SCIAMACHY Quality Working Group (SQWG-3):

Project Overview

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Introduction

- Tasks of the SCIAMACHY Quality Working Group (SQWG):
  - Focus on all activities around the evolution of the **operational processing** of SCIAMACHY data.
  - **Pool all necessary expertise in one group** who takes the responsibility for the evolution and improvements of the operational data processing chain from Level 0 to Level 2.
- First SQWG was formed in **2007**, following the exercise successfully applied to the evolution of data processing of other ENVISAT instruments
- Demonstrated since then the efficient maintenance and evolution of the operational SCIAMACHY processors under *ESA contract* and with *national co-funding*.

SQWG-3 Project History

- After the unexpected **end of the ENVISAT operational phase in April 2012** it was agreed between all agencies that a continuation of the SQWG activities is needed.

- A **work plan for Phase F** has been set up, reviewed and recommended for implementation by the SCIAMACHY Science Advisory Group and was agreed to be implemented by all parties.

- **RfQ** begin of December 2013

- **Proposal** submitted begin of February 2014

- Project start **July 2014**, original duration **30 months** (i.e. until **January 2017**)

- Extension via a two **CCNs** (validation and L1 maintenance activities) and several cost-neutral extensions until **June 2019**.

- Current members of the SQWG are the University of Bremen (**IUP**) (Lead), **BIRA**, **DLR-IMF**, **SRON** and **ESS**.

- The expertise of **KNMI** is brought in via an association with SRON/ESS.

SQWG-3 Project Goals

- **Update the Level 0-2 processing chain** so it reflects the current scientific knowledge.
  Special emphasis is put on **improvements in the Level 0-1 area** (instrument calibration and corrections), since this task requires expert instrument knowledge that is not available outside the SQWG.

- **Deliver the processor baseline** (processors including documentation and user tools) that enables the generation of a **quality controlled Level 1b and Level 2 data** sets for the whole mission that can be used by scientific and institutional users.

- Ensure **long-term usability of the data** by
  - (1) reviewing the complete documentation
  - (2) providing the data in a standard format.

Project Structure
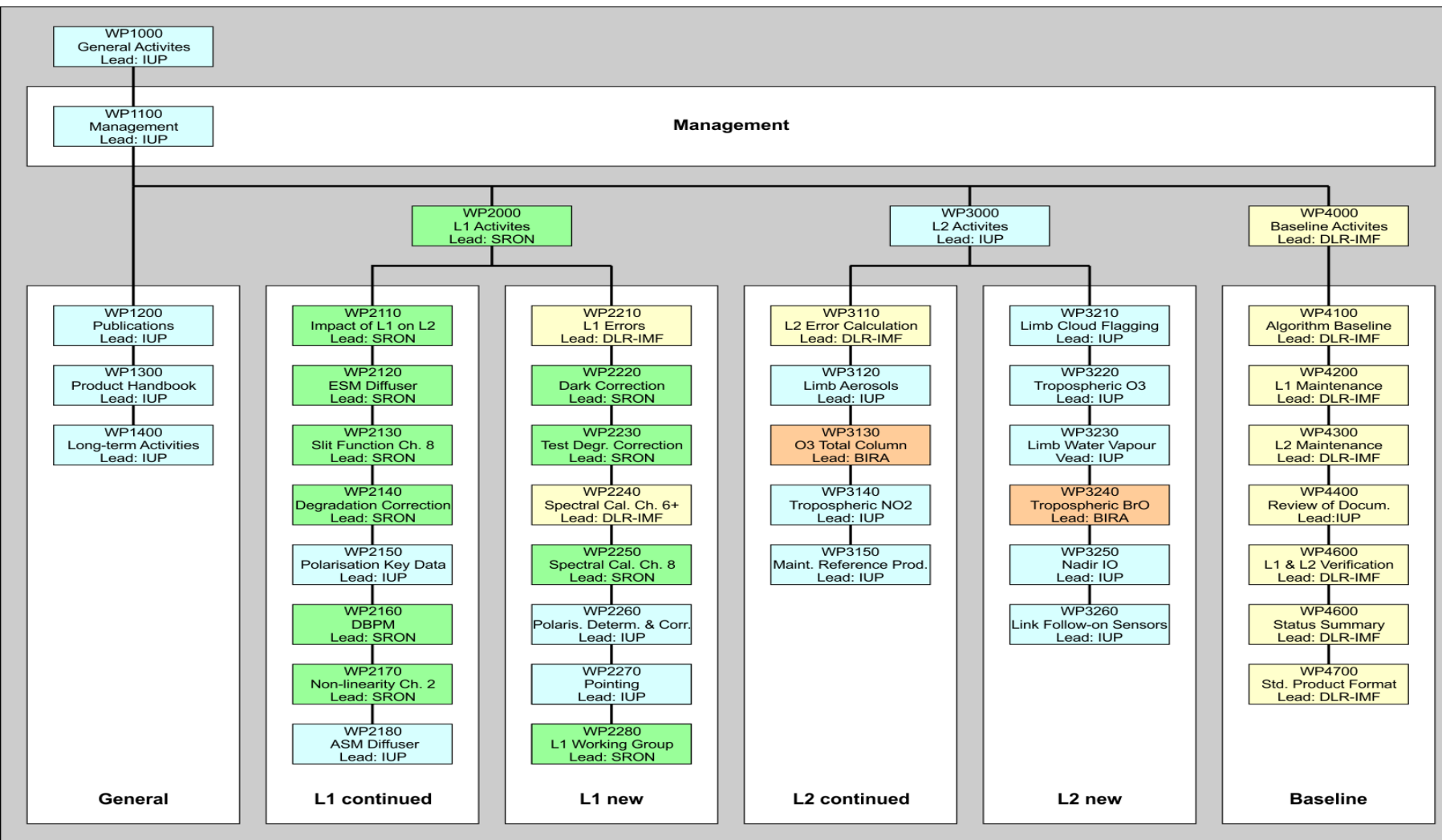
- Work packages include:
  - Finalisation of previous baseline (L1V8, L2V6)
  - Generation of new baseline (L1V9, L2V7)

- Tight schedule:
  - Focus on L1
  - Only few new operational L2 products
  - Additional scientific L2 products

- Later added:
  - CCN1 (BIRA-IASB / IUP):
    - WP5xxx (Validation)
  - CCN2 (ESS/IUP):
    - WP6xxx (L1 maintenance)

Overall schedule

- Following the requirement in the Statement of Work, the project was organized in two phases.

- Focus of Phase 1:
  - Investigate and implement improvements of L1 and L2 algorithms into the corresponding baselines
  - Results were presented at the Mid Term Review (MTR)

- Focus of Phase 2:
  - Finalization of verification activities
  - Collect and consider feedback from validation
  - Produce the required documentation for the baselines and the data products
  - CCN activities

- Significant delay mainly due to more effort for finalisation of previous baseline and complexity of improved polarisation correction (implemented in Phase 2)

Project Overview: Activities

- Activities performed in the SQWG-3 project are broken down in the following main tasks (described in following slides):

  – General Activities (including especially management activities)
  – L1 Activities (covering planned improvements of the L1 products)
  – L2 Activities (covering planned improvements of the L2 products)
  – Baseline Activities (covering the generation of the new operational L1 and L2 baselines)
  – CCN1 Activities (covering L2 validation)
  – CCN2 Activities (covering L1 maintenance / quality assessment)

- Note: Generation of operational products is covered by separate (DLR) project

- Details on improvements of operational L1 and L2 products and CCN results in dedicated presentations

General Activities

- Management of the project
- Publications related to the project
- Maintenance of the SCIAMACHY Product Handbook
- Recommendations for long-term activities

L1 Activities (investigated/implemented improvements)

- Check impact of L1 on specific L2 products
- Investigate/improve ESM diffuser solar reference spectra
- Investigate/improve degradation correction
- Investigate/improve polarisation key data
- Individual pixel characterization for DBPM characterization
- Investigate/improve and consolidate L1 errors
- Investigate/improve dark correction
- Test degradation correction
- Investigate/improve spectral calibration for channel 8
- Investigate/improve polarisation determination and correction
- Investigate/improve pointing

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L1 Activities – not implemented

- Investigate/improve spectral calibration for channel 6+:
    - Prepared but not implemented for time reasons
- Time dependent spectral slit function ch. 8:
    - CO algorithm developers recommended no implementation
- Investigate/improve absolute radiometric calibration of ASM diffuser:
    - Suggested algorithm (scaling of ASM to ESM diffuser) resulted in unknown product quality; no time/resources for full approach (include ASM diffuser in mirror model)
- Non-linearity correction for ch. 2:
    - Implementation already not foreseen in proposal; only documentation required
- Support of the L1 Working Group established by ESA:
    - No L1 working group meetings during project time
- Optional activities from SoW (not possible due to limited resources)
    - Time dependent slit function for channel 6+
    - Spike correction
    - Stray light correction using blinded pixels

L2 Activities (investigated/implemented improvements)

- Documentation and improvement of error calculation
- Further improvement of the O3 total column product
- Further improvement of the tropospheric NO2 product
- Maintenance of the scientific reference products (to be used e.g. during verification)
- Improvement of the limb cloud flagging
- Link SCIAMACHY time series to follow-on sensors

- Optional L2 activities not addressed in this study due to limited resources:
    – Full physics approach for CO, CH4, CO2
    – Synergetic CH4 from channel 6 and 8

L2 Activities: Scientific Products

- Development of a scientific limb aerosol product
- Development of a scientific tropospheric O3 product from Limb-Nadir matching
- Feasibility study for a limb water vapour product
- Development of a tropospheric BrO product
- Development of a scientific Nadir IO product

-> see later slides for results

Baseline Activities

- Maintenance and evolution of the L1 and L2 Algorithm Baselines

- L1 products maintenance

- L2 products maintenance

- Review of documentation with the aim to identify missing information and update/extend documentation as necessary

- Verification of the new L1 and L2 data sets

- Summary of the L1 and L2 baseline status; especially list any remaining open issues which might affect the data product quality and could be tackled in a potential follow-on study.
  -> recommendations: see later presentation

- Implementation of a standard product format to facilitate use of the data (especially for future projects)

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Validation Activities (CCN1)

- Management support for validation (IUP)

- Multi-TASTE validation activities (BIRA-IASB), including:

  - Ground-based data handling

  - Ground-based validation of L1 V8 / SGP V6: full mission

  - Technical verification of first L1 V9 / SGP V7 data

  - Ground-based validation of L1 V9 / SGP V7: full mission

  - Reporting and valorisation

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L1 Maintenance Activities (CCN2)

- Management support for maintenance (IUP/ESS)
- Support to external users (ESS/IUP)
- Reflectance investigations (ESS) -> see later presentation
- Solar irradiance investigations (IUP) -> see later presentation
- Level 1 product content investigations (IUP)

Deliverables (details see final report)

- SQWG-3:

Deliverables	Periodicity	Requirement
Contribution to the SPPA SCIAMACHY Reporting	On-demand	[R-33]
Presentations of results	At QWG progress meetings	[R-34]
Progress report	3-monthly, at QWG progress meetings	[R-35]
Final Report	End of Project	[R-36]
Contributions to presentations and publications by the Agency	On-demand	[R-40]
Input to Agencies web story	Annual	[R-41]
Anomaly Reports	On demand	[R-37]
Technotes and SCRs on proposed baseline changes	Continuous	[R-13], [R-18], [R-21], [R-26]
SPR/SCR/CIF databases	Continuous	[R-11]
Investigation plan for SPR resolution	Continuous	
Input for Product Handbook update	Upon processor or calibration baseline update	[R-31]
SQWG Part of Baseline Documentation (Disclaimer)	Upon processor baseline update	[R-10]
Baseline status summary report	End of Project	[R-74]

- DLR/ESL:

Deliverables	Periodicity	Requirement
Baseline Documentation (except Disclaimer)	Upon processor baseline update	[R-10]
Configuration ADFs	Upon processor baseline update	[R-12]
Binary of operational processors (Level 1b and Level 2)	Upon processor baseline update	
User tool SciaL1C	Upon SciaL1c baseline update	[R-25]

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Open SQWG-3 Deliverables

- L2V7 Full Validation Report (draft available; final expected 6 Dec)

- Inputs L2 README file (delivered, tbc ESA acceptance)

- Final Report (delivered, tbc ESA acceptance)

- Documents for project closure (in preparation)

Progress Meetings

Meeting	Date	Location
Kick-Off (KO)	22 July 2014	Telecon
Progress Meeting 1 (PM1)	20 October 2014	Bremen
Progress Meeting 2 (PM2)	28 January 2015	Telecon
Progress Meeting 3 (PM3)	5-6 May 2015	DLR Oberpfaffenhofen
Progress Meeting 4 (PM4)	22 September 2015	Telecon
Progress Meeting 5 (PM5)	24-25 November 2015	SRON
Mid-term Review (MTR)	February 2016	ESRIN
Progress Meeting 6 (PM6)	14-15 June 2016	Telecon
Progress Meeting 7 (PM7)	21-22 September 2016	Bremen
Status Telecon	15 December 2016	Telecon
Status Telecon	2 March 2017	Telecon
Status Telecon	23 May 2017	Telecon
Status Telecon	11 July 2017	Telecon
Status Telecon	14 June 2018	Telecon
Final Presentation (FP)	6 December 2019	Bremen

- The minutes of the progress meetings and the monthly reports are available on the web
- Additionally project telecons etc. were performed

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SQWG3 FP 6 December 2019

Summary: Improvements

Level 1

Planned Improvement	Operational Implementation		
	not planned	done in Phase 1	done in Phase 2
ESM diffuser solar reference spectra		x	
Time dependent spectral slit function ch 8		investigated	
Degradation correction		x	
Polarisation key data		x	
Individual pixel characterization for dead/bad pixel mask		x	
Non-linearity correction for ch. 2	x	documentation only	
Absolute radiometric calibration of ASM diffuser		investigated	
Consolidation of L1 errors			x
Dark correction		x	
Test degradation correction			x
Spectral calibration ch 6+			x
Spectral calibration ch 8		x	
Polarisation determination and correction			x
Pointing		x	

Level 2

| Planned Improvement	Operational Implementation		
	Scientific product	done in Phase 1	done in Phase 2
O3 total column *		x	
Tropospheric NO2 *		x	
Limb cloud flagging (update)			x
Tropospheric BrO			x
Documentation and improvement of L2 error calculation			x
Nadir IO	x		
Tropospheric O3 from Limb-Nadir matching	x		
Limb water vapour	x		
Limb aerosols	x		
Limb cloud flagging (new extended algorithm)	x		

* (for L2V6)

Scientific data products

- Developed in the context of the SQWG-3 project.

- Not implemented into the operational processing, mainly because of limited resources / time, or because of the special character of the product (for example, the Nadir IO product is only available as monthly slant column data).

- Processed at IUP based on available L1 and L2 data (usually L1V8, L2V6).

- Data and corresponding documentation are provided via the IUP web pages (see final report for details and references)

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Scientific Product: Nadir IO

- Atmospheric IO amounts are comparably small; nadir measurements of IO are mostly close to the detection limit.

- Therefore, the nadir IO product is provided as monthly average slant columns data (January 2003 to April 2012).

- Care in interpretation of absolute amounts is necessary.

- Usually, further averaging of the monthly data is required for scientific applications.

- Basic algorithm is described in Schönhardt et al. (2012)
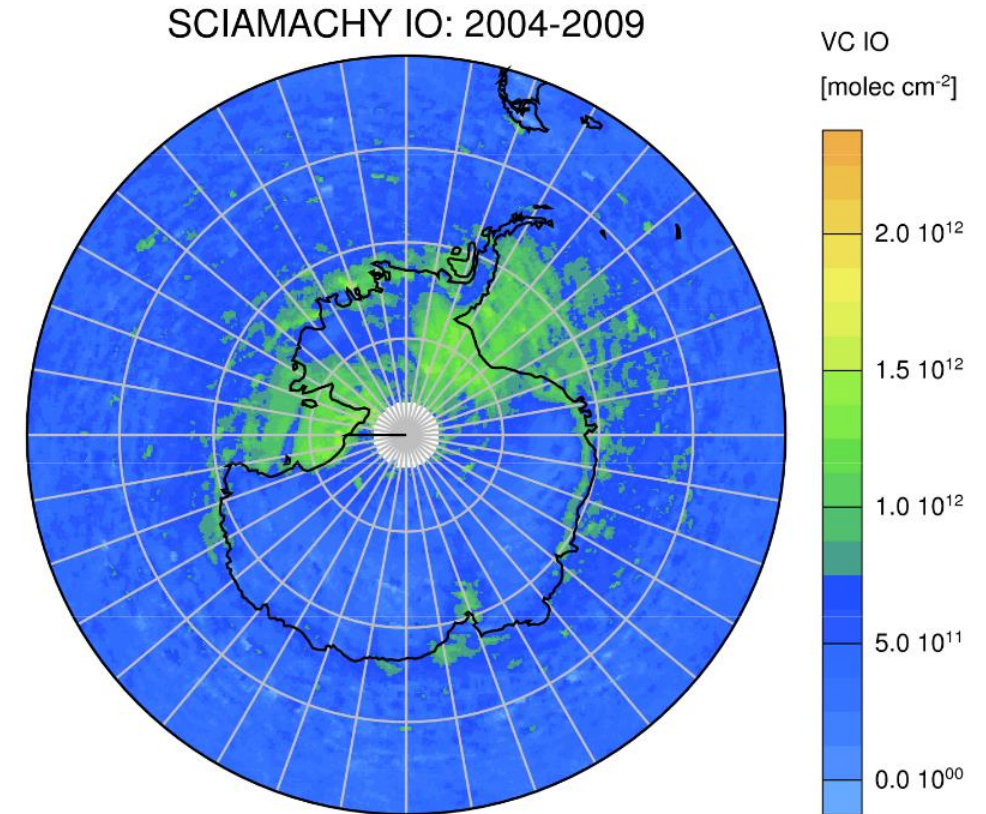
IO vertical columns above the Antarctic region averaged over the period of six years, from 2004 to 2009. Different types of areas show enhanced IO amounts – sea ice regions, ice shelves, coast lines, and parts of the continent. (Figure from Schönhardt et al., 2012)

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Scientific Product: Tropospheric O3 from limb-nadir matching

- Generated by using the Limb-Nadir Matching method, following the algorithm described in Ebojie et al. (2014).

- Based on combination of operational nadir and limb ozone products from L2V6.

- Generally by 5-10 DU lower than the IUP scientific product.

- Expected since validation showed a positive bias of operational L2V6 ozone product in the stratosphere.

- Available from IUP web site as Level 2 and Level 3 (monthly zonal means)

5x5 O3_TROP LIMONAD_SCIA_SCIA_ESA_V2JJ_E in DU200807
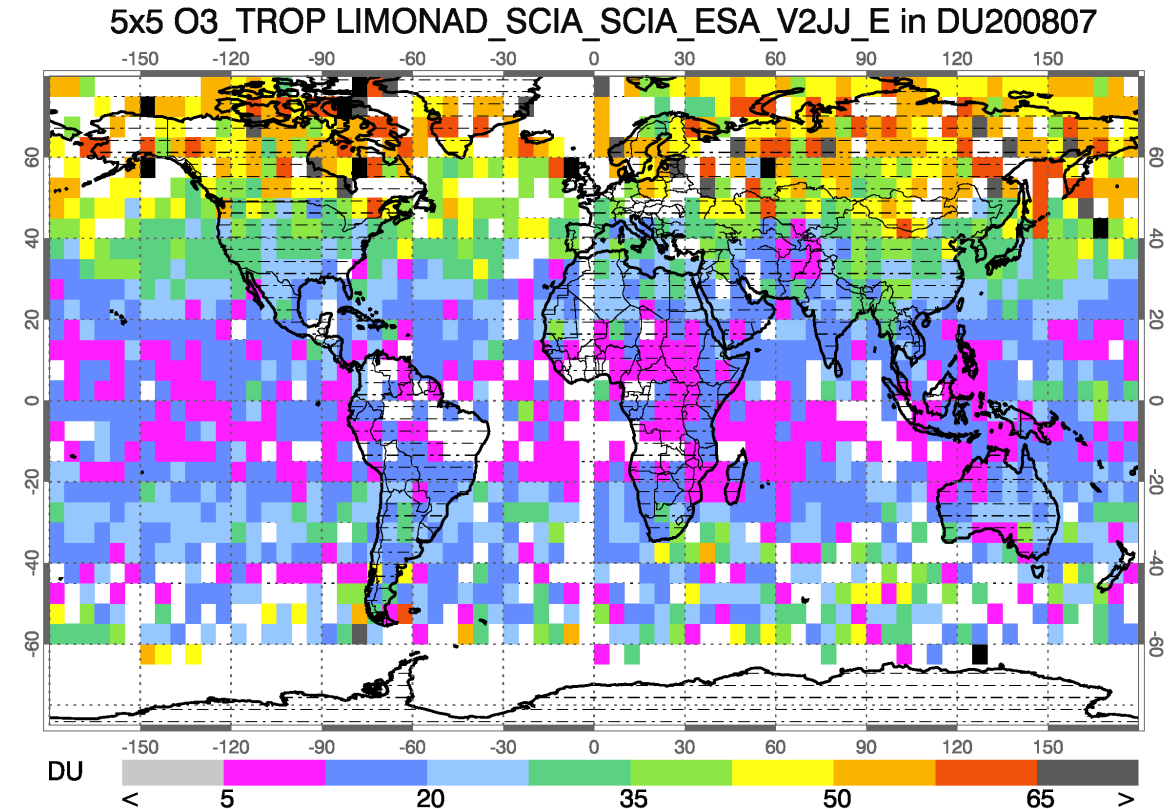
Global contour plot of monthly mean tropospheric ozone values with grid cells of 5°x5° for the month July 2008.

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Scientific Product: Limb H2O

- Originally only feasibility study foreseen because of high computational effort.

- Nevertheless, complete SCIAMACHY time series could be processed.

- Retrieval algorithm is improved version of the one described in Weigel et al, (2016).

- Product V4.2 comprises data in the upper troposphere / lower stratosphere (UTLS) region.

- Data have been filtered for clouds, availability of aerosol extinction and retrieval convergence.
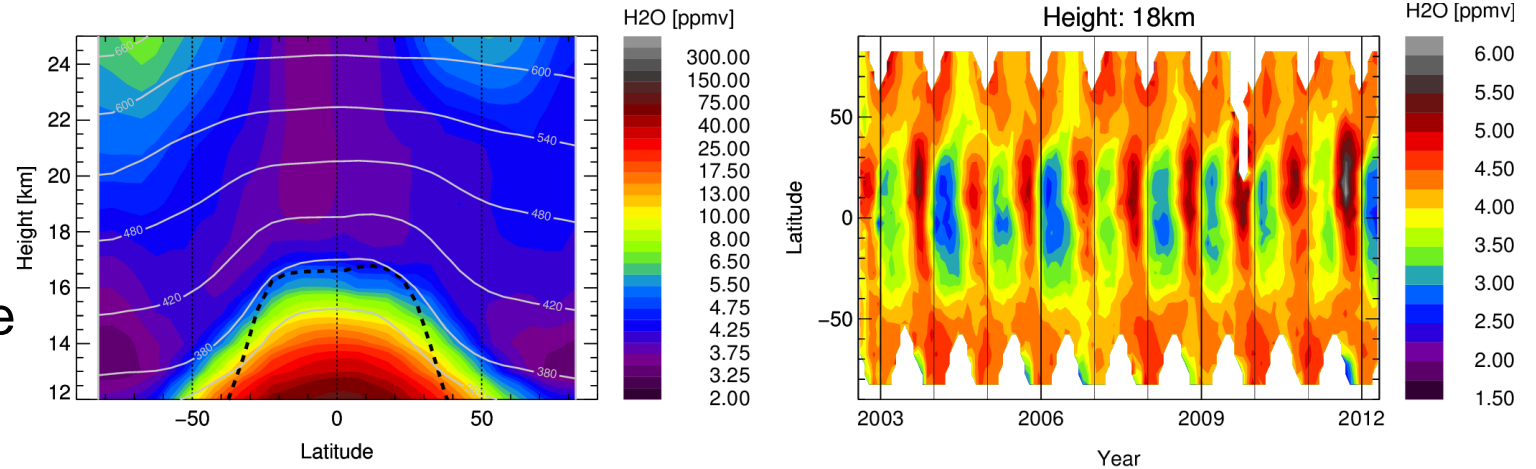
Left: zonal mean data for 12 to 25km for the complete data set V4.2 including lines of constant potential temperature (gray lines) and the position of the blended tropopause (black dashed line) calculated from collocated ECMWF Interim data. Right: zonal mean time series at 18 km height

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# Scientific Product: Limb aerosol extinction

- Contains Level 2 data set of the aerosol extinction coefficient retrieved from SCIAMACHY limb measurements
- Detailed description of the retrieval algorithm V1.4 is given in Rieger et al. (2018).
- Data are provided without specific filtering
- Recommendations for data filtering are given in the accompanying README file.
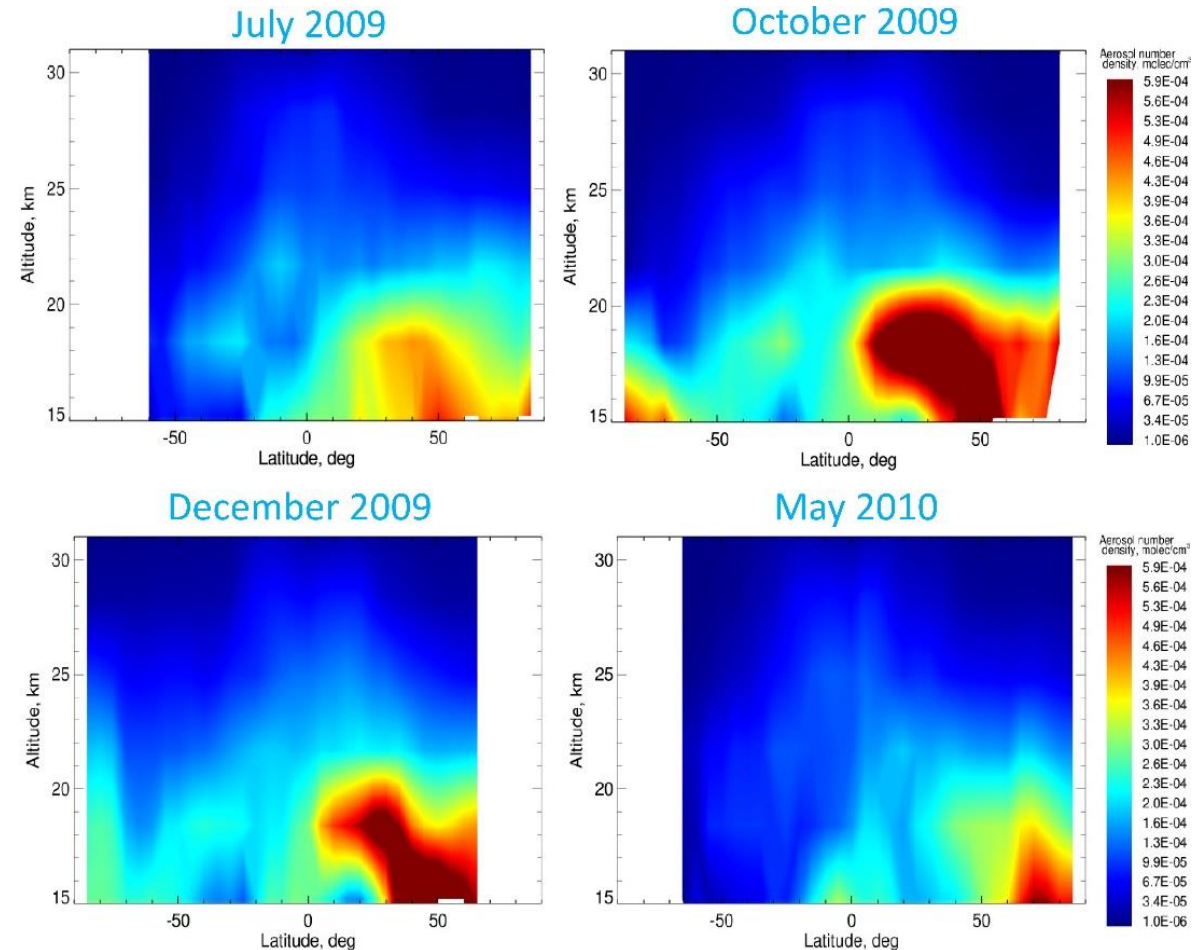
Example: Zonal monthly mean aerosol extinction coefficients at 750 nm showing the evolution of the volcanic plume after the Sarychev Peak eruption (June 2009).

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Scientific Product: Limb clouds

- Completely new development done in the context of SQWG-3.

- Basic idea is to assign to each limb measurement a probability that it is affected by a cloud.

- Then, determine the cloud top height or, rather, the highest tangent height at which a cloud is likely present in a limb profile.

- The new retrieval method especially provides a better distinction between aerosols and clouds than then operational algorithm.
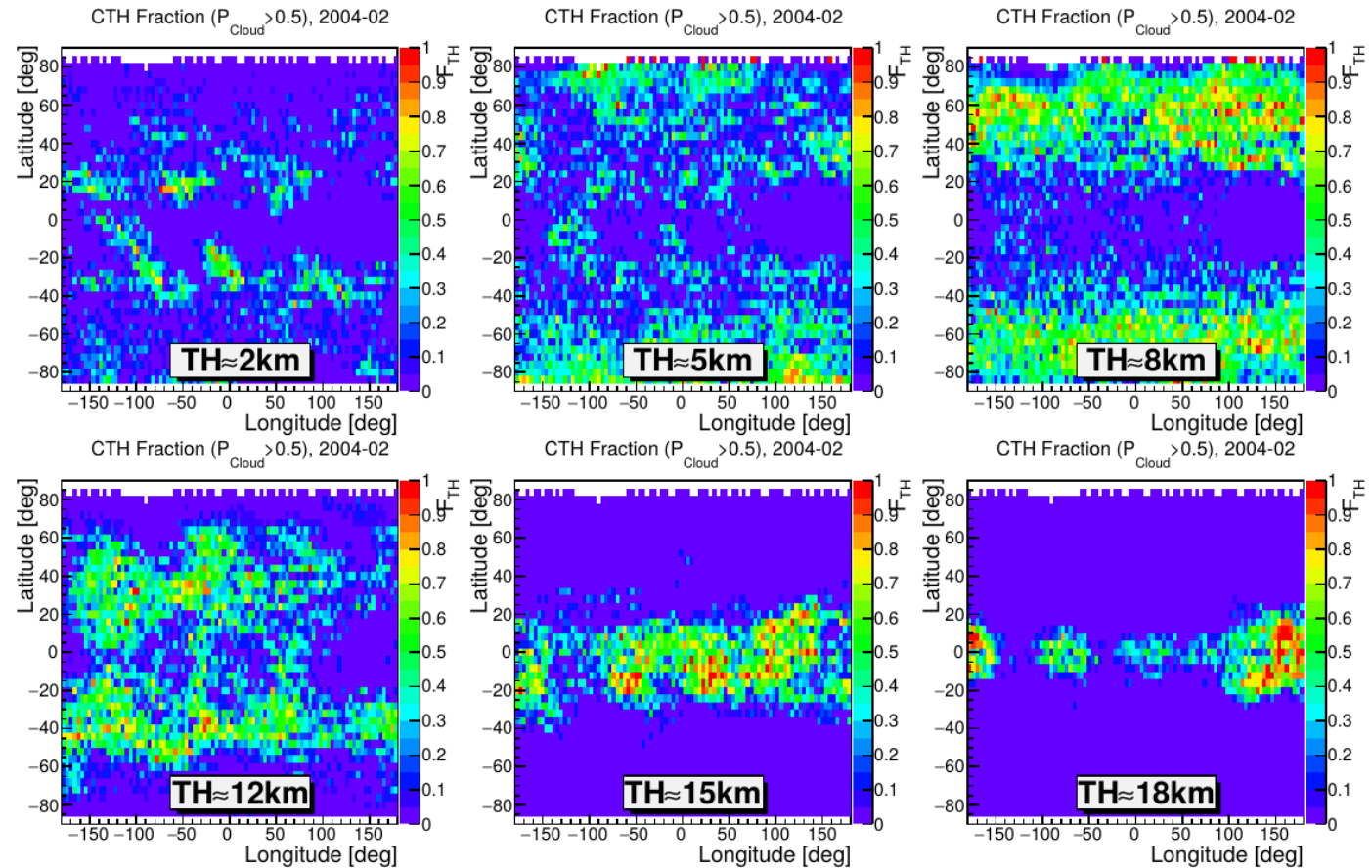
Latitude–longitude distribution of the occurrence rate for clouds with cloud TH at the measured TH, for February 2004.
Clockwise from upper left: 2km, 5 km, 9 km, 12km, 15 km and 18 km.

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Conclusions

- All work as described before has been performed

- All required deliverables have been provided, for some final acceptance by ESA is required

- L1V9 and L2V9 baselines have been delivered, verified and validated

- Validation detected an unforeseen trend in total ozone columns L2V7, which is possibly related to the new L1V9 (possibly also O3 profiles issues)

- As a consequence, it was decided not to release L1V9 and L2V7 to the public

- Improvements of L1 (to remove the O3 trend) will be investigated in the context of the FDR4ATMOS project, where many SQWG partners are involved.

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