The MLS instrument aboard UARS has demonstrated the MLS capability of measuring upper tropospheric water vapour profiles (Read *et al.*, 1995; Sandor *et al.*, 1998), knowledge of which is essential for understanding climate variability and global warming but which previously has been extremely difficult to observe reliably on a global scale. MLS is unique in its ability to provide these measurements in the presence of tropical cirrus, where important processes affecting climate variability occur. MLS also provides unique measurements of cirrus ice content. The simultaneous MLS measurements of upper tropospheric water vapour, ice content, and temperature, under all conditions and with good vertical resolution, will be of great value for improving our understanding of large scale meteorological systems (such as El Niño) affecting the distribution of atmospheric water, climate variability, and tropospheric-stratospheric exchange. The simultaneous measurements of dynamical tracers CO and $N_2O$ enhance the value of this data set by helping identify stratospheric or tropospheric source regions of the air masses being observed.

*Current status*: The MLS instrument was turned on shortly after launch because there is no requirement for outgassing, and the MLS team was able to produce data within 15 days of launch. Figure 4 (see colour plate VII) shows the tropical water vapour "tape recorder" (see Mote *et al.*, 1996) as seen by MLS. The instrument has shown no problems and is operating flawlessly.

## *OMI*

The OMI instrument is a contribution of the Netherlands's Agency for Aerospace Programmes (NIVR) in collaboration with the Finnish Meteorological Institute (FMI) to the EOS Aura mission. OMI will continue the TOMS record for total ozone and other atmospheric parameters related to ozone chemistry and climate (Levelt, 2006). OMI measurements will be highly synergistic with measurements from the other instruments on the EOS Aura platform. The OMI instrument employs hyperspectral imaging in a "push-broom" mode to observe solar backscatter radiation in the visible and ultraviolet. The Earth will be viewed in 740 wavelength bands along the satellite track with a swath large enough to provide global coverage in 14 orbits (1 day). The nominal 13 x 24 km spatial resolution can be zoomed to 13 x 13 km for detecting and tracking urban-scale pollution sources. The hyperspectral capabilities will improve the accuracy and precision of the total ozone amounts and will also allow for accurate radiometric and wavelength self-calibration over the long term. Aside from the measurements listed in Table 1, the OMI instrument will distinguish between aerosol types, such as smoke, dust, and sulfates, and can measure cloud pressure and coverage, which provide data to derive tropospheric ozone. A combination of algorithms including TOMS version 7, Differential Optical Absorption Spectroscopy (DOAS), hyperspectral BUV retrievals and forward modelling will be used to extract the various OMI data products.

*Current status*: After an outgassing and cool down period, OMI began to produce data in October 2004. Figure 5 (see colour plate VII) shows an $NO_2$ map produced by the OMI science team. Additional discussion of the OMI instrument is given by Levelt *et al.* (2006).

### *TES*

TES is a high-resolution infrared-imaging Fourier transform spectrometer with spectral coverage of 3.2 to 15.4 $\mu$m at a spectral resolution of 0.025 $cm^{-1}$, thus offering line-width-limited discrimination of essentially all radiatively active molecular species in the Earth's lower atmosphere (Beer *et al.*, 2006). TES has significantly higher spectral resolution than the AIRS instrument aboard EOS Aqua. TES was designed with the capability to make both limb and nadir observations. In the limb mode, TES has a height resolution of 2.3 km, with coverage from 0 to 34 km. In the down-looking modes, TES has a spatial resolution of 0.53 x 5.3 km with a swath of 5.3 x 8.5 km. TES is a pointable instrument and can access any target within 45° of the local vertical, or produce regional transects up to 885 km length without any gaps in coverage. TES employs both the natural thermal emission of the surface and atmosphere and reflected sunlight, thereby providing day-night coverage anywhere on the globe. TES operates in a combination of limb and nadir mode (called global survey mode) every other scan. On alternate days, TES does special observations including "step-and-stare" mode and assessment of special targets like volcanoes. In the global survey mode, TES will provide global measurements of tropospheric ozone and its photochemical precursors such as the other measurements listed in Table 1.

Because TES retrieves the entire spectrum from 3.2 to 15.4 µm, the opportunity exists to make measurements of a large number of other gases (*i. e.* ammonia and organics). Although the retrieval of these gases will be done in a research mode, the existence of this capability provides a resource for the tropospheric chemistry community.

*Current status*: After launch, TES went through a lengthy outgassing procedure to minimize the ice build up on the detectors. Initial results from TES are shown in Figure 6 (see colour plate VII). After seven months of operation, the translator mechanism (which moves the reflecting surfaces of the spectrometer) began to show signs of bearing wear. The TES Instrument Team commanded the instrument to skip the limb sounding modes in May 2005. This will increase the bearing life of the translator and the life of the instrument. In any event, both HIRDLS and MLS provide limb measurement products redundant to TES. Further information on the TES instrument can be found in Beer (2006).

### *Validation*

Aura scientists along with the stratospheric and tropospheric measurement community are currently engaging in an extensive validation programme. This programme includes aircraft missions (one in 2004, two in 2005, two planned for 2006 and one planned for 2007), high altitude balloon launches, additional ground-based measurements and additional sonde launches. The validation programme will continue through 2008. Aura has also developed the Aura Validation Data Center (AVDC) that facilitates the exchange of data and provides instrument field of view predictions for the validation programme. Our first validation workshop was held on September 9, 2005 and presentations can be found on the AVDC website.

### *Data Release*

Aura data is being released through the Langley (TES) and Goddard (MLS, OMI, HIRDLS) Distributed Active Archive Centers. Nearly all MLS data is publicly available, but data users should carefully read the MLS data users guide. OMI data products will be provisionally released in stages from late 2005 to mid-2006. TES tropospheric data products are scheduled for public release in mid-2006. HIRDLS data will be released in mid-2006.

## Summary

The EOS Aura mission was successfully launched on July 15, 2004. With the exception of HIRDLS, all of the instruments are functioning as designed, although to preserve instrument life, TES is now operating only in the nadir mode. Aura will provide the next level of measurements needed by the stratospheric and tropospheric community to advance the science and to answer the crucial questions: Is the stratospheric ozone layer recovering? How is the chemistry of the troposphere changing? What are the roles of upper tropospheric aerosols, water vapour and ozone in climate change? Although there are only four instruments on Aura, they will provide the needed sets of measurements to answer these broad questions. Furthermore, the breadth of these instrument capabilities will allow us to use Aura data to attack future science questions.

For more information on the Aura platform and instruments, please refer to the website http://aura.gsfc.nasa.gov. Other websites of interest include :
Aura Validation Data Center (AVDC) : http://avdc.gsfc.nasa.gov
Aqua : http://aqua.nasa.gov
CALIPSO : http://www-calipso.larc.nasa.gov
CloudSat : http://cloudsat.atmos.colostate.edu
CNES PARASOL : http://smsc.cnes.fr/PARASOL/GP_mission.htm
OCO : http://oco.jpl.nasa.gov

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# A Highlight of the First-Year Aura MLS Observations

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Since its launch in July 2004, the Aura MLS (Microwave Limb Sounder) has been working perfectly and providing new insights on dynamics in the upper troposphere and lower stratosphere (UT/LS). This report highlights some interesting features revealed in the first-year MLS observations (Version 1.5 data).

UARS MLS and HALOE data show that water vapour entering the tropical LS continues to rise as a result of the Brewer-Dobson circulation, producing the so-called tape-recorder effect (Mote *et al.*, 1998). The Aura MLS provides greatly improved sensitivity and sampling in the UT/LS region such that not only the tape-recorder effect is captured, but other important transport processes can be observed. In particular, the Aura MLS $H_2O$ exhibits a somewhat different morphology from UARS observations at 100 hPa. As shown in Figure 1 (see colour plate VIII), a large amount of $H_2O$ entering the tropical LS during the summer monsoon season (June-September), is transported to higher latitudes in the subsequent months. This gradual poleward transport is not evident in the UARS MLS and HALOE data, but appears quite clearly in the Aura MLS data. The poleward transport is evident in both hemispheres but shows a slight asymmetry about the equator. The mid-latitude mixing, such as that produced by cut-off anticyclones, plays an important role in the transport of $H_2O$ at 100 hPa from the subtropics to mid-latitudes during the period from June to September. As shown in Figure 2 (see colour plate VIII), the summer jet divides tropospheric and stratospheric air quite well in most of the 20°N-60°N latitude zone, producing overall anti-correlated CO and $O_3$ distributions at 100 hPa. South of the jet, however, the anticyclone tends to blur the barrier by mixing high $H_2O$ concentration values to mid- and high latitudes, and high $O_3$ concentration values from high latitudes to the subtropics.

The gradual poleward transport following the Asian summer monsoon can be explained using the Stratosphere-Troposphere Exchange framework outlined in Holton *et al.* (1995). Parcels of air entering the "middle world", which are likely to maintain their entry mixing ratio water vapour because of the warmer temperatures there, will be spread poleward by the "extratropical pump"; part of the downward control mechanism of the Brewer Dobson circulation. By January, when the tropics is largely dehydrated at 100 hPa, $H_2O$ is abundant at mid- and high latitudes. At this time, the subtropical jet acts as a transport barrier, preventing high-latitude $H_2O$ from entering the subtropics until the next monsoon season. In summary, the features observed in Aura MLS $H_2O$, $O_3$ and CO are consistent with the STE scheme in Holton *et al.* (1995), although detailed data validation and model calculations are yet to be carried out in the future to quantify transport and mixing processes in the extratropical UT/LS.



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# The Assessment of Stratospheric Aerosol Properties

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The SPARC's Assessment of Stratospheric Aerosol Properties (ASAP) (see SPARC Newsletter No. 24, July 2004) has been completed and the associated SPARC Report will appear ***in early 2006 as SPARC Report No.4, and will be available in printed form and by download from the SPARC web site***. In the past, stratospheric aerosols have only been integrated into assessments in the context of their effects on ozone chemistry, and have not been critically evaluated themselves. Thus, the objective of this first effort was to perform a systematic analysis of the state of knowledge of stratospheric aerosols. It includes an examination of precursor concentrations and trends, measurements of stratospheric aerosol properties, trends in those properties, and modelling their formation, transport, and distribution under both background and volcanically perturbed conditions.

The ASAP Report covers this material in 350 pages with 150 Figures. In addition, data comprising the basis for the analysis are archived in the ASAP Data Archive at the SPARC Data Center (http://www.sparc.sunysb.edu/) including altitude/latitude gridded fields of aerosol extinction and derived quantities such as surface area densities, and a 'gap-filled' data set for the period 1979 through 2004 based on the SAGE record, which should be of particular interest for future modelling work.

## Excerpt from the ASAP Executive summary:

### *Key Findings*

- **The vast bulk of existing aerosol data does not comprise a complete measurement set and, as a result, many parameters required for scientific or intercomparison purposes are derived indirectly from the base measurements**. This is true for space-based measurements where only bulk extinction is measured but is also true in degree for most ground-based and *in situ* systems. Unlike gas species, aerosol cannot be characterized by a single quantity but has a size distribution and variable composition. The fact that each system measures a different set of parameters greatly complicates almost every stage of measurement comparisons, accentuating the need for aerosol models.

- **Disagreements between the various data sets and models indicate that significant questions remain regarding the ability to characterize stratospheric aerosol during volcanically quiescent periods, particularly in the lower stratosphere**. Space-based and *in situ* measurements of aerosol parameters tend to be consistent following significant volcanic events like El Chichón and Pinatubo. However, during periods of very low aerosol loading, this consistency breaks down and significant differences exist between systems for key parameters including aerosol surface area density and extinction. Comparisons of models and satellite observations of aerosol extinction are generally fairly good at visible wavelengths above the 20-25 km altitude region under non-volcanic conditions, but are less satisfactory for infrared wavelengths. Although integrated aerosol quantities such as surface area density and effective radius can be calculated without approximation from a known size distribution, the satellite and *in situ* observational bases for size distributions are controlled by *a priori* assumptions regarding the distribution itself or by having coarse size resolution, respectively. During volcanically quiescent periods, models and observations disagree significantly mainly due to the fraction of the surface area density produced by models residing in particles too small to be measured, especially near nucleation regions. While there are some model short-comings relative to observations particularly in the lower stratosphere, it seems likely that space-based data sets underestimate, perhaps significantly, aerosol surface area density in the lower stratosphere.

- **The analysis of non-volcanic stratospheric aerosol, although hampered by very limited periods without volcanic influence since systematic measurements began, indicates no long-term trend**. Since the beginning of systematic stratospheric aerosol measurements in the early 1970s there have been three periods with little or no volcanic perturbation, although only the period from 1999 onwards can be confidently identified as free of volcanic aerosols. The other periods (late 1970s and late 1980s) are difficult to evaluate, given their brevity and the complex variability observed. In particular, the period in the late 1980s seems likely to have not reached a stable non-volcanic level. Trends derived from six long-term data sets for the late 1970s to the current period are not significantly different from zero.

- **The dominant stratospheric aerosol precursor gases are OCS and $SO_2$ and, through $SO_2$, human-related activities may influence the observed background stratospheric aerosol**. There is general agreement between measured OCS and modelling of its transformation to sulfate aerosol, and observed aerosols. However, there is a significant dearth of $SO_2$ measurements, and the role of tropospheric $SO_2$ in the stratospheric aerosol budget, while significant, remains a matter of some guesswork. In addition, it is not well understood whether decreasing global, human-derived $SO_2$ emissions, or increasing emissions in low latitude developing countries, such as China, dominate the human component of $SO_2$ transport across the tropical tropopause.

## *Recommendations*

- **The importance of stratospheric aerosol in climate and atmospheric chemistry strongly supports a commitment to continuing both space-based and *in situ* observations of aerosols into the foreseeable future**. Both types of measurements are necessary because neither approach seems likely to independently produce a robust depiction of global, stratospheric aerosol properties.

- **Observations of $SO_2$ in the upper troposphere and lower stratosphere and of $H_2SO_4$ and $SO_2$ in the middle and upper stratosphere would be extremely valuable to improve our modelling and predictive capabilities of stratospheric aerosol**. Currently, there is a general scarcity of measurements of key sulfur-bearing gases during their transport from the upper troposphere into the upper stratosphere.

- **A more complete understanding of the detailed structure of the underlying aerosol size distribution is required to facilitate improvement in the closure between measurement data sets and confidence in derived properties like surface area density**. This is becoming increasingly important as measurement systems change and robust conversion between data sets is required to maintain data sets amenable to trend analysis. It is also important to improve aerosol size distribution and composition knowledge in the vicinity of the tropical tropopause where such information is crucial input to microphysical models of stratospheric aerosol. In addition, aerosols in the upper troposphere are not composed purely of $H_2SO_4/H_2O$ but include organics (up to 50 % by mass), mineral dust, soot, and other compounds. Organics are also found in stratospheric aerosols in small quantities. Since the role of non-sulfate aerosols in serving as sites for chemical reactions and as condensation nuclei with concomitant effects on the stratospheric aerosol is not well known, measurements focused on these aerosols are desirable.

- **The upper troposphere and lower stratosphere, particularly, in the tropics is a crucial region for understanding stratospheric aerosol and warrants detailed scientific investigation**. Sensitivity studies in this report show that the lower stratospheric aerosol layer is strongly dependent on input from the tropical upper troposphere.

- **Future modelling studies should strive to include important but as yet missing or poorly treated elements, such as upper tropospheric and meteoritic particles, and various relevant chemical and dynamical processes**. The stratospheric aerosol could be quite sensitive to aerosol input through the tropical tropopause, as suggested in the present report. Also, meteoritic material descending into the stratosphere from the mesosphere may be important to the morphology of stratospheric aerosols, particularly in polar air and perhaps globally. Chemically, in particular the photolysis of sulfuric acid affecting the upper edge of the aerosol layer especially in the polar regions should be included in the models. In addition, a more robust 3-D representation of transport and cloud processes is required to reproduce aerosol observations in the troposphere-stratosphere transition region, as well as to face the challenge of reproducing the seasonal variability of aerosols.

# Future SPARC and SPARC-related Meetings

## 2006

**January 9-12:** **Chapman Conference on Jets and Annular Structures in Geophysical Fluids**, Savannah, Georgia, USA (http://www.agu.org/meetings/cc06acall.html)

**January 7-11:** **The routes for organics oxidation in the atmosphere and its implications to the atmosphere (Workshop)**, Alpe d'Huez, France

**January 29-February 2: 86th AMS Annual Meeting**, Atlanta, Georgia
The Jim Holton Symposium
18th Conference on Climate Variability and Change,
10th Symposium on Integrated Observing and Assimilation Systems for Atmosphere, Oceans and Land Surface (IOAS-AOLS)
(http://www.ametsoc.org/meet/annual/index.html)

**April 2-7 :** **EGU General Assembly**, Vienna, Austria (http://meetings.copernicus.org/egu2006/index.html)

**May 23-26:** **AGU Joint Assembly**, Baltimore, USA (http://www.agu.org/meetings/ja06/)

**May 29-June 1:** **40th Annual CMOS Congress**, Toronto, Canada (http://www.cmos2006.ca)
Special SPARC Session

**June 12-15:** **Modelling of Deep Convection and its Role in the Tropical Tropopause Layer SPARC-GEWEX/GCSS-IGAC Workshop**, Victoria, Canada

**16-23 July:** **36th COSPAR Scientific Assembly and Associated Events,** Beijing, China (http://www.cospar2006.org)






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