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11 workshop

**Atmospheric Science from Space using
Fourier Transform Spectrometry**

**Bad Wildbad (Black Forest), Germany
8th to 10th of October 2003**

**Programme
Abstracts
List of Participants**

Programme

Wednesday, 8 October 2003

Programmatic Session

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| 09:00-09:30 | O-P-1 | Reinhard Beer, California Institute of Technology, Pasadena, USA
The EOS AURA tropospheric emission spectrometer (TES) |
| 09:30-10:00 | O-P-2 | Herbert Fischer, Forschungszentrum Karlsruhe, Germany
The MIPAS/ENVISAT experiment: Status and results |
| 10:00-10:30 | O-P-3 | Claude Camy-Peyret, Université Pierre et Marie Curie, Paris, France
IASI status (tbc) |
| 10:30-11:00 | | Coffee break |
| 11:00-11:30 | O-P-4 | Haruhisa Shimoda, Earth Observation Res. Center, NASDA, Japan
Greenhouse gas measuring instrument for GOSAT |
| 11:30-12:00 | O-P-5 | Jean-Marie Flaud, Johannes Orphal, Université Paris-Sud, Orsay, France
The Geostationary Fourier Imaging Spectrometer (GeoFIS) as part of the Geostationary Tropospheric Pollution Explorer (GeoTROPE) mission: Objectives and capabilities |
| 12:00-12:30 | O-P-6 | Markus Melf, EADS Astrium GmbH, Germany
AMIPAS – concepts and technologies for an advanced MIPAS instrument |
| 12:30-13:00 | | Discussion |
| 13:00-14:30 | | Lunch break |

Calibration Session

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| 14:30-14:50 | O-II-1 | Manfred Birk, German Aerospace Center (DLR), Germany
Radiometric characterisation of MIPAS/ENVISAT |
| 14:50-15:10 | O-II-2 | Helen Worden, Jet Propulsion Laboratory, USA
Calibration and characterization of the tropospheric emission spectrometer |
| 15:10-15:30 | | Discussion |
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| 16:00-18:30 | | Poster session |
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Thursday, 9 October 2003

Programmatic Session

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The atmospheric chemistry experiment (ACE): mission overview

Retrieval Techniques Session

09:30-09:50 **O-I-1** **Marco Ridolfi, University of Bologna, Italy**
MIPAS-ENVISAT measurements:
Study of the trade-off between accuracy and horizontal resolution

09:50-10:10 **O-I-2** **Juliette Hadji-Lazaro, University of Paris, France**
Operational retrieval of trace gases concentrations from IASI spectra

10:10-10:30 **O-I-3** **Tatsuya Yokota, Nat. Inst. For Environmental Studies, Japan**
Preliminary study on a nadir looking SWIR FTS of GOSAT project to monitor CO₂ column density from space

10:30-11:00 Coffee break

11:00-11:20 **O-I-4** **Christopher Boone, University of Waterloo, Canada**
Analysis of the atmospheric chemistry experiment FTS spectra

11:20-11:40 **O-I-5** **Helen Worden, Jet Propulsion Laboratory, Pasadena, USA**
Characterization of AURA-TES (Tropospheric Emission Spectrometer) NADIR and LIMB Retrievals

11:40-12:10 Discussion

12:10-13:45 Lunch break

Spectroscopy Session

13:45-14:05 **O-I-6** **Prasad Varanasi, State University of New York at Stony Brook, USA**
The Current Status of the Infrared Spectroscopic Database Applicable to ASSFTS

14:05-14:25 **O-I-7** **Shephard A. Clough, Atmospheric and Environmental Research Inc., USA**
A New Water Vapor Continuum Model: MT_CKD_1.0

14:25-14:45 **O-I-8** **Richard A. Tipping, University of Alabama, USA**
Recent progress in the theoretical calculation of continuum absorptions

14:45-15:15 Discussion

15:15-15:45 Coffee break

15:45-18:45 **Poster session**

19:00 Conference Dinner

Friday, 10 October 2003

MIPAS

- 09:00-09:20 **O-III-1** **Thomas von Clarmann, Forschungszentrum Karlsruhe, Germany**
Retrieval of temp. and pointing information from MIPAS limb emission spectra
- 09:20-09:40 **O-III-2** **Piera Raspollini, IFAC of the National Research Council, Italy**
MIPAS LEVEL 2 near real time processor performance
- 09:40-10:00 **O-III-3** **Vivienne Payne, University of Oxford, England**
Analysis of monthly mean profiles of water vapour and methane from MIPAS
- 10:00-10:20 **O-III-4** **Michael Höpfner, Forschungszentrum Karlsruhe, Germany**
MIPAS measurements of ClONO₂ and polar stratospheric clouds during the Antarctic vortex split in September 2002
- 10:20-10:50 Coffee break
- 10:50-11:10 **O-III-5** **Bernd Funke, Instituto de Astrofísica de Andalucía (CSIC), Spain**
Non-LTE retrieval of NO, NO₂, and CO from MIPAS-ENVISAT
- 11:10-11:30 **O-III-6** **Chiara Piccolo, University of Oxford, England**
Oxford retrievals of MIPAS data during the 2002 Antarctic winter
- 11:30-11:50 **O-III-7** **Martine De Mazière, Belgian Institute for Aeronomy, Brussels, Belgium**
Validation of MIPAS operational LEVEL 2 products using ground-based network data
- 11:50-12:45 Discussion, next meeting

End of workshop

Abstracts

Abbreviations

O = Oral

P = Programmatic

I = Retrieval

II = Calibration/Validation

III = MIPAS

O-P-1

The EOS AURA TROPOSPHERIC EMISSION SPECTROMETER (TES)

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The Tropospheric Emission Spectrometer (TES) is a high-resolution infrared Fourier Transform spectrometer that operates in both limb and nadir viewing modes for the investigation of the physics and chemistry of the Earth's lower atmosphere.

TES is currently being integrated onto the AURA spacecraft in readiness for launch into Sun-synchronous polar orbit early in 2004.

The talk will focus on pre-delivery system tests and calibrations as they impact the expected on-orbit performance.

O-P-2

The MIPAS/ENVISAT experiment: status and results

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Abstract not available

O-P-3

IASI status (tbc)

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Greenhouse gas measuring instrument for GOSAT

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The mission of GOSAT (former GCOM-A1) is to clarify sources and sinks of CO₂ in sub-continental scales. The first candidate sensor to satisfy this mission was SOFIS (Solar Occultation Fourier Interferometric Sounder: ILAS follow on). SOFIS can measure stratospheric and upper tropospheric (higher than 5km) CO₂ in 1% accuracy.

However, analyses using inverse atmospheric transport model revealed that those data, which will be provided from SOFIS, are not sufficient to increase the accuracy of continental scale sources and sinks, because of the uncertainty incidental to transport models. The candidate sensor to satisfy the mission discussed were, 1) Fabry-Perot near IR spectrometer which measures the sun glint of water surfaces, 2) Near IR spectrometer which measures land surface scattering and 3) Thermal IR FTS. The conclusion of was as follows.

- 1) Recommend a sensor which covers from near IR to thermal infrared using FTS.
- 2) It should cover O₂-A band, 1.6 μ m and 2.0 μ m CO₂ lines, and CO₂, CO and CH₄ lines in thermal infrared.
- 3) The spectral resolution should be 0.1 - 0.2 cm⁻¹.
- 4) The signal to noise ratio should be 100 - 300.
- 5) IFOV should be 5 - 8km.

The detailed specifications of this sensor would be specified until Mar. 2004. In addition to the core sensor, one more sensor will be on-board GOSAT. It is called SWIFT, which will be provided by ESA (European Space Agency) and CSA (Canadian Space Agency). SWIFT (Stratospheric Wind Interferometer For Transport studies) measures stratospheric winds by observing Doppler shift of ozone absorption line near 9 μ m using Fourier transform spectrometer.

The Geostationary Fourier Imaging Spectrometer (GeoFIS) as part of the Geostationary Tropospheric Pollution Explorer (GeoTROPE) mission: Objectives and capabilities

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One of the major challenges facing atmospheric sciences is to assess, understand and quantify the impact of natural and anthropogenic pollution on air quality on Earth at a local, regional and continental scale. In the troposphere the characteristic time of chemical processes, of source strengths and of the dynamics induce important short term, i.e. sub-hourly, variations, and significant horizontal and vertical variability of constituents and geophysical parameters. To study tropospheric composition and processes it is therefore required to link diurnal with seasonal and annual timescales, as well as local with regional and continental spatial scales, by performing sub-hourly measurements at appropriate horizontal and vertical resolution. Tropospheric observations from low-Earth orbit (LEO) platforms have already demonstrated the potential of detecting constituents relevant for air quality but they are limited by the daily revisit time and local cloud cover statistics. The net result is that from LEO the troposphere is significantly under-sampled. In fact measurements from Geostationary Orbit (GEO) limit the observation to half hemisphere but offer the only practical approach to the observation of diurnal variation from space with the pertinent horizontal resolution. As a consequence the Geostationary Tropospheric Pollution Explorer (GeoTroPE) mission has been proposed. It consists of two instruments: The Geostationary Fourier Imaging Spectrometer (GeoFIS) covering the thermal infrared (TIR) and the Geostationary Scanning Imaging Absorption spectrometer for atmospheric cartography (GeoSCIA) covering the ultraviolet-visible (UV-VIS) and short-wave-infrared (SWIR) regions. Indeed the simultaneous measurements of the thermal emission in the TIR (which provides also night time measurements) and of the backscattered radiation in the UV-VIS-SWIR lead to an optimal combination as far as the relevant species, the vertical resolutions, the time scales, are concerned. This talk is dedicated, both to the scientific objectives and capabilities, and to the technical description of the GeoFIS instrument which is an imaging Fourier-transform spectrometer using large focal-plane arrays as detectors.

AMIPAS – concepts and technologies for an advanced MIPAS instrument

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For the Future Atmospheric Chemistry Sensors, Astrium investigated on behalf of ESA a Phase A-study of an Advanced MIPAS (AMIPAS) including a limb-viewing IR cloud imager (LCI) instrument concept in support of AMIPAS product quality. The required task focussed on the investigation of concepts for new generation sensors, encompassing configuration, system, subsystems and assemblies.

This activity was initiated by ESA following a recommendation of the Earth Sciences Advisory Committee to continue scientific studies on candidate Earth Explorer Atmospheric Chemistry missions. The need for an IR limb sounder working in the medium infrared built on the heritage of MIPAS for the sake of continuity was identified because chemistry missions may become relevant during the next years in the frame of the ESA's Earth watch programme.

The reduction of the costs compared to the ACECHEM mission was the keystone of the revision of the requirements for the AMIPAS instrument. The outcome of the study is a compact instrument which would be well suited also for a small satellite platform. The instrument concept is based on a single port dual slide imaging Michelson interferometer. In the course of the study the conceptual design was derived for an instrument with higher spatial resolution and reduced spectral demands with respect to the MIPAS instrument on ENVISAT. It was shown that the requirements given by ESA can be met with a very compact, simple and thus cost effective design.

This paper will address the outcome of the AMIPAS concept design, including the preliminary architecture and the expected radiometric and geometric performances.

Radiometric characterisation of MIPAS/ENVISAT

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MIPAS on ENVISAT was investigated regarding radiometric accuracy. Commissioning phase in-flight measurements of the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) FT-spectrometer on ENVISAT (ENVironmental SATellite) were analysed with a dedicated IDL tool.

This included FT instrument characterisation as well as parts of level 1b processing, both independent from the nominal ESA data processing and in-flight characterisation. At the present state of analysis MIPAS was found to operate close to the physical sensitivity limit with radiometric errors not exceeding the specifications which, however, are not very demanding.

The presentation will focus on detector non-linearity, micro- vibrations in the interferometer, and pointing jitter.

Calibration and characterization of the tropospheric emission spectrometer

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Prior to shipment of the Tropospheric Emission Spectrometer (TES) to the AURA spacecraft in late April, 2003, the instrument was put through an extensive series of thermal vacuum tests, over an 8-month period, to characterize and calibrate the instrument performance.

During these tests, measurements were made to characterize the field-of-view, radiometric and spectral performance of the instrument. The measurements were highly successful in for quantifying key instrument parameters and also permitted the characterization of many unexpected, but important instrument features. This presentation will describe the measurements and results of the TES pre-flight calibration.

The atmospheric chemistry experiment (ACE): mission overview

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The ACE mission goals are:

- (1) to measure and to understand the chemical and dynamical processes that control the distribution of ozone in the upper troposphere and stratosphere, with a particular emphasis on the Arctic region;
- (2) to explore the relationship between atmospheric chemistry and climate change;
- (3) to study the effects of biomass burning in the free troposphere;
- (4) to measure aerosol number density, size distribution and composition in order to reduce the uncertainties in their effects on the global energy balance.

ACE will make a comprehensive set of simultaneous measurements of trace gases, thin clouds, aerosols, and temperature by solar occultation from a satellite in low earth orbit. A high inclination (74 degrees) low earth orbit (650 km) will give ACE coverage of tropical, mid-latitudes and polar regions. The solar occultation advantages are high sensitivity and self-calibration.

A high-resolution (0.02 cm^{-1}) infrared Fourier Transform Spectrometer (FTS) operating from 2 to 13 microns ($750\text{-}4100\text{ cm}^{-1}$) will measure the vertical distribution of trace gases, and the meteorological variables of temperature and pressure. The ACE concept is derived from the now-retired ATMOS FTS instrument, which flew on the Space Shuttle in 1985, 1992, 1993, 1994.

Climate-chemistry coupling may lead to the formation of an Arctic ozone hole. ACE will provide high quality data to confront these model predictions and will monitor polar chemistry as chlorine levels decline. The ACE-FTS can measure water vapor and HDO in the tropical tropopause region to study dehydration and strat-trop exchange. The molecular signatures of massive forest fires will be evident in the ACE infrared spectra. The CO_2 in our spectra can be used to either retrieve atmospheric pressure or (if the instrument pointing knowledge proves to be satisfactory) for an independent retrieval of a CO_2 profile for carbon cycle science.

Aerosols and clouds will be monitored using the extinction of solar radiation at 0.525 and 1.02 microns as measured by two filtered imagers as well as by their infrared spectra. A dual spectrograph called MAESTRO has been added to the mission to extend the wavelength coverage to the 280-1000 nm spectral region. The broad-band atmospheric extinction measured with high signal-to-noise ratio by MAESTRO is particularly useful for the derivation of aerosol

and cloud physical properties. The PI for the MAESTRO instrument is T. McElroy from the Meteorological Service of Canada (MSC).

ACE is unique in that MAESTRO, the ACE-FTS and the imagers all share the same suntracker and make simultaneous measurements of the same scene. The FTS and imagers have been built by ABB-Bomem in Quebec City, while the satellite bus has been made by Bristol Aerospace in Winnipeg. ACE was selected in the Canadian Space Agency's SCISAT-1 program, and was successfully launched by NASA on August 12, 2003 for a 2 year mission. The main international partners for ACE are NASA, for the launch and algorithm work at NASA-Langley, and Belgium/ESA, for the CMOS imaging arrays and scientific support.

MIPAS-ENVISAT measurements: Study of the trade-off between accuracy and horizontal resolution

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MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is a mid-infrared emission limb-scanning spectrometer operating, since March 1st, 2002, onboard the ESA's ENVironmental SATellite. Common features of limb-scanning experiments are both high vertical resolution and poor horizontal resolution. In this paper we exploit the 2-dimensional retrieval approach developed in M. Carlotti, M. Dinelli, P. Raspollini, M. Ridolfi, "Geo-fit approach to the analysis of satellite limb-scanning measurements", *Appl. Opt.*, **40**, No. 12, 1872-1875, (2001) to investigate the possibility of improving the horizontal resolution of MIPAS measurements.

Two different strategies are considered for this purpose: the first one exploiting the possibility (offered by the Geo-fit analysis method) of an arbitrary definition of the retrieval grid; the second one is based on the possibility to degrade the spectral resolution of the MIPAS interferometer. The performances of the two strategies are compared in terms of the trade-off between the attained horizontal resolution and the retrieval accuracy. We find that, for some target species, it is possible to improve (double) the nominal horizontal resolution of MIPAS measurements while maintaining a good retrieval accuracy.

Operational retrieval of trace gases concentrations from IASI spectra

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The IASI (Infrared Atmospheric Sounding Interferometer) instrument will be launched in 2005 aboard the European satellite MetOp. It is designed to provide temperature and water vapor vertical profiles for operational meteorology. From spectra measured by IASI, it is also possible to retrieve concentrations of several trace gases for chemistry and climate studies.

In the framework of the preparation of the IASI mission, we develop an inversion algorithm based on neural network techniques to estimate columns of ozone (O₃), methane (CH₄), and carbon monoxide (CO) from the spectra. The first version of this algorithm is implemented by EUMETSAT in the EPS (EUMETSAT Polar System) ground segment.

The inversion algorithm is a transfer function between IASI Level 1 radiances and Level 2 temperatures on the one hand, and column values on the other hand. The neural architecture chosen is the multi-layer feedforward network which allows the modelisation of non-linear functions. The algorithm is presented together with its performance on simulations sets.

The algorithm sensitivity is characterized and the inversion errors are estimated using Rodger's classical formalisms.

The trace gas inversion algorithm was applied to the analysis of spectra provided by the IMG (Interferometric Monitor for Greenhouse gases) instrument that was carried aboard the Japanese satellite ADEOS and provided about eight months of data between November 1996 and June 1997. The CO, O₃ and CH₄ distributions are compared with available independent data: ground based, sondes, and satellite measurements.

Preliminary study on a nadir looking SWIR FTS of GOSAT project to monitor CO₂ column density from space

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It is planned that Greenhouse gases Observing Satellite (GOSAT) of Japan will be launched in 2007. GOSAT will mount a sensor to monitor CO₂ column density globally. These data measured by a GOSAT sensor and ground-based monitoring station data will be used into an atmospheric transport inverse model to identify source/sink distribution of CO₂ in a sub-continental scale. The Committee for GOSAT Project Research Promotion has recommended to adopt a nadir looking FTS, which covers Short Wavelength Infrared (SWIR) region, as one of the practicable candidates of the instruments to measure column density of CO₂. National Institute for Environmental Studies (NIES) has just started preliminary researches on CO₂ sensitivity analysis, error analyses, data retrieval algorithm study, ground-based/air-borne validation strategy, and a plan of inverse model study.

The SWIR FTS will measure 1.6 micrometer and 2.0 micrometer spectral regions to monitor CO₂, H₂O and aerosols. An oxygen A-band in 0.76 micrometer region will be also measured to monitor air mass and to identify cloud effects. The 1.64 micrometer absorption band of CH₄ would be possibly used to estimate methane column abundance, too.

This presentation will report the latest research status on the nadir looking SWIR FTS, especially on the error source identification, error analysis, estimation of albedo variation effects in one FTS scanning with a movement of the FOV on spectra. A validation experiment plan by of an air-borne nadir looking SWIR FTS will also be shown.

Analysis of the atmospheric chemistry experiment FTS spectra

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SciSat-1, also known as the Atmospheric Chemistry Experiment (ACE), is a satellite mission for remote sensing of the Earth's atmosphere. The mission is the first in a planned series of small science satellites to be flown by the Canadian Space Agency. The primary measurement technique to be used for ACE is solar occultation, with the measurements extending from 10 to 100 km in altitude. The main focus for the mission is the study of Arctic ozone.

The instrument suite on board ACE consists of a high resolution (0.02 cm^{-1} unapodized resolution) Fourier Transform Spectrometer (FTS) operating in the infrared ($750 - 4100\text{ cm}^{-1}$), a UV/Visible spectrometer operating between 0.3 and 1.0 microns with resolution 1 to 2 nm, a pair of filtered imagers (one measuring at 0.525 microns and the other at 1.02 microns) taking snapshots of the sun, a suntracker to keep the instruments pointed at the sun, and a startracker to provide information on satellite orientation.

The SciSat-1 satellite was successfully launched into the target orbit (altitude 650 km, inclination 74 degrees) on August 12th, 2003. Following early orbit activities, the commissioning of the satellite bus and science instruments began and will continue through September and possibly into early October 2003. Science measurements from the SciSat-1 satellite await the completion of these commission activities.

Science calibration and testing of the ACE instruments took place February through March 2003 at the University of Toronto. Results of this test campaign relating to the analysis of ACE-FTS data will be described.

Analysis software for the ACE mission makes use of a global fit type approach for the processing of FTS measurements, employing non-linear least squares fitting of the occultation spectra. Two analysis approaches have been developed, one for the case of good pointing knowledge from the satellite and one for the case of poor pointing knowledge. The decision of which approach to use awaits assessment of the quality of pointing information available from the satellite.

If occultation measurements from the SciSat-1 satellite are available in time, early spectra and results will be shown. Otherwise, examples will be shown for the processing of ATMOS spectra. ATMOS (the Atmospheric Trace MOlecule Spectroscopy experiment) was flown by NASA four times on space shuttle missions, and it featured an FTS taking measurements in the solar occultation configuration.

Characterization of AURA-TES (Tropospheric Emission Spectrometer) NADIR and LIMB Retrievals

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The TES Level 2 algorithm retrieves vertical profiles of atmospheric temperature and trace gases from radiometrically calibrated measured spectra. The retrieval is based on minimizing the difference between a measured spectrum and a model spectrum, which is calculated for an estimated atmospheric state. This minimization is subject to smoothness constraints imposed on the atmospheric profiles being retrieved and is applied iteratively using a non-linear least squares solver.

Algorithm descriptions and simulation results are presented. Simulations of the data acquired by TES along different orbit tracks were generated in order to test the TES nadir and limb retrieval algorithms for different spatial and temporal (seasonal and day/night) regimes. Noise added to simulated radiances is representative of the noise measured during TES instrument calibration. Retrieval results, including error analysis and expected vertical resolution, are shown for both the nadir and limb viewing modes of TES.

The Current Status of the Infrared Spectroscopic Database Applicable to ASSFTS

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Since its inception as a useful compilation of molecular spectroscopic parameters needed in the detection of plume signatures in the atmosphere, the *AFCRL* compilation by McClatchey et al (1973), the line list has been an indispensable tool for the laboratory spectroscopist as well as the atmospheric scientist. What began as a modest venture by a few engaging practical molecular spectroscopists as Benedict and Kaplan, among others, in the 1960's has since evolved into *HITRAN-2002*, the globally popular spectroscopic database developed by Rothman et al (2002). Despite its growing pains this indispensable catalog, along with its many clones such as *GEISA*, has now become the major archive of not only molecular spectroscopic parameters for the entire gamut of wavelengths of interest to the atmospheric scientist but also of aerosols and other constituents of the atmosphere.

The evolution of the database is a reflection of the internationally coordinated effort that was invested into expanding and improving the database through carefully conceived and performed laboratory experiments, which were aided by the state-of-the-art improvements made in the spectroscopic tools, and advanced theoretical studies that were much aided by the advent of the computer age. The improvement in the database, however meritorious, over the past four decades is but a mere drop in the vast ocean of atmospheric spectroscopy.

Much still needs to be done and known in order to properly assess atmospheric transmission of shortwave and longwave radiation. While many of the important spectral lines have been assigned reasonably accurately and their intensities determined along with their dependence upon temperature, the segment of the database devoted to line broadening parameters is hardly adequate. The parameterization of the variation of the air-broadened half-widths, air-induced shifts, and shapes of spectral lines is available only for a few lines of a few molecules. The temperature- and pressure- dependent absorption cross-sections of many greenhouse gases whose spectra cannot be resolved have begun to be reported only recently.

Proper understanding of and parameterization of continua is a continuing challenge, replete with controversial methodologies. Recently "discovered" enhanced shortwave absorption by the atmosphere has spawned many a theory including that of "anomalous" absorption by known absorbers and unmeasured absorption by unknown molecular complexes. This presentation ventures to comment on the current status of the database and to identify the outstanding problems in atmospheric transmission spectroscopy.

A New Water Vapor Continuum Model: MT_CKD_1.0

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For the first time since its inception, a new formulation for the CKD approach to the water vapor continuum has been generated. This new version is designated MT_CKD_1.0. The original CKD formulation, derived in 1980 based upon laboratory measurements due to Burch and collaborators, applied an empirically derived multiplicative factor (different for the self and foreign continua) to the line wing of the impact line shape. This resulted in a line shape that was super-Lorentzian in the near and intermediate line wings and exhibited sub-Lorentzian behavior in the far wings. The self and foreign line shapes were consistently applied to all lines from the microwave to the shortwave, which, when summed, produced the coefficients for the original CKD_0 self and foreign continuum models. This formulation of the CKD continuum was consistent with the interpretation that the water vapor continuum was due to the intermediate and far wings of allowed transitions of the water vapor monomer. In the years since the generation of CKD_0, the continuum coefficients in certain spectral regions have been modified due to new continuum measurements, but the generating functions for the continuum have never been equivalently adjusted.

This poster presents the features of the recently released water vapor continuum model MT_CKD_1.0, which utilizes a new formulation of the continuum and is based on the most highly regarded measurements of continuum coefficients, both field- and laboratory-based. The model's formulation is of a different functional form than the CKD formulation, with the contribution from each spectral line being the sum of two terms: a) a sub-Lorentzian line shape, the product of the impact line shape and a function with values less than unity; and b) a small, broad additional line shape that provides the needed super-Lorentzian absorption in the intermediate line wings. The MT_CKD_1.0 formulation is consistent with the interpretation that the water vapor continuum is due to two distinct effects, the far wings of allowed transitions (dominant in between water vapor bands) and collision-induced absorption (dominant within bands) resulting from the generation of a short-lived dipole moment due to the collision.

Also presented will be a discussion of recent validations of the modifications to the carbon dioxide line shape and associated continuum recently incorporated into the MT_CKD continuum model.

Recent progress in the theoretical calculation of continuum absorptions

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Recent progress in the theoretical calculation of the water continuum, for both the self- and foreign-continua in the 8-12 micron infrared window and for the foreign-continuum in the millimeter wave region, will be presented.

The theoretical results will be compared with laboratory measurements and with empirical continua. Collision-induced absorptions for N₂-N₂, N₂-O₂ and O₂-O₂ in the translation-rotation and the fundamental vibration-rotation regions have been calculated, and the absorptions can easily be obtained for any temperature of interest. Because there are no experimental measurements for N₂-O₂ pairs in the far infrared, the theoretical calculations can supplement the results available for N₂-N₂ that are implemented in many radiative transfer codes. For air, the O₂-O₂ absorption is very small, but the N₂-O₂ absorption increases the N₂-N₂ absorption by 35% or more, depending on the frequency and temperature.

Finally, results for the collision-induced absorption, arising from transient dipole-induced dipoles during the collision of H₂O and N₂ pairs, have been made. Below 2500 cm⁻¹, these absorptions are negligible compared with the foreign-continuum. Our results are in disagreement with the latest MT-CKD empirical formulation, in which it is claimed that collision-induced absorption is responsible for much of the absorption within the bands.

Retrieval of temperature and pointing information from MIPAS limb emission spectra

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Retrieval of abundances of atmospheric species from limb infrared emission spectra requires accurate knowledge of the pointing of the instrument in terms of elevation, as well as temperature and pressure profiles. An optimal estimation-based method is presented to infer these quantities from measured spectra. The successful and efficient joint retrieval of these largely correlated quantities depends strongly on the proper selection of the retrieval space, the selection of spectral microwindows and the choice of reasonable constraints which force the solution to be stable. The proposed strategy was applied to limb emission spectra recorded with the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) onboard the ENVISAT research satellite in order to validate the instrument pointing information based on the satellite's orbit and attitude control system which uses star tracker information as a reference.

Both systematic and periodic pointing calibration errors were detected, which meanwhile have been corrected to a major part. Furthermore occasional pitch jumps were detected, which could be assigned to parameter uploads to the satellite's orbit and attitude control system. It has been shown that in general it is justified to assume local thermodynamic equilibrium below 60 km for these purposes. The retrieval method presented has been proven to be suitable for independent monitoring of MIPAS line-of-sight pointing.

MIPAS LEVEL 2 near real time processor performance

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Starting from the end of March 2002, MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is measuring atmospheric middle-infrared limb-emission spectra from the sun-synchronous, nearly-polar orbit ENVISAT satellite.

The limb-emission measurements are acquired continuously during both day and night, providing a 3-dimensional, almost global, map of the atmospheric emission every 24 hours. From the inversion of the spectra measured by MIPAS it is possible to infer the spatial distribution of many atmospheric constituents.

The processing steps necessary for the inversion of MIPAS measurements constitute the so called "Level 2 data analysis". The algorithm for Level 2 near real-time analysis of MIPAS spectra was developed by an international consortium of scientists supported by the European Space Agency (ESA) and was implemented in the ENVISAT Payload Data Segment. This code is designed to provide, in an automated and continuous mode, atmospheric vertical profiles of temperature, pressure and concentration of six key species: O₃, H₂O, CH₄, HNO₃, N₂O and NO₂, in the range 6-68 km.

The performances of both the instrument and the Level 2 algorithm were tested and validated during the MIPAS commissioning phase. Recently some modifications were implemented in the retrieval code, leading to an improvement of the accuracy of MIPAS data products. These improvements are being assessed by means of intercomparison of MIPAS products with external measurements. In this paper we will show examples of MIPAS products and will report an updated assessment of MIPAS performances.

Analysis of monthly mean profiles of water vapour and methane from MIPAS

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Water vapour and methane are two of the species retrieved operationally from the MIPAS instrument on the European Space Agency's ENVISAT satellite.

Methane oxidation is the main source of water vapour in the stratosphere. The oxidation of methane produces approximately two molecules of water vapour for each destroyed methane molecule. The quantity $\text{H}_2\text{O} + 2\text{CH}_4$ is therefore expected to be reasonably constant with altitude in the lower stratosphere, providing a useful internal validation test.

Monthly mean profiles of water vapour, methane and the quantity $\text{H}_2\text{O} + 2\text{CH}_4$ have been calculated for one year's worth of MIPAS data. The profiles have been separated into six latitude bands and the results compared with climatology.

MIPAS measurements of ClONO₂ and polar stratospheric clouds during the Antarctic vortex split in September 2002

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During end of September 2002 the Antarctic polar vortex split after an unusual major warming. Due to persisting chlorine activation on 475 K, ClONO₂ measured by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) on ENVISAT showed a pronounced collar structure with high mixing ratios at the vortex edge and low values in the inner region on September 20.

MIPAS data reveal a fast deactivation of inner-vortex chlorine until September 25 by increasing ClONO₂ and decreasing ClO mixing ratios and by the last detection of polar stratospheric clouds on September 21. Until mid October ClONO₂ decreased, indicating conversion into HCl. Recovery had already taken place on 625 K on September 20 and in the following ClONO₂ mixing ratios were decreasing. The data are compared with the only continuous measurements of ClONO₂ in the Antarctic polar vortex before MIPAS by the CLAES instrument on UARS in September 1992.

O-III-5

Non-LTE retrieval of NO, NO₂, and CO from MIPAS-ENVISAT

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The Michelson Interferometer for Passive Atmosphere Sounding (MIPAS) on board of the polar orbiter ENVISAT, launched on March 1st, 2002, detects non-LTE emissions of NO (5.3 μm), NO₂ (6.2 μm), and CO (4.5 μm) with high spectral resolution. Vertical profiles of NO, NO₂, and CO have been retrieved from a large set of MIPAS data measured between July and October 2002 in order to study the dynamical coupling of mesosphere and stratosphere and the downward transport of mesospheric/thermospheric NO_x.

Non-LTE effects have been considered by means of a novel retrieval scheme which includes a generic non-LTE population model. Derived data gives evidence for a large amount of mesospheric air in the South polar stratosphere over the whole period.

The presentation will report on recent validation activities and summarise preliminary results.

The IMK/IAA MIPAS/ENVISAT group:

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Oxford retrievals of MIPAS data during the 2002 Antarctic winter

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At the end of September 2002 the Antarctic underwent a stratospheric warming in which the polar vortex split up into two parts, that led to a corresponding splitting of the ozone hole.

The MIPAS instrument has acquired infrared limb emission spectra during this period. From these measurements profiles of atmospheric temperature and composition can be retrieved. OPTIMO, the Oxford retrieval code, uses an iterative fit with a priori constraints (optimal estimation method) to invert MIPAS spectra.

Here we present some results of OPTIMO analysis during the polar vortex splitting event and a comparison with the near real time L2 analysis provided by ESA. The near real time L2 products of September 2002 do not provide a complete coverage mainly because at that time they were still under validation. The OPTIMO retrieval is more robust and therefore provides better coverage, according to the availability of MIPAS L1B spectra.

Validation of MIPAS operational LEVEL 2 products using ground-based network data

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Data from a quasi-global network of ground-based instruments are being used for the validation of MIPAS vertical profiles of atmospheric species. The ground-based instruments are almost all part of the international Network for Detection of Stratospheric Change (NDSC). The network instruments used here include O₃ lidars, microwave radiometers and sondes, Dobson and Brewer spectrophotometers, and UV-Vis DOAS and FTIR spectrometers.

The deliverables of the network that can be compared to MIPAS operational data products range from high vertical resolution O₃ profiles, as provided by the O₃ sondes and lidars, to total column amounts of species like O₃, HNO₃, CH₄ and N₂O from the FTIR instruments. Some FTIR stations in the network also retrieve distinct tropospheric and stratospheric abundances, or even low vertical resolution profiles. New retrieval algorithms for UV-Vis DOAS instruments can provide low vertical resolution profiles of NO₂ in the stratosphere: preliminary data are available for Harestua, Norway.

Depending on the characteristics of the ground-based correlative data, in particular the independent elements of information in the different types of measurements, different approaches for comparisons with MIPAS data are being investigated. Several examples will be discussed. It is shown, for example, that for stratospheric species like HNO₃, the total column ground-based data allow useful comparisons with MIPAS integrated profile data. For species like CH₄ that have a strong tropospheric contribution, the MIPAS integrated profile data have been compared with ground-based retrievals of stratospheric abundances. Ground-based, low vertical resolution profiles are compared to MIPAS profiles taking into account the respective averaging kernels.

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Poster

P Programmatic

ACE-FTS instrument: 2 first months on-orbit

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The Atmospheric Chemistry Experiment (ACE) is the mission selected by the Canadian Space Agency for its next science satellite, SCISAT-1. ACE consists of a suite of instruments in which the primary element is an infrared Fourier Transform Spectrometer (FTS) coupled with an auxiliary 2-channel visible (525 nm) and near infrared imager (1020 nm).

A secondary instrument, MAESTRO, provides spectrographic data from the near ultra-violet to the near infrared, including the visible spectral range. In combination the instrument payload covers the spectral range from 0.25 to 13.3 micron. A comprehensive set of simultaneous measurements of trace gases, thin clouds, aerosols and temperature will be made by solar occultation from a satellite in low earth orbit.

The ACE mission will measure and analyse the chemical and dynamical processes that control the distribution of ozone in the upper troposphere and stratosphere. A high inclination (74 degrees), low earth orbit (650 km) allows coverage of tropical, mid-latitude and polar regions.

This paper presents the instrument-related activities for on-orbit commissioning of the ACE-FTS instrument on-board SciSat-1. In particular, activities related to the interferometer sub-system, cryocooler module and suntracker module will be covered. The first on-orbit results will be presented. The latest status of the spacecraft will also be presented.

Inversion of NADIR looking spectra performed at the resolution of IASI-balloon (0.1cm^{-1}) and of IASI-MetOp (0.5cm^{-1})

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In the framework of the Infrared Atmospheric Sounding Interferometer (IASI) mission onboard the MetOp satellite, the Laboratoire de Physique Moléculaire et Applications (LPMA) has developed a balloon-borne Fourier transform infrared (FTIR) instrument called IASI-balloon to record high resolution (0.1cm^{-1} apodised) spectra of the atmosphere/surface system in the nadir looking geometry.

The flight IASI02 of this experiment which took place on Aug. 5, 2002 from ESRANGE near Kiruna (Sweden), provided a large number of thermal emission nadir looking FTIR spectra in the region $650\text{-}2700\text{ cm}^{-1}$ recorded from float at about 30 km altitude. Inversion of columns and profiles of O_3 , CH_4 , N_2O and CO are presented. By degrading the observed IASI-balloon spectra to the spectral resolution of IASI-MetOp (0.5 cm^{-1} apodised), we have been able to compare the impact of the spectral resolution and assess the expected performances of the IASI instrument, which should be operational by the end of 2005.

Potential of observations from the tropospheric emission spectrometer to constrain estimates of continental sources of carbon monoxide

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We have conducted an observing system simulation experiment for the Tropospheric Emission Spectrometer (TES) satellite instrument to determine the potential of nadir retrievals of carbon monoxide (CO) from this instrument to constrain estimates of the strengths of continental sources of CO.

We use the GEOS-CHEM global chemical transport model to produce a pseudo-atmosphere in which the relationship between sources and concentrations of CO is known. Linear profile retrievals of CO are calculated by sampling this pseudo-atmosphere along the orbit of TES. These retrievals are used as pseudo-observations with a maximum *a posteriori* inverse algorithm to estimate the CO source strengths from the different continents starting from an *a priori* estimate of the sources.

This algorithm explicitly accounts for the finite vertical resolution of the retrieval, instrument errors, and representation and transport errors in the GEOS-CHEM simulation of CO. Transport errors are estimated using pairs of successive chemical forecasts of CO to characterize the global error pattern, which is then scaled by the residual relative error in the model simulation of aircraft observations over the NW Pacific.

We show that just a few days of observations from TES have the potential to accurately estimate the specified “true” sources of CO: *a posteriori* uncertainties on the sources are typically less than 10%, as compared to 50% assumed for the *a priori*. We demonstrate that with proper characterization of observation errors, TES could provide valuable information to help quantify sources of CO.

Laboratory characterisation of the radiation explorer in the far infrared breadboard (REFIR/BB) for the atmospheric emission measurement in the 100-1100 cm⁻¹ spectral range

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A spectrometer named Radiation Explorer in the Far InfraRed (REFIR) is being proposed for a future space mission aimed at the spectral measurement in the far infrared of the Earth outgoing emission from 100 to 1100 cm⁻¹ wavenumber, with particular attention at the spectral regions that are not covered by any current or planned space mission. In preparation for a possible space mission, a BreadBoard version (REFIR/BB) of the Fourier transform spectrometer has been built. REFIR/BB will allow us to study the trade-off between all instrument parameters, to test the optical layout and to optimise the data acquisition strategy.

This work describes the laboratory results on REFIR/BB with particular attention to the instrument characterisation. Tests were performed both in air, at ground level, and under a vacuum chamber. In perspective the breadboard could be flown for test flight on aircraft or balloon platforms.

Remote detection and analysis of high temperature events (HTE)

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High Temperature Events (HTE), such as volcano gas emissions or forest fires, occur very frequently. They do not only cause damage to people and infrastructure, but are also contributing to global warming. There is an increasing demand to reliably detect HTE and monitor the gases they emit, which makes it possible to prevent disasters and model HTE impact on climate.

However, permanent observation of wide areas can only be achieved by airborne or spaceborne measurements, so remote sensing methods are of great interest.

For this reason, the Remote Sensing Department of the German Aerospace Center has designed a new and unique measurement arrangement for airborne measurements. It consists of two sensor systems: a camera system which has one visible and two IR channels, all of them featuring very high spatial resolution, and a Fourier Transform Spectrometer of very high spectral resolution. Combined evaluation of the data of the sensor systems (Data Fusion) will enable to detect HTE, classify the observed scenery and calculate vertical gas profiles.

In summer 2003, measurements above Etna and Stromboli volcanos (Italy) as well as above a forest fire near Cottbus (Germany) have been performed. First results will be presented.

Information content analysis of combined IR-imager and FTIR measurements for CO₂ and CO columns over inhomogeneous vegetation fire scenes

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Spaceborne nadir FTIR measurements require a large instrument field of view to yield sufficient signal to noise ratio. The corresponding diameter on ground may be several km for a spaceborne instrument. In case of vegetation fires, this means that there will always be a mixed signal composed from varying fractions of flaming fire lines, smoldering area behind the fire, undisturbed background, and smoke over background.

If emissions of trace gases as CO₂ and CO are to be retrieved and assigned to the appropriate fire parts, knowledge of the relative area of these surface types is necessary since the area fractions are used to model the mixed signal in the retrieval process. In the measurement system investigated here, the area types are classified and their fractions and temperature determined by a broad band IR imaging spectrometer. We consider this information known in the further retrieval of CO₂ and CO columns using a non linear least squares algorithm with simple bounds.

The information content of such a mixed signal with respect to CO₂ and CO column retrieval over the flaming, smoldering, and undisturbed (background) parts of a forest fire scene is investigated with help of the Jacobian matrix and the averaging kernels.

Poster

I Retrieval

Retrievals of trace gases from IMG/ADEOS spectra for chemistry and climate applications

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Space-borne thermal infrared instruments working in the nadir geometry are providing spectroscopic measurements of species that impact on the chemical composition of the atmosphere and on the climate forcing.

Here we present the retrieval of several trace gases from the high-resolution spectra recorded by the Interferometric Monitor of Greenhouse gases (IMG), launched aboard the ADEOS platform in august 1996. The retrieval algorithm, which combines a general least-squares spectral fitting approach and the optimal estimation method, is presented. The emphasis is placed onto the retrieval of weakly absorbing molecules (CFC-11, CFC-12 and HNO₃) in the atmospheric window and onto the retrieval of vertical CO and ozone profiles. The latter are compared with profiles retrieved using neural network techniques as well as with those measured locally by ozone sondes.

The results are used to illustrate the potential scientific return to be expected from future missions using advanced infrared nadir sounders, operating both from a polar and geostationary orbit.

Characteristics of spectral emissivity for various types of the surface derived from IMG spectrum data

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Emissivity of the surface in the thermal infrared region, particularly in the atmospheric window region, is an important parameter when we consider the energy budget in the surface-atmosphere system. Recently, global mapping of broad band infrared emissivity have been obtained from MODIS and ASTER data analyses. However, spectral emissivity data are still necessary for characterizing the surfaces more precisely.

In this study, we have developed a procedure to derive spectral emissivity in 8-12 micron region from IMG data. Principally, it is not possible to completely separate the surface temperature and emissivity at each wavelength because the number of independent parameter is $N+1$ for N channel observation (one thermodynamical temperature plus emissivities at N wavelength), but that can be obtained from the measurement is N (radiances at N channels). That means that we need one additional information or assumption to solve the equations.

In this study, we set an assumption depending on the surface type derived from visible imagery simultaneously observed with high resolution radiance spectra. This method have been applied to the analysis of IMG data, and some interesting characteristics of spectral emissivity have been obtained for various types of the surface such as desert sand and sea ice.

A method for retrieving columnar CO₂ concentration from thermal infrared radiation spectrum

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Recently, some attempts to retrieve atmospheric CO₂ concentration profile from the thermal infrared radiation spectrum have been made mainly based on simulation studies (e.g., Chedin et al., 2003; Engelen et al., 2001). In most of these studies, a lot of effort has been made to improve retrieval accuracy in the lower atmosphere and that in the columnar concentration, i.e. combining some different CO₂ absorption bands or taking spatial and temporal average of retrieved concentration data. However, the spectral resolution was assumed only to be about 1 cm⁻¹ in most of these studies supposing the usage of IASI data.

In this study, one retrieval method using a set of strong and weak absorption CO₂ bands has been examined. The usage of a weak absorption band of which each line is separated at a high spectral resolution in the order of 0.1 cm⁻¹ is expected to be useful for deriving the columnar CO₂ concentration. Some results from IMG data analysis using this method and error estimation results will be presented.

Radiative transfer modelling for TES

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The forward model to be used for the Tropospheric Emission Spectrometer (TES) retrievals of constituents and temperature is built from the Line-By-Line Radiative Transfer Model (LBLRTM). Forward model validations against high quality airborne and surface interferometer measurements demonstrate that the residuals between the calculations and observations are being reduced from "degrees to tenths of a degree". This reduction in forward model systematic error is critical in order to attain the retrieval accuracy capabilities of the next generation of passive remote sensors.

There have been a number of key improvements to the TES forward model that have reduce the systematic errors in the spectral line calculation. The model incorporates the new MT_CKD_1.0 water vapor continuum where the self and foreign water vapor continuum models are each based on the contributions from two components: a collision induced component and a line shape component. The CO₂ line shape and associated CO₂ continuum have been modified and incorporated into the forward model as part of MT_CKD_1.0. CO₂ line coupling is also being investigated and is presently treated to second order at 618, 667, 720, 721, 742, and 792 cm⁻¹ and to first order for CO₂ at the 1932, 2076, 2093, 2193 cm⁻¹ Q-branches. The forward model for the TES absorption coefficients uses a more accurate algorithm for the Voigt line shape function, providing a slight difference on high altitude limb retrievals as the Doppler limit is approached.

Recent improvements in the line parameters have significantly reduced systematic errors associated with the forward model calculation. In order to keep generality for cross-platform comparisons, and incorporate recent spectroscopic line parameter improvements, the TES (tes_v_1.0) spectroscopic line file is built from HITRAN2000 with the updates available as of 08/2003 (last update 09/2001). The TES line file also includes additional updates to CH₄, CO, and O₃, which are expected to be included in HITRAN updates in the near future. Presented are validations of the TES forward model against aircraft upwelling radiation from the High resolution Interferometric Sounder (HIS) Convection and Moisture EXperiment (CAMEX) and Scanning-HIS ARM/FIRE Water vapor EXperiment (AFWEX), and surface Atmospheric Emitted Radiance Interferometer (AERI) downwelling radiation from the ARM Southern Great Plains (SGP) and North Slope of Alaska (NSA) sites. Also provided is an ozone retrieval that utilizing the improved forward model spectral line parameters and upwelling aircraft observations.

Calculation of altitude-dependent Tikhonov constraints for TES NADIR retrievals

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Constraints are a standard retrieval tool used by TES to regularize retrievals of atmospheric profiles. Standard constraints that are currently used for atmospheric profile retrievals include the inverse of a climatology and Tikhonov constraints. However, these types of constraints currently have some less than optimal properties. Climatological constraints may include unphysical correlations, for example correlations between stratosphere/troposphere; are sometimes finely tuned to a particular climatology; and are not optimized for interfering species error for a standard retrieval. Tikhonov constraints of a single type or with a single strength value can introduce artifacts because different strengths and types are sometimes needed for different parts of the atmosphere.

This paper describes a method for creating and evaluating constraints that are altitude-dependent hybrid combinations of 0th, 1st, and/or 2nd derivative constraints. The constraint strengths are determined by minimizing a combination of the a posteriori error and the degrees of freedom using the simplex method. The estimated errors resulting from these altitude-dependent constraints are compared to the inverse a priori covariance for both the climatology that was used to develop them, and for a different climatology to measure the robustness of the constraint to a different climatology. Constraints are calculated for three representative atmospheres: mid-latitude, tropics, and polar, and for five species: water, ozone, carbon monoxide, methane, and atmospheric temperature.

This paper shows that the altitude-dependent hybrid Tikhonov constraints have comparable error to the inverse covariance for the climatology for which they were developed, and can in some cases do significantly better than the inverse covariance when applied to an unexpected climatology.

Two dimensional characterization of atmospheric profile retrievals from limb sounding observations

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Limb sounders measure atmospheric radiation that is dependent on atmospheric temperature and constituents that have a radial and angular distribution in Earth-centered coordinates. In order to evaluate the sensitivity of a limb retrieval to radial and angular distributions of trace gas concentrations, we perform and characterize one-dimensional (vertical) and two-dimensional (radial and angular) atmospheric profile retrievals.

Our simulated atmosphere for these retrievals is a distribution of carbon monoxide (CO), which represents a plume off the coast of south-east Asia. Both the one dimensional (1D) and two dimensional (2D) limb retrievals are characterized by evaluating their averaging kernels and error covariances on a radial and angular grid that spans the plume. We apply this 2D characterization of a limb retrieval to a comparison of the 2D retrieval with the 1D (vertical) retrieval.

By characterizing a limb retrieval in two dimensions the location of the air mass where the retrievals are most sensitive can be determined. For this test case the retrievals are most sensitive to the CO concentrations about 2 degrees latitude in front of the tangent point locations. We find the information content for the 2D retrieval is an order of magnitude larger and the degrees of freedom is about a factor of two larger than that of the 1D retrieval primarily because the 2D retrieval can estimate angular distributions of CO concentrations.

This 2D characterization allows the radial and angular resolution as well as the degrees of freedom and information content to be computed for these limb retrievals. We also use the 2D averaging kernel to develop a strategy for validation of a limb retrieval with an in-situ measurement.

Iteratively regularized Gauss-Newton methods for quadratic and bound constraint problems in atmospheric remote sensing

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The retrieval of atmospheric profiles (nb. temperature and concentrations etc) from spectroscopic measurements is an ill-posed inverse problem, and additional information (e.g., 'smoothness', climatological data, etc.) has to be provided to stabilize the solution. For linear inverse problems Tikhonov regularization is a well established approach, and criteria such as the L-curve give a means to automatically select the appropriate amount of regularization.

However, nonlinear inverse problems present further challenges. Here we discuss an Iterative Regularized Gauss-Newton algorithm for the quadratically constrained nonlinear least squares problem. Furthermore an extension using bound constraints additionally to avoid negative solutions is presented.

The performance of the algorithms is studied by means of simulations of temperature and molecular concentration retrievals from MIPAS type high resolution limb emission infrared spectra.

Windows-based line-by-line radiative transfer computation using Mathcad

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MCLBL (tentative name) is a new Windows-based software environment for line-by-line radiative transfer computation. Formerly, only a few software programs of this type was available because standard line-by-line computations are too slow to be implemented in interactive applications.

We have developed a special algorithm to accelerate the speed of line-by-line computations by factors of 50-100 without significant loss of accuracy. The user-friendly, intuitive interface and flexibility realized by incorporating this algorithm into Mathcad may completely change the R&D styles of researchers who work on spectroscopic analyses.

MCLBL can easily be used for many types of applications (including small-scale retrieval problems) by utilizing the powerful built-in functions in Mathcad. A simulation of infrared transmission spectra observed in the solar occultation geometry by a Fourier transform spectrometer is presented as an example.

Fast approximation of line-wing absorptions in high-resolution infrared spectra

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When performing line-by-line simulations of atmospheric high-resolution infrared spectra, a large portion of the computation time is spent in the calculation of the absorptions by the far wings of the absorption lines.

For applications in which one is interested mainly in evaluating the effective absorption in a small microwindow in between lines, a computationally less expensive method has been developed. The method is faster than the explicit line-by-line calculation by a factor proportional to the number of line-wings that contribute to the absorption in the simulated microwindow.

This paper presents the method and demonstrates its performances for an application of high-resolution infrared nadir radiances in the 700 – 1200 cm^{-1} band. Typically one obtains a gain in computation time of order 10 to 100.

EOF approach to physical inversion of spectral radiance for geophysical parameters

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One of the main problems we are concerned with new generation sensors such as space-borne Fourier Transform Spectrometers is the huge amount of spectral radiance data points these instruments yield. This characteristic is in contrast with the need of real time processing of the spectral radiance for inversion of geophysical parameters, e.g. temperature, water vapour, ozone needed for Numerical Weather Prediction.

Although, physical inversion schemes are the ideal candidate to be used along with FTS radiance, the time requirement imposed, e.g. by Numerical Weather Prediction applications will likely hamper their full exploitation for operational end uses. Alternative statistical inversion approaches, such as Neural Network and EOF (Empirical Orthogonal Functions) regression, have been tested because of: their computational efficiency. While fast, these methods seem not to be able to reach the goal accuracy needed, e.g. for water vapour and ozone.

In this study we present a novel inversion approach which combines the computational efficiency of EOF representation to the robustness of physical inversion. The idea is to develop the Radiative Transfer Equation (RTE) into an appropriate EOF basis, to retain only the most significant principal components and, finally, to produce the physical inversion in the EOF space rather than into the usual radiance space. The advantages are manifold: 1) a truncated EOF representation of the RTE acts like a regularization process when producing inverse products, therefore there is no need to further regularize the inversion process; 2) there is no additional regularization parameter to be selected in the process; 3) in principle we could use a forward model to yield only those few principal components used in the EOF expansion, so that improving the fastness of the procedure.

The new approach has been checked and exemplified by inverting IMG spectral radiance for temperature, water vapour and ozone and the results have been compared to ECMWF analyses for the same location and date as those of the IMG soundings.

The Next HITRAN Edition: Description of New Parameters and Formats

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The current HITRAN compilation¹ consists of several components useful for radiative transfer calculation codes: high-resolution spectroscopic parameters of molecules in the gas phase, absorption cross-sections for molecules with very dense spectral features, aerosol refractive indices, ultraviolet line-by-line parameters and absorption cross-sections, and associated database management software. The line-by-line portion of the database contains spectroscopic parameters for thirty-eight molecules and their isotopologues suitable for calculating atmospheric transmittance and radiance properties.

The total length of a record (line transition) is 100 characters, which has been adopted since the edition of 1986 through to the current edition. In the upcoming edition, the number of parameters will be increased, and the record length will be 160. It should be noted that the parameters are independent quantities, valuable as input to various computer codes that simulate transmission or radiance in gaseous media. They have been chosen with respect to internationally accepted modeling schemes. This poster describes the future format for the line-by-line portion of the HITRAN database, especially for a coherent vibrational and rotational quanta identification, as well as the description of the calculation of the Einstein-A coefficient and the statistical weights of the upper and lower states of the transition (these new parameters being useful for non-local thermodynamic equilibrium problems, astrophysics, and other applications).

Acknowledgements:

1. Rothman LS, Barbe A, Benner DC, Brown LR, Camy-Peyret C, Carleer MR, Chance KV, Clerbaux C, Dana V, Devi VM, Fayt A, Flaud JM, Gamache RR, Goldman A, Jacquemart D, Jucks KW, Lafferty WJ, Mandin JY, Massie ST, Nemtchinov V, Newnham D, Perrin A, Rinsland CP, Schroeder J, Smith K, Smith MAH, Tang K, Toth RA, Vander Auwera J, Varanasi P, Yoshino K, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001" *JQSRT* **82**, 5-44 (2003).

See

HITRAN

web-site:

<http://cfa-www.harvard.edu/HITRAN>

Millenium HITRAN Compilation

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The current edition of the HITRAN molecular absorption compilation has been made available on an anonymous ftp-site located at the Harvard-Smithsonian Center for Astrophysics (<ftp://cfa-ftp.Harvard.edu/pub/HITRAN>). The compilation consists of five main folders: The traditional line-by-line parameter database; IR cross-sections; UV cross-sections and line-by-line parameters; Aerosol refractive indices; and tables of globally applicable quantities (partition sums, isotopic abundances, molecular masses, etc), algorithms (for line-coupling corrections), and references to parameters and cross-sections. There is also a high-temperature analog of HITRAN called HITEMP. Some updates or corrections have been posted since the official release of the archival data in the ftp-site. These improvements are given in the public HITRAN web-site (<http://cfa-www.Harvard.edu/HITRAN>) and will be incorporated into the next edition.

Collaborations with many research teams throughout the world have enabled great improvements in providing more accurate parameters, extended spectral coverage, and documentation. The improvements not only will provide increased capabilities for atmospheric transmittance/radiance calculations and remote sensing, but also will allow access and analytical tools for related molecular databases. Besides the line-by-line absorption parameters, significant progress has been made for pressure-temperature sets of absorption cross-sections as well as increased tables of aerosol properties. A new edition of the HITRAN compilation is now in preparation.

Poster

II Cal/Val

High resolution measurements of the instrument line-shape function of Fourier transform spectrometers

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Applications of Fourier transform spectroscopy in atmospheric science often implies high resolution, high accuracy measurement of spectral lines. To obtain meaningful retrieval of physical quantities such as temperature, pressure and concentration, one requires a precise knowledge of the effect of the instrument on the acquired data. The instrument line-shape (ILS) of a Fourier transform spectrometer (FTS) is governed by the angular distribution of light in the interferometer. This influence is sometime referred to as off-axis effect. Radiant intensity distribution is mainly determined by field of view configuration but can also be affected by several types of misalignment, optical aberrations and diffraction. Experimental validations of these ILS models have been performed but never with a high enough resolution to clearly show the predicted divergence contribution.

The reason is simple, common FTS designs usually impose that the divergence contribution is to be at most comparable to the interferogram truncation contribution. This poster presents line-shape measurements obtained from a reconfigurable FTS specifically designed to resolve the divergence contribution to the ILS. The FTS records double-sided interferograms with a maximum path difference of 18 cm. It is capable of sustaining a maximum off-axis angle of 18 mrad without vigneting across the entire optical path difference scan. The optical path is folded in each arm of the interferometer by a moving cube-corner retroreflector and sent onto a flat end mirror. Optical path difference variation is accomplished by moving the folding retroreflectors. The instrument is thus essentially a flat mirror interferometer. The field stop is located in the focal plane of the input optics. This allows us to perform measurements at different wavelengths using two different oversized detectors without affecting the field of view configuration. ILS corresponding to different field of view geometries are obtained by placing an arbitrary shaped aperture in the focal plane of the input optics.

Spectra from two radiation sources are measured. A diffuse, uniform circular monochromatic light source is obtained from a 6450 cm^{-1} DFB laser and an integrating sphere. The spectral line width of the DFB laser being much narrower than the FTS resolution, spectra obtained from this source are direct measurements of the ILS. A more conventional line-shape characterization setup consisting of a 12 cm absorption cell is also used to provide comparison between the two characterization methods as well as experimental transmission spectra to develop and test ILS correction algorithm.

Measurements show to be in excellent agreement with the geometrical model. Future work will focus on refining the instrument models to explain the remaining discrepancies as well as testing the limits of correction algorithms on real data.

Field widening effects on modulation efficiency and ILS resulting from the use of uncompensated beam splitter

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Our presentation deals with the behavior of Fourier-transform spectrometers (FTS) using an uncompensated beam splitter. As expected, the lack of compensation results in strong dispersion over the spectral band, spreading the zero-path difference (ZPD) region of the interferograms.

In fact, the exact position of the ZPD varies with wavenumber. It is very interesting to notice that operating with an uncompensated beam splitter is equivalent to use a field-widening configuration. The latter enables to achieve an infinite Haidinger fringe pattern for a given non-zero optical path difference (OPD). This configuration involves necessarily that fringes are observed at ZPD.

Symmetrical operation about ZPD therefore suffers increased limitations due to the tighter fringe pattern resulting from supplementary phase accumulation into the beam splitter substrate. The fringe pattern integration over the instrument field-of-view (FOV), for single pixel as well as for imagers, results in apparent loss of modulation efficiency. In fact, global impact on instrument line shape (ILS) (or equivalent self-apodization) is expected, with both contributions to the ILS phase and amplitude. All these effects are presented to show the impact on performance of using an uncompensated beam splitter.

Theoretical predictions obtained through an analytical model and through a complete 3D numerical model agree.

The instrumental line shape of TES as deduced from gas cell measurements using the software `linefit`

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The instrumental line shape (ILS) is among the key parameters specifying the performance of a spectrometer. The ILS has to be characterised accurately for the retrieval of geophysical variables from measured spectra, otherwise unrecognized ILS imperfections might be a source of substantial systematic errors.

We present an ILS characterisation for each pixel of the spectrometer TES derived from low pressure gas cell measurements. The software LINEFIT has been used to generate the constrained fits. Whereas the fits are performed in spectral domain, the constraints on the ILS parameters are applied in the interferogram domain, which is appropriate for a Fourier spectrometer as TES. The a-priori for the ILS parameters of each pixel have been determined using LINEFIT's auxiliary software ALIGN.

Some results on MIPAS/ENVISAT inflight instrument calibration

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Results on some inflight calibration tasks performed at IMK and CSIC during the MIPAS/ENVISAT calval phase are presented. The instrument performance w.r.t. NESR, spectral noise covariance, ILS shape, spectral offset and shift, and LOS are addressed.

The influence of the high atmosphere on deep space spectra, used for the gain calibration, is dealt with too. As a general result the MIPAS instrument seems to meet the specifications quite well.

However unexplained features of e.g. the spectral noise covariances still remain and are discussed.

MIPAS-B observations for the validation of target parameters of MIPAS-ENVISAT and ILAS-II

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Embedded in the ENVISAT validation programme of the chemistry instruments MIPAS, GOMOS, and SCIAMACHY two balloon flights were carried out with MIPAS-B, the balloon borne version of MIPAS. The first one at mid-latitudes during the night of 24/25 September 2002 from Aire sur l'Adour, France, adjusted to the night-time overpass of orbit 2975.

Here, a perfect match in terms of time and location of air masses sounded by MIPAS and GOMOS could be achieved. The second flight was carried out in the late winter arctic vortex on 20/21 March 2003 from Kiruna, Sweden, matching evening and morning overpasses of ENVISAT (orbits 5508 and 5515). Prior to this MIPAS-B observation, a limb scan of the Japanese sensor ILAS-II aboard ADEOS-II was performed some degrees east of the MIPAS-B measurement with a temporal offset of about 4.5 hours.

This paper compares MIPAS-B data to results obtained from MIPAS on ENVISAT (both operational data and profiles retrieved at IMK) as well as first results from ILAS-II that have been available so far.

Measurement capabilities and applications of the high resolution Fourier Transform Spectrometer SAFIRE-A

(SPECTROSCOPY OF THE ATMOSPHERE BY USING FAR-INFRARED EMISSION - AIRBORNE)

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We present here the main instrumental features, measurement capabilities and perspectives for future applications of a high resolution Fourier transform spectrometer that was specifically designed and built to operate onboard the high altitude aircraft M-55 Geophysica and that has already measured the atmospheric signal during more than 25 flights, as part of the M55 payload, in different test and scientific campaigns.

The instrument, named SAFIRE-A (Spectroscopy of the Atmosphere by using Far Infrared Emission - Airborne), is a passive remote-sensor capable to perform limb-sounding observations of the atmospheric emission in the Far-Infrared region (20 - 200 cm^{-1}) with a spectral resolution of 0,004 cm^{-1} unapodized. The radiation from the atmosphere and from a cold or hot blackbody is collected by the input optics and analysed by a polarising interferometer; the output of the interferometer is sent to the Cold Optics and Detector Module, where it is split into two channels and, after passing through narrow-band filters (approximately 2 cm^{-1} wide), detected by photon-noise limited detectors. Sequences of individual spectra acquired at different limb angles are processed using an inversion algorithm specifically developed for the airborne measurements (RAS, Retrieval Algorithm for SAFIRE-A), to retrieve the VMR (Volume Mixing Ratio) vertical profiles of minor atmospheric constituents whose spectral features are present in the measured frequency intervals.

The capability of the instrument to measure the geographical and vertical distribution of several target species belonging to the most important catalytic families involved in Ozone chemistry, with a vertical resolution of approx. 2 km and a horizontal resolution of approx. 100 km, has been already proven in several field campaigns carried out at mid (Italy, 1996, 1998/99 and 2002) and high latitudes (Arctic region, 1996/97 and Antarctic, 1999). Here the most recent results will be shown as an example of the level achieved by the instrument performances. Special emphasis will be given to the observations carried out in October 2002 from Northern Italy, and in March 2003 from Kiruna (Arctic region), with the aim of validating the level-2 products of MIPAS, GOMOS and SCIAMACHY onboard the European satellite ENVISAT-1, since this activity is going to be one of the key task of the instrument in the short and medium term.

Validation of MIPAS Temperature Profiles with other satellite measurements

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MIPAS on ENVISAT measures vertical profiles of atmospheric temperature and various species with nearly global coverage and high accuracy/precision. The MIPAS data analysis processor at Institut für Meteorologie und Klimaforschung (IMK) provides simultaneous retrieval of temperature and line-of-sight parameters, as well as, indirectly, pressure from measured spectra and the spacecraft ephemerides.

This step precedes the species abundance retrievals, because an accurate knowledge of the observational geometry and the physical state of the atmosphere is an essential requirement for any space-based limb-viewing remote sensing experiment attempting to characterize the chemical composition of our environment.

The MIPAS IMK temperature data products are compared with a number of satellite observations, including ECMWF and UKMO assimilation, SABER near-to-mid infrared radiometry, HALOE solar occultation, and CHAMP and SAC-C radio occultation. The individual profiles and zonal means measured by MIPAS and other instruments at different locations and times show reasonable agreement, though deviations may exist due to characteristics of the instruments and observation scenarios. This indicates the reliability of MIPAS-IMK data products and their capability for providing valuable scientific information.

Validation of ozone measurements from MIPAS-ENVISAT: First results

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Vertical profiles of ozone are retrieved with the IMK scientific semi-operational processor from spectra measured by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) aboard the environmental satellite ENVISAT. The results are intercompared with those obtained by the MIPAS balloon instrument (Aire sur l'Adour) and the ground-based FTIR (Kiruna).

The intercomparison strategy follows the quantitative description of Rodgers/Connor (2003) including transformation of the retrieved profiles to the same a priori profile and estimation of noise errors, systematic errors, as well as errors due to different smoothing.

Analysis of MIPAS residual spectra

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Residual spectra are the difference between spectra measured by the instrument spectra generated by the retrieval forward model at the final iteration. Ideally, these should contain only measurement noise but in practice a number of features are present indicating systematic errors either in the forward model or the instrument characterisation. Residual spectra for each microwindow are included in the distributed MIPAS Level 2 product.

Residual and Error Correlation (REC) analysis is a statistical technique for analysing such data. The principle is to identify correlations between persistent features in the residual spectra and the signatures expected from known sources of error such as calibration uncertainties or interference from non-retrieved species. This is now performed routinely as part of the monitoring of MIPAS data quality.

Here we present some results from the REC analysis of the first year of MIPAS data.

MIPAS-B VALIDATION STRATEGY

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Balloon measurements with the established and well characterised balloon version of MIPAS are used for a number of satellite instruments like ILAS and ILAS-II on the Japanese ADEOS satellites, the chemistry-dedicated instruments GOMOS, MIPAS and SCIAMACHY on ESA'S ENVISAT, and the Canadian ACE mission.

As a limb sounder, MIPAS-B can be launched at any time of the day and the measurement scenario can be optimised to the validation task without being restricted by the position of the sun. The strategy used for the validation flights to obtain the best possible coincidence in time and space between the satellite measurement and the correlative balloon observation will be illustrated including the tools used. Back trajectory and trajectory hunting methods are applied to increase the number of matches.

Poster

III MIPAS

Advanced MIPAS-Level-2 Data Analysis (AMIL2DA)

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The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), which is a core instrument of the Envisat polar platform launched on 1 March 2002 by the European Space Agency (ESA), is a powerful tool to measure vertical profiles of trace species on a global scale. While operational data processing by ESA covers only analysis of pressure, temperature, and the mixing ratios of the species O₃, H₂O, HNO₃, CH₄, and N₂O, MIPAS infrared spectral limb emission measurements contain much more information not explored in by real time processing. The goal of AMIL2DA is to generate and validate data analysis tools for these supplemental data products.

Instead of merging the contributions of all participants to one data analysis algorithm which fits all purposes, the AMIL2DA strategy is to maintain the diversity of different computer codes by each group which are custom-tailored to their specific scientific needs, and prove their reliability by thorough cross-validation. As a first step, forward radiative transfer algorithms, which are the core part of each data processor, have been cross-validated. In a second step, the inversion underwent a blind-test intercomparison based on synthetic measurements.

In the third step, the codes have been applied to real MIPAS measurements. Deficiencies in forward radiative transfer as well as inversion algorithms have been detected and removed. Along with these activities, the spectroscopic database was improved and contributions to the MIPAS instrument characterization were made.

The AMIL2DA consortium is:

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2D-retrieval approach and diagnostics for MIPAS-Envisat

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The Fourier transform spectrometer MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) on ENVISAT measures infrared emission of the Earth's atmosphere in a limb viewing mode. Due to the long ray path, limb sounders are sensitive to even little abundant species. However, horizontal gradients cause systematic errors within the retrieval if a horizontally homogeneous atmosphere is assumed.

A dedicated method of taking full 2D fields of state parameters into account is presented. The 2D state vector is updated sequentially for each limb scan. The diagnostics comprise estimated random error, vertical and horizontal degrees of freedom for retrieval, as well as vertical and horizontal resolution.

Retrievals of trace species in the UTLS region from MIPAS/ENVISAT

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ENVISAT with MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) on board was successfully launched on 1 March, 2002. Since 24 March 2002, MIPAS measures high-quality mid-infrared limb emission spectra with 0.035 cm^{-1} spectral resolution. The non-operational scientific level-2 data analysis of MIPAS/ENVISAT to be performed at IMK has been developed. The work of this project was focussed on various retrieval aspects in the upper troposphere/lowermost stratosphere region. Theoretical work on basis of synthetic spectra led to the expectation that up to 20 species in the upper troposphere region should be detectable with total accuracy (including all relevant systematic error sources) better than 100 %, many of them better than 10 %. The approaches developed were applied to early MIPAS/ENVISAT data.

Example retrievals from real data will be presented and their characteristics will be discussed in terms of usefulness for UTLS science issues, for example vertical transport, trop/strat exchange, horizontal mixing, or upper troposphere ozone photochemistry.

The IMK MIPAS/ENVISAT team:

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Retrieval of SF₆ profiles from the MIPAS satellite instrument

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Sulphur Hexafluoride (SF₆) is a highly symmetric octagonal molecule with its main vibrational-rotational transition centred around a single ν -3 Q branch at 947.9cm⁻¹, with band limits 915-960cm⁻¹. This intense spectral feature gives rise to a strong radiative effect, a thousand times stronger than that of CO₂, making it one of the most efficient greenhouse gases.

We demonstrate retrievals of SF₆ profiles over the altitude range 6-36 km from atmospheric spectra taken by MIPAS, a limb-viewing infrared Fourier Transform Spectrometer on ESA's ENVISAT satellite. Due to low S/N, some coaddition is required. A mean mid-latitude profile shows expected tropospheric (4 +/- 0.7 ppmv) mixing ratio, in agreement with recent measurements and in line with accepted trends from anthropogenic emission.

Multi-target-retrieval of the volume mixing ratio of SF₆ from MIPAS spectra

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A retrieval approach for the simultaneous determination of the altitude distributions of pressure (p), temperature (T) and Volume Mixing Ratio (VMR) of atmospheric constituents from limb scanning measurements of the atmosphere has been developed and implemented in a computer code for the analysis of MIPAS-ENVISAT observations [B.M.Dinelli, D.Alpaslan, M.Carlotti, L.Magnani, M.Ridolfi, 'Multi-target retrieval (MTR): the simultaneous retrieval of pressure, temperature and volume mixing ratio profiles from limb-scanning atmospheric measurements', *Journal of Quantum Spectroscopy and Radiative Transfer*, in press, (2003)].

This analysis method, named Multi-Target Retrieval (MTR), has been used to retrieve the altitude distribution of the SF₆ VMR in the troposphere, from selected MIPAS orbits. The SF₆ profile was retrieved simultaneously with the p, T, water and ozone profiles analysing selected spectral features of SF₆ jointly with the spectral intervals used by the ESA Level 2 processor for the sequential analysis of the MIPAS key species.

MIPAS retrievals of UTLS O₃ and H₂O

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The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) provides global infrared limb measurements covering a large spectral range (685-2410 cm⁻¹) at 0.035 cm⁻¹ (unapodised) spectral resolution. The nominal-mode measurements span tangent altitudes from 6 to 68 km.

A retrieval processor is being developed at RAL to complement the ESA operational processor, with particular emphasis on retrievals of ozone and water vapour in the upper troposphere/lower stratosphere (UT/LS) region. The selection of sections of spectrum (microwindows) for use in retrievals is also being optimised for accurate retrievals at UTLS altitudes.

This poster will describe the RAL MIPAS retrieval processor and show some example results.

Observations of polar stratospheric clouds with MIPAS

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Due to the limb-emission measurement method, MIPAS is very sensitive to thin clouds. This is especially valuable for the detection of polar stratospheric clouds (PSCs), also during polar night.

In the first part we will discuss the evolution of PSCs during the northern polar winter 2002/2003 and during the southern winter 2003. In the north, during nearly all days of December 2002 large PSCs were present in the polar vortex. In the following months, some PSCs occurred in January, nearly none in February and the last were detected end of March. In the south, first PSCs appeared on May 21, 2003 and after a few days the whole Antarctic area was covered with PSCs.

In the second part of this contribution the spectral signatures of PSCs in the broad-band spectra of MIPAS will be discussed. Different types will be distinguished.

By means of radiative transfer simulations, including scattering, we will show what can be inferred about composition and microphysical parameters from MIPAS PSC observations.

Wave forcing estimated from MIPAS stratospheric temperature and ozone measurements during the Southern Polar Vortex split-up event of 2002

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The temperature and ozone profiles observed by MIPAS on ENVISAT in the southern hemisphere during the late September of 2002 show significant longitudinal variations. The amplitudes and phases of the zonal variations are derived by harmonics analysis on a daily basis for individual latitude bands and each altitude level. Their latitude, height, and day-to-day variabilities are investigated.

The zonal variations show drastic increases at latitudes 60S - 80S around 23 and 24 September, with maximum amplitudes of 2 - 3 ppmv and 30 - 40K in the region of 20 and 35 km for ozone mixing ratio and temperature, respectively. The large-amplitude disturbances break down in one or two days, with the wavenumber one amplitudes decreasing much more significantly. The amplitudes of wavenumber one and two then become comparable in the latitude and altitude regions, resulting in an apparent wavenumber two pattern of the observed temperature and ozone fields.

These features of polar vortex break-down are in agreement with other observations. A simple model is suggested to estimate planetary wave forcing, which is as large as +/- 500 m/s/day and may be responsible for the split-up event.

Measurements of water vapour during the vortex split up in September/October 2002 with MIPAS/ENVISAT

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The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) onboard ENVISAT is a limb viewing mid-infrared high-resolution spectrometer. At IMK a non-operational MIPAS level 2 processor is used to derive geophysical data from the MIPAS observations. Among numerous atmospheric parameters, water vapor and temperature profiles are retrieved in an altitude range from 5 km up 68 km.

In September and October 2002 a major stratospheric warming in the antarctic region lead to an unusual early split up of the south polar vortex. MIPAS measurements in the polar vortex are available for the period from mid to end of September and mid of October.

The water vapor measurements for the polar stratosphere show lower volume mixing ratios inside the vortex than outside for altitudes covering the lower stratosphere. These low water vapor mixing ratios with values between 2 and 3 ppmv in the lower stratosphere are related to cold temperatures. The formation of PSC in these altitudes lead to a dehydration of the air masses. The sum of water vapor and 2 times methane for these measurements shows strongly decreased values inside the vortex, indicating that the observed air masses are affected by dehydration.

As a consequence of the strong cooling in the lower stratosphere the Antarctic air masses in higher altitudes are subject to subsidence. Water vapor volume mixing ratios measured in the middle stratosphere inside the vortex show larger values than outside. These larger mixing ratios are related to air masses that subsided from higher altitudes with larger water vapor mixing ratios.

The evolution of the water vapor distribution inside and outside of the polar vortex during the major warming in September 2002 has been observed with MIPAS/ENVISAT and will be discussed.

NO_y from Michelson Interferometer for Passive Atmospheric Sounding on environmental satellite in the South hemisphere vortex split in September/October 2002

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Reactive nitrogen species HNO₃, ClONO₂, NO, NO₂, and N₂O₅ were derived from the analysis of high resolution atmospheric limb emission spectra measured by MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) on board ENVISAT during the split of the southern polar vortex in September/October 2002. The retrieval of N₂O₅, the chemical and transport processes leading to NO_y deficit, and NO_y partitioning are investigated. The retrieval of N₂O₅ is complicated by its continuum-like emission feature covering a wide spectral region.

The method of constraining N₂O₅ continuum to its value in N₂O₅ free spectral region was found to give better results. Most of the available NO_y in the polar vortex is in the form of HNO₃ and NO_x in the lower stratosphere, typical midlatitude feature at this time, with the exception of 22 - 27 September which is characterized by HNO₃ and ClONO₂ dominating NO_y partitioning between 400 K and 475 K levels.

This is a strong evidence that chlorine activation has already taken place at the beginning of the period while the changes in the partitioning from HNO₃ and NO_x to HNO₃ and ClONO₂ dominance during the split vortex is due to the conversion of NO_x into N₂O₅ in this altitude range. The [NO_y]:[N₂O] correlation inside the vortex was found to deviate from its early winter relation (compact canonical relation).

The total [NO_y] inside the vortex is lower than reference values by 8.3 to 9.5 ppbv during the whole period on 475 K level. The observed NO_y deficit during the period is attributed to descent followed by quasic-horizontal mixing and denitrification in proportion of approximately 40 % and 60 % respectively. The variation in the deficit from beginning of the period to early mid-October is within the range of the uncertainties which is about 1.0 ppbv thereby indicating that the vortex was fairly isolated from the ex-vortex in the lower stratosphere during the period despite the major warming.

Study of the Antarctic vortex split-up in September/October 2002 by means of trace species from MIPAS/ENVISAT

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In late September 2002 an Antarctic major stratospheric warming occurred, which led to a split-up of the polar vortex. Such an event had never before happened since the beginning of regular antarctic stratospheric temperature observations in the 1950's. The split-up is studied by means of CH₄, N₂O, CFC-11 and O₃ data of September 20-27 and October 11-13, 2002, retrieved at the Institute for Meteorology and Climate Research Karlsruhe (IMK) from level 1-B spectra from MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) on board of the European research satellite ENVISAT (ENVironmental SATellite). For this purpose, horizontal and vertical CH₄ and N₂O distributions of selected orbits are presented. Further, outside-vortex N₂O and CH₄ data from before and after the split-up as well as outside- and inside-vortex N₂O and CH₄ data are correlated. By correlation of ozone with CFC-11 we attempt to gain information on ozone variations during the split-up.

Observation of ClO by MIPAS/ENVISAT before and during the Antarctic vortex split in September/October 2002

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We present ClO measurements by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) on board of the European research satellite ENVISAT (ENVironmental SATellite) between September 8 and October 13, 2002. Retrievals were performed at the Institute for Meteorology and Climate Research Karlsruhe (IMK), using level 1-B spectra provided by the European Space Agency (ESA). The results shown here are the first ClO profiles retrieved from MIPAS spectra.

During the investigated period the Antarctic polar vortex encountered an unusual major warming, which started around September 20 and led to a vortex-split at September 25 and subsequent dissolution of one of the vortex fragments into midlatitude air. Such an event had never before been observed since the beginning of regular Antarctic measurements in the 1950's.

MIPAS measured high ClO volume mixing ratios of up to 2.5 ppbv from September 8 until September 20 in the dayside lower antarctic stratosphere, i.e. before and at the beginning of the major warming. Thereafter, the PSCs disappeared and ClO rapidly decreased. After September 23 MIPAS did no longer observe significant amounts (> 1 ppbv) of ClO.

The temperature and CO₂ abundance of the mesosphere and lower thermosphere as measured by MIPAS/ENVISAT

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The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) is a high-resolution limb sounder on board the ENVISAT satellite, successfully launched on March 1, 2002. MIPAS has a wide spectral coverage, high spectral resolution (0.05 cm^{-1} , apodised), and high sensitivity, which allows to measure, simultaneously, the kinetic temperature, the CO₂ volume mixing ratio, and non-LTE populations of vibrational levels emitting at 15, 10 and 4.3 μm in the upper atmosphere.

This data set is very useful for better understanding the non-LTE in CO₂ and also the composition and energetics of the upper atmosphere. MIPAS scan the limb operationally from 6 km up to 68 km and up to higher altitudes for special modes of observations.

In this paper we present preliminary retrievals of temperature, CO₂ abundances and non-LTE CO₂-related parameters from MIPAS data taken in the upper atmosphere mode.

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