# Remote Sensing Technology Institute

Institut für Methodik
der Fernerkundung

**Status Report 2007 – 2013**

DLR

# Spectrometric Sounding of the Atmosphere

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**IMF carries out research on methods for extracting atmospheric state variables from remote sensing data. Based on these, we develop and implement algorithms and operational software systems for the continuous generation of data products.**

## Missions and Sensors

Since the quality of the derived atmospheric parameters not only depends on the capabilities of the retrieval procedures but also on the quality of the input data we invest considerably into acquiring the detailed knowledge of the construction and functioning of spaceborne atmospheric instruments.

### ENVISAT/SCIAMACHY

For spaceborne spectrometers, SCIAMACHY onboard ENVISAT can be regarded as a blueprint. GOME and GOME-2 are scaled-down versions of the highly sophisticated SCIAMACHY design.

SCIAMACHY observed scattered and reflected spectral radiances in nadir and limb geometry, the spectral radiance transmitted through the atmosphere in solar and lunar occultation geometry and the extraterrestrial solar irradiance and lunar radiance in the UV-VNIR-SWIR range.

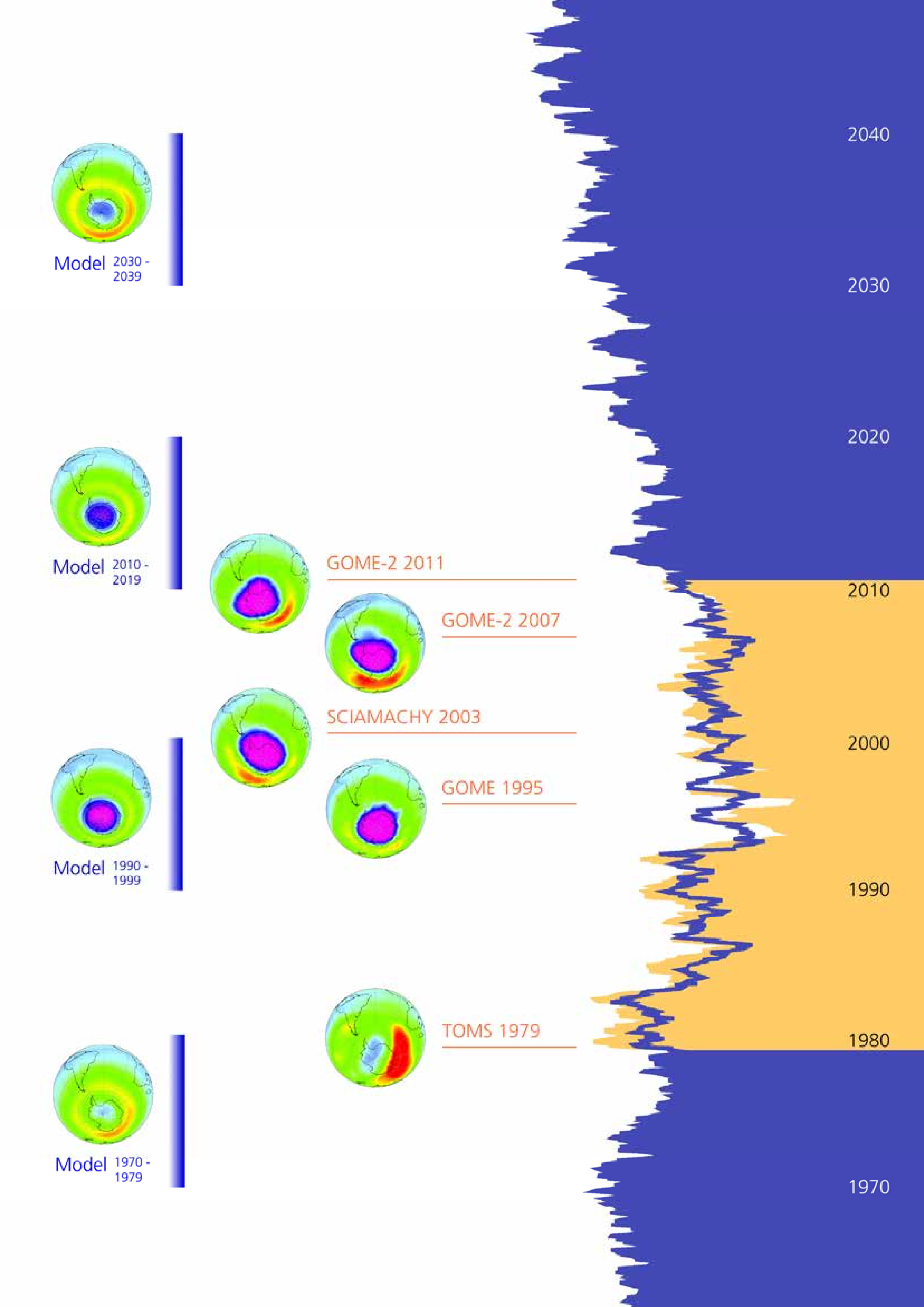
The nadir mode yields total column measurements. From limb observations height resolved profiles of atmospheric parameters as well as cloud height and cloud type information are retrieved. A unique feature of SCIAMACHY was the ability to operate the instrument in such a way that nadir and limb observations could be combined to yield tropospheric information, known as limb/nadir matching.

Because of the AO character of SCIAMACHY with DLR being one of the sensor providers, a large share of instrument operations and data processing tasks were assigned to IMF. This occurred in collaboration with ESA and other scientific facilities in Germany, the Netherlands and Belgium.

Rather challenging is the SCIAMACHY level 1b-2 processing since it combines different retrieval methods and code modules in one operational processor. It also has to reflect SCIAMACHY's multiple viewing geometries. The individual algorithms were developed by IMF, University of Bremen, BIRA Belgium and KNMI and were implemented by us. A rigorous verification scheme ensures that all algorithms are correctly operationalized, i.e. converted from the scientific prototype into an implementation that fulfills the requirements of the operational processing environment.

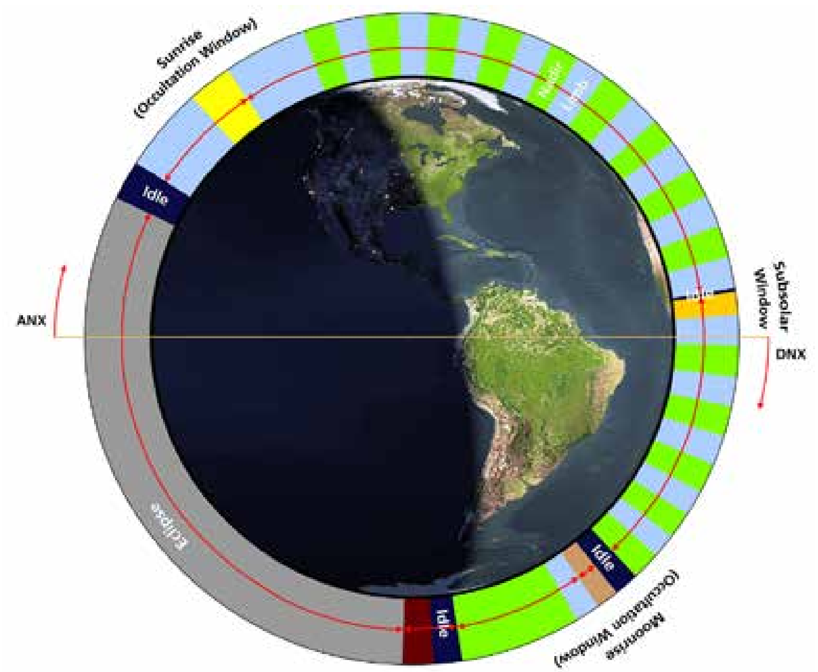
For the entire mission duration, IMF contributed considerably to the tasks of SCIAMACHY operations including mission planning, instrument configuration control configuration status and instrument performance monitoring. For this purpose the national SCIAMACHY Operations Support Team (SOST) had been established with personnel from IMF and University of Bremen. In the routine mission phase SOST was ESA’s single technical counterpart for SCIAMACHY instrument operations.

**Time profile of the ozone anomaly between 60°N and 60°S from spaceborne measurements for the period 1979 – 2011 (yellow), compared to the prediction of a climate-chemistry model (Institute of Atmospheric Physics) between 1960 and 2050 (blue). For selected years the observed ozone hole over Antarctica is illustrated together with model displays spanning one decade each.**



2040
2030
2020
2010
2000
1990
1980
1970
Model 2030 - 2039
Model 2010 - 2019
Model 1990 - 1999
Model 1970 - 1979
GOME-2 2011
GOME-2 2007
SCIAMACHY 2003
GOME 1995
TOMS 1979


SCIAMACHY availability between 2002 and 2012. The very high duty cycle was an outstanding achievement and made SCIAMACHY a reference sensor on ENVISAT.




Complex measurement sequence within a SCIAMACHY orbit consisting of nadir, limb and Sun occultation observations with occasional subsolar and lunar occultation data acquisitions

In 2007 SCIAMACHY reached its specified mission lifetime and the mission extension, running until the end of 2013, commenced. Up until October 2010, routine SOST tasks did not differ considerably from those of the first five years of the mission. The high duty cycle of > 90 % could be maintained. Of particular importance was our quantitative estimate of additional roll, pitch and yaw mispointing angles which reduced the error of line-of-sight pointing knowledge to ±150 – 200 m, about an order of magnitude better than originally specified. Thus the capabilities of the limb data could be fully exploited.

In October 2010 the ENVISAT mission extension required lowering the platform orbit by about 17 km. In cooperation with EADS-Astrium we re-configured SCIAMACHY thus maintaining the excellent optical and pointing performance in the operational phase following the orbit maneuver. When the ENVISAT platform was struck by a fatal anomaly on April 8, 2012, causing the loss of the mission, SCIAMACHY was still in very good shape.

Throughout the mission new science requirements, e.g. regular observations of the mesosphere and lower thermosphere, were successfully implemented considerably improving SCIAMACHY's science output. One of the most challenging tasks occurred when we prepared and executed spectral studies of the atmosphere of Venus. Originally intended for calibration purposes they also delivered science information about the Venusian atmosphere with surprisingly detailed IR spectra of our nearest neighboring planet.

Selected publications: [141], [413], [426], [491], [615], [626], [713], [807], [849], [979]

### ERS-2/GOME

Acknowledging the fact that a European spaceborne mission had urgently been required at the end of last century, ESA embarked on a 'fast-track' activity GOME onboard the ERS-2 platform. Only a nadir mode for the UV-VNIR range was implemented. While the nominal swath width of 960 km remained identical to that of SCIAMACHY, the ground pixel resolution was inferior at 320 × 40 $km^2$ as compared to SCIAMACHY’s 26 × 30 $km^2$.

Between 1995 and 2011, IMF, in collaboration with partner institutes, developed the algorithms and operated the processors for the generation of operational near-realtime, offline and reprocessed GOME level 1 and level 2 products.

The data from GOME continues to be used as the reference for the generation of climate data records and also as test-bed for the development and validation of new retrieval algorithms and improved versions of our UPAS level 2 processor.

Selected publications: [113], [204], [259], [262], [303], [461], [775], [828], [854]

### MetOp/GOME-2

By operating GOME-2 on MetOp, a satellite series consisting of three platforms, GOME-type measurements will be available far into the 21st century. The GOME-2 swath can reach up to 1,920 km and the spatial resolution, when the swath is reduced by a factor of 2, reaches 40 × 40 $km^2$.

The operational GOME-2 trace gas column and cloud products are provided by EUMETSAT’s Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M-SAF). During the first Continuous Development and Operations Phase (CDOP) of the O3M-SAF, which started in 2007 and lasted for five years, we developed GOME-2 trace gas column algorithms and cloud parameters. The operational retrieval of these products used our well-established GOME Data Processor (GDP). Services provided by the O3M-SAF at EOC occur in near realtime, offline and reprocessing mode. They focus on climate and air quality monitoring applications.

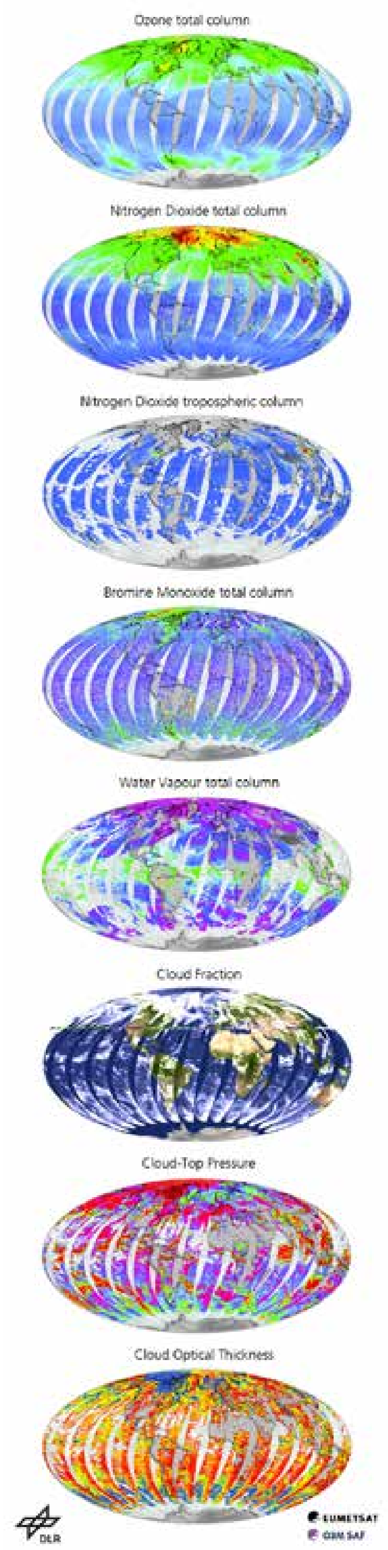
In February 2012, the CDOP-2 started, which will run until 2017. During CDOP-2 we will develop new and improved products, implement new dissemination methods and enhance user services.

Selected publications: [112], [124], [151], [170], [225], [445], [461], [828], [836], [856]

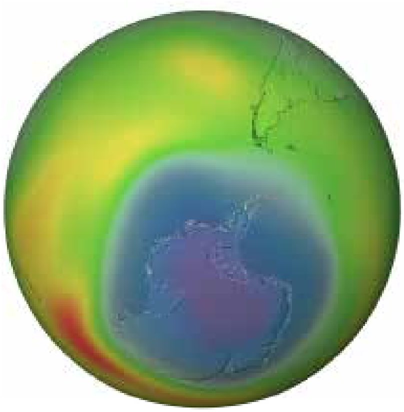
### Sentinel-5 Precursor

With GOME-2, we successfully made the transition from ESA research missions (GOME and SCIAMACHY) to operational EUMETSAT missions and services. All experience gained with the O3M-SAF can be regarded as a big asset in the preparation for our engagement in future Copernicus atmospheric missions, such as Sentinel-5 Precursor (S5p), Sentinel-4 and -5, aiming at the provision of global information on atmospheric composition for operational applications on air quality and climate. The first of these will be S5p. Its TROPOMI payload will measure solar radiance and irradiance in the UV-VNIR-SWIR range with an unprecedented spatial resolution of 7 × 7 $km^2$ at nadir in a 2,600 km wide swath.

IMF plays a central role in the processing and handling of the S5p data. Our main involvement in the development of the payload data ground segment concerns the provision of one of the level 2 processors. Level 2 algorithm and processor development occurs in the framework of a European-wide working group where we contribute our GDP expertise by:




**Atmospheric parameters operationally retrieved by IMF’s GOME-2 processing system UPAS in the framework of the O3M-SAF**



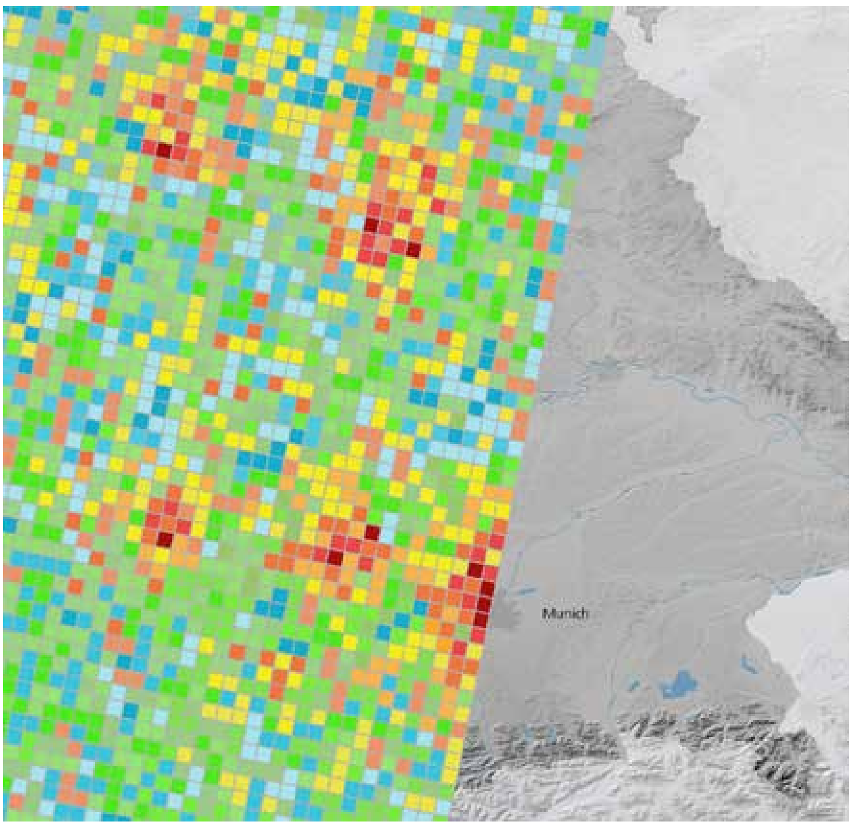
Ozone hole in 2009 over Antarctica as derived from GOME-2 data

- developing prototype algorithms and operational processors
- validating data products using independent retrieval algorithms.

In this context the new version of our level 2 UPAS processor (see below) must cope with a data rate exceeding that of GOME-2 by a factor of 100.

**Sentinel-4 and -5, CarbonSat**

Sentinel-5 Precursor will set the stage for the Sentinel-5 mission with its UV-VIS-NIR-SWIR spectrometer which is to be launched about half a decade later. Its prime focus lies on air quality and composition-climate interactions.




Simulation of a S5p track over Bavaria. For Munich the city boundary is given illustrating the very high spatial resolution of S5p.

The Sentinel-4 mission shall be launched one year prior to Sentinel-5. The platform carries two instruments, the thermal infrared sounder IRS and the Ultraviolet Visible Near-infrared spectrometer (UVN) taking measurements in the UV-VNIR range. With Sentinel-4, absorption spectroscopy for the purpose of atmospheric remote sensing will be made from a geostationary orbit for the first time. The observation repeat cycle period will be one hour, enabling the instrument to detect short-term changes of the atmosphere.

Even further into the future, CarbonSat may measure the global concentrations of the greenhouse gases carbon dioxide and methane under the provision that it is selected by ESA as one of the future Earth Explorer missions. With CarbonSat, the greenhouse status of the Earth's atmosphere will be available on short timescales and at very high spatial resolution of 2 × 2 $km^2$.

For all three planned missions, Sentinel-4 and -5 together with CarbonSat, IMF contributes to the definition of the level 0-1 processors, including generation of the Algorithm Theoretical Basis Documents, and key aspects of instrument calibration. It is our intention, once specific payload data ground segment functions are assigned, to play a central role in the areas of algorithm development and processing with particular focus on development of the level 2 processors.

| Mission/Sensor | Wavelength (nm) | Species |
|---|---|---|
| **ENVISAT/SCIAMACHY** | UV-VIS-NIR: 215 – 1063<br>SWIR: 1934 – 2044<br>2259 – 2386 | nadir: **$O_3$**, **$NO_2$**, **BrO**, **$H_2O$**, **$SO_2$**, **HCHO**, **OClO**,**CHOCHO**, **CO**, **$CH_4$**, **AAIA**, **clouds**<br>limb: **$O_3$**, **$NO_2$**, **BrO**, **clouds**<br>limb/nadir matching: **tropospheric $NO_2$** |
| **ERS-2/GOME** | UV-VIS-NIR: 237 – 794 | **$O_3$**, **$NO_2$**, **$H_2O$**, BrO, $SO_2$, HCHO, OClO, tropospheric $O_3$, tropospheric $NO_2$, **clouds** |
| **MetOp/GOME-2** | UV-VIS-NIR: 240 – 790 | **$O_3$**, **$NO_2$**, **$H_2O$**, **BrO**, **$SO_2$**, **HCHO**, **tropospheric $NO_2$**, **tropospheric $O_3$**, OClO, CHOCHO, **clouds** |
| **Sentinel-5 Precursor** | UV-VIS-NIR: 270 – 775<br>SWIR: 2305 – 2385 | **$O_3$**, **$SO_2$**, **HCHO**, **tropospheric $O_3$**, $NO_2$, tropospheric $NO_2$, BrO, **clouds** |
| **Sentinel-5** | UV-VIS-NIR: 270 – 775<br>SWIR: 1590 – 1675<br>2305 – 2385 | **$O_3$**, **$NO_2$**, **$H_2O$**, **BrO**, **$SO_2$**, **HCHO**, **tropospheric $NO_2$**, **tropospheric $O_3$**, OClO, CHOCHO, **clouds** |
| **Sentinel-4** | UV-VIS-NIR: 305 – 775 | **$O_3$**, **$NO_2$**, **$H_2O$**, **BrO**, **$SO_2$**, **HCHO**, **tropospheric $NO_2$**, **tropospheric $O_3$**, OClO, CHOCHO, **clouds** |
| **CarbonSat** | NIR: 757 – 775<br>SWIR: 1559 – 1675<br>2043 – 2095 | $CO_2$, $CH_4$ |
| **ADM-Aeolus** | UV: 355 | wind profiles |
| **MERLIN** | SWIR: 1645 | $CH_4$ |

**Suite of sensors used at IMF for the spectrometric sounding of the Earth's atmosphere. The listed target species are those where IMF contributed to the operational (bold) or scientific products either in processor or algorithm development. For future missions intended parameters are provided.**

## ADM-Aeolus

ADM-Aeolus is Europe's first lidar mission for atmospheric wind profiling. The Doppler instrument ALADIN will illuminate the atmosphere off-track from nadir with UV pulses at 355 nm and record the light backscattered by molecules and particles.

IMF's responsibilities for ADM-Aeolus are twofold. Firstly, on the basis of recent instrument characteristics IMF developed and refined several modules of the end-to-end instrument simulator. With our contributions, the laser pulse model is now able to handle backscatter on a single-pulse level. This enables a broad field of scientific investigations into heterogeneous atmospheric conditions and the impact of laser frequency jitter on measurement accuracy. In addition, instrument imperfections in the Fizeau-/Fabry-Pérot interferometers and the accumulation CCD can be modeled. Secondly, IMF has further improved and optimized the level 1b algorithms. Because of our scattering expertise, including exploitation of the IMF developed scattering database for spheroidal particles, one focus is on lidar signal scattering by aerosols, polar stratospheric and thin cirrus clouds. From this, recommendations for optimizing the algorithms and software of the operational level 1b processor will be set.

Selected publications: [106], [250], [322]

## MERLIN

Currently, DLR develops its first active spaceborne atmospheric sensor in the context of the Franco-German MERLIN mission. The goal is high precision retrieval of methane concentration. This requires accurate in-orbit performance of the differential absorption lidar instrument in combination with novel aspects for processor development. IMF contributes considerably to instrument related tasks. The success of MERLIN relies on optimum selection of the laser SWIR wavelengths at about 1.65 µm. By using our Py4CAtS line-by-line tool we performed atmospheric transmittance calculations and identified a suitable spectral region with strong methane absorption and minimal interference from other gases. Since a precise knowledge of the behavior of the instrument is of paramount importance for level 0-1 processing, we will invest considerably into the monitoring of MERLIN's in-orbit performance. Based on our experience with SCIAMACHY, IMF develops and implements a concept which provides the required information over long time scales.

We are also responsible for the level 0-1a and level 1a-1b processors. They will be based on algorithms established within MERLIN's science community. From these the reference prototype processor will be developed and implemented in a preoperational test environment. By adding ground segment specific interfaces and scheduling, the reference prototype will become the operational processor and will undergo a Factory Acceptance Test before final implementation.

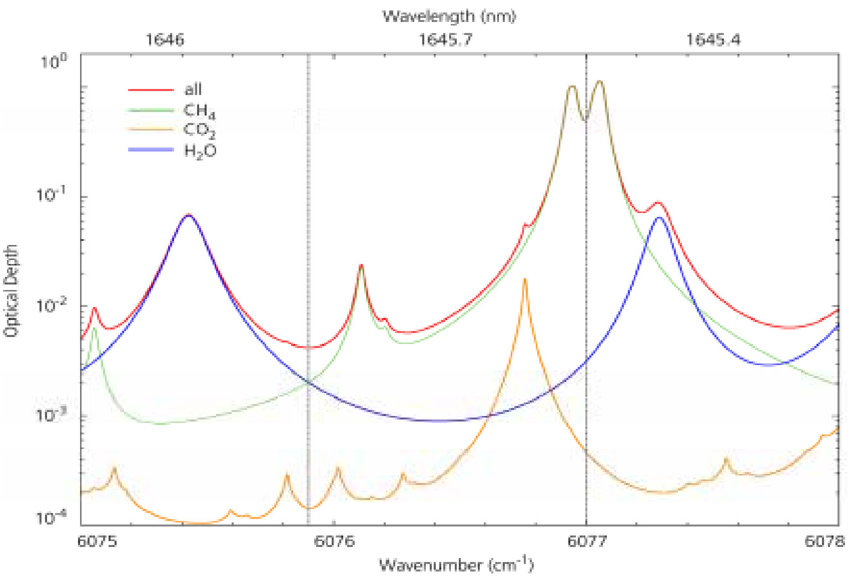
Selected publications: [41], [431]

**ENVISAT/MIPAS**

Our experience in this area includes e.g. Fourier transform laboratory spectroscopy and is long-standing. Therefore we contributed to investigating the in-orbit performance of MIPAS on ENVISAT. Our work characterized the detector degradation that causes a change in the nonlinearity. A corrective algorithm was implemented in the update of the MIPAS level 0-1 processor, thus facilitating analyses of drift effects such as temperature or water concentration.

Selected publications: [266], [301], [493]

**Optical depth for a vertical path through a tropical atmosphere. In addition to methane, water and carbon dioxide contribute significantly to the total optical depth. The vertical lines indicate the on- and offline wavelengths for MERLIN.**




**TELIS**

IMF operates TELIS, the terahertz and submillimeter limb sounder. This is a helium-cooled three-channel heterodyne spectrometer for trace gas measurements in the stratosphere. It was developed by IMF with major support from SRON. The detectors consist of a far-infrared (FIR) channel (1,790 – 1,870 GHz) and a submillimeter channel (450 – 650 GHz provided by SRON). The high spectral resolution and short exposure time result in a high vertical resolution of about 2 km, a pre-requisite for dynamical process studies.

To reach observer altitudes of up to 38 km, TELIS is part of the stratospheric balloon gondola provided by the Institute for Meteorology and Climate Research, KIT, together with the Fourier spectrometer MIPAS-B2. This TELIS/MIPAS-B2 platform is a unique chemistry mission allowing a practically complete coverage of all species relevant to stratospheric ozone. TELIS focuses on short lived species such as OH, ClO, BrO, HCl, $O_3$, HOCl, and $HO_2$. In addition, TELIS also measures species relevant for climate change such as water vapor and its isotopomeres ($H_2O$, $H_2{}^{17}O$, $H_2{}^{18}O$, HDO) or tracers (e.g. CO).

TELIS has successfully participated in three campaigns in Kiruna, Sweden, in the winters of 2009, 2010 and 2011. A further mid-latitude campaign is planned for 2014 in Canada.

The raw data for both channels is processed by us to yield radiometrically calibrated radiances together with the required auxiliary data. Extensive gas cell measurements allowed a front-end to back-end radiometric characterization under close to atmosphere conditions. Our instrument model enabled correction of radiometric errors caused by nonlinearities within the intermediate frequency chain. Other radiometric error sources, i.e. the unknown sideband ratios of the receivers, have been characterized in a series of quality-improving measurements, greatly profiting from IMF's new FT spectrometer BRUKER IFS 125 HR.

For the retrieval of geophysical parameters, i.e. molecular concentrations, we use the PILS code developed at IMF. It is based on the GARLIC forward model and DRACULA regularization modules and is applicable for microwave to mid IR limb emission spectra. For a quantitative assessment we have performed an exhaustive sensitivity study indicating that for OH nonlinearity effects, inaccurate sideband ratios and pointing are the dominant error sources. Furthermore, multichannel retrieval exploiting FIR and submillimeter data concurrently showed significant improvements for hydrogen chloride compared to single channel retrieval. The concentration profiles retrieved so far show good agreement with other instruments such as MIPAS-B2 or SMILES.

Selected publications: [27], [42], [78], [334], [577], [687]

# Generic Processing Systems

### Universal Processor for Atmospheric Sensors – UPAS

Operational level 2 processing systems translate the theoretical basics of radiative transfer, inversion and scattering into software tools applicable to calibrated level 1 data. Their structures require flexibility because ongoing research produces new retrieval algorithms which have to be incorporated to maintain state-of-the-art performance. IMF decided to develop UPAS, the Universal Processor for Atmospheric UV/VIS/NIR Sensors as a generic multi-mission system for the retrieval of trace gases and cloud properties. Since its operational readiness back in 2004, UPAS has been continuously improved and forms the backbone level 2 retrieval system at IMF.

UPAS follows an object oriented design and is implemented in C++ under Linux. It uses a client/server architecture for fast processing of satellite data on a cluster of multi-core computers. The settings of the retrieval algorithms can be easily changed using XML configuration files.

**Balloon campaign 2009, Kiruna/Sweden: TELIS and MIPAS-B (KIT) ready for lift-off**

Retrievals in UPAS are performed with the GOME Data Processor (GDP) version 4, which was implemented from the outset. We develop the corresponding algorithms together with the partner institutes BIRA (Belgium), University of Bremen and RTS Inc. (USA). Independent geophysical validation is performed by AUTH (Greece) and BIRA. The GOME total ozone products, generated by GDP4/UPAS, reached accuracies at the percentage level, comparable to that of ground-based sensors. The first version of UPAS was available for use in 2004 for the generation of operational GOME products. Presently, UPAS is being used for the reprocessing of SCIAMACHY nadir measurements and for the operational processing of GOME-2 data from MetOp-A and MetOp-B. The GOME-2 near-realtime products are generated in 10 minutes, thus achieving the challenging requirement of level 2 product dissemination in less than 2 hours from sensing. UPAS has turned out to be very robust and stable, it runs standalone in a 24/7 environment and already fulfills the operational requirements of the Copernicus program. A second generation of UPAS is under development in order to cope with the hundredfold increase in data volume expected from future missions.

Selected publications: [113], [151], [283], [303]

**Generic Calibration Processing System – GCAPS**

The design of level 0-1 processors should provide operational flexibility to ensure adaptability to different sensors while still possessing lean, programmer-friendly structures. The existing prototype processor for SCIAMACHY is IDL based and does not support bulk processing as required by ESA's reprocessing campaigns. Therefore we decided to transfer the corresponding algorithms existing at IMF into a new generic level 0-1 processing framework, GCAPS, the Generic Calibration Processing System. Its requirements include:

– provision of structures for controlling the data flow and configuring calibration chains
– instrument independency
– internal data representation independency from the input/output data formats
– full configurability by the user, i.e. switchable and changeable calibration steps
– processor multithreading.

These requirements led to a lean structure providing the basic functionality needed for level 0-1 processing. From this, one can build instrument specific processors by coding the relevant plug-ins and defining calibration chains in the configuration file. This framework also facilitates the cross-calibration of sensors. Because algorithms are easily exchangeable, one can use identical algorithms for a given calibration step and compare the results. Any remaining differences can then only be caused by different input data, but not by a given instrument specific algorithm.

Currently, we are implementing the plug-ins needed for the reprocessing of SCIAMACHY level 0 data. The resulting GCAPS version has been selected by ESA to become the new operational level 0-1 processor. It will also be used for the GOME level 0-1 processor update and will be the system of choice whenever IMF handles level 0-1 algorithm and processor development for future sensors.

# Methods and Applications

**Retrieval, or determining atmospheric characteristics from electromagnetic spectra, requires input data of the highest quality. For this reason we develop calibration algorithms for the entire suite of atmospheric sensors exploited at IMF. Furthermore, a deep understanding of radiative transfer, inversion and scattering is needed. We perform research activities aimed at either deriving known atmospheric state variables with the highest precision or at retrieving new parameters from remote sensing data.**

## Sensor Calibration Algorithms

The first step in the derivation of geophysical parameters from remote sensing data is the generation of level 1 data by applying the full sequence of calibration steps to the instrument raw data. At the end of this step the raw measurements have to be converted to physical quantities. IMF is actively pursuing:

– development of calibration algorithms

– conceptual design and development of operational processors.

The typical calibration chain for spectral imagers consists of:

– correction of detector effects such as nonlinearity, memory effect, pixel-to-pixel gain and etalon, smear and dark signal

– correction of instrument stray light

– spectral and radiometric calibration

– polarization correction

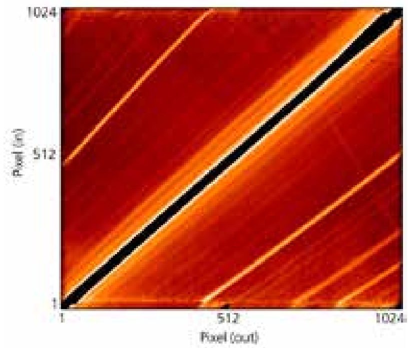
– correction/monitoring of any degradation effects such as dead and bad pixel mask.

Stray light correction and spectral calibration usually turn out to be the most difficult to implement. A full resolution stray light calculation requires a multiplication for each pixel of the CCD array with all other pixels and a subsequent addition of all contributions. However, this would consume too much time in level 0-1 processing. In addition, the corresponding on-ground reference measurements necessary as input would last much longer than what is usually assigned to calibration campaigns. Therefore practical solutions have to be found not jeopardizing the accuracy, e.g. finding a suitable reduction for the stray light matrix. For the Sentinel-4 UVN instrument, IMF is currently working on a solution to this problem.

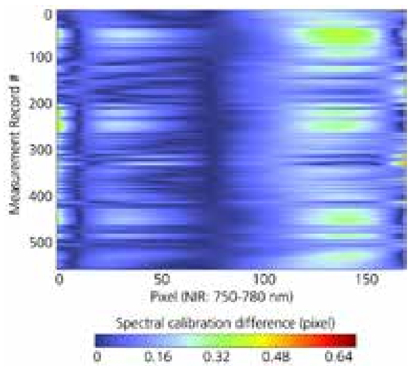
The main challenge in spectral calibration is that it has to use the spectrum itself together with a model to obtain the high accuracies needed for retrieval. Hence, non-observable characteristics such as an inhomogeneous illumination of the instrument slit already lead to an unacceptably high uncertainty in the spectral position of the detector pixels. Our studies aim at developing algorithms for spectral calibration, mitigating the impact of heterogeneous scenes and at performing corresponding error analyses.

For GOME and SCIAMACHY the level 0-1 processors have been developed by IMF and are still maintained and improved for post-mission reprocessing campaigns. Additionally, for several upcoming absorption spectroscopy type missions IMF has already adopted the task of developing the level 0-1 chain. Extending this work to active spectral instruments will even allow us to contribute the level 0-1 processing for MERLIN.

Selected publications: [262], [451], [453], [796]




**SCIAMACHY stray light in channel 5 on a logarithmic scale. Each row shows the stray light spectrum caused by unit input (y axis). The diagonal black region is defined as part of the slit function and free of stray light. Diagonal lines are caused by focus reflections of one part of the spectrum to another ('ghosts'). Since stray light introduces spectral artifacts which spoil retrievals, its portion in a spectrum has to be reduced to < 1 % of the relative signal changes. Stray light algorithms are instrument-specific. The experience gained from SCIAMACHY supports our efforts to establish solutions for Sentinel-4.**




**Comparison between spectral calibration of the GOME-2A nadir range using the onboard spectral line source and a spectral calibration derived from the spectrum itself. The latter method might be used to correct for spectral shifts caused by inhomogeneous scene illumination. Differences between the two approaches are shown in units of spectral pixels for measurements along one orbit.**

## Radiative Transfer

Inverse problems in atmospheric remote sensing are frequently solved by nonlinear optimization where forward models play a central role. Modeling the radiative transfer (RT) through the atmosphere along with the instrument response and the performance of the model has a crucial impact on the success of the retrieval. The accuracy of the model is decisive for the quality of the retrieved atmospheric state parameters, however, approximations are mandatory to speed up the code especially for operational level 1-2 processing where millions of spectra have to be analyzed.

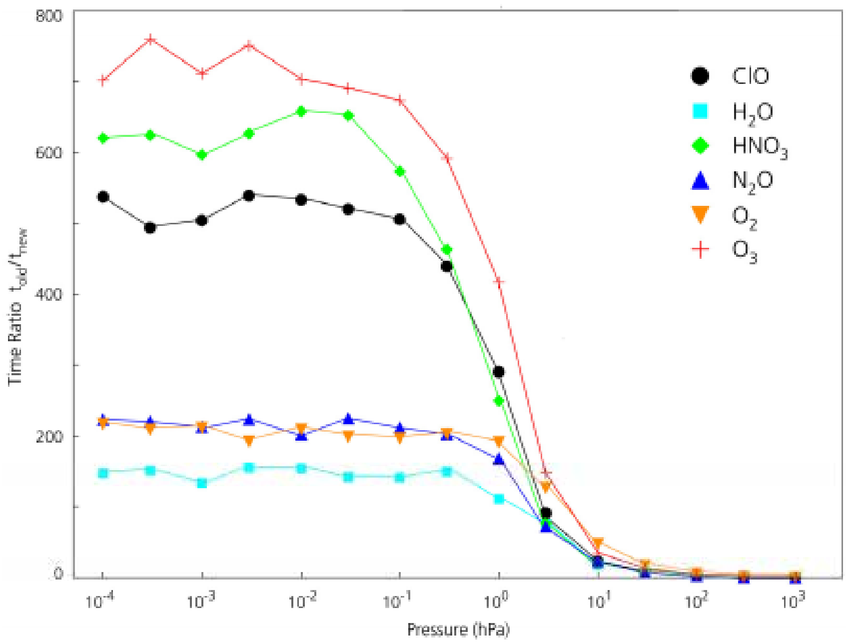
The challenges for RT modeling depend on the spectral region of interest. In the UV band multiple scattering of radiation requires the solution of an integro-differential equation, whereas in the microwave and IR bands molecular absorption has to be evaluated using time consuming line-by-line (LBL) models. An example for an IR LBL radiative transfer with multiple scattering is outlined later in the section on exoplanets.

*Infrared and Microwave*

In the infrared and microwave range, LBL models are essential tools for the analysis of high resolution spectra, and are mandatory for generating and verifying fast parameterized RT models. They are computationally demanding because the combined effect of collisional and Doppler broadening described by the Voigt profile has no analytical expression. Dozens of algorithms have been developed in the past, usually exploiting different approximations for different regimes of the function arguments. However, this conditional evaluation makes code optimization difficult or impossible, so we developed a new algorithm combining two rational approximations for small and large argument values.

Even with a highly optimized Voigt function algorithm, the large number of function evaluations required for high resolution RT modeling necessitates further optimization, and we have further accelerated our codes using a multigrid approach where the function is evaluated on a dense grid only near the line center and coarser grids are used elsewhere. Using three grids increased the speed by about two orders of magnitude for typical IR/microwave applications.

In the last decade novel computing architectures have gained increasing attention and we have investigated field programmable gate arrays to accelerate LBL modeling. First tests with a version currently under development show a speed-up of almost two orders of magnitude compared to conventional CPUs.




**Computational gain, i.e. ratio of execution time of the three-grid algorithm for evaluation of molecular cross-sections in the microwave spectral regime. The pressure range corresponds to altitudes up to 100 km. Because spectral lines become narrower with increasing altitude, the computational savings are especially important for small pressures.**

The multigrid Voigt algorithm constitutes the core of our LBL program GARLIC that is used extensively for a variety of Earth remote sensing applications and, more recently, also for the modeling and analysis of planetary spectra. A Python implementation of the LBL routines enabling cross-section and optical depth calculations from HITRAN and GEISA data has been made publically available in the context of an ESA study.

For the iterative solution of nonlinear inverse problems, derivatives of the spectra with respect to the parameters to be fitted are required in addition to the spectra themselves. Finite difference approximations are time-consuming and subject to truncation or cancellation errors, whereas hand-coding derivatives in the forward model are tedious and error-prone. The retrieval codes built up using GARLIC as the forward model utilize automatic differentiation techniques that allow for quick implementation of the exact Jacobians.

*Ultraviolet and Visible*

In anticipation of the huge amount of data to be delivered by the new generation of European UV/VNIR atmospheric composition sensors such as S5p, fast and accurate RT models for simulating satellite-based measurements in a cloudy atmosphere are required. We developed DOME, a software tool that includes as a forward model the discrete ordinate method with matrix exponential, and SAM, the small-angle modification of the RT equation. In the latter approach, the solution of the RT equation under the small-angle approximation is subtracted from the total radiance; the resulting radiance field is much smoother than the diffuse radiance and the method is more appropriate for modeling strongly anisotropic scattering.

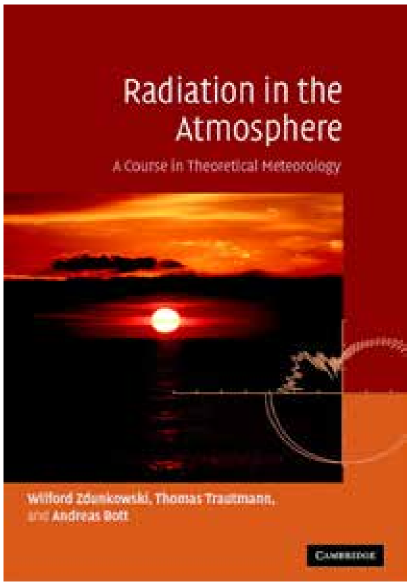
The discrete ordinate method with matrix exponential and the small-angle modification of the RT equation have been equipped with several acceleration techniques. These include:

- the left eigenvectors matrix approach for computing the inverse of the right eigenvectors matrix
- the telescoping technique
- the method of false discrete ordinate

and provide a considerable increase in relative speed.

A further reduction of the computational time by a factor of 4 – 6 has been achieved by using various dimensionality reduction techniques for the optical parameters of an atmospheric system. Besides principal component analysis, these techniques include local linear embedding methods (locality pursuit embedding, locality preserving projection, locally embedded analysis) and discrete orthogonal transforms (cosine, Legendre, wavelet).

For a better understanding of the influence of real cloud fields on trace gas retrievals, we developed deterministic and stochastic multi-dimensional RT models. The deterministic model solves the integral form of the RT transfer equation by the Picard iterative method. This method, which is a successive order of scattering solution method, computes the radiance field on a discrete spatial grid with the angular distribution represented in a spherical harmonic series. The radiance field can be computed by using first- and high-order difference schemes equipped with interpolation and flux conservation error calculations, or by employing the Galerkin method. Moreover, the adaptive grid technique improves the solution accuracy by increasing the spatial resolution in regions where the source function is changing more rapidly.




**Monography on Radiative Transfer co-authored by Thomas Trautmann, IMF**

The multi-dimensional scalar SHDOM for solving the radiative transfer equation

$$\frac{d\mathbf{I}}{ds}(\mathbf{r},\mathbf{\Omega}) = -\sigma_{ext}(\mathbf{r})[\mathbf{I}(\mathbf{r},\mathbf{\Omega}) - \mathbf{J}(\mathbf{r},\mathbf{\Omega})]$$

has also been extended to the vector case. The vector model uses complex and real generalized spherical harmonics in the energetic representation of the Stokes vector,

$$\mathbf{J}_{nm} = \frac{\omega}{2}\mathbf{G}_n\mathbf{I}_{nm} + \frac{\omega}{2}\mathbf{G}_n\mathbf{Y}_{nm}^{H}(-\mu_0,\varphi_0)\mathbf{F}_0\boldsymbol{e}^{-\tau_{ext}^{sun}}$$

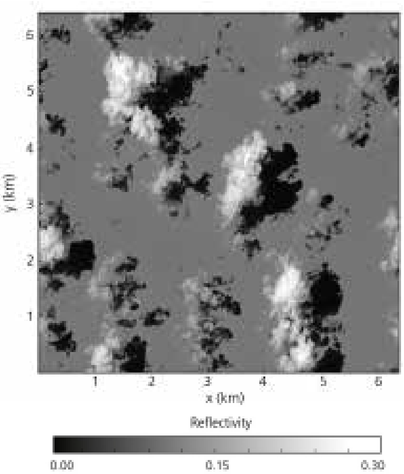
and retains some powerful features of the scalar model, as e.g. the combination of the generalized spherical harmonic and the discrete ordinate representations of the radiance field, the use of a linear short characteristic method for computing the corner-point values of the Stokes vector, and the application of the adaptive grid technique.

*Monte Carlo Methods*

Deterministic methods solve the radiative transfer equation by discretizing the spatial coordinates, thus enabling accurate solutions of approximate models. On the other hand, Monte Carlo methods simulate radiation-matter interactions according to their probability and hence find approximate solutions of (stochastically) accurate models. Monte Carlo methods are especially suited for RT simulations in arbitrarily complex scenes, e.g. including inhomogeneous 3D clouds and surfaces.

We have developed MoCaRT, a flexible Monte Carlo Radiative Transfer model with special focus in 3D radiation effects. Variance reduction, e.g. stratified maximum cross-section, weighted scattering, continuous absorption, regionalization, and further acceleration techniques, such as parallelization and Russian roulette, are used to achieve fast and accurate convergence. Using MoCaRT together with stochastic generation of subscale variability enabled us to characterize cloud heterogeneity effects on radiances and fluxes and to reduce the radiation biases.

Selected publications: [3], [16], [17], [19], [20], [21], [33], [147], [148], [149], [155], [166], [229], [252], [277], [450], [452]




**MoCaRT-simulated reflectivity in a cumulus field with 10 × 10 m² resolution provided by the Parallelized Large-Eddy Simulation model. The size of the domain is 6.4 × 6.4 km². The reflectivity field was convolved with the instrumental response function of MERIS channel 6 around the oxygen A-band.**

**Inversion and Retrieval**

The retrieval problems arising in atmospheric remote sensing belong to the class of discrete ill-posed problems. These problems are unstable under data perturbations and can be solved by numerical regularization methods where the solution is stabilized by taking additional information into account.

IMF has developed the DRACULA (aDvanced Retrieval of the Atmosphere with Constrained and Unconstrained Least squares Algorithms) regularization tool for retrieval of atmospheric state parameters from a variety of atmospheric sounding instruments. The regularization tool communicates with the forward model via a subroutine which computes the spectra and the Jacobian matrix at any given iteration.

DRACULA includes direct and iterative regularization methods, based on different principles. The rationale for this is twofold: Firstly, for a specific application, we may select the optimal approach from the point of view of accuracy and efficiency. Secondly, for the operational use the control parameters of a specific regularization can be determined in advance by a comparison of several methods.

From the class of direct methods Tikhonov regularization is the most representative. In this approach the objective function involves an additional penalty term which depends on the regularization matrix and the regularization parameter. In the

DRACULA implementation of Tikhonov regularization, the regularization matrix can be chosen as the Cholesky factor of an a priori profile covariance matrix, or as discrete approximations to the first- and second-order derivative operators. An appropriate estimate of the regularization can be computed by using a priori, a posteriori and error-free parameter choice. From the second category, we mention the discrepancy principle, the error consistency method, and the unbiased predictive risk estimator method, while the third category comprises the generalized cross-validation, the maximum likelihood estimation, the quasi-optimality criterion, and the L-curve method. The efficiency of the algorithm is increased by using step-length and trust-region methods for minimizing the Tikhonov function. In these methods, the new iterate can be computed by means of several algorithms based on the singular value decomposition of the standard-form transformed Jacobian matrix, the bi-diagonalization of the Jacobian matrix, and on iterative methods using a special class of preconditioners constructed by means of the Lanczos algorithm.

In some applications, the Tikhonov function may have many local minima, and a decent method for solving the optimization problem tends to get stuck especially for severely ill-posed problems. In this case, iterative regularization methods are a good alternative. In iterative regularization methods the number of iteration steps plays the role of the regularization parameter, and the iterative process is stopped after an appropriate number of steps in order to avoid an uncontrolled expansion of the noise error. DRACULA incorporates several iterative approaches, including:

– the nonlinear Landweber iteration
– the iteratively regularized Gauss-Newton method
– the regularizing Levenberg-Marquardt method
– the Newton-CG method
– asymptotic regularization methods.

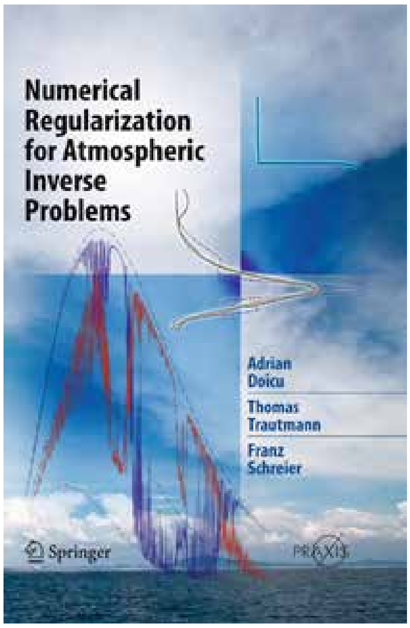
These approaches are insensitive to overestimation of the regularization parameter, do not depend on a priori information, and can be applied to large-scale problems.

Additionally, the regularization tool contains special direct regularization methods such as:

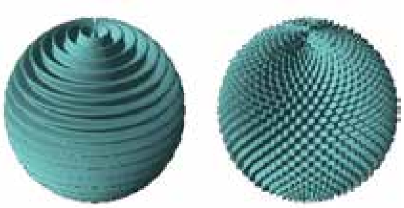
– the regularized total least squares method which is attractive when the Jacobian matrix is inexact,
– mollifier methods, in which the generalized inverse is constructed by means of a priori information,
– the maximum entropy regularization, which uses the relative or cross entropy as non-quadratic penalty terms.

DRACULA has been applied to data processing for SCIAMACHY, MIPAS, GOME, and more recently, for GOME-2 and IASI. Furthermore it is used for the analysis of observations of the balloon-borne FIR limb sounder TELIS mentioned before.

In some cases only vertical column densities rather than altitude dependent concentration profiles are needed and the complexities of regularization can be avoided. Accordingly, for analysis of SCIAMACHY SWIR nadir observations we have developed the Beer Infrared Retrieval Algorithm (BIRRA) that embraces an optimized forward model built from our GARLIC code embedded in a separable nonlinear least squares fit. It takes into account that some of the unknowns enter the forward model linearly. BIRRA is part of the operational SCIAMACHY level 1-2 processor and is used for retrieval of carbon monoxide and methane vertical column densities. Furthermore, we use BIRRA in a prototype fashion for scientific purposes, e.g. for retrieval of methane from Japan's




**Monography on regularization for atmospheric inverse problems by IMF authors Adrian Doicu, Thomas Trautmann and Franz Schreier**



Chebyshev particles with 2D (left) and 3D (right) surface geometry used to model light scattering on particles with a small-scale surface roughness

GOSAT. Likewise variants of BIRRA are applied to the exploitation of thermal IR nadir sounding data from AIRS and IASI.

Selected publications: [190], [230], [231], [290], [334], [429], [716], [813], [972]

**Electromagnetic Scattering**

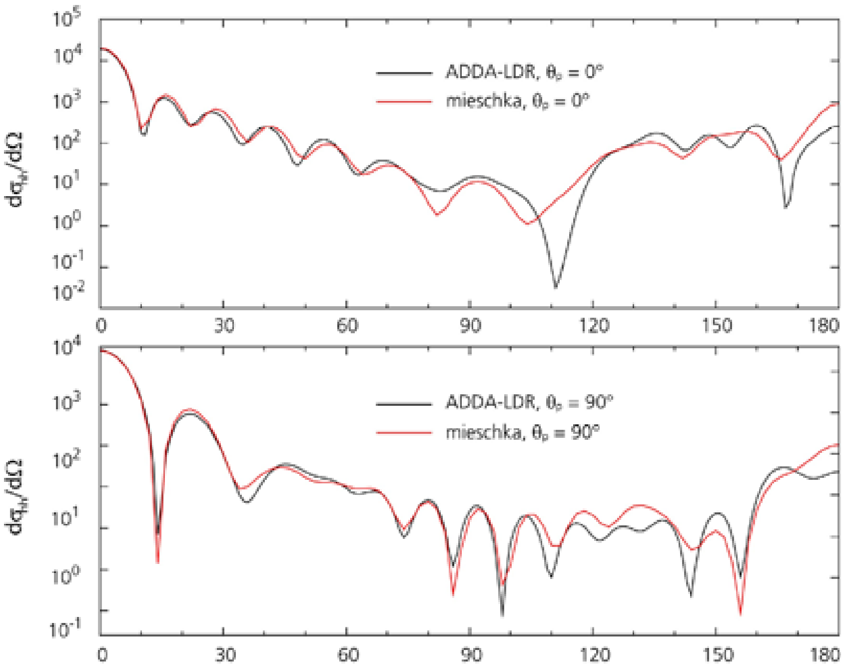
Electromagnetic wave scattering is a basic physical process which has to be considered in a wide variety of different remote sensing techniques. At IMF emphasis has been put on light scattering modeling at non-spherical particles. Based on a sophisticated Green's function approach a reliable T-matrix code was developed that has proven to be quite flexible. This software was used to establish a scattering database aimed at relieving the user of the large numerical effort and the complex accuracy considerations which are necessary in the context of non-spherical light scattering modeling. It was applied to several realistic scattering situations, and compared to other approaches to increase its reliability.

The scattering database contains more than 100,000 precalculated light scattering data sets of randomly oriented spheroidal particles in the resonance region. These entries possess a specified accuracy permitting their use as a benchmark for other methods. The database also provides a sophisticated user interface that was developed to facilitate data access. It provides additional functionalities such as interpolation between data or the computation of size-averaged scattering quantities.

A rather subtle issue of non-spherical particle geometry is small-scale surface roughness. 2D and 3D Chebyshev particles are used as a first geometric approach to study such surface effects in light scattering. T-matrix computations are usually plagued by ill-conditioning problems, especially for large size parameters. A combination of group theoretical methods with a Green's function approach which has the form of the Lippmann-Schwinger equation,

$$G(x,x') = G_0(x,x') + \oint_{\partial\Gamma} \Sigma_{\partial\Gamma}(x,\overline{x}) \cdot G(\overline{x},x')\, d\overline{x}$$

was successfully developed for the iterative solution of the T-matrix to overcome this problem. It was demonstrated that neglecting such surface effects in the interpretation of remote sensing data (e.g. lidar data) may result in large errors.




Polarized differential scattering cross sections (horizontal-horizontal) of an oblate spheroid with a volume-equivalent size parameter of 15, an aspect ratio of 0.67, and a complex refractive index of 1.6 + i · 0.0005 at a plane wave incidence along the minor semi axis (top: $\theta_p = 0°$) and the major semi axis (bottom: $\theta_p = 90°$). Results have been obtained by using the discrete dipole approximation code ADDA (black) and MIESCHKA (red).

Together with colleagues from the University of Novosibirsk (Russia) and SMHI (Sweden), calculations for different particle geometries have been performed to test the range of applicability and reliability of our own T-matrix program as well as other publicly available scattering programs. The programs under consideration were either different implementations of T-matrix methods or of the discrete dipole approximation. We could show that the fulfillment of the reciprocity condition can be used with benefit to estimate the accuracy of the scattering results obtained by the different programs. It turned out that reciprocity is highly sensitive to numerical inaccuracies, and that it is a much stronger criterion than energy conservation. We further demonstrated that the widespread discrete dipole approximations are more intricate due to the complex interplay between the different polarizability models needed in these approximations and the considered scattering configuration. Simply relying on the latter methods may lead to highly erroneous results, especially if higher size parameters and higher refractive indices of the particles are considered.

Selected publications: [106], [144], [250], [430]

**Spectroscopic References**

The retrieval of atmospheric parameters from remote sensing data requires quantitative knowledge of molecular absorption features for radiative transfer calculations. Therefore, a number of databases (HITRAN, GEISA, etc.) exist, providing the necessary information such as line parameters or absorption cross-sections. These databases must undergo permanent update, either for improving their completeness and accuracy or because new missions have additional needs.

IMF operates a spectroscopic laboratory for contributing parameters with defined uncertainties to spectroscopic databases covering the range from UV to millimeter wavelengths. One of the key topics of our laboratory work concerns the quality of the data. Numerous sources contribute to it. Their characterization requires expertise in many fields such as instrumentation, preparation of gaseous samples and data analysis procedures. Our laboratory belongs to the few world-wide capable of providing spectroscopic data with well-defined error bars. Our team is part of the HITRAN scientific advisory committee.

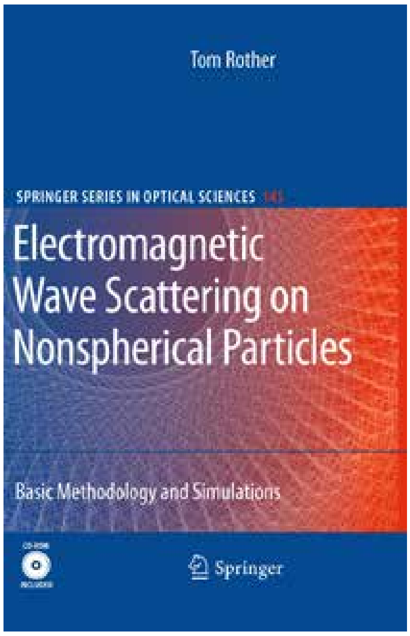
The laboratory spectroscopy facility was utilizing a commercial high resolution Fourier transform spectrometer (Bruker IFS 120HR, spectral range from NIR to millimeter wave) until 2009, which meanwhile has been replaced by the successor model IFS 125HR (UV to millimeter wave). When laboratory work is aiming at highest quality particular attention has to be paid to the absorption cells. In our laboratory four cells are available, all designed by ourselves. They cover the temperature range of 190 – 1,000 K and absorption path lengths from 0.16 m to 120 m. One cell is equipped with two window pairs for measuring different spectral regions such as UV/MIR or MIR/FIR for the same gas sample. A flow system and gas handling system allows synthesizing all relevant atmospheric constituents. An 800 liter mixing chamber and calibrated pressure and temperature sensors permit generating defined gas/air mixtures.

Software for data processing has been developed for:

– correction of instrument errors including detector nonlinearity, channeling and sample/instrument thermal emission

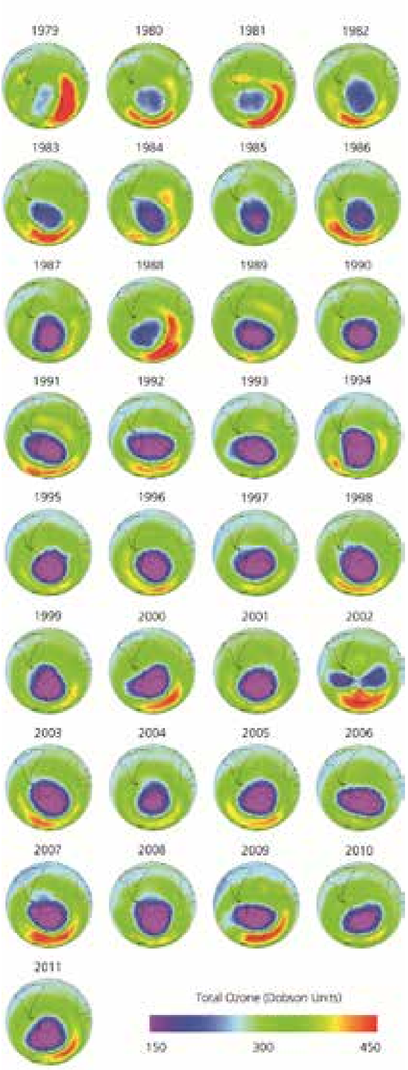
– line fitting building on more than 10 years of experience with the FitMAS code

– calculation of line positions, line strengths, pressure broadening and




**Monography on Electromagnetic scattering on nonspherical particles by Tom Rother, IMF**

**IMF-developed absorption cell for the Bruker IFS 125HR sample compartment with an absorption path of 22 cm, applicable to a temperature range 190 – 350 K. The cell body is a double-jacketed glass tube. The windows are mounted on stainless steel flanges coated with PFA. The window openings with baffles can be seen.**




**Evolution of the ozone hole over Antarctica derived from satellite measurements between early October 1979 until 2011. From 1995 on data from GOME, SCIAMACHY nad GOME-2 are used. Earlier measurements are provided by US missions.**

line shifting from line fit results of multiple spectra. The resulting certified data can be stored in an extended HITRAN database format.

Of the results obtained in the past years, a few are particularly worth mentioning:

- new NIR $H_2O$ database: Within the framework of DLR's WALES project measurements of water/air mixtures in the temperature range 230 – 318 K at 80 m absorption path were carried out. Data reduction required the speed-dependent Voigt line profile in order to model the spectral features to the noise level.
- Reanalysis of MIR $H_2O$ regarding pressure broadening with consolidated error bars.
- ClOOCl cross-sections: Application to arctic balloon-borne measurements permitted, for the first time, retrieval of concentration profiles. The proof of ClOOCl constitutes an important milestone in the understanding of polar ozone loss.
- HITRAN updates: The content of this database could be improved for $H_2O$ line intensities and broadening in the mid- and near-infrared, MIR ClO line intensities, and ClOOCl mid-infrared absorption cross sections.

Present work includes improvement of the spectroscopic database for $BrONO_2$, $H_2O$ and $CH_4$ in the mid-infrared. The current absorption cross sections for $BrONO_2$, a reservoir for bromine, are only known to 20 % accuracy. Improved spectroscopic data will help to quantify the inorganic bromine budget in the atmosphere which is important for mid-latitude ozone chemistry.

Selected publications: [68], [221], [249]

**Long-term Observation of Ozone**

The Global Climate Observing System identified a number of Essential Climate Variables (ECVs) required to support the climate research community. The ECVs largely depend on satellite observations from several missions covering different domains of the Earth system: atmospheric, oceanic and terrestrial.

Today European satellite missions provide 18 years of atmospheric composition data. Using these, a first version of a homogenized global ECV, total ozone, was created at EOC. It covers the period 1995 – 2011 and uses data from GOME, SCIAMACHY and GOME-2, supplemented by NASA data starting in 1979. This formed the basis for a first comparison with ground-based measurements and an initial evaluation of a coupled climate-chemistry model in collaboration with DLR's Institute of Atmospheric Physics (IPA).

The evaluation of results derived from numerical modeling with observations provides indications about the quality of the applied model which partly reflects our current understanding of atmospheric processes, their causes and how interactions lead to changes in atmospheric behavior. We could show that the ozone anomalies are well reproduced by the E39C-A climate model from IPA. There is a good agreement between the latitudinal, global, seasonal and decadal effects measured by the satellites and predicted by the model. Having verified that the model prediction is a reliable forecast for past and current stratospheric ozone, we could thus use the model simulations as an indicator for when the ozone layer will build up again such that the conditions for ozone depletion over Antarctica will vanish. Our calculations indicate that we have just left the overall minimum in ozone concentrations and are beginning a slow recovery. In about 30 – 40 years we can expect that the state of stratospheric ozone will be similar to the status assumed for the early 20th century.

This work was awarded the DLR's Science Prize in 2011.

In the ESA ozone CCI project we are responsible for the generation of the total ozone ECV and system engineering tasks. The second version of the total ozone ECV using improved retrieval algorithms reaches accuracies at the percent level per decade.

Selected publications: [241], [436], [444]

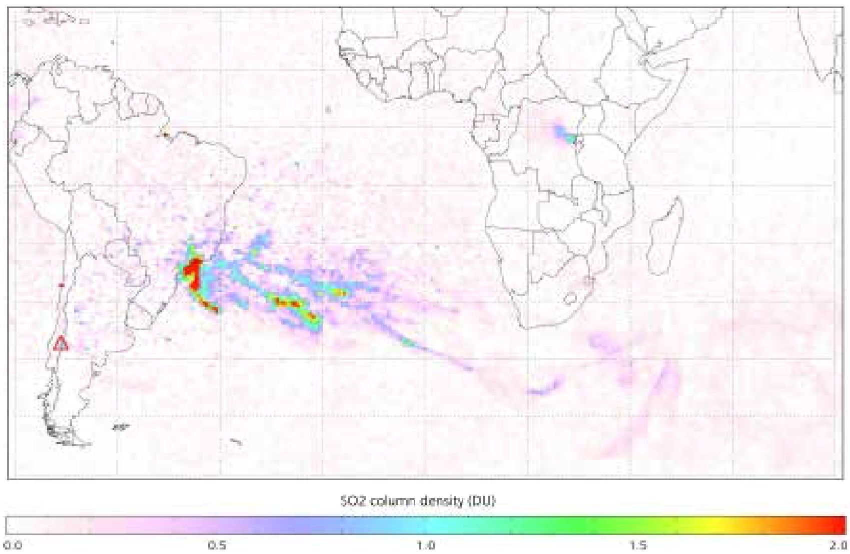
**Volcanic Sulphur Dioxide from Space**

Spaceborne atmospheric sensors like GOME-2 on the MetOp satellites enable the detection of the emissions of volcanic gases such as sulphur dioxide ($SO_2$) and aerosols, and hence the monitoring of volcanic activity and eruptions on a global scale. This is of great importance since volcanic eruptions are a major natural hazard, not only to the local environment and populations near large volcanoes but also to aviation.

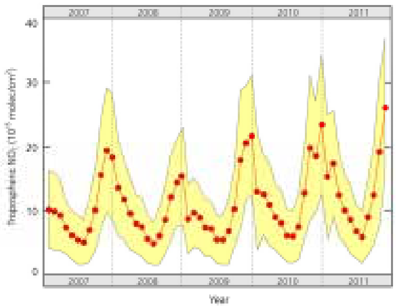
The retrieval of volcanic $SO_2$ emissions using the GOME-2 instrument is performed by IMF within the framework of EUMETSAT's Satellite Application Facility. The high spectral resolution of the instrument allows the retrieval of the total column density of $SO_2$ from solar backscatter measurements in the UV wavelength region (around 320 nm) by applying the DOAS method.

We have studied several major volcanic eruptions that deposited large amounts of volcanic gases and ash into the atmosphere. Three eruptions of the Kasatochi volcano in August 2008 in Alaska transported volcanic $SO_2$ and ash particles to a height of at least 10 km, where they became a major hazard to aviation. GOME-2 measured very large $SO_2$ column amounts of about 150 DU the first day after the eruption. Although the Kasatochi eruption was rather strong, the ejected ash concentrations were low, making it difficult to track the volcanic plume by ash retrieval techniques. However, our studies demonstrated in this case that volcanic cloud tracking is also possible using $SO_2$ measurements.

The Eyjafjallayökull eruption in southern Iceland from April to May 2011 had a severe impact on global mobility. Prevailing winds carried volcanic ash to the European continent and caused European-wide disruption to aviation for several days. The GOME-2 near-realtime retrieval performed at IMF allowed continuous monitoring of the volcanic plume. We also tested a new algorithm to retrieve both the total $SO_2$ column density as well as the height of the volcanic plume. Plume height is essential information for aviation safety and forecasting of the trajectory of the volcanic cloud. The retrieved $SO_2$ plume heights from the Eyjafjallayökull eruption estimated from GOME-2 observations on May 5 ranged from 8 – 13 km, in good agreement to within 1 – 3 km of visual observations, radar data and modeling




**$SO_2$ distribution over the Atlantic Ocean after the eruption of the Copahue volcano in Chile (red triangle) on 22 December 2012. The image is an eight days composite of GOME-2 $SO_2$ retrievals.**




**Monthly average tropospheric $NO_2$ columns measured by GOME-2 over northeast China 2007 – 2012. The yellow area indicates the error range. Note the general increase except in the economic recession period 2008/2009.**

results. Meanwhile IMF's expertise in retrieval of volcanic $SO_2$ from space is used in several national and international projects dealing with the monitoring of volcanoes. We deliver $SO_2$ data retrieved from GOME-2 to:

– ESA SACS and SMASH projects: These support the Volcanic Ash Advisory Centers in providing expertise to civil aviation authorities in case of significant volcanic eruptions.

– EU-FP7 GMES downstream service EVOSS: Its main goal is the monitoring of potentially active volcanoes in Europe, Africa and the Caribbean by gathering data from multiple satellites, as well as ground-based data.

– BMBF Geotechnology project Exupéry: Our measurements are used for the development of a mobile volcano fast response system which can be quickly deployed in case of a volcanic crises or volcanic unrest. In combination with ground-based data and state-of-the-art particle dispersion models, volcanic plumes can thus be monitored and forecasted up to three days in advance.

The retrieval of $SO_2$ using GOME-2 satellites enables continuous monitoring of volcanic events. With the recent launch of MetOp-B in 2012 and the upcoming MetOp-C satellite, scheduled for 2017, monitoring of volcanic eruptions will continue beyond 2020.

Currently, new methods to improve the quality of the retrieved $SO_2$ column densities and volcanic plume height are being developed. This improvement will be directly implemented in our operational level 1-2 processors for upcoming satellite missions. The work is performed in close collaboration with international leading research organizations such as, e.g., the Belgian Institute for Space Aeronomy and NASA.

Selected publications: [103], [246]

### Tropospheric Nitrogen Dioxide and Air Quality

Satellite remote sensing of air quality on urban, regional and global scales is of great importance since air pollutants are responsible for strong environmental and health impacts, and also play an important role in global climate change.

GOME-2 measurements offer the possibility to study the large scale temporal and spatial variability of tropospheric nitrogen dioxide ($NO_2$) and formaldehyde (HCHO) with better spatial resolution than GOME, permit the detection of anthropogenic $SO_2$ emissions over polluted regions and provide access to the tropospheric $O_3$ column for the (sub)-tropical region. Measurements of HCHO can be used to constrain non-methane volatile organic compound (VOC) emissions in current state-of-the-art chemical transport models. Using the ratio of HCHO columns to tropospheric $NO_2$ column, GOME-2 can determine the spatial and temporal variations in surface ozone-$NO_x$-VOC sensitivity on urban scales. We showed that large parts of Europe are $NO_x$-limited as indicated by an HCHO/$NO_2$ ratio larger than two, while major urban and industrial centers tend to be VOC-limited.

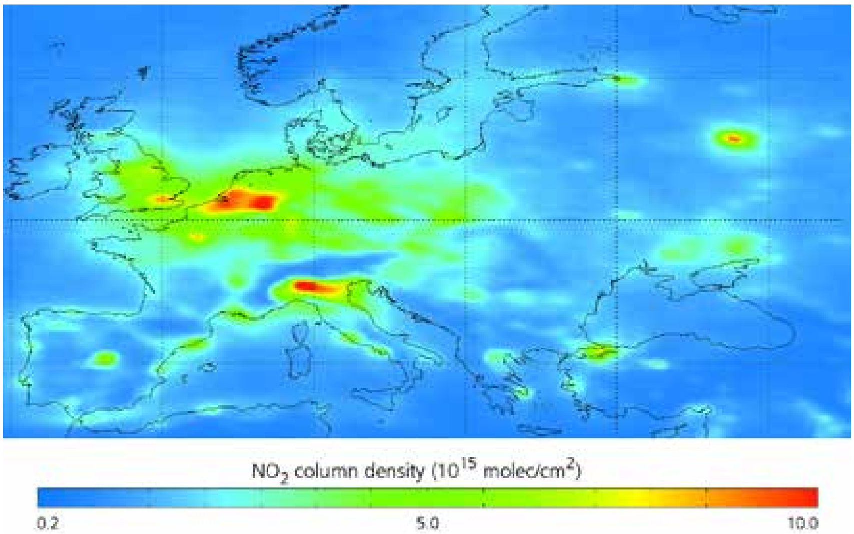
In the last three decades, air pollution has become a major environmental issue in metropolitan areas of China as a consequence of fast industrialization and urbanization. The world's largest area with high $NO_2$ pollution is found over east China. Apart from the economic recession period 2008/2009, a clear increase of tropospheric $NO_2$ over northeast China is found from 2007 to 2012. In contrast, a reduction of $SO_2$ is found over northeast China from 2007 to 2009, mainly related to the installation of desulphurization equipment in coal-fired power plants and boilers and the shutting down of small coal-fired boilers which started in 2007.

The 2008 Olympic Games, EXPO 2010 and the 2010 Asian Games have been held in the Chinese megacities Beijing, Shanghai and Guangzhou respectively. To improve the air quality during these mega-events, many emission control measures focusing on energy, industry, transport and construction were implemented by host cities before and during the mega-events. We have assessed the effectiveness of these measures and studied the impact on pollutants over these host cities using our GOME-2 trace gas products:

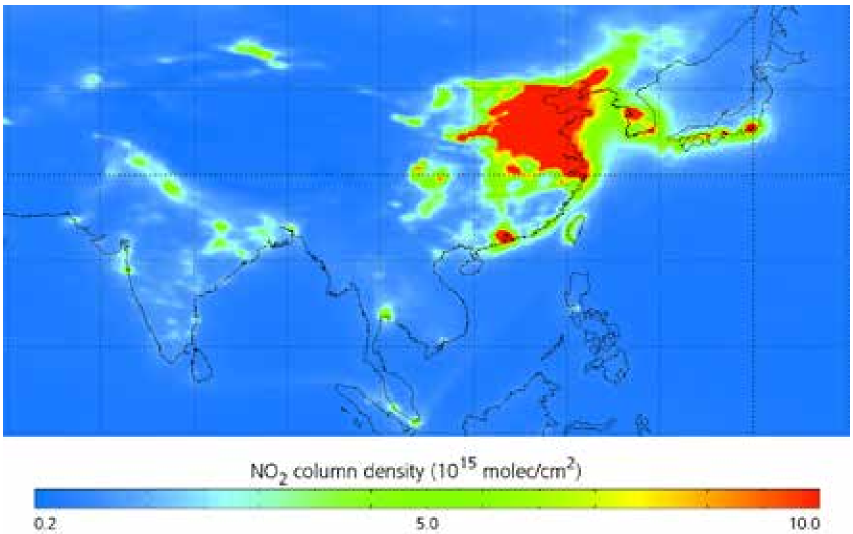
- Olympic period in 2008: Tropospheric $NO_2$ has decreased by up to 38 % in Beijing
- EXPO period in 2010: Tropospheric $NO_2$ columns over Shanghai showed a significant reduction when they decreased about 8 % compared to the same period in the previous year, while the tropospheric $NO_2$ columns increased about 20 % during the post Expo period.

IMF's expertise on satellite observations of important trace gases is also used to monitor air quality changes over China caused by the East Asian monsoon circulation within the framework of the ESA-MOST Dragon 3 project. The East Asian monsoon is a major atmospheric system affecting air mass transport, convection and precipitation and studies showed that it plays a significant role in characterizing the temporal variation and spatial patterns of air pollution over China. The project will also contribute to explore the potential impact of air pollutants over China on a regional climate change.

Selected publications: [114], [142], [170]




**Average tropospheric $NO_2$ columns measured by GOME-2 over Europe for 2007 – 2012. High concentrations are obvious above large urban and industrial areas including the Po Valley, the Benelux, South-East England and Germany's Ruhr area. Also the city-size polluted areas around Paris, Madrid and Moscow can be identified as hot spots.**




**Average tropospheric $NO_2$ columns measured by GOME-2 over East Asia for 2007 – 2012**

### Atmospheres of Exoplanets

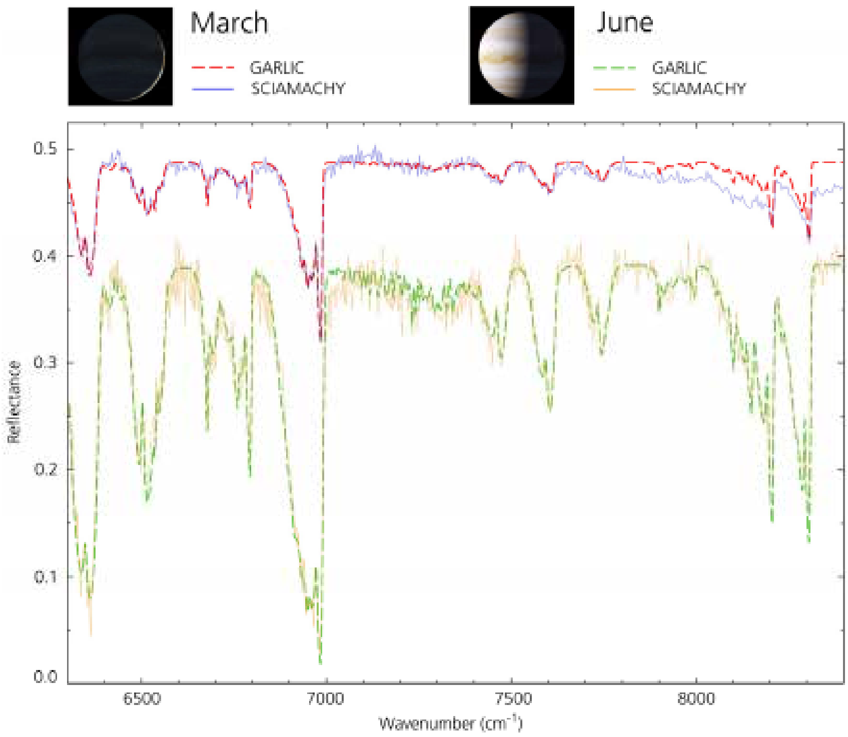
More than 880 exoplanets have been discovered in the past 20 years. A few dozen have a mass lower than 10 Earth masses and some of them are orbiting in the habitable zone of their central star. The spectroscopic characterization of the Earth-like planets' atmosphere is becoming increasingly interesting. Particular attention is drawn to the feasibility of detecting bio-signatures, i.e. spectral features indicating the presence of molecules related to life.

DLR has taken a leading role in such studies when the Helmholtz Research Alliance 'Planetary Evolution and Life' was founded in 2008. Under the lead of DLR's Institute for Planetary Research we contribute our experience in atmospheric radiative transfer modeling. For studies of planetary spectra our LBL code GARLIC turned out to be an important tool due to its efficiency and flexibility. In a first application we successfully modeled ground-based observations of the Venus transit in 2004. Another study was devoted to early Earth: A radiative-convective atmosphere model updated by our LBL molecular absorption data significantly improved the models' performance and indicates that carbon dioxide might be an important factor in what is known as 'Faint Young Sun' paradox.

Planetary atmospheres probably have clouds that influence atmospheric chemistry, dynamics and radiation. Hence for atmospheric remote sensing it is important to study the impact of clouds on the spectra. To enable a rigorous modeling of radiative transfer in scattering atmospheres with high spectral resolution, we have coupled GARLIC with DISORT and used Venus observations by SCIAMACHY for validation. The central star's radiation influences the planet's atmosphere, and hence its spectral appearance, so we investigated the IR emission of clear-sky and cloudy atmospheres of Earth-like planets around F, G, K, and M class stars. In general, different clouds have different effects, with low clouds cooling and high clouds warming the troposphere.

Moreover, clouds modify the spectral signatures. The water and ozone bands are highly reduced, indicating that clouds may produce false-negative detection. Increasing cloud coverage also hampers estimates of the surface temperatures, especially for high-level clouds.

Analysis of radiation source regions can provide valuable information about the detectability of molecular signatures, i.e. radiation mainly coming from the upper atmosphere is less likely to be hidden by clouds. Weighting functions, originally introduced for temperature sounding in meteorology and planetary science, visualize the altitude regimes contributing to the upwelling radiation.



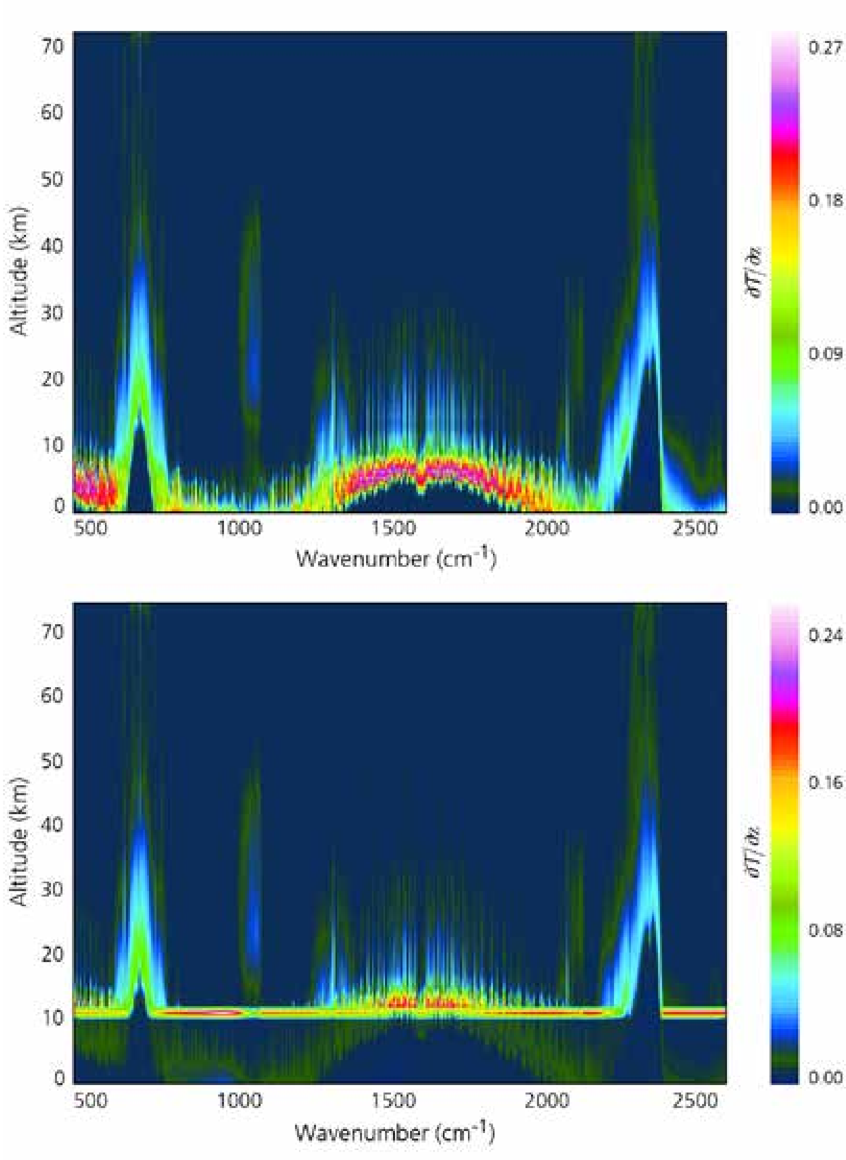

Venus SWIR spectra measured by SCIAMACHY in 2009 and modeled by GARLIC

The red dwarf Gliese 581 is one of our closest galactic neighbors at a distance of only 20 light years. It has attracted increasing attention because at least three potentially low-mass planets are orbiting this M class star, one of which, GL 581d, could be a habitable Super-Earth. Atmospheric model scenarios of GL 581d with moderate surface temperatures were used to calculate high resolution spectra with GARLIC. Assuming a transiting system, we studied the detectability of species directly or indirectly related to biology, i.e. $O_2$, $O_3$, CO, $CO_2$ and $H_2O$. The spectra indicate that without careful examination, $CO_2$ bands could be erroneously interpreted as evidence for ozone or methane, indicating the risk of false-positive or false-negative detection of biomarkers.

In first retrieval studies we have investigated whether signatures of atmospheres indicating a habitable exoplanet can be detected in the near future. In one study GARLIC was used to create transmission and emission spectra of an Earth-like exoplanet for a large set of scenarios involving different stellar types and orbital distances. Signal-to-noise ratios for instruments planned for the ground-based European Extremely Large Telescope and the James Webb Space Telescope were calculated. We were able to show that with transmission spectroscopy, signal-to-noise ratios for some photometric filters could be high enough to detect biosignatures under favorable conditions.

Another study concluded that for spaceborne mission concepts such as DARWIN and EChO, emission spectroscopy alone may perhaps not be capable of characterizing the atmospheres of potentially habitable planets. A combination with other techniques or exploitation of multiple observations will be necessary.

Selected publications: [26], [58], [59], [60], [64], [86], [143], [161], [172], [281]




**Weighting functions for a clear sky (top) and a high cloud ($H_2O$ ice) covered (bottom) planet orbiting an F-star**