SCIAMACHY Level 1b-2 Data Processing
Status & Changes

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SCIAMACHY Level 1b-2: Data Processors

**ENVISAT PDS**
- SGP NRT L0-1b
- SGP NRT L1b-2
  - Industrial Implementation
- SGP OFL L1b-2

**DLR-IMF’s Development Environment**
- Prototype NRT L0-1b
- Prototype NRT L1b-1c
- Prototype NRT L1c-2
- Prototype OFL L1b-2

**Abbreviations**
- SGP: SCIAMACHY Ground Processor
- NRT: Near Real Time
- OFL: Offline
SCIAMACHY Level 1b-2: Algorithm Overview - Status

**NADIR UV / VIS**
- DOAS GDP 2.4 / 2.7
- AMF from Look-up tables based on RTM GOMETRAN
- Vertical column density
- Cloud fraction by Optical Cloud Recognition Algorithm
- AAIA

**NADIR IR**
- BIAS Algorithm
- Cloud-top reflectance height
- Vertical column density retrieval
- Combination of both retrievals possible

**LIMB**
- Original prototype by SAO
  - Single scattering forward model
  - Optimal estimation or Generalized Marquardt-Levenberg
- Extensions by DLR-IMF
  - Multiple Scattering LUTs based on RTM of IFE/Bremen (CDI-PI)
  - Modifications on Numeric and System Engineering
SCIAMACHY Level 1b-2 Data Processor Changes: Origins

Data processor changes are due to

- Algorithm Changes
- Altering of auxiliary information
- Software adjustment  NRT: Prototype ↔ IPF
  - Extra action introduced after ACVE-1 to ensure development baseline
  - Outcome from commissioning phase
  - Adjustment requirements
    - Agreement in floats must be $10^{-5}$ relative or better
    - All others exact

- System Engineering Changes to enhance the processor performance
  (Performance enhancement of Level 2 OFL: ~ 40 %, t < 20 min / orbit)
• Re-organisation of internal data structure
  ‣ Until 2003, the internal data structure was an image of the spectral cluster structure. This led to restrictions for some applications for nadir and limb sounding observations.
  ‣ Now, the neighboured clusters with identical integration time are concatenated. Thus, the data processors are now more flexible in extensive usage of the broad bandwidth of the detectors.

• The adjustment between IPF and prototype has been successfully finished for Level 0-1b and Level 1b-2 (as well). Successful FAT: End of 2003

• Coming within this year
  ‣ Solar reference spectra from all sources as calibrated and un-calibrated, as well.
SCIAMACHY Level 1b-2 Data Processor Changes: Nadir UV / VIS

- **Slant Column Density**
  - In principle, unchanged for prototype: DOAS as GDP Version 2.4/2.7
  - O₃ reference spectra is determined from a set of 5 T-dependent spectra. The reference spectra is now interpolated wrt T (instead Nearest Neighbour)
  - Under-sampling spectra are now calculated and installed
  - Restriction to two fitting windows in IPF removed
  - Coming within this year: DOAS to GDP Version 3.X
  - In addition, extension of reference spectra data base
  - Application to minor trace gases
    - Re-fined application settings (fit window, reference spectra, etc.)
    - Availability of all Solar spectra (calibrated and un-calibrated)

- **Air Mass Factor**
  - Cut-off solar zenith angle is now set to 90 degree
  - Correction of Geo location computation within Level 0-1b

- **Vertical Column Density**
  - Coming within this year: Update to GDP Version 3.X
SCIAMACHY Level 1b-2 Data Processor Changes: Nadir UV / VIS

- **Cloud Cover Detection**
  - Deduction of cloud cover from PMD (rgb)
  - Scaling factors are now adapted to SCIAMACHY measurement data (instead to GOME as at begin of life)
  - Re-organization within IPF
  - Coming within this year: Minor correction of line-of-sight dependency

- **Absorbing Aerosol Index**
  - Unchanged for both, prototype and IPF
  - But: OFL and NRT are based on different interpolation routines. Slight deviations between both versions must be expected.
  - Algorithm lacks from the level 1b absolute calibration.

- **Cloud-top pressure**
  - Climatological information is given per shortest integration time of the state within the Cloud & Aerosol MDS
SCIAMACHY Level 1b-2 Data Processor Changes: Nadir IR

- **BIAS Algorithm**
  - Implementation bug located and removed
  - Adjustment between prototype and IPF finished
  - Upgrade / change of Bad Pixel Mask in preparation
  - Upgrade of fitting windows
**UV/VIS**

- \( \text{NO}_2 \) and minor trace gases are affected by unsufficient calibration of the spectra. This leads to shifts in column density, but it has to be exactly analyzed for each application. The next upgrade of the processors will provide all solar spectral information available from SCIAMACHY measurements.
- The Absorbing Aerosol Index (AAIA) is also affected by off-sets in the irradiance and radiance calibration which is under intensive study.
- Ozone is based on original GOME Data Processor Version 2.4/2.7. To advance the product quality of \( \text{O}_3 \), the GDP Version 3.X which is an extension of the current operational GDP Version 3.0, will be implemented in the SCIAMACHY Offline Processor within this year.

**IR**

- Applications in IR are affected by the Ice-layers which contaminates the detector channel 7&8.
- Beside the above mentioned upgrades, retrieval knowledge from limb retrieval methods (see below) will be transferred (within DLR-IMF)
Limb retrieval can be performed at the DLR-IMF development team with different systems:

- The (operational) version of the SCIAMACHY Level 1b-2 OFL processor
- An experimental system which provides various retrieval methods, but is slow compared to the operational processor
- Prototype of the SCIAMACHY Level 1b-2 OFL which has been extended by
  - Gaussian / Exponential Covariance Scheme
  - Geophysical (season and latitude) variation of initial & a priori profile
- And which will be extended
  - Several “lessons learnt” from the experimental system
- In addition, the Flittner approach is now also available in the prototype.

The different retrieval schemes will be discussed in a poster contribution during this workshop on Wednesday.
SCIAMACHY Level 1b-2 Data Processor: Limb Profile Retrieval Flow

Input
Preparation Measurement Vector
Set-up of Database, Geometry, Atmospheric Properties

Retrieval
Set-up of Multiple-Scattering, Slit function, Ring, Polarisation, Optical Properties
Convolution Preparation
State Vector Initialization
Regularization Initialization
Retrieval Method
Forward Model

Output

Colour Coding indicates deviation from operational processor:
Flittner Approach & Experimental System
Experimental System
SCIAMACHY Level 1b-2 Data Processor: Limb Profile Retrieval

- **Baseline for the retrieval**
  - Partial column density (PCD) is the quantity to be retrieved
  - VMR at several heights is read as input from climatology (US-Standard, AFGL)
  - From that values, VMR is averaged per layer
  - Those values are taken for the PCD retrieval initialization
  - Retrieved PCD is then converted to VMR, but note
    - The dependency between PCD and VMR is given by an integration equation.
    - The conversion is based on an interpolation for each layer
    - The result for each layer is given for the lower boundary limit of the layer

- **Recommendation for comparisons**
  - The most appropriate retrieval result is covered in the PCD entry
• Status of Limb processing
  ‣ First version for $O_3$ profile retrieval in UV
    - Allows global profile retrieval
    - Verification with profiles from IFE Bremen (Flittner approach) showed good coincidence
    - To be improved since of strong mixing with a priori
    - In addition, $O_3$ profile retrieval in VIS will be added

  ‣ First version for $NO_2$ profile retrieval in VIS
    - $NO_2$ profile retrieval has been stabilized compared to recent verification
    - The usage of the experimental system allows the optimal set-up of the operational processor (see poster contribution for more information)
    - Some minor extensions must be added to the operational processor

  ‣ Currently, the results are affected by wrong tangent height input
    - Profiles can be shifted up to higher altitudes and the maximum can be drastically decreased/increased. Both effects are mixed!
The application of Method (B) allows to determine the regularization and weighting factor input for Method (A) (Operational processor). Thus, a fast operational processor can be optimized by the usage of a rather slow but more sophisticated system.
SCIAMACHY Level 1b-2 Data Processor Changes: Outlook

- Currently, most Nadir products are strongly dependent on Level 1b product quality.
- The availability of all solar spectra (calibrated and un-calibrated) measured by SCIAMACHY is one step to more flexibility to overcome with some of the calibration challenges, especially for Nadir UV/VIS.
- The extension of the reference spectra database will complement the flexibility.
- The Ozone (Nadir) product quality in UV will be improved within this year by the implementation of GDP Version 3.X, first in the SCIAMACHY Level 1b-2 OFL data processor.
- Additional profile information wrt Ozone will be provided within this year for the VIS spectral region.
- The NO$_2$ profile retrieval will be enhanced.
- Experience gained from the experimental system will flow into the Limb data processing and improve the products.
Everybody is invited for algorithm proposals.

Please note that there is introduced - equivalent to the operation support - a change request system with a dedicated formalism and form (PCR).

Forms are available at DLR-Bonn and have to be sent to DLR-Bonn and EO-Help (DLR-Bonn: German Space Agency, Christian.Chlebek@dlr.de)
• We highly acknowledge all institutions, entities, and research sites which contribute to the master plan which have been established for the SCIAMACHY data processing last year.

• We like to thank the verification team for helpful discussions, inputs, and proposals.

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