QA_4ECV HCHO and NO_2 MAXDOAS reference data sets: Product description

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List of QA$_4$ECV MAXDOAS stations

Station	Lat, Long	Class	Data Source	Time coverage
De Bilt/Cabauw (NL)	52°N, 5°E	Sub-urban	KNMI	03/2011-11/2017
Uccle (BE)	50°N, 4°E	Urban	BIRA	04/2011-06/2015
OHP (FR)	44°N, 5.5°E	Rural	BIRA	02/2005-12/2016
Xianghe (CHN)	39°N, 117°E	Sub-urban	BIRA	04/2010-01/2017
Bujumbura (BU)	3°S, 29°E	Sub-urban	BIRA	01/2014-12/2016
Bremen (DE)	53°N, 9°E	Urban	IUP-UB	02/2005-12/2016
Nairobi (KEN)	1°S, 37°E	Rural / Urban	IUP-UB	01/2004-11/2014
Athens (GR)	38°N, 23°E	Urban	IUP-UB	09/2012-10/2016
Mainz (DE)	50°N, 8°E	Urban	MPIC	06/2013-12/2015
Thessaloniki (GR)	41°N, 23°E	Urban	AUTH	01/2011-05/2017

MAXDOAS harmonisation procedure

QA_4ECV harmonisation procedure is based on a 4-step approach:

1. **Intercomparison of NO_2 and HCHO slant column densities (SCDs) retrieved from common spectra in order to assess the overall consistency of the retrievals performed within the MAXDOAS community and to derive recommendations for standardized analysis settings**
2. **Development of NO_2 and HCHO airmass factor (AMF) look-up tables in order to harmonize the conversion of SCDs into vertical column densities (VCDs)**
3. **Error budget harmonisation**
4. **Data and metadata reporting in the Generic Earth Observation Metadata Standard (GEOMS) HDF4 format**

Further details available in QA_4ECV deliverables D3.8 and D3.9

I.Recommended DOAS settings for NO_2

(a) Fit settings: **An alternative wavelength range in the UV should be used if the instrument does not cover the visible range**

Reference Spectrum	Window (nm)	Cross sections	Intensity Offset	Polynomial order	Wavelength calibration	Additional adjustment
Sequential (**average** zenith before and after the scan)	425-490	1,2,3,4,5,6 (see Table 2b below)	Order 1 (constant)	5 (6 coefficients)	Based on reference SAO solar spectra (Chance and Kurucz, 2010)	All spectra shifted and stretched against the reference spectrum

(b) Cross sections:

Molecule number	Molecule	Reference + remarks
1	NO_2 (298 K)	Vandaele et al., 1997; I0-correction optional (using appropriate SC)
2	Orthogonalized NO_2 (298 K)	Vandaele et al., 1997; NO_2 cross section (interpolated to 0.01 nm) multiplied with lambda and orthogonalized against the original cross section and a polynomial of order 5 (6 coefficients) in the range 423-492 nm (2 nm more at the edges for convolution with slit function).
3	O_3 (223 K)	Bogumil et al., 2003
4	O_4 (296 K)	http://www.oma.be/BIRA-IASB/Scientific/Topics/Lower/LaboBase/Laboratory.html
5	H_2O (296 K)	Rothman et al., 2010
6	Ring	Chance and Spurr (1997)

Table 2: Recommended DOAS settings for NO_2.

I.Recommended DOAS settings for HCHO

(a) Fit settings:

Reference Spectrum	Window (nm)	Cross sections	Intensity Offset	Polynomial order	Wavelength calibration	Additional adjustment
Sequential (**average** zenith before and after the scan)	(1) 336.5-359 (2) 324.6-359	1,2,3,4,5,6,7 (see Table 3b below)	Order 1 (constant)	5 (6 coefficients)	Based on reference SAO solar spectra (Chance and Kurucz, 2010), include O_3 and optimize slit function	All spectra shifted and stretched against the reference spectrum

(b) Cross sections:

Molecule number	Molecule	Reference + remarks
1	O_4	Thalman and Volkamer, 2013
2	Ring	Calculated with QDOAS according to Chance and Spurr (1997) and normalized as in Wagner et al. (2009)
3	O_3 (223 K, Io corr. 1e20 molec/cm^2)	Serdyuchenko et al., 2014
4	O_3 (243 K, Io corr. 1e20 molec/cm^2)	Serdyuchenko et al., 2014
5	NO_2, (298 K, Io corr. 1e17 molec/cm^2)	Vandaele et al., 1997
6	BrO	Fleischmann et al., 2004
7	HCHO	Meller and Moortgat (2000)

Table 3: Recommended DOAS settings for HCHO. Two different data sets will be generated using two different wavelength range: 336.5-359 and 324.6-359 nm.

2.Vertical columns inversion

- **Use of SCDs measured at 30° elevation in order to minimize the impact of aerosols:**

$$VCD_{\theta,30°,\varphi} = \frac{DSCD_{\theta,30°,\varphi}}{DAMF_{\theta,30°,\varphi}} = \frac{SCD_{\theta,30°,\varphi} - SCD_{\theta,90°,\varphi}}{AMF_{\theta,30°,\varphi} - AMF_{\theta,90°,\varphi}}$$

- **The only exception is OHP where 18°, 16°, and 15° elevation angles are used for the 02/2005-05/2007, 06/2007-12/2011, and 01/2012-12/2016 periods, respectively.**

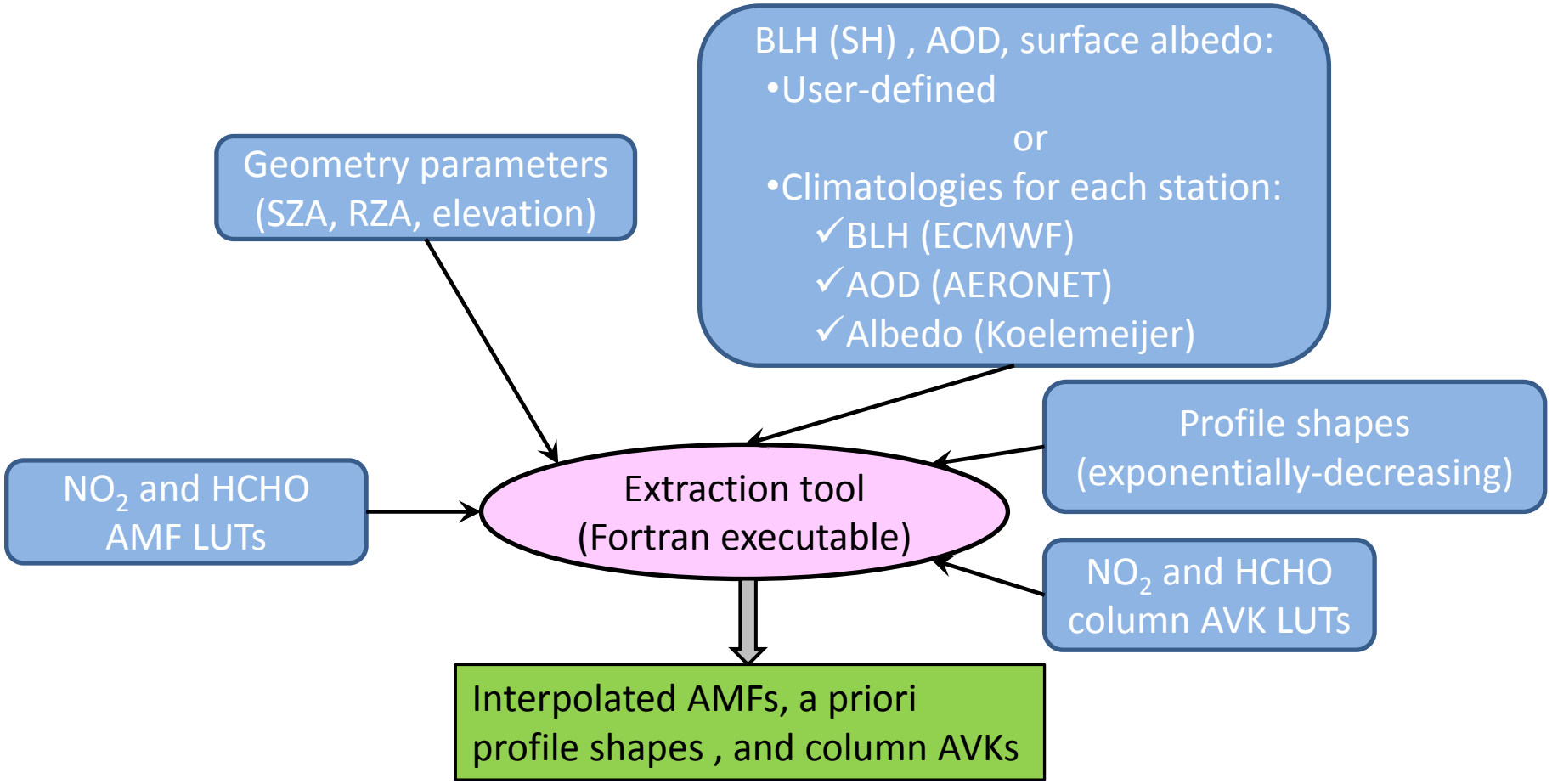
- **DAMF are extracted from LUTs using station-based climatologies for BLH, AOD, and surface albedo (see next slide)**

- **LUTs also provide vertical profiles and column averaging kernels corresponding to the extracted AMFs.**

Further details available in QA$_4$ECV deliverables D3.8

2.Vertical column inversion

DAMF, vertical profile, and column averaging kernel extraction procedure:



3.Error budget harmonisation

a)Systematic uncertainty:

- Uncertainty related to the NO_2 and HCHO XS (9 and 3%, respectively)

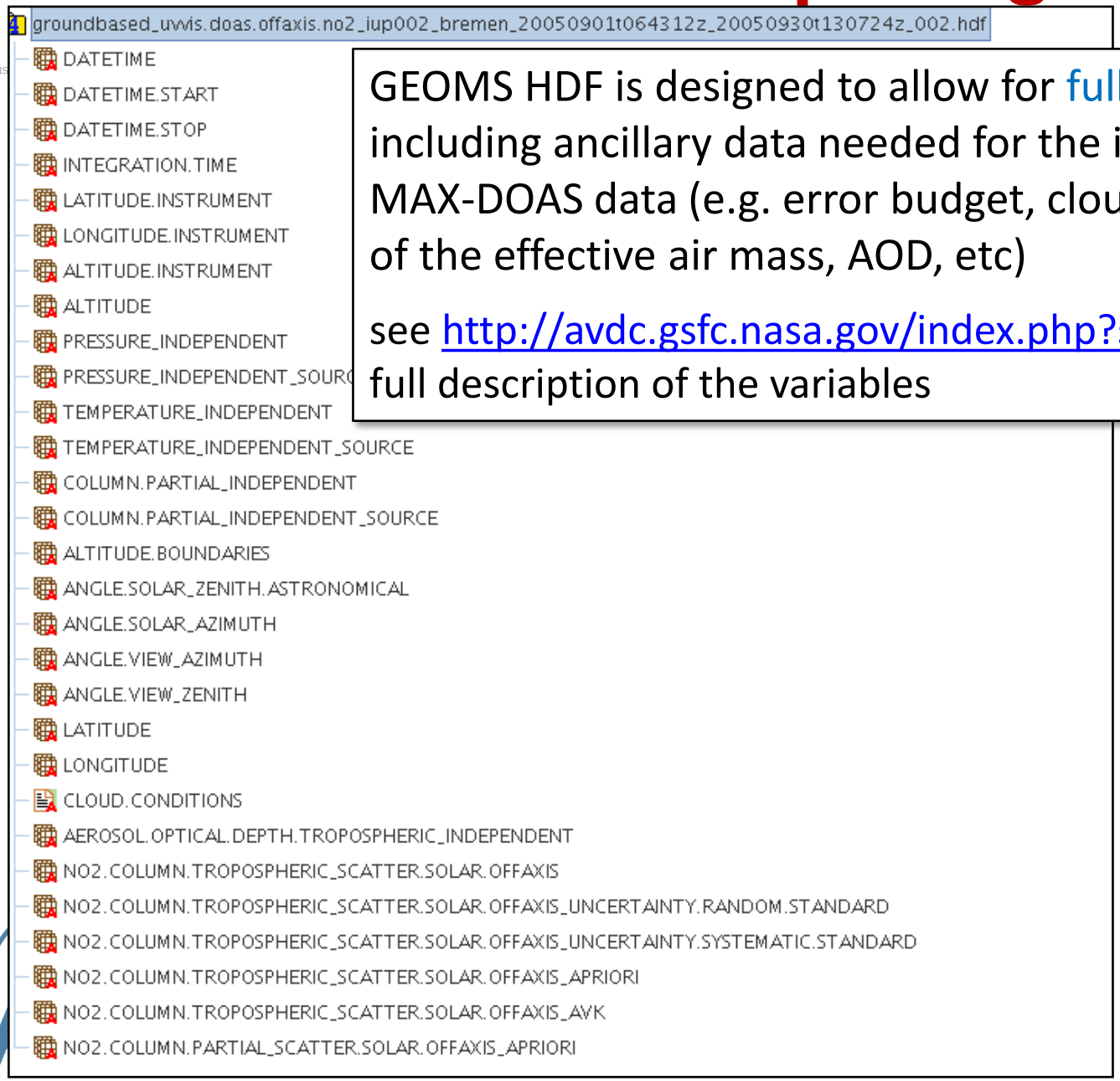
b)Random uncertainty (added in quadrature):

- 1-sigma standard deviation of the statistical error from the DOAS fit
- Uncertainty on AMFs:

Parameter	NO_2 (in %)				HCHO (in %)			
	Xianghe (2011)		Uccle (2012)		Xianghe (2011)		Uccle (2012)	
	15°	30°	15°	30°	15°	30°	15°	30°
AOD	14(55)	9(29)	4(22)	3(11)	18(62)	10(31)	4(20)	1(7)
Profile shape	10(12)	8(10)	7(9)	5(6)	8(12)	7(11)	8(12)	5(8)
BLH	3(5)	2(3)	4(6)	1(3)	8(13)	5(9)	8(11)	4(6)
Surface albedo	<1	<1	<1	<1	<1	<1	<1	<1
Aerosol - AS	<4	<4	<4	<4	<4	<4	<4	<4
Aerosol - SSA	<1	<1	<1	<1	<1	<1	<1	<1
	NO_2 DAMF				HCHO DAMF			
	15° elevation		30° elevation		15° elevation		30° elevation	
Total uncertainty (%)	41		22		45		23	

Further details available in QA_4ECV deliverables D3.9

4. Standardized data reporting



GEOMS HDF is designed to allow for full traceability of data, including ancillary data needed for the interpretation of MAX-DOAS data (e.g. error budget, cloud conditions, location of the effective air mass, AOD, etc)

see http://avdc.gsfc.nasa.gov/index.php?site=1876901039 for a full description of the variables

Further information

For further information on the QA_4ECV MAXDOAS reference data sets, see the following documents:

- **Deliverable D3.8 'Historical record of independent reference data for NO_2, HCHO, and CO':**

  http://www.qa4ecv.eu/sites/default/files/QA4ECV_D3.8_v1.0_web.pdf

- **Deliverable D3.9 'Quality indicators on uncertainties and representativity of atmospheric reference data':**

  http://www.qa4ecv.eu/sites/default/files/D3.9.pdf

- **Deliverable D3.10 'Report on independent validation of atmospheric reference data sets':**

  http://www.qa4ecv.eu/sites/default/files/QA4ECV_D3.10_v2.pdf

Disclaimer

It is strongly recommended to contact corresponding instrument PI for any usage of the QA$_4$ECV MAXDOAS data sets. Instrument PI's e-mail address is available in the main attributes of the GEOMS HDF files.