Changes to the SGP OL V5.01 Processor after Validation

SCIAMACHY Level 1b to 2 processing

ENV-TN-QWG-SCIA-0111

Issue 1

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Change Record

Issue	Date	Page	Description of Change
1	19/04/11	all	completely new

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1 Introduction

1.1 Purpose and Scope of the document

SCIAMACHY is a joint project of Germany, The Netherlands and Belgium for atmospheric measurements. SCIAMACHY has been selected by the European Space Agency (ESA) for inclusion in the list of instruments for Earth observation research for the ENVISAT polar platform, which has been launched in 2002. The SCIAMACHY programme is currently in mission under the supervision of the SCIAMACHY science team (SSAG), headed by the Principal Investigators Professor J. P. Burrows (University of Bremen, Germany), Professor I.A.A. Aben (SRON, The Netherlands) and Dr. C. Muller (BIRA, Belgium).

The Quality Working Group has been installed in 2007 to intensify the development and implementation of the Algorithm Baseline for the operational data processing system of SCIAMACHY. Current members of the QWG are the University of Bremen (IFE) (Lead), BIRA, DLR, and SRON. The expertise of KNMI is brought in via an association with SRON.

This document describes the changes that were made to the processor version 5.01 which went operational in February 2010. It is intended as the basis for decision of the implementation of an improved operational processor version 5.02.

After validation some deficiencies of the Level 2 products became obvious, which were not seen in verification because of the larger data set used for validation. The changes were made with two priorities in mind:

1. Improve the product significantly.
2. Do minimal changes to the processor.

The reason for the latter is to enable a fast track implementation of the new version of the processor without delivering a complete new baseline documentation. Changes were made to the algorithms of the following nadir products:

- SO_2 background correction
- OClO slant column
- (x)CO retrieval

If the processor change is accepted by ESA this document, together with the Algorithm Baseline Documentation of version 5.01 and an updated ATBD will form the new baseline of the operational processor.

1.2 Documents

1.2.1 Applicable Documents

Following documents are applicable for this technical note:

[A1] ENVISAT-1 Ground Segment Concept, ESA/PB-EO(94)75, Issue 5, 20 September 1994

[A2] ESA Software Engineering Standards, ESA PSS-05-0, Issue 2, Feb. 1991

[A3] ENVISAT Product Specification Volume 15, Rev. 3k

[A4] IECF Technical Description, PO-TN-ESA-GS-1142

1.2.2 References

[R1] Validation Report,...

[R2] Verification Report OL V 6.0, SCIAMACHY Level 1b to 2 processing, ENV-VPR-QWG-SCIA-0095, issue 3, 8.6.2010

1.3 Abbreviations and Acronyms

BIRA	Belgisch Instituut voor Ruimte-Aëronmie
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V.
ENVISAT	Environmental Satellite
ESA	European Space Agency
IECF	Instrument Engineering and Calibration Facility
IUP-UB	Institut für Umweltphysik der Universität Bremen
SCD	Slant Column Density
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SGP	SCIAMACHY Ground Processor
SQWG	SCIAMACHY Quality Working Group
SRON	Netherlands Institute for Space Research
SSAG	SCIAMACHY Science Advisory Group
VCD	Vertical Column Density

1.4 Document Overview

The following sections can be found in this document:

- **Section 1** : Introduction (this section)
- **Section 2** : Here the update method, the checks performed and the individual processor changes are described.
- **Section 3-5 :** These sections describe the verification of the changes made for the Nadir retrieval of OClO, SO_2 and CO
- **Section 6** : Contains the result of the regression test to prove that the result of other products are still the same after the processor change
- **Section 7** : Summary of results

2 Description of Processor Changes

Processor V 5.02 will replace operational V 5.01. V 5.02 offers improvements for SO_2 and CO products, which became necessary after the validation of V 5.01. The changes to the processor and the new results are described for each product in the subsequent sections after an explanation of the procedure to update the processor on a fast track without a complete update of the algorithm baseline.

2.1 Update Method

The reference processor that is used to come to a new operational processor is the *internal* version 5.2. This version was not released to the public, but was an intermediate version which was in the scope of the new verification scheme fully verified and accepted (see [R2]). The difference between the operational version 5.01 and the internal version 5.2 are

- the change to 64bit system and
- an up-to-date gcc compiler version 4.3.1.
- correction of the polynomial degree of OClO
- Various background database fixes

These changes make it easier to implement the new processor and takes advantage of the 64bit architecture and modern libraries.

In order to ensure that the switch to the new processor version does not introduce regressions that degrade the quality of successfully validated products, a regression test is made where all end products of the new operational version are compared to the reference version 5.2. In this test, only the improved products should have changed.

For the changed product we will show a comparison of the operational version 5.01 and the new version 5.02 using the versification data set. In the case of CO, an extended data set of several months is used since the product is only intended to build long term averages.

2.1.1 Data Set

Where not otherwise specified, the verification data set was used:

Table 2.1: *Level 1b verification data set. It consists of data from the previous SGP version 4 verification data and 12 additional orbits from 2007 and 2008.*

Orbit #	Level 1b Product
2209	SCI_NL__1PPLRA20020802_093420_000057082008_00151_02209_6028.N1
2321	SCI_NL__1PPLRA20020810_051658_000059332008_00263_02321_6224.N1
2946	SCI_NL__1PPLRA20020922_211146_000059542009_00387_02946_5191.N1
3358	SCI_NL__1PPLRA20021021_155758_000059312010_00298_03358_0195.N1
3502	SCI_NL__1PPLRA20021031_172353_000060152010_00442_03502_1460.N1
4520	SCI_NL__1PSLRA20030110_201324_000060152012_00458_04520_0605.N1

Orbit #	Level 1b Product
4618	SCI_NL__1PPLRA20030117_163251_000059612013_00055_04618_1553.N1
4673	SCI_NL__1PPLRA20030121_124504_000059822013_00110_04673_1532.N1
4720	SCI_NL__1PSLRA20030124_193330_000059612013_00157_04720_0740.N1
4757	SCI_NL__1PSLRA20030127_093541_000059382013_00194_04757_0777.N1
4812	SCI_NL__1PPLRA20030131_054818_000059382013_00249_04812_0261.N1
4830	SCI_NL__1PSLRA20030201_115858_000060212013_00267_04830_0312.N1
4868	SCI_NL__1PSLRA20030204_034212_000059772013_00305_04868_0063.N1
4953	SCI_NL__1PSLRA20030210_021227_000059772013_00390_04953_0135.N1
4995	SCI_NL__1PSLRA20030213_003742_000060092013_00432_04995_0171.N1
5033	SCI_NL__1PSLRA20030215_162052_000059662013_00470_05033_0209.N1
5147	SCI_NL__1PSLRA20030223_152900_000059832014_00083_05147_0324.N1
5202	SCI_NL__1PSLRA20030227_114155_000060062014_00138_05202_0379.N1
5257	SCI_NL__1PSLRA20030303_075437_000060172014_00193_05257_0513.N1
5326	SCI_NL__1PSLRA20030308_033623_000059702014_00262_05326_0824.N1
5373	SCI_NL__1PSLRA20030311_102423_000059332014_00309_05373_0868.N1
5411	SCI_NL__1PSLRA20030314_020647_000060172014_00347_05411_0498.N1
5482	SCI_NL__1PSLRA20030319_010920_000059732014_00418_05482_0778.N1
5636	SCI_NL__1PSLRA20030329_192131_000059682015_00071_05636_0850.N1
5677	SCI_NL__1PSLRA20030401_160721_000059352015_00112_05677_0853.N1
5789	SCI_NL__1PPLRA20030409_115325_000059792015_00224_05789_0622.N1
5845	SCI_NL__1PSLRA20030413_094713_000059792015_00280_05845_1186.N1
5859	SCI_NL__1PSLRA20030414_091529_000059792015_00294_05859_1212.N1
5972	SCI_NL__1PSLRA20030422_064249_000059902015_00407_05972_0559.N1
6027	SCI_NL__1PSLRA20030426_025607_000059862015_00462_06027_0616.N1
6197	SCI_NL__1PSLRA20030508_000258_000056592016_00131_06197_0848.N1
6298	SCI_NL__1PSLRA20030515_012255_000056852016_00232_06298_1194.N1
6467	SCI_NL__1PSLRA20030526_204328_000056472016_00401_06467_1178.N1
6468	SCI_NL__1PSLRA20030526_222404_000056792016_00402_06468_1276.N1
6505	SCI_NL__1PSLRA20030529_122606_000056472016_00439_06505_1222.N1
6534	SCI_NL__1PSLRA20030531_130323_000056782016_00468_06534_1361.N1
6586	SCI_NL__1PSLRA20030604_041422_000056782017_00019_06586_1316.N1
6649	SCI_NL__1PSLRA20030608_135157_000056462017_00082_06649_1429.N1
6651	SCI_NL__1PSLRA20030608_171309_000056462017_00084_06651_1433.N1
6739	SCI_NL__1PSLRA20030614_204544_000056462017_00172_06739_1552.N1
6810	SCI_NL__1PSLRA20030619_194811_000056802017_00243_06810_0044.N1
6881	SCI_NL__1PSLRA20030624_185041_000056502017_00314_06881_0122.N1
6935	SCI_NL__1PSLRA20030628_132301_000056522017_00368_06935_0180.N1
6991	SCI_NL__1PSLRA20030702_111635_000056542017_00424_06991_0249.N1
7076	SCI_NL__1PSLRA20030708_094735_000056902018_00008_07076_0363.N1
7103	SCI_NL__1PSLRA20030710_070348_000056592018_00035_07103_0392.N1
7201	SCI_NL__1PSLRA20030717_032244_000056972018_00133_07201_0511.N1

Orbit #	Level 1b Product
7286	SCI_NL__1PSLRA20030723_015356_000056692018_00218_07286_0827.N1
7399	SCI_NL__1PSLRA20030730_232204_000057082018_00331_07399_0831.N1
7480	SCI_NL__1PSLRA20030805_151059_000056802018_00412_07480_0931.N1
7505	SCI_NL__1PSLRA20030807_090605_000057132018_00437_07505_0964.N1
7831	SCI_NL__1PSLRA20030830_033631_000059802019_00262_07831_1438.N1
7834	SCI_NL__1PSLRA20030830_083809_000060042019_00265_07834_1443.N1
7884	SCI_NL__1PSLRA20030902_202746_000059642019_00315_07884_1506.N1
7896	SCI_NL__1PSLRA20030903_163503_000059652019_00327_07896_1522.N1
7993	SCI_NL__1PSLRA20030910_111410_000059362019_00424_07993_1648.N1
8077	SCI_NL__1PSLRA20030916_080347_000059752020_00007_08077_1758.N1
8161	SCI_NL__1PSLRA20030922_045448_000059312020_00091_08161_1876.N1
8231	SCI_NL__1PSLRA20030927_021533_000059742020_00161_08231_2086.N1
8330	SCI_NL__1PSLRA20031004_001602_000058872020_00260_08330_2108.N1
8401	SCI_NL__1PSLRA20031008_231804_000059342020_00331_08401_2218.N1
8422	SCI_NL__1PSLRA20031010_103030_000059712020_00352_08422_2244.N1
8449	SCI_NL__1PSLRA20031012_074712_000059342020_00379_08449_2294.N1
8483	SCI_NL__1PSLRA20031014_164626_000060182020_00413_08483_2468.N1
8582	SCI_NL__1PSLRA20031021_144611_000059742021_00011_08582_2486.N1
8666	SCI_NL__1POLRA20031027_113618_000059772021_00095_08666_0114.N1
8707	SCI_NL__1POLRA20031030_082053_000059742021_00136_08707_0167.N1
8835	SCI_NL__1POLRA20031108_065742_000059342021_00264_08835_0354.N1
8877	SCI_NL__1POLRA20031111_052250_000059662021_00306_08877_0413.N1
8903	SCI_NL__1POLRA20031113_005833_000059662021_00332_08903_0457.N1
8913	SCI_NL__1POLRA20031113_174436_000059662021_00342_08913_0472.N1
9057	SCI_NL__1POLRA20031123_191039_000059832021_00486_09057_0843.N1
9127	SCI_NL__1POLRA20031128_163232_000059612022_00055_09127_0799.N1
9168	SCI_NL__1POLRA20031201_131645_000059832022_00096_09168_0861.N1
9189	SCI_NL__1POLRA20031203_002955_000059612022_00117_09189_0899.N1
9253	SCI_NL__1POLRA20031207_114757_000059822022_00181_09253_1147.N1
9309	SCI_NL__1POLRA20031211_094209_000059612022_00237_09309_1114.N1
9336	SCI_NL__1POLRA20031213_065709_000060262022_00264_09336_1146.N1
9391	SCI_NL__1POLRA20031217_031011_000060272022_00319_09391_1331.N1
9816	SCI_NL__1POLRA20040115_194539_000059612023_00243_09816_1790.N1
9987	SCI_NL__1POLRA20040127_182730_000060002023_00414_09987_2025.N1
10584	SCI_NL__1PPLRA20040309_112444_000059692025_00009_10584_0235.N1
10597	SCI_NL__1PPLRA20040310_091242_000059332025_00022_10597_0260.N1
11382	SCI_NL__1PPLRA20040504_052223_000060032026_00306_11382_1287.N1
12521	SCI_NL__1PPLRA20040722_190912_000056432028_00443_12521_0516.N1
13328	SCI_NL__1PPLRA20040917_040756_000059922030_00248_13328_1494.N1
13560	SCI_NL__1PPLRA20041003_090641_000059522030_00480_13560_1718.N1
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Orbit #	Level 1b Product
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16884	SCI_NL__1PPLRA20050523_141702_000059962037_00297_16884_6790.N1
17574	SCI_NL__1PPLRA20050710_191429_000057092038_00486_17574_0119.N1
18499	SCI_NL__1PPLRA20050913_100425_000060032040_00409_18499_1289.N1
19811	SCI_NL__1PNPDE20051214_024739_000062162043_00218_19811_1262.N1
20693	SCI_NL__1PPLRA20060213_163755_000059392045_00098_20693_1073.N1
21754	SCI_NL__1PPLRA20060428_193304_000060232047_00157_21754_2226.N1
22306	SCI_NL__1PPLRA20060606_090800_000056942048_00208_22306_2834.N1
22330	SCI_NL__1PPLRA20060608_012219_000056942048_00232_22330_2935.N1
22331	SCI_NL__1PPLRA20060608_030255_000057342048_00233_22331_2937.N1
22332	SCI_NL__1PPLRA20060608_044331_000056952048_00234_22332_2939.N1
22333	SCI_NL__1PPLRA20060608_062406_000057342048_00235_22333_2941.N1
22334	SCI_NL__1PPLRA20060608_080442_000056942048_00236_22334_2863.N1
22335	SCI_NL__1PPLRA20060608_094518_000057342048_00237_22335_2864.N1
22336	SCI_NL__1PPLRA20060608_112554_000056942048_00238_22336_2865.N1
22337	SCI_NL__1PPLRA20060608_130630_000057342048_00239_22337_2866.N1
22338	SCI_NL__1PPLRA20060608_144705_000056952048_00240_22338_2867.N1
22339	SCI_NL__1PPLRA20060608_162741_000057342048_00241_22339_2868.N1
22340	SCI_NL__1PPLRA20060608_180817_000056952048_00242_22340_2869.N1
22341	SCI_NL__1PPLRA20060608_194853_000057342048_00243_22341_2870.N1
22342	SCI_NL__1PPLRA20060608_212929_000056942048_00244_22342_2871.N1
22343	SCI_NL__1PPLRA20060608_231005_000057342048_00245_22343_2872.N1
22416	SCI_NL__1PPLRA20060614_013340_000056952048_00318_22416_2955.N1
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22420	SCI_NL__1PPLRA20060614_081604_000056952048_00322_22420_2959.N1
22421	SCI_NL__1PPLRA20060614_095640_000057352048_00323_22421_2960.N1
22422	SCI_NL__1PPLRA20060614_113716_000056952048_00324_22422_2961.N1
22423	SCI_NL__1PPLRA20060614_131751_000057352048_00325_22423_2962.N1
22424	SCI_NL__1PPLRA20060614_145827_000056952048_00326_22424_2963.N1
22425	SCI_NL__1PPLRA20060614_163903_000057352048_00327_22425_2964.N1
22426	SCI_NL__1PPLRA20060614_181939_000056952048_00328_22426_2965.N1
22427	SCI_NL__1PPLRA20060614_200015_000057352048_00329_22427_2966.N1
22428	SCI_NL__1PPLRA20060614_214051_000056952048_00330_22428_2967.N1
22429	SCI_NL__1PPLRA20060614_232127_000057352048_00331_22429_2968.N1
23246	SCI_NL__1PPLRA20060811_010646_000059902050_00146_23246_0835.N1
23247	SCI_NL__1PPLRA20060811_024721_000060042050_00147_23247_0836.N1
23248	SCI_NL__1PPLRA20060811_042759_000059902050_00148_23248_0837.N1
23249	SCI_NL__1PPLRA20060811_060834_000060042050_00149_23249_0838.N1

Orbit #	Level 1b Product
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23251	SCI_NL__1PPLRA20060811_092947_000060042050_00151_23251_0840.N1
23252	SCI_NL__1PPLRA20060811_111024_000059902050_00152_23252_0841.N1
23253	SCI_NL__1PPLRA20060811_125059_000060042050_00153_23253_0842.N1
23254	SCI_NL__1PPLRA20060811_143137_000059902050_00154_23254_0843.N1
23255	SCI_NL__1PPLRA20060811_161212_000060042050_00155_23255_0844.N1
23256	SCI_NL__1PPLRA20060811_175250_000059902050_00156_23256_0845.N1
23257	SCI_NL__1PPLRA20060811_193325_000060042050_00157_23257_0846.N1
23258	SCI_NL__1PPLRA20060811_211402_000059902050_00158_23258_0847.N1
23361	SCI_NL__1PPLRA20060819_015541_000060042050_00261_23361_0954.N1
24149	SCI_NL__1PPLRA20061013_030746_000059972052_00047_24149_1706.N1
24150	SCI_NL__1PPLRA20061013_044906_000059482052_00048_24150_1707.N1
24151	SCI_NL__1PPLRA20061013_062859_000059962052_00049_24151_1708.N1
24152	SCI_NL__1PPLRA20061013_081019_000059482052_00050_24152_1709.N1
24153	SCI_NL__1PPLRA20061013_095012_000059962052_00051_24153_1710.N1
24154	SCI_NL__1PPLRA20061013_113132_000059482052_00052_24154_1711.N1
24155	SCI_NL__1PPLRA20061013_131124_000059962052_00053_24155_1712.N1
24156	SCI_NL__1PPLRA20061013_145245_000059482052_00054_24156_1713.N1
24157	SCI_NL__1PPLRA20061013_163237_000059972052_00055_24157_1714.N1
24158	SCI_NL__1PPLRA20061013_181358_000059482052_00056_24158_1715.N1
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24160	SCI_NL__1PPLRA20061013_213511_000059482052_00058_24160_1717.N1
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24992	SCI_NL__1PPLRA20061211_003228_000060022053_00389_24992_3150.N1
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24994	SCI_NL__1PPLRA20061211_035340_000060032053_00391_24994_3154.N1
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24998	SCI_NL__1PPLRA20061211_103605_000060022053_00395_24998_4778.N1
24999	SCI_NL__1PPLRA20061211_121652_000059912053_00396_24999_4902.N1
25000	SCI_NL__1PPLRA20061211_135717_000060032053_00397_25000_5000.N1
25001	SCI_NL__1PPLRA20061211_153804_000059912053_00398_25001_5034.N1
25002	SCI_NL__1PPLRA20061211_171829_000060032053_00399_25002_5136.N1
25003	SCI_NL__1PPLRA20061211_185916_000059912053_00400_25003_5236.N1
25004	SCI_NL__1PPLRA20061211_203941_000060022053_00401_25004_5761.N1
25331	SCI_NL__1PPLRA20070103_165509_000059912054_00227_25331_3320.N1
25414	SCI_NL__1PPLRA20070109_120441_000059922054_00310_25414_6224.N1
26176	SCI_NL__1PPLRA20070303_174059_000059862056_00070_26176_2621.N1
26411	SCI_NL__1PPLRA20070320_034214_000059912056_00305_26411_7214.N1

Orbit #	Level 1b Product
27221	SCI_NL__1PPLRA20070515_175210_000056972058_00113_27221_4648.N1
28094	SCI_NL__1PPLRA20070715_173353_000057522059_00485_28094_3011.N1
28982	SCI_NL__1PPLRA20070915_182114_000059922061_00371_28982_8151.N1
29855	SCI_NL__1PPLRA20071115_180453_000059602063_00242_29855_3284.N1
30399	SCI_NL__1PPLRA20071223_180949_000059922064_00285_30399_1787.N1
31258	SCI_NL__1PPLRA20080221_182435_000059592066_00142_31258_5349.N1
32102	SCI_NL__1PPLRA20080420_172928_000060232067_00485_32102_4119.N1
32961	SCI_NL__1PPLRA20080619_174750_000056972069_00342_32961_9057.N1
33805	SCI_NL__1PPLRA20080817_164920_000060042071_00184_33805_5238.N1
34664	SCI_NL__1PPLRA20081016_170345_000060042073_00041_34664_2255.N1

2.2 Nadir OClO Retrieval

Changes in the source code:

No changes compared to V 5.2.

Changes in the initialization file:

- *degree_of_additive_polynomial* was changed from 4 to 5.
- *sza_cutoff* changed from 95 deg to 92 deg

2.3 Nadir SO_2 Retrieval

Changes in the source code:

All bug fixes concerning the background database from V 5.2 to V 5.6 were incorporated.

Changes in the initialization file:

- *max_sza* changed from 89 to 80
- for *SOL_ASM_UNCAL* squeeze changed from *max=1.0 min=1.0* to *max=1.01 min=0.99*
- species *ds_name="RING_IFE_SO2"* changed to *ds_name="SCIA_RING__KPNO_ch2_BIRA"*, and the according is_absolute from *"false"* to *"true"*
- species *ds_name="ETA_NADIR_BREMEN_2"* changed to ds_name=*"ETA_NADIR_BREMEN_1"*

2.4 Nadir CO Retrieval

Changes in the source code:

Wavelength stretch has been implemented in addition to the shift.

Changes in the initialization file:

- *fixed_shift* removed from bias *fit_control* and
- *<wl_shift> -0.0447 </wl_shift> <wl_stretch> -0.00498 </wl_stretch> <wl_reference> 2324.43 </wl_reference>* added instead

3 Nadir OClO Verification and Analysis Results

3.1 Data Set Used

See Table 2.1

3.2 Reason for the Processor Change

In the course of the SCIAMACHY validation campaign initiated by ESA an offset between the scientific and operational SCIAMACHY products was revealed. The reason was the inappropriate polynomial degree used in DOAS fit in the SGP. The polynomial was corrected by adjusting its degree in the configuration file.

3.3 Results

3.3.1 Comparison to Reference Algorithm

Histograms of abolute differences between the reference algorithm and the corrected SGP can be seen in Figure 3.1.

Absolute differences between the improved version of the SGP and the reference algorithm decreased from ~ $2.6 \cdot 10^{13}$ molec·cm^{-2} to $1.6 \cdot 10^{13}$ molec·cm^{-2} (from 53 to 24 %).

Differences as a function of latitude are shown in Figure 3.2. There was no obvious latitudinal dependence in the differences in the SGPv5.0. Although in the improved version the differences are generally smaller, however they increase slightly with a latitude.

As OClO is photochemically unstable species, it is present in twilight conditions only (see Figure 3.3).

As can be seen in Figure 3.3 non-zero SCD values are expected for SZA > 90°. Therefore, only corresponding SCDs (90° < SZA < 93°) were taken for a scatter plot, which is presented in Figure 3.4. The scatter between the reference and the operational algorithms gets smaller (correlation coefficient increased from 0.886 to 0.949), the SCDs retrieved by the improved SGP version are closer to X=Y-line (corresponding to an ideal case).

Application of the correct degree polynomial improved naturally the DOAS fit quality. This fact is illustrated in Figure 3.5. Although SGP residuals are still slightly higher then those of IUP, the difference between them are obviously decreased (in average from 11 to 8 %).

3.3.2 Disclaimer Input

The following text for the product quality disclaimer is recommended:

- There is indication for a low bias of about $2 \cdot 10^{13}$ molec·cm^{-2}
- Don't use OClO values measured in the ascending node (the satellite moving northwards)
- Beyond 90 degree SZA data get noisy and sometimes spurious high OClO values are also observed in the absence of chlorine activation

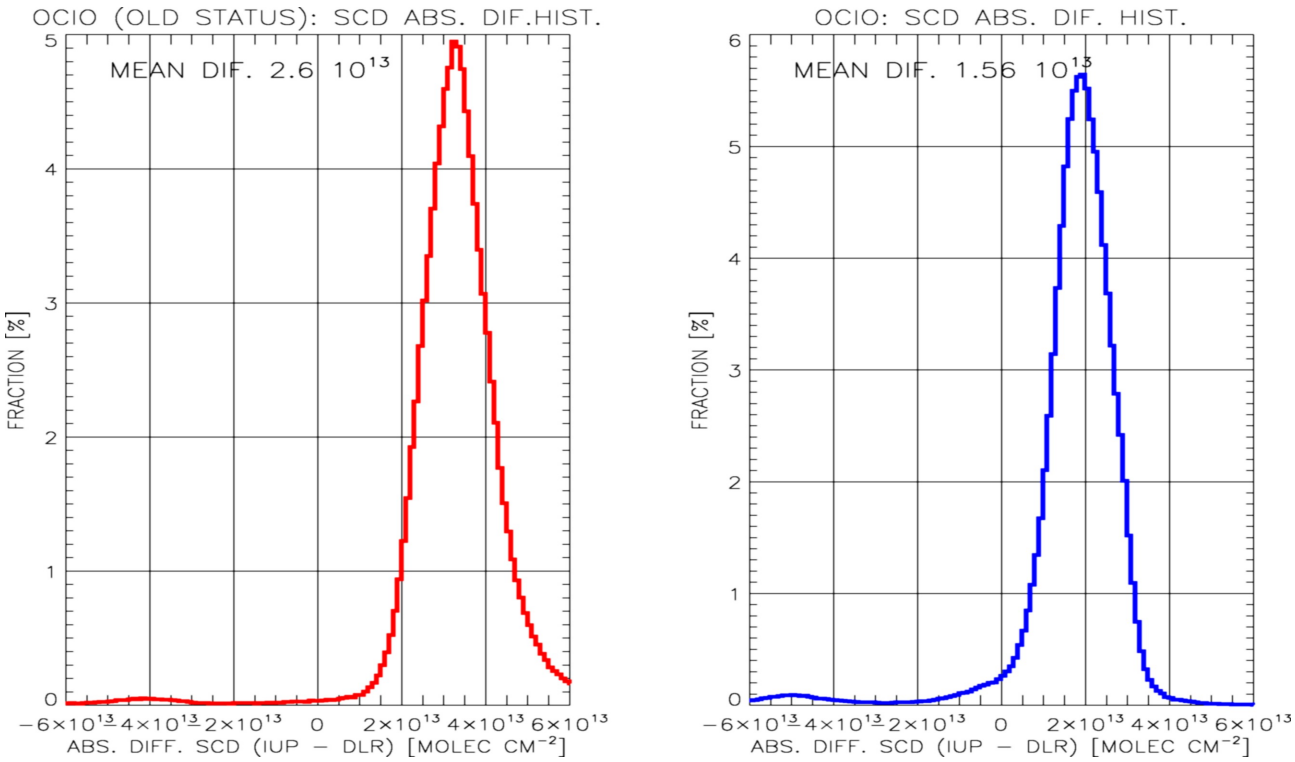


Figure 3.1: *Histogram of absolute differences between the reference algorithm and SGPv5.01 (left panel); and the improved SGP version (right panel)*

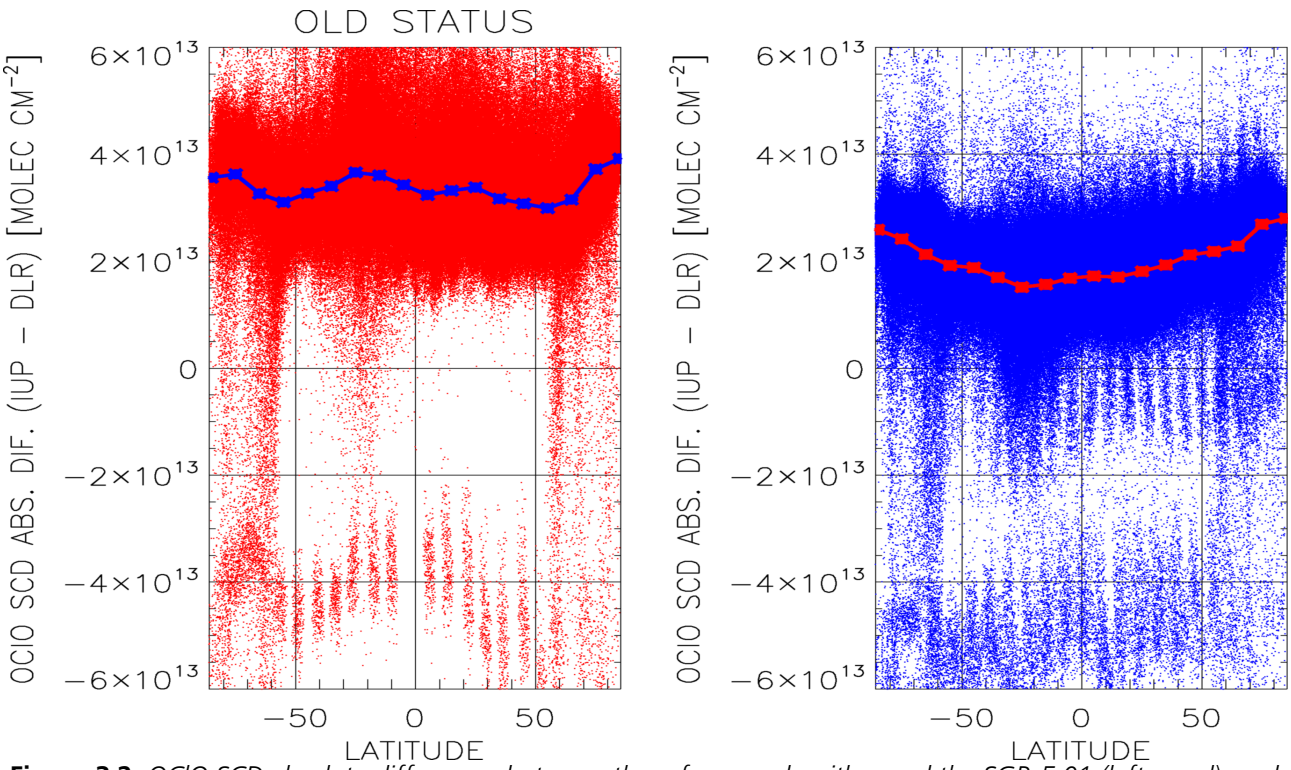


Figure 3.2: *OClO SCD absolute differences between the reference algorithm and the SGPv5.01 (left panel); and the improved SGP version (right panel) as a function of latitude*

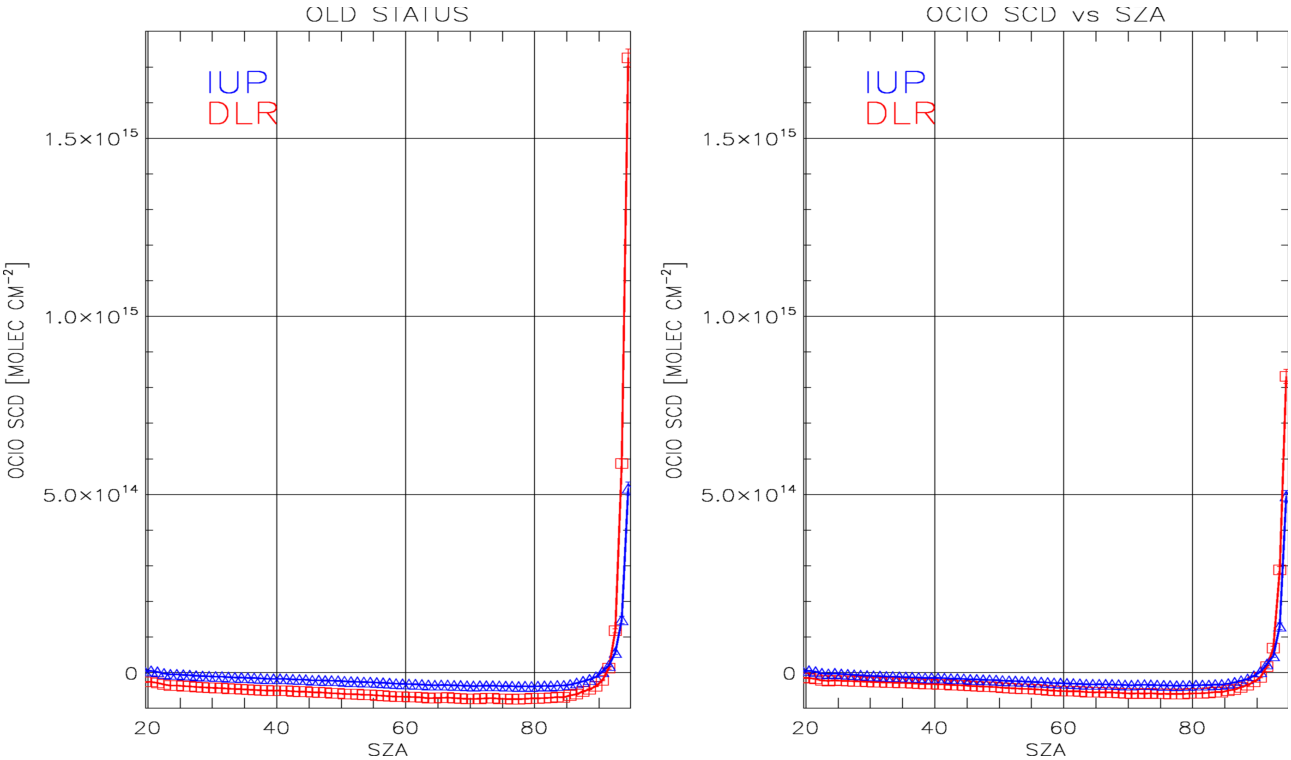


Figure 3.3: *Averaged OClO SCD retrieved by the reference algorithm, SGPv5.01 (left panel) and the improved SGP version (right panel) as a function of SZA*

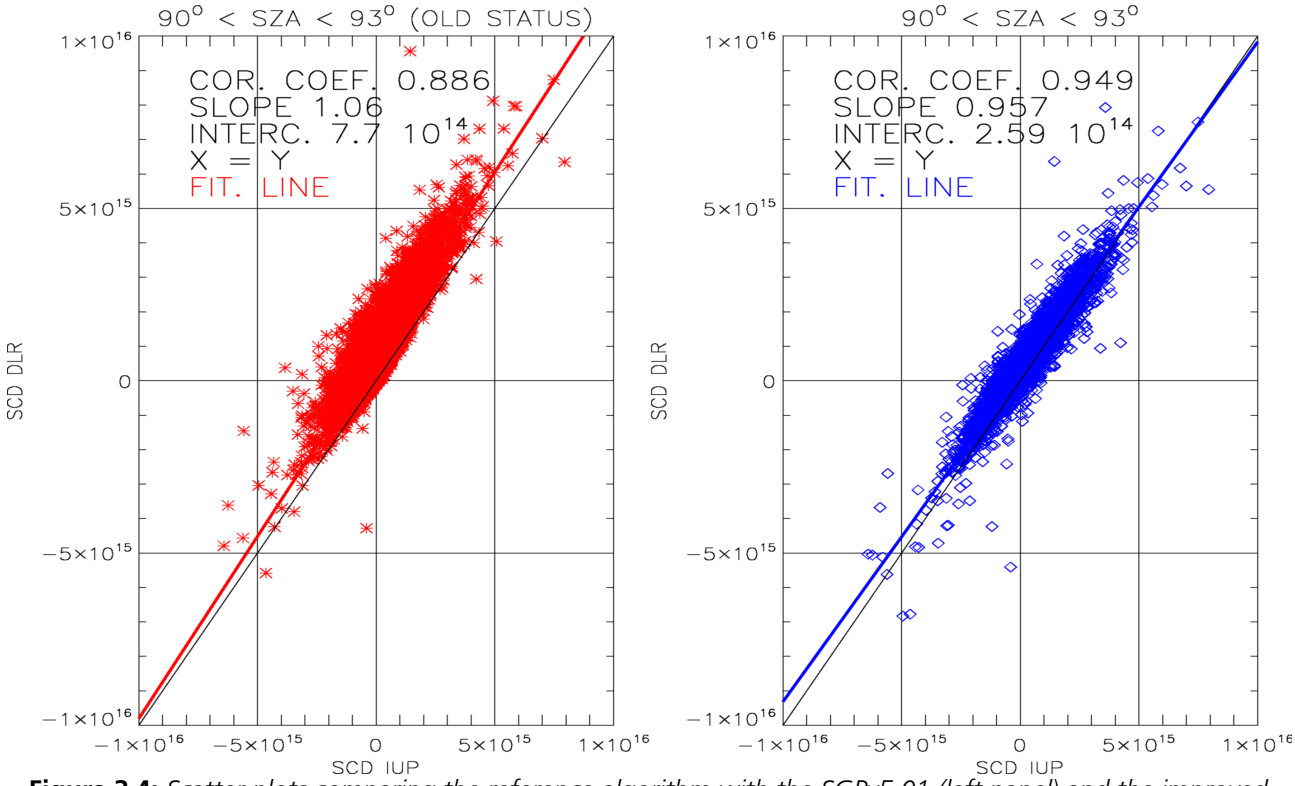


Figure 3.4: *Scatter plots comparing the reference algorithm with the SGPv5.01 (left panel) and the improved version of the SGP (right panel)*

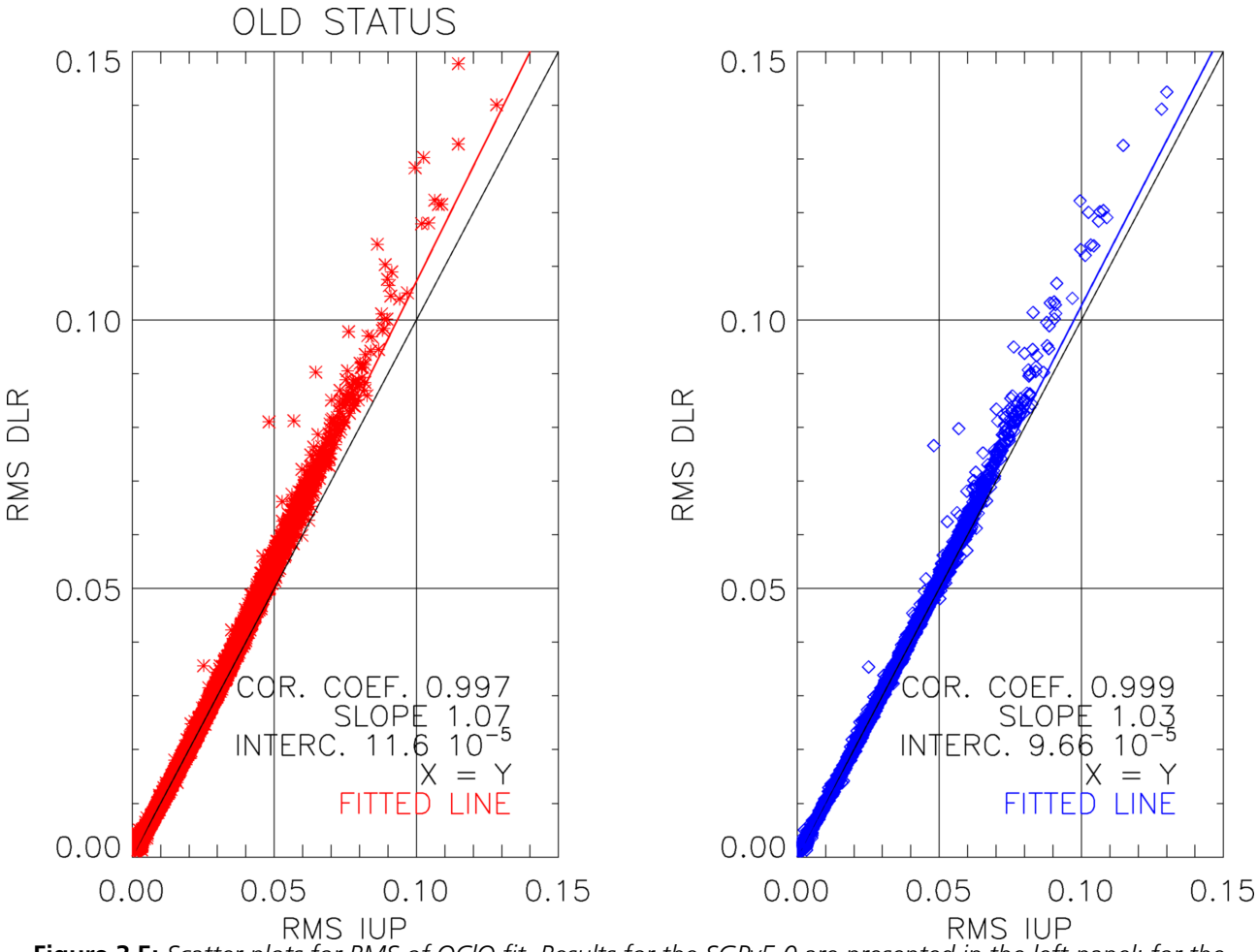


Figure 3.5: *Scatter plots for RMS of OClO fit. Results for the SGPv5.0 are presented in the left panel; for the improved SGP version in the right one*

4 Nadir SO_2 Verification and Analysis Results

4.1 Data Set Used

See Table 2.1

4.2 Reason for the Processor Change

The SCIAMACHY validation campaign initiated by ESA gave an opportunity for overall quality check for the products, which currently cannot be validated on a global scale. One such product is vertical columns of sulphur dioxide (SO_2). The IUP team checked a much larger dataset of SO_2 than used in the verification campaign and revealed the following deficits:

- strongly negative values at high latitudes;
- occasional „stripes“ with very large values

These problems were caused by a bug in the background correction algorithm: not all the orbits touching the reference sector were taken into account for the calculation of correction value. Another bug was found in the calculation of the quality flag for the background correction. Due to a rather strict conditions for SCDs to be taken for calculation of the correction value it happens often that in high latitudes no correction value can be calculated. As a consequence SCDs remain uncorrected. The values were placed in the product and asserted with the aforementioned quality flag. But in the past the flag always equaled zero. This was fixed. Now the quality flag varies between 0 and 7 and a user can see which SCDs are uncorrected.

In addition to the debugging of the algorithm for the reference sector correction, a careful check of the DOAS retrieval setting was performed. Several improving changes were suggested and approved by the developer of the reference algorithm (A. Richter):

- Allow the Earthshine stretch
- Use the Ring spectrum provided by BIRA for ozone retrieval instead of the Ring correction provided by IUP

4.3 Results

4.3.1 Comparison to Reference Algorithm

There are two types of the SO_2 vertical columns placed in the official SCIAMACHY L2 product: one converted from the slant columns assuming SO_2 is situated in the boundary layer between an earth surface and 1 km (this represents an anthropogenic pollution scenario and is named VCD_{BL}); and another one – assuming SO_2 is situated between 10 and 11 km (volcanic eruption scenario; $VCD_{VOLCANIC}$).

Allowance of the Earthshine stretch helped to decrease an offset between the reference algorithm and the SGP at high latitudes (characterised by high SZA), whereas usage of the BIRA Ring spectrum instead of the IUP one significantly improved a situation in tropics and mid-latitudes (lower SZA). The

improvements are illustrated in Figure 4.1.

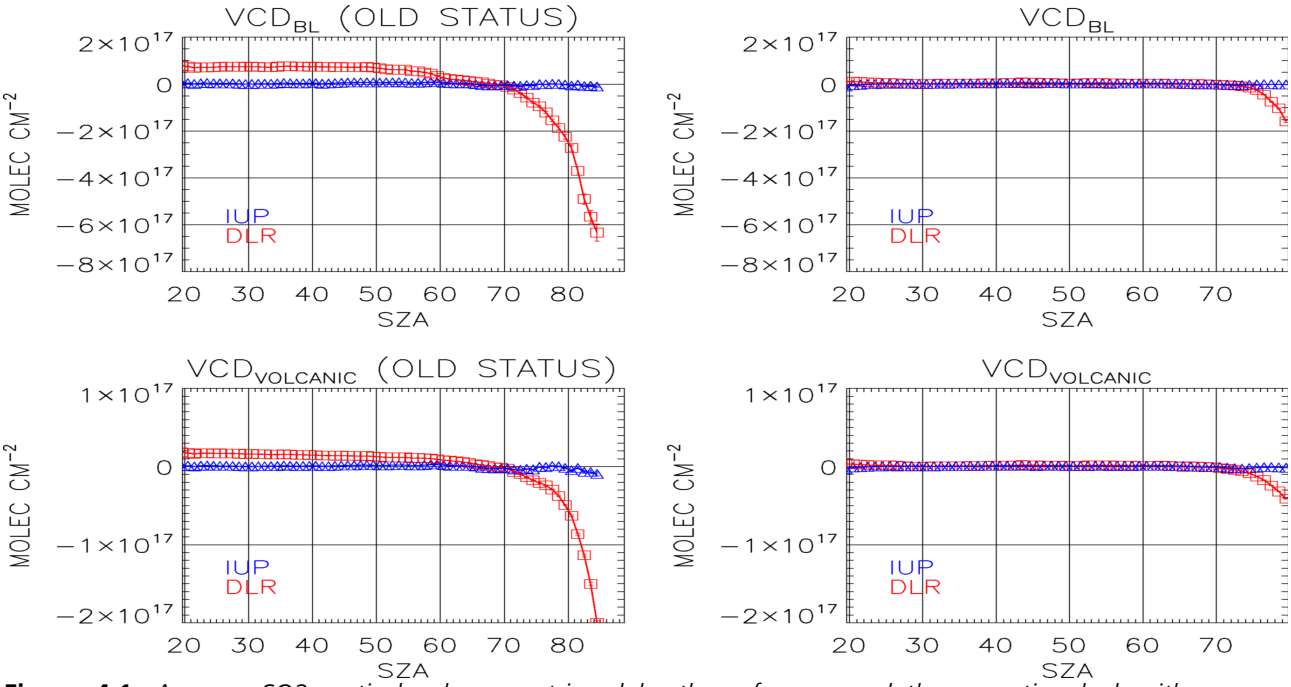


Figure 4.1: *Average SO2 vertical columns retrieved by the reference and the operational algorithms as a function of SZA. Top left panel: anthropogenic scenario for SGPv5.01; bottom left panel: volcanic scenario for SGPv5.01; top right panel: anthropogenic scenario for the improved SGP; bottom right panel: volcanic scenario for the improved SGP.*

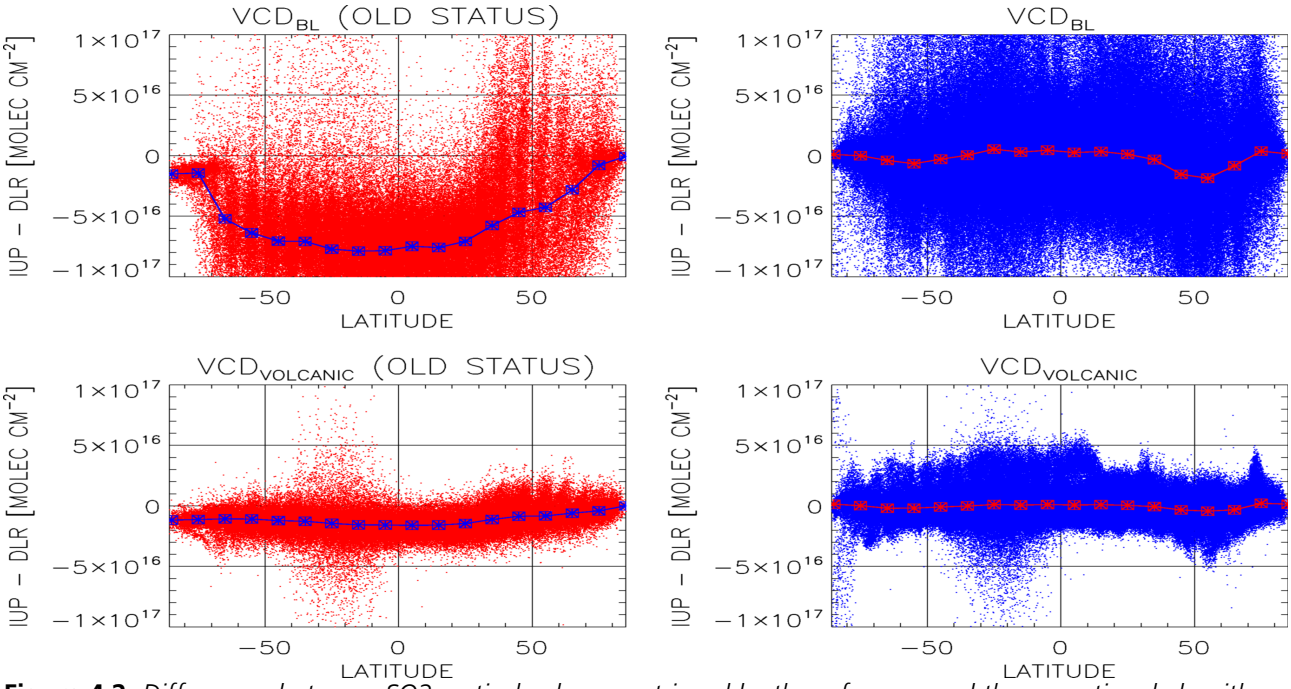


Figure 4.2: *Differences between SO2 vertical columns retrieved by the reference and the operational algorithms as a function of latitude. Top left panel: anthropogenic scenario SGPv5.01; bottom left panel: volcanic scenario SGPv5.01; top right panel: anthropogenic scenario improved SGP; bottom right panel: volcanic scenario improved SGP*

In Figure 4.2 differences between the reference and the operational algorithms are shown as a function of latitude. Although there is still large scatter for individual values, average differences are now much closer to zero with almost no latitudinal dependence in contrast to the situation with the SGPv5.0.

The improvements are additionally underlined by Figure 4.3, where differences are plotted as histograms.

All processor changes mentioned above did not have any impact on air mass factors.

Summarizing, the average difference between the reference and the operational algorithm decreased from $7 \cdot 10^{16}$ molec·cm^{-2} to $5 \cdot 10^{14}$ molec·cm^{-2} in case of VCD_{BL}; for $VCD_{VOLCANIC}$ previously the average difference was $1 \cdot 10^{16}$ molec·cm^{-2}, now it is $2 \cdot 10^{14}$ molec·cm^{-2}. On a relative scale this means that difference decreased from 80 to 2 % (on average!!!).

4.3.2 SO_2 offset correction database

An important prerequisite for the SO_2 product of high quality is a sufficiently filled database for the offset correction. In ideal case the database has to contain correction values for each day of the SCIAMACHY measurements. To achieve this goal, a processing of the full SCIAMACHY dataset is necessary, which is very time consuming.

However, during this verification procedure the database filled with the orbits of the verification data set (~ 180 orbits) was created. This database can be taken to start reprocessing. *It is also desirable to add the correction values from the day the reprocessing will start from (e.g. 2nd August 2002 or 1st January 2003).* If this is not done, the processor will use correction values for this day from a "nearest

neighbour" day (which in the verification set database could lay as far as 10 – 15 days away) leading not to the best result (see Figure 4.4 with SO_2 measurements on 1st January 2003 corrected using both methods: the database filled with the verification orbits only and the very same database but with 1st January 2003 additionally preprocessed).

4.3.3 Disclaimer Input

The following text for the product quality disclaimer is recommended:

The user is strongly advised to use the SO_2 quality flag placed in the L2 product (for more details consult SCIAMACHY L2 OL I/O DD and SCIAMACHY Offline Processor Level1b-2 Algorithm Theoretical Baseline Document). The quality flag value varies between 0 and 7 meaning:

- 0 - SO_2 product is NOT CORRECTED for an offset. Don't use it!
- 1..7 - SO_2 product is corrected and usable (the higher the quality flag value, the better a correction values used)

Don't use SO_2 values measured in the ascending node (the satellite moving northwards), since offset correction values applied are not appropriate for this measurement geometry.

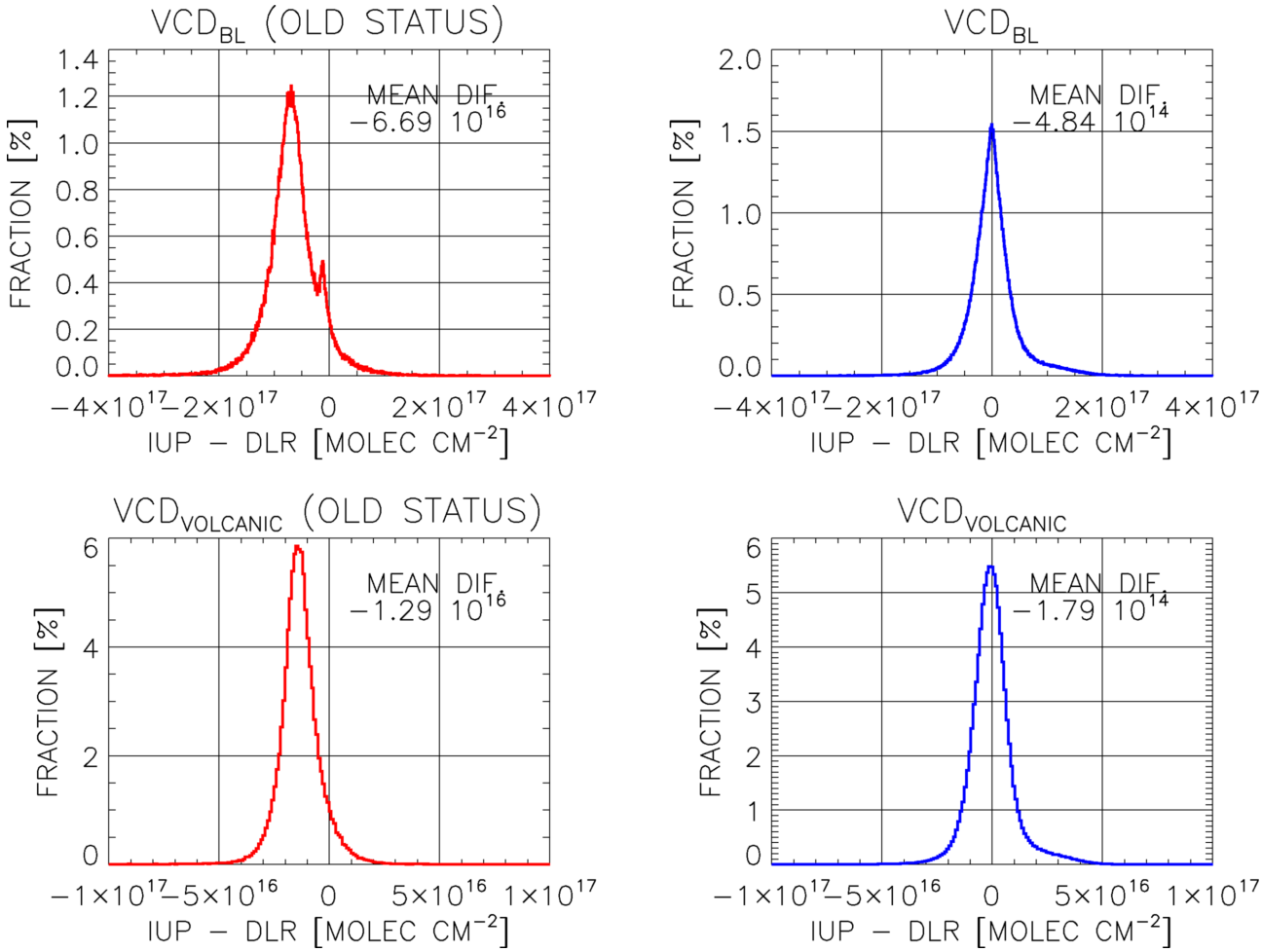
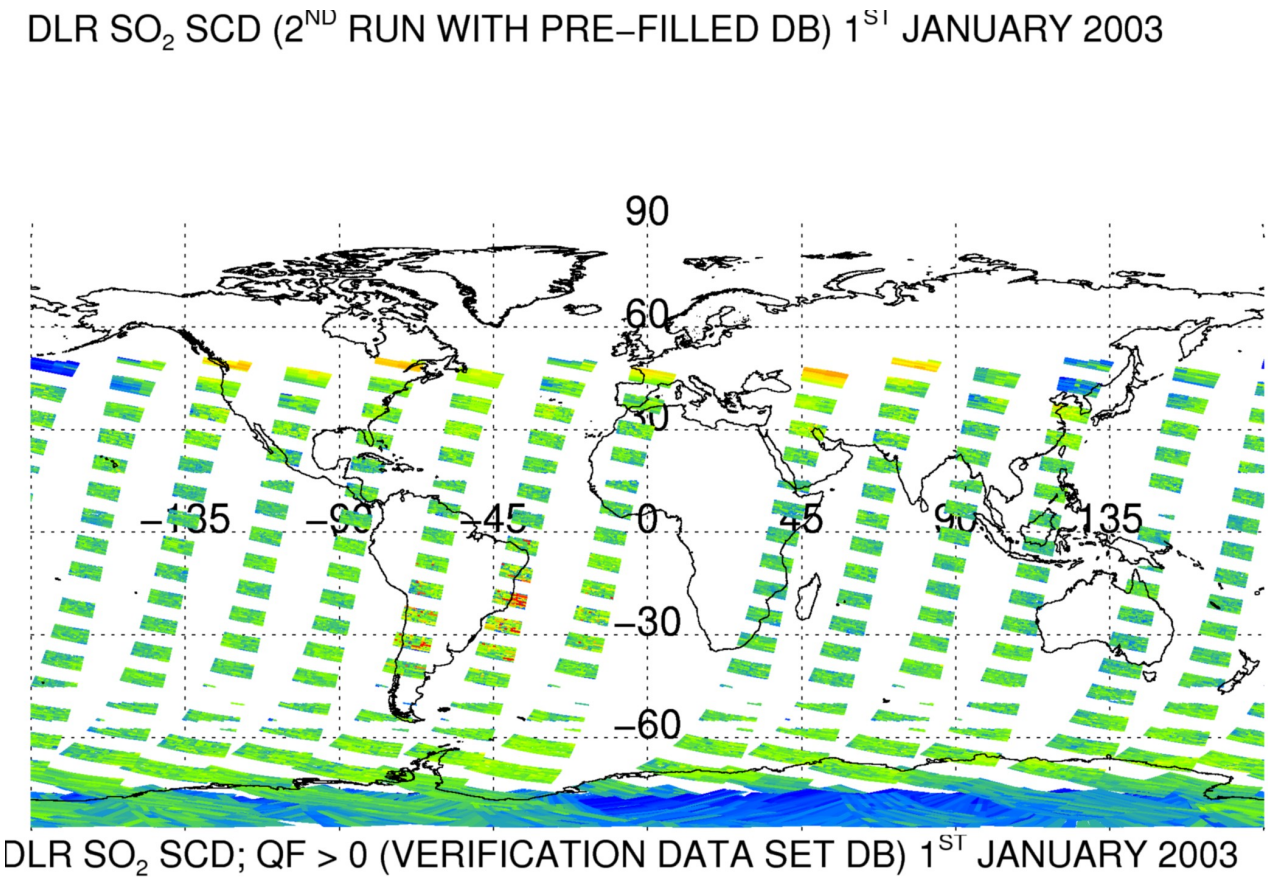


Figure 4.3: *Histogram of the differences between SO2 vertical columns retrieved by the reference and the operational algorithms. Top left panel: anthropogenic scenario for SGPv5.01; bottom left panel: volcanic scenario for SGPv5.01; top right panel: anthropogenic scenario for improved SGP; bottom right panel: volcanic scenario for improved SGP*



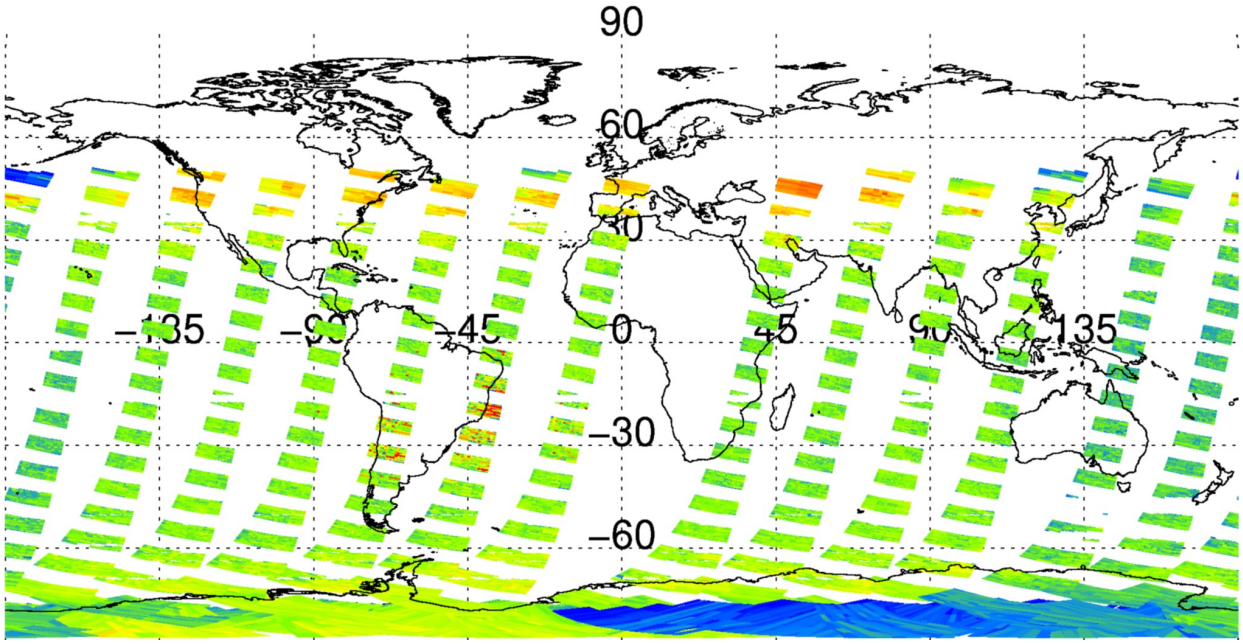


Figure 4.4: *Maps with SO2 SCDs for 1st January 2003. Top panel: corrected using the database filled with the verification orbits and the orbits from the 1st January 2003; bottom panel: the same but without the orbits from the 1st January 2003*

5 Nadir CO Verification and Analysis Results

Individual CO retrievals in channel 8 have low quality, since the CO spectral information contained in the spectra is comparable to the noise level and much lower than other overlapping species (H_2O and CH_4). In turn, the retrieval error is reduced by time-averaging the CO product. Accordingly, it is more convenient to assess the quality of the CO product according to time-averaged CO distributions than for individual observations.

5.1 Data Set Used

For the test, all data from 2003 to 2005 were processed. The quality checks were performed on monthly mean, since this is the intended use case for the data (still, individual data for each orbit will be provided).

5.2 Reason for the Processor Change

During the SCIAMACHY quick validation programme, it was found that the CO product from SGP v5.01 did not fulfil the quality requirements. In particular, the probability distribution functions (PDFs) of CO SGP v5.01 were biased to unrealistically low values. Additionally, global maps of CO turned out to be very noisy and did not exhibit realistic distributions. The main reason for this was identified to be the omission of a wavelength correction for the level 1b spectra in SGP v5.01 and the inclusion of some bad pixel in the fit.

The Spectral Line Source (SLS) on-board SCIAMACHY is not suitable for an in-flight spectral calibration of channel 8 due to the lack of enough SLS spectral lines within this channel. Consequently, the pixel-to-wavelength relationship of channel 8 in level 1b product is still set to the on-ground calibration.

In the mean time, the wavelength dependency of the channel 8 spectral correction has been investigated at DLR by using absorption signatures of atmospheric methane, water vapour and carbon monoxide. The spectral correction found can be well approximated by a 1st degree polynomial within the CO fitting window (2nd degree polynomial over the whole channel 8). The neglect of this correction has a dramatic impact on the quality and the absolute values of the CO retrievals (as it was the case of CO SGP v5.01).

In CO SGP v5.02, a linear spectral correction for the CO fitting window has been incorporated. Additionally, the Level 0-1 processing was corrected in times around the decontamination by providing a regular updated Dead and Bad Pixel Mask (DBPM).

5.3 Results

In this section, monthly means of the CO SGP product are analysed. In Sec. 5.3.1, results of the former version (5.01) of the operational SGP are presented. In sections 5.3.2 and 5.3.3, plots of global distributions, PDFs and time series of the mean and of the occurrence density are shown for the months of February, April and September of the years 2003, 2004 and 2005. Some statistics (mean, median, standard deviation, skewness and kurtosis) are presented in Sec. 5.3.4 and the results compared to the SCIAMACHY scientific products WFMD (IUP) and - where possible - IMLM (SRON).

The VCD (vertical column density) field of the CO SGP v5 product has two entries. The first one

represents "XCO", defined as

$$XCO := \frac{\alpha_{CO}}{\alpha_{CH4}} VCD_{CO}^{ref},$$

where α_{CO} is the scaling factor of the a-priori CO VCD (VCD_{CO}^{ref}) and α_{CH4} the scaling factor of the a-priori CH4 VCD. The second one is the uncorrected CO VCD:

$$VCD_{CO} := \alpha_{CO} VCD_{CO}^{ref}.$$

In the results presented hereafter only measurements satisfying the following criteria where considered:

- Convergence reached (first bit of quality flag == True),
- Solar zenith angle less than 80° (second bit of quality flag == True),
- only observations over land,
- only observations with cloud fraction less than 20% (from SGP v5.02 dataset "clouds_aerosol"), and
- retrieval error of CO VCD less than 1.5E+18.

The SGPv5.01 products were gridded into 1°x1° lon/lat bins, whereas for all other cases a 2°x2° lon/lat grid was used.

5.3.1 Comparison to operational SGP 5.01

In order to point out the improvements included in SGP version 5.02 with respect to version 5.01, some results of the former version (5.01) are presented in this subsection. The results obtained with both versions do not match exactly in time. With the SGP version 5.01 the validation dataset was processed, whereas with version 5.02 the processed orbits comprised all months of the years 2003, 2004 and 2005. Despite the temporal mismatch, the improvements in version 5.02 are clearly visible (see subsections 5.3.2 and 5.3.3).

Figure 5.1 shows the binned time series of the scaling factors of CO (left) and CH4 (middle), as well as of VCD_CO (right) SGP version 5.01. Notice the unrealistically low values of the CO scaling factor and VCD_CO. The variability of the CH4 scaling factor is due to a dependence on the instrument transmission.

Figure 5.2 shows global distributions of SGP v5.01 XCO (left) and VCD_CO (middle) for the whole validation dataset. The maps are unrealistic. The right panel shows PDFs of VCD_CO (blue) and XCO (light yellow). The distributions are centred around zero, confirming what was shown in Figure 5.1: the distributions are biased to negative values.

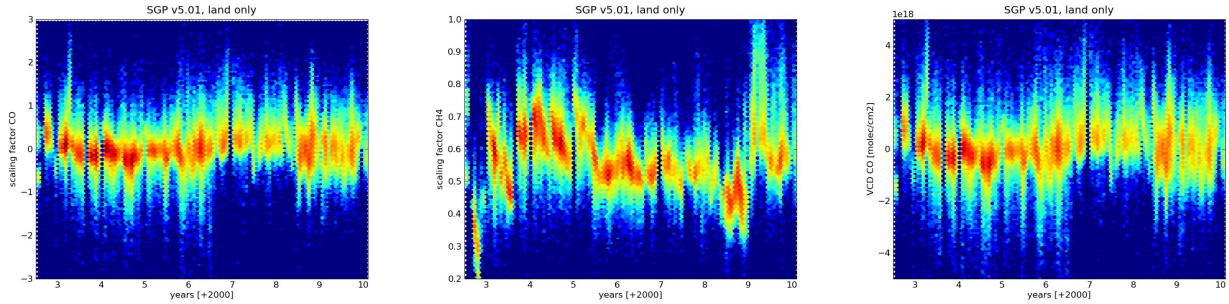


Figure 5.1: From left to right: Time series of the fitted scaling parameters of CO and CH4 vertical columns, and VCD_CO SGP v5.01. The colour labels represent the number of values that fall inside a given bin. Blue means low and red high density.

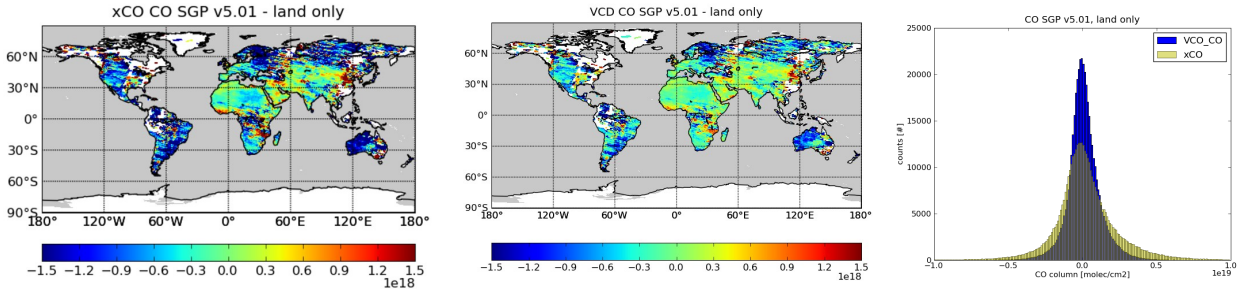


Figure 5.2: Global distributions of SGP v5.01 XCO (left) and VCD_CO (middle). All data from the validation dataset was gridded in 1°x1° lon/lat bins. Right: (not normalized) Probability density function of VCD_CO (blue) and XCO (yellow).

5.3.2 *SGP v5.02* XCO Columns

In this subsection, a representative selection of graphical illustrations of the SGP v5.02 XCO product are shown. The selected months are February, April and September and the results are shown for each of the years of 2003, 2004 and 2005. Each of the figures shows (from top down): Global distributions of XCO, (not normalized) PDFs, time series of the mean and time series of the density of occurrence. Note that the error bars in the time series (daily mean) plots do not represent the standard deviation of the mean, but the standard deviation of the population. The XCO results will not be commented individually but they will be explained together with those of VCD_CO in subsection 5.3.5.

2003

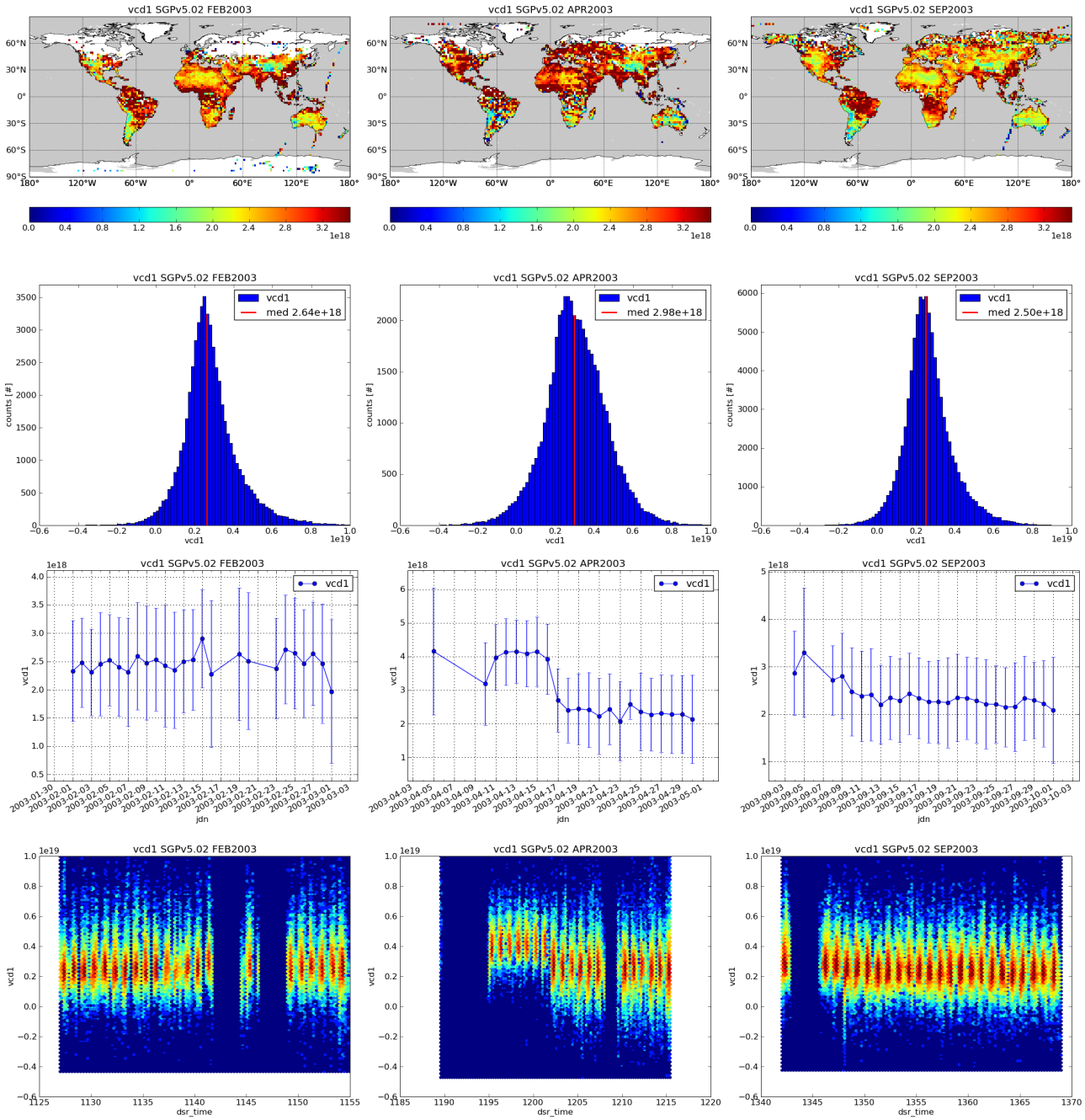


Figure 5.3: From top down: SGP v5.02 XCO global distributions, (not normalized) PDFs, time series and density time series of February (left), April (middle) and September (right) 2003.

2004

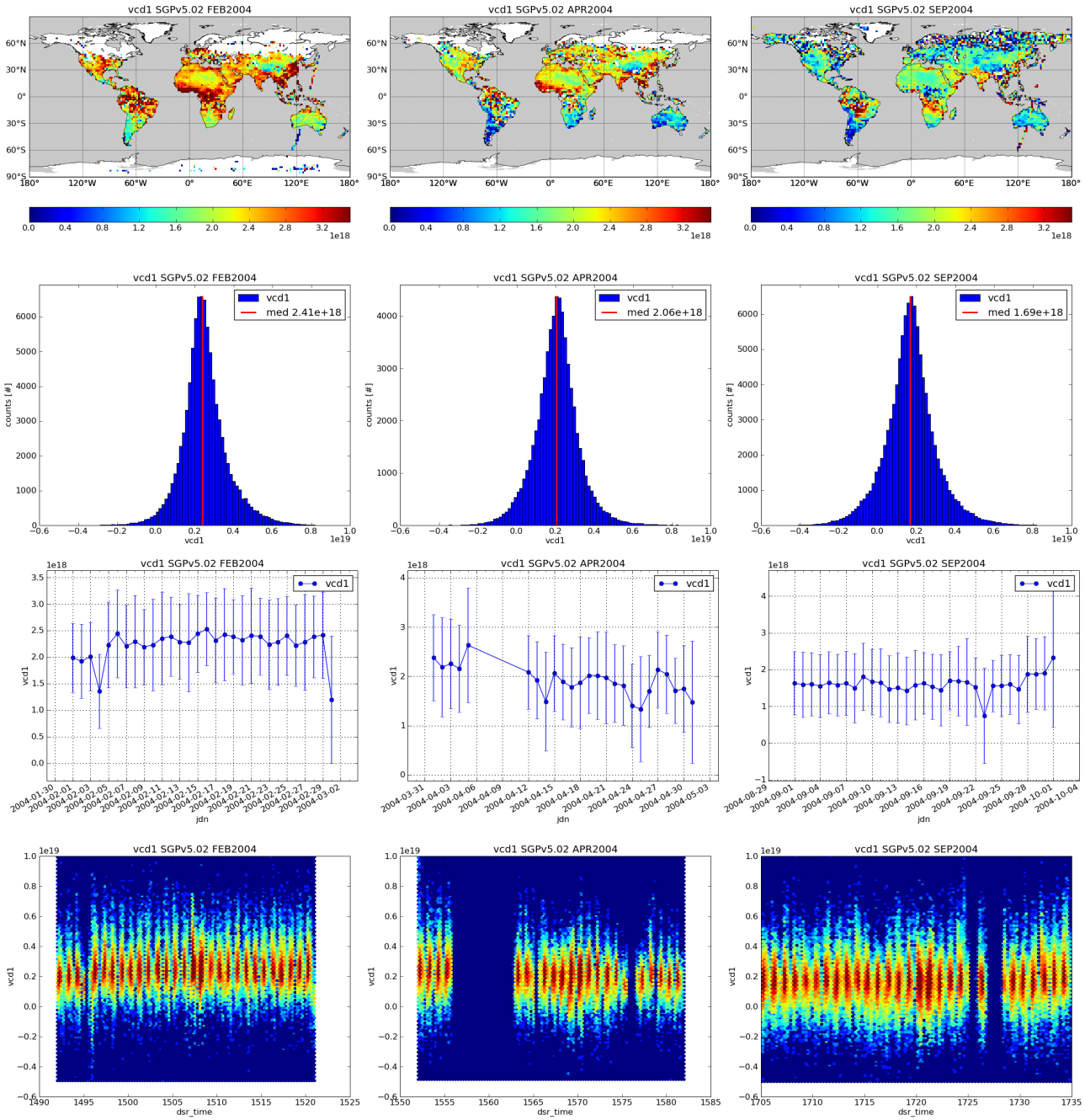


Figure 5.4: From top down: SGP v5.02 XCO global distributions, (not normalized) PDFs, time series and density time series of February (left), April (middle) and September (right) 2004.

2005

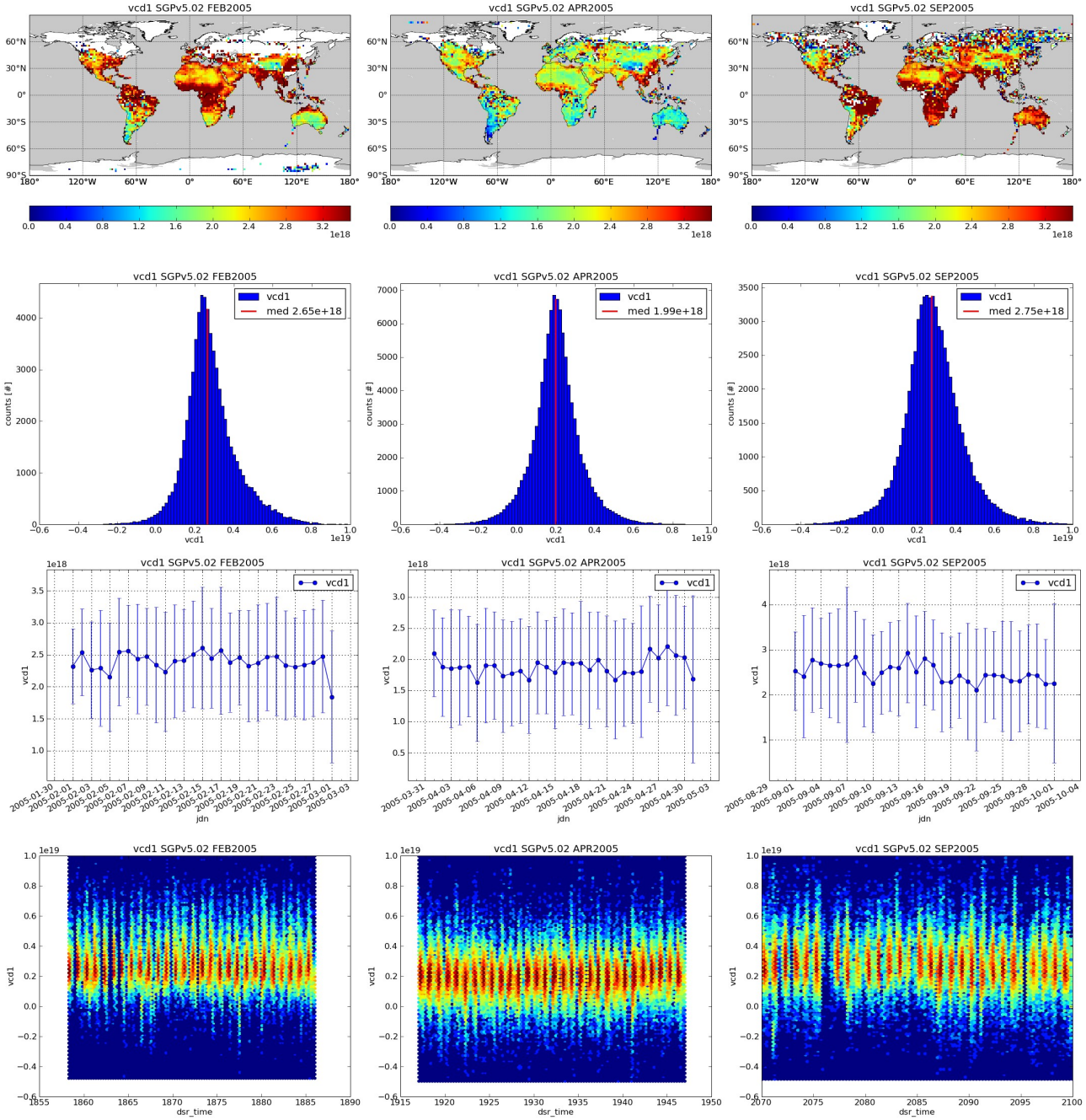


Figure 5.5: From top down: SGP v5.02 XCO global distributions, (not normalized) PDFs, time series and density time series of February (left), April (middle) and September (right) 2005.

5.3.3 SGP v5.02 CO Vertical Columns

Same as previous section but for SGP v5.02 VCD_CO product.

2003

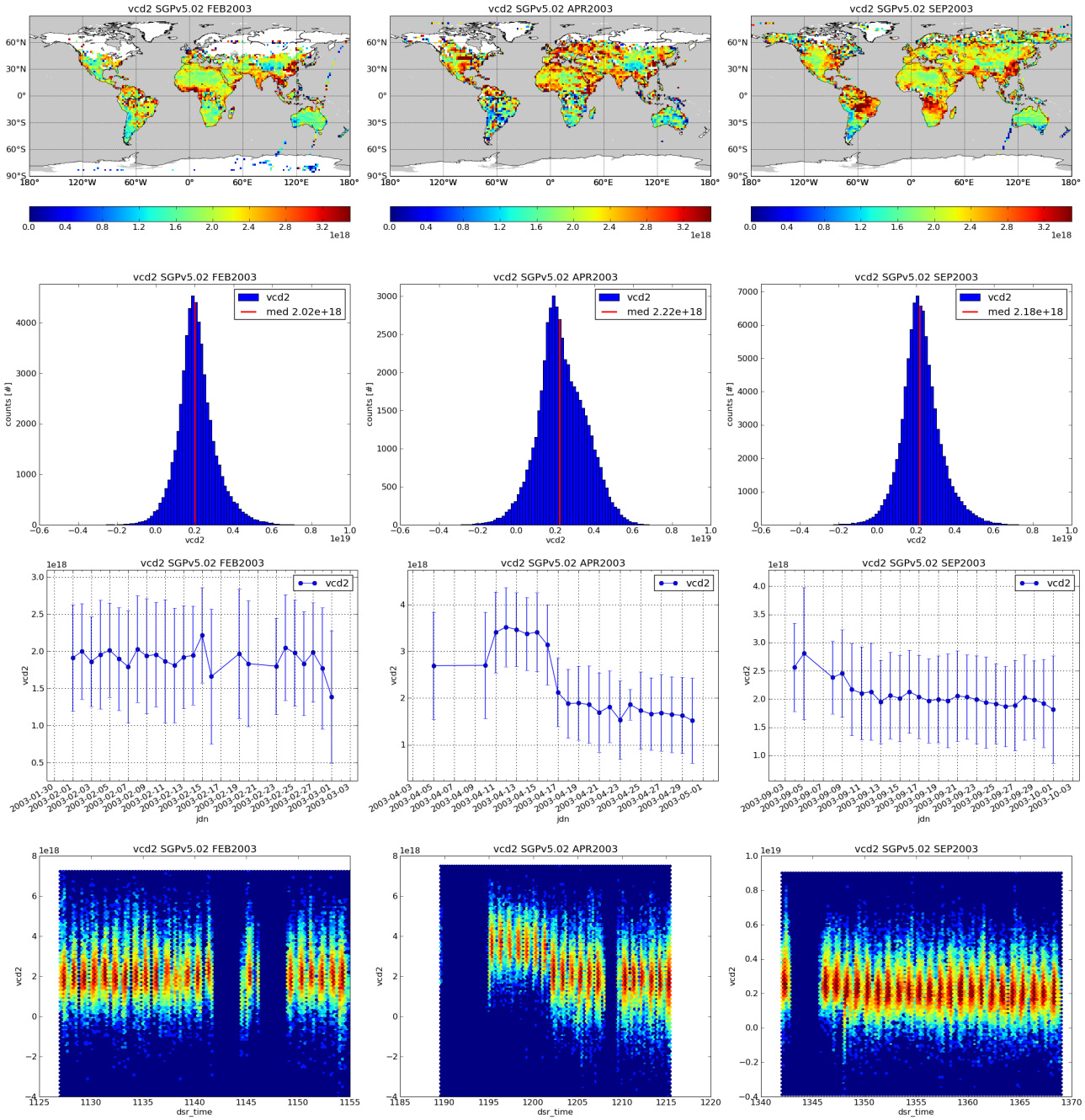


Figure 5.6: From top down: SGP v5.02 VCD CO global distributions, (not normalized) PDFs, time series and density time series of February (left), April (middle) and September (right) 2003.

2004

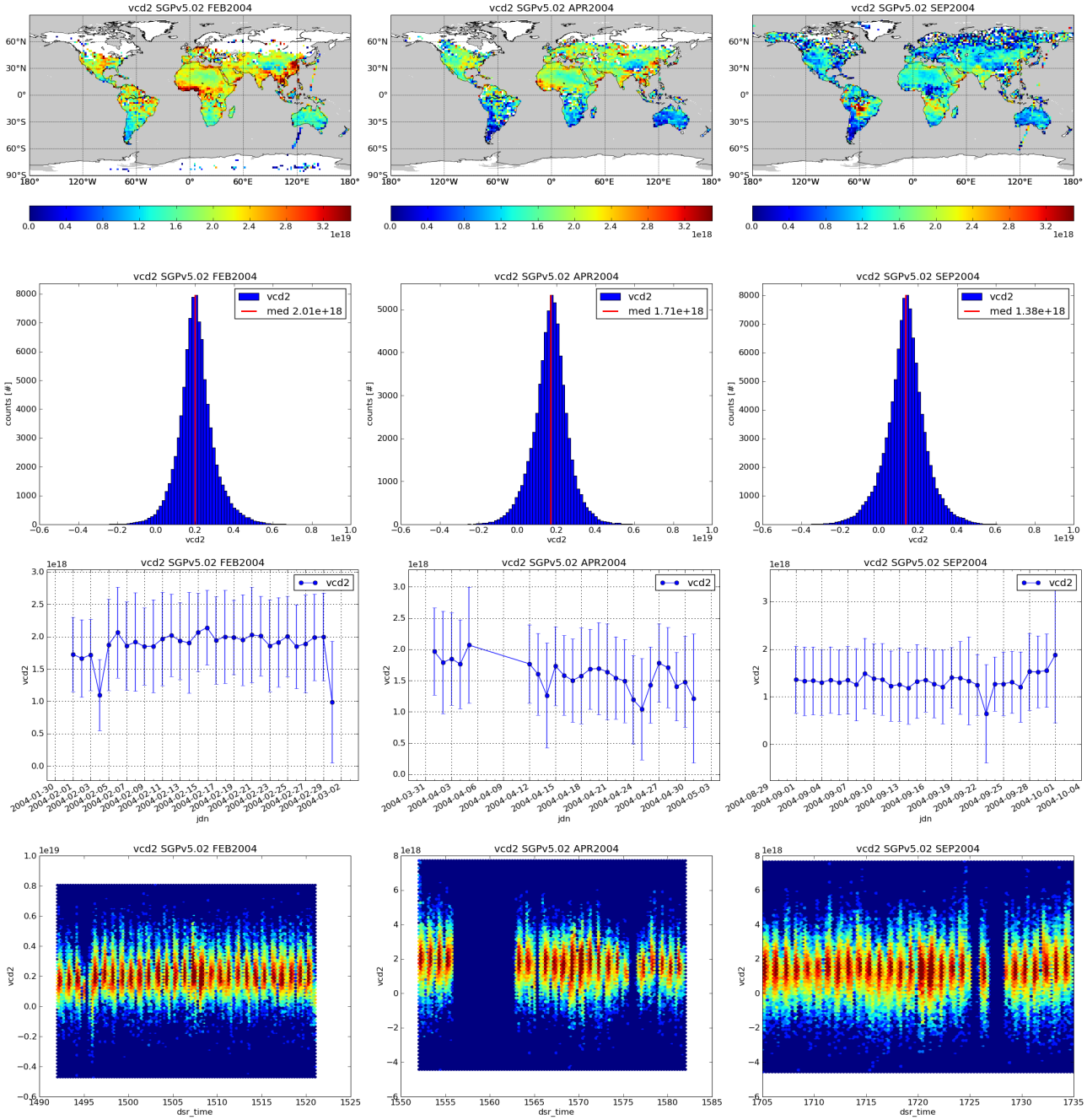


Figure 5.7: From top down: SGP v5.02 VCD CO global distributions, (not normalized) PDFs, time series and density time series of February (left), April (middle) and September (right) 2004.

2005

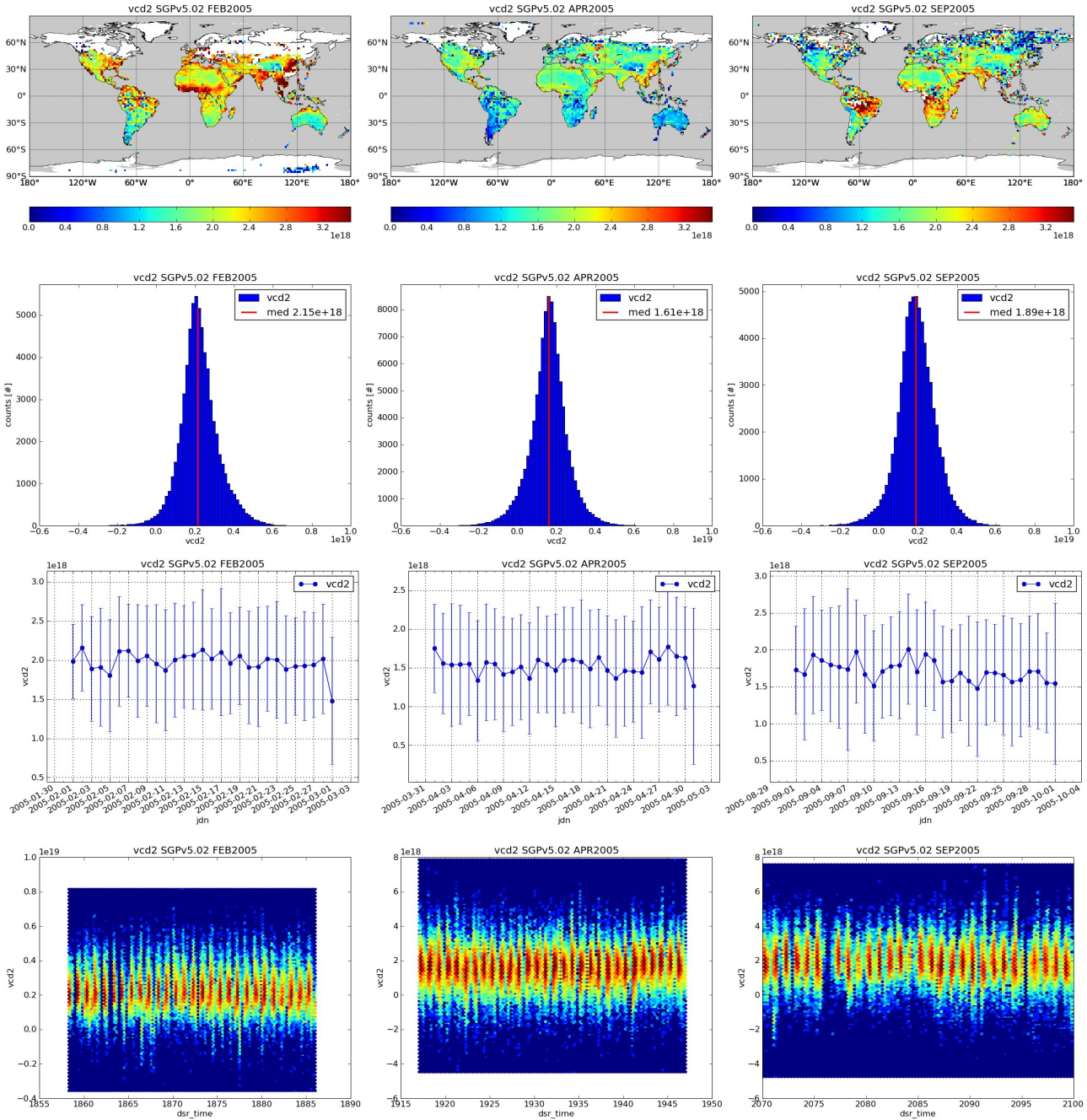


Figure 5.8: From top down: SGP v5.02 VCD CO global distributions, (not normalized) PDFs, time series and density time series of February (left), April (middle) and September (right) 2005.

5.3.4 Statistics

In this section the overall statistics for the calculated monthly mean are shown. The following table shows

- the number of valid points **N**,
- the median $\tilde{\mathbf{x}}$,
- the mean $\bar{\mathbf{x}}$,
- the standard deviation σ
- the relative difference (SGP-Algo)/SGP $\Delta\tilde{\mathbf{x}}$ for the median and for the mean $\Delta\bar{\mathbf{x}}$

for the monthly means from 2003 to 2005 in units of 1e18. "SGP" marks the results of the operational processor, "WFMD" is the algorithm of the university of Bremen, "IMLM" the algorithm of SRON. Differences larger than +/-20% are highlighted in grey, those smaller than +/-10% are bold faced. SGP and WFMD algorithms provide xCO (in *italics)* and CO, IMLM provides CO only. A plot of the time dependence of the mean and median for the SGP and for the WFMD algorithm can be found in Figure 5.9 and Figure 5.10. For the global mean most of the values are within 10% relative difference.

The SGP values show generally a larger point-to-point variability than the WFMD values, since only a standard filtering was applied to the operational data. A closer look at the individual data sets might lead to a better result, but this out of the scope in this investigation. Very roughly, both algorithms follow the same trends. From 2005 onwards, the agreement gets worse, most likely due to the detector degradation and the loss of important spectral points.

At the current stage at least the averaging of values over a month is recommended. Seasonal or yearly averages will be of better quality than the monthly means.

	2003						2004						2005					
	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$
JAN																		
SGPv5.02_XCO	*39781*	2.57	2.73	1.34			*32372*	2.19	2.23	1.21			*42324*	2.07	2.15	1.34		
SGPv5.02_CO	39781	2.10	2.18	1.00			32372	1.86	1.87	0.97			42324	1.78	1.79	1.04		
wfmd0.6_l2b_XCO	*64279*	2.49	2.46	0.91	***3.06%***	*10.07%*	*63307*	1.96	1.96	0.75	*10.26%*	*12.26%*	*47383*	2.07	2.03	0.72	***-0.07%***	***5.50%***
wfmd0.6_l2b_CO	64279	2.29	2.26	0.90	**-8.76%**	**-3.43%**	63307	1.80	1.82	0.77	**3.11%**	**2.32%**	47383	1.94	1.90	0.75	**-8.44%**	**-6.43%**
FEB																		
SGPv5.02_XCO	*55803*	2.64	2.81	1.45			*84530*	2.40	2.49	1.20			*68365*	2.66	2.85	1.38		
SGPv5.02_CO	55803	2.02	2.09	1.00			84530	2.00	2.04	0.95			68365	2.16	2.24	1.00		
wfmd0.6_l2b_XCO	*53286*	2.60	2.59	0.85	***1.52%***	***7.69%***	*73382*	2.12	2.12	0.74	*11.54%*	*15.06%*	*48092*	2.22	2.18	0.68	*16.65%*	***23.62%***
wfmd0.6_l2b_CO	53286	2.23	2.21	0.79	-10.44%	**-6.00%**	73382	1.95	1.95	0.73	**2.77%**	**4.63%**	48092	2.00	1.96	0.66	**7.63%**	12.38%
IMLMv6.4_CO							57291	1.46	1.30	1.44	**26.89%**	**36.48%**		0.00	0.00	0.00		
MAR																		
SGPv5.02_XCO	*62250*	2.77	2.99	1.72			*51525*	2.17	2.24	1.18			*91976*	2.50	2.65	1.41		
SGPv5.02_CO	62250	2.02	2.10	1.11			51525	1.82	1.85	0.92			91976	2.02	2.07	1.02		
wfmd0.6_l2b_XCO	*94105*	2.77	2.81	0.90	***0.05%***	***6.22%***	*97137*	2.31	2.32	0.77	***-6.35%***	***-3.19%***	*61949*	2.27	2.26	0.68	***8.91%***	*14.76%*
wfmd0.6_l2b_CO	94105	2.28	2.30	0.77	-13.09%	**-9.32%**	97137	2.10	2.11	0.74	-15.36%	-13.70%	61949	2.05	2.03	0.65	**-1.39%**	**2.16%**
APR																		
SGPv5.02_XCO	*50850*	2.98	3.04	1.60			*57544*	2.07	2.06	1.17			*102481*	2.00	2.03	1.30		
SGPv5.02_CO	50850	2.22	2.32	1.25			57544	1.72	1.69	0.92			102481	1.62	1.60	0.97		
wfmd0.6_l2b_XCO	*94190*	2.53	2.54	0.81	*15.08%*	*16.22%*	*122948*	2.31	2.31	0.74	*-11.39%*	*-12.00%*	*66367*	2.32	2.32	0.68	*-15.51%*	*-13.93%*
wfmd0.6_l2b_CO	94190	2.15	2.17	0.76	**3.43%**	**6.55%**	122948	2.05	2.06	0.71	-19.22%	**-21.84%**	66367	2.07	2.06	0.65	**-27.60%**	**-28.87%**
IMLMv6.4_CO							69787	1.67	1.61	1.49	**2.76%**	**4.50%**						

	2003						2004						2005					
	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$
MAY																		
SGPv5.02_XCO	*81359*	2.63	2.64	2.02			*73756*	2.03	2.05	1.26			*102516*	2.46	2.56	1.45		
SGPv5.02_CO	81359	1.83	1.78	1.28			73756	1.64	1.62	0.96			102516	1.92	1.93	1.02		
wfmd0.6_l2b_XCO	*66646*	2.44	2.51	0.92	***6.92%***	***4.92%***	*77457*	2.21	2.22	0.74	***-8.54%***	***-8.75%***	*68926*	2.41	2.41	0.72	***2.24%***	***5.64%***
wfmd0.6_l2b_CO	66646	2.01	2.09	0.83	**-9.97%**	-17.29%	77457	1.89	1.92	0.68	-15.53%	-18.32%	68926	2.10	2.10	0.67	**-9.15%**	**-8.73%**
JUN																		
SGPv5.02_XCO	*96103*	2.54	2.61	1.70			*67087*	2.39	2.54	1.60			*106657*	2.39	2.48	1.52		
SGPv5.02_CO	96103	1.82	1.82	1.15			67087	1.80	1.84	1.09			106657	1.81	1.82	1.05		
wfmd0.6_l2b_XCO	*82737*	2.19	2.29	0.87	*13.88%*	*12.29%*	*2729*	2.12	2.16	0.68	*11.20%*	*14.90%*	*61433*	2.31	2.33	0.69	***3.25%***	***6.08%***
wfmd0.6_l2b_CO	82737	1.72	1.80	0.73	**5.54%**	**1.13%**	2729	1.81	1.85	0.67	**-0.54%**	**-0.36%**	61433	1.96	1.97	0.62	**-8.38%**	**-8.33%**
JUL																		
SGPv5.02_XCO	*73166*	2.33	2.34	1.98			*100313*	2.11	2.16	1.36			*111078*	2.24	2.29	1.70		
SGPv5.02_CO	73166	1.45	1.41	1.17			100313	1.81	1.81	1.11			111078	1.54	1.50	1.04		
wfmd0.6_l2b_XCO	*33311*	1.87	2.01	0.79	*19.90%*	*14.00%*	*20415*	1.82	1.88	0.69	*13.87%*	*12.72%*	*43935*	2.06	2.12	0.67	***8.15%***	***7.58%***
wfmd0.6_l2b_CO	33311	1.31	1.41	0.56	**9.23%**	**0.44%**	20415	1.60	1.66	0.64	11.92%	**8.22%**	43935	1.65	1.70	0.56	**-7.40%**	-13.19%
AUG																		
SGPv5.02_XCO	*28481*	2.40	2.40	2.03			*87344*	2.10	2.12	1.33			*89730*	2.96	3.08	1.63		
SGPv5.02_CO	28481	1.43	1.39	1.15			87344	1.74	1.71	1.04			89730	1.95	1.98	0.97		
wfmd0.6_l2b_XCO	*21915*	2.18	2.27	0.86	***9.20%***	***5.61%***	*37754*	1.87	1.93	0.69	*11.19%*	***8.72%***	*26854*	1.93	2.01	0.63	*34.78%*	*34.74%*
wfmd0.6_l2b_CO	21915	1.66	1.80	0.82	-16.57%	-29.42%	37754	1.61	1.67	0.63	**7.19%**	**2.35%**	26854	1.50	1.56	0.49	23.40%	21.37%
SEP																		
SGPv5.02_XCO	*91636*	2.50	2.62	1.27			*96456*	1.70	1.71	1.36			*69183*	2.77	2.86	1.57		
SGPv5.02_CO	91636	2.18	2.25	1.05			96456	1.38	1.36	1.05			69183	1.91	1.93	1.01		

	2003						2004						2005					
	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$	N	$\tilde{x}$	$\bar{x}$	σ	$\Delta\tilde{x}$	$\Delta\bar{x}$
wfmd0.6_l2b_XCO	*126180*	2.31	2.37	0.89	***7.77%***	***9.61%***	*59814*	1.86	1.95	0.72	***-9.90%***	*-13.98%*	*17333*	2.16	2.25	0.72	***22.16%***	***21.21%***
wfmd0.6_l2b_CO	126180	2.12	2.17	0.86	**2.87%**	**3.56%**	59814	1.62	1.68	0.64	-17.46%	**-23.48%**	17333	1.71	1.78	0.57	10.50%	**7.97%**
IMLMv6.4_CO		0.00	0.00	0.00			70401	1.54	1.66	1.45	-11.08%	**-21.90%**		0.00	0.00	0.00		
OCT																		
SGPv5.02_XCO	*81907*	2.27	2.39	1.33			*59803*	2.15	2.31	1.55			*87056*	2.26	2.23	2.04		
SGPv5.02_CO	81907	1.90	1.96	1.04			59803	1.68	1.76	1.12			87056	1.55	1.50	1.30		
wfmd0.6_l2b_XCO	*116402*	2.34	2.42	0.93	***-3.15%***	***-1.22%***	*52942*	1.96	2.05	0.77	***8.66%***	*11.20%*	*37701*	2.18	2.32	0.87	***3.38%***	***-4.01%***
wfmd0.6_l2b_CO	116402	2.13	2.19	0.88	-12.00%	-11.78%	52942	1.65	1.72	0.67	**2.07%**	**2.20%**	37701	1.73	1.83	0.68	-11.54%	**-22.57%**
NOV																		
SGPv5.02_XCO	*48177*	2.10	2.19	1.29			*51098*	1.77	1.84	1.64			*62583*	1.29	1.26	2.42		
SGPv5.02_CO	48177	1.74	1.79	1.01			51098	1.29	1.29	1.11			62583	0.88	0.86	1.58		
wfmd0.6_l2b_XCO	*83315*	2.05	2.09	0.80	***2.41%***	***4.39%***	*33786*	1.86	1.94	0.71	***-5.05%***	***-5.28%***	*35828*	1.95	2.13	0.93	***-51.03%***	***-68.37%***
wfmd0.6_l2b_CO	83315	1.82	1.86	0.75	**-4.33%**	**-4.00%**	33786	1.50	1.56	0.59	-16.34%	**-20.88%**	35828	1.55	1.69	0.73	**-76.63%**	**-96.91%**
DEC																		
SGPv5.02_XCO	*36785*	1.94	1.99	1.41			*43252*	2.19	2.34	1.78			*57272*	2.11	2.24	2.17		
SGPv5.02_CO	36785	1.55	1.55	1.07			43252	1.54	1.60	1.17			57272	1.45	1.51	1.41		
wfmd0.6_l2b_XCO	*29827*	2.09	2.15	0.83	***-7.38%***	***-8.08%***	*20193*	2.00	2.06	0.75	***8.64%***	*11.92%*	*34571*	2.20	2.35	0.98	***-4.32%***	***-5.05%***
wfmd0.6_l2b_CO	29827	1.82	1.88	0.78	-17.87%	**-21.38%**	20193	1.56	1.61	0.62	**-1.63%**	**-0.67%**	34571	1.75	1.86	0.77	**-20.43%**	**-23.43%**

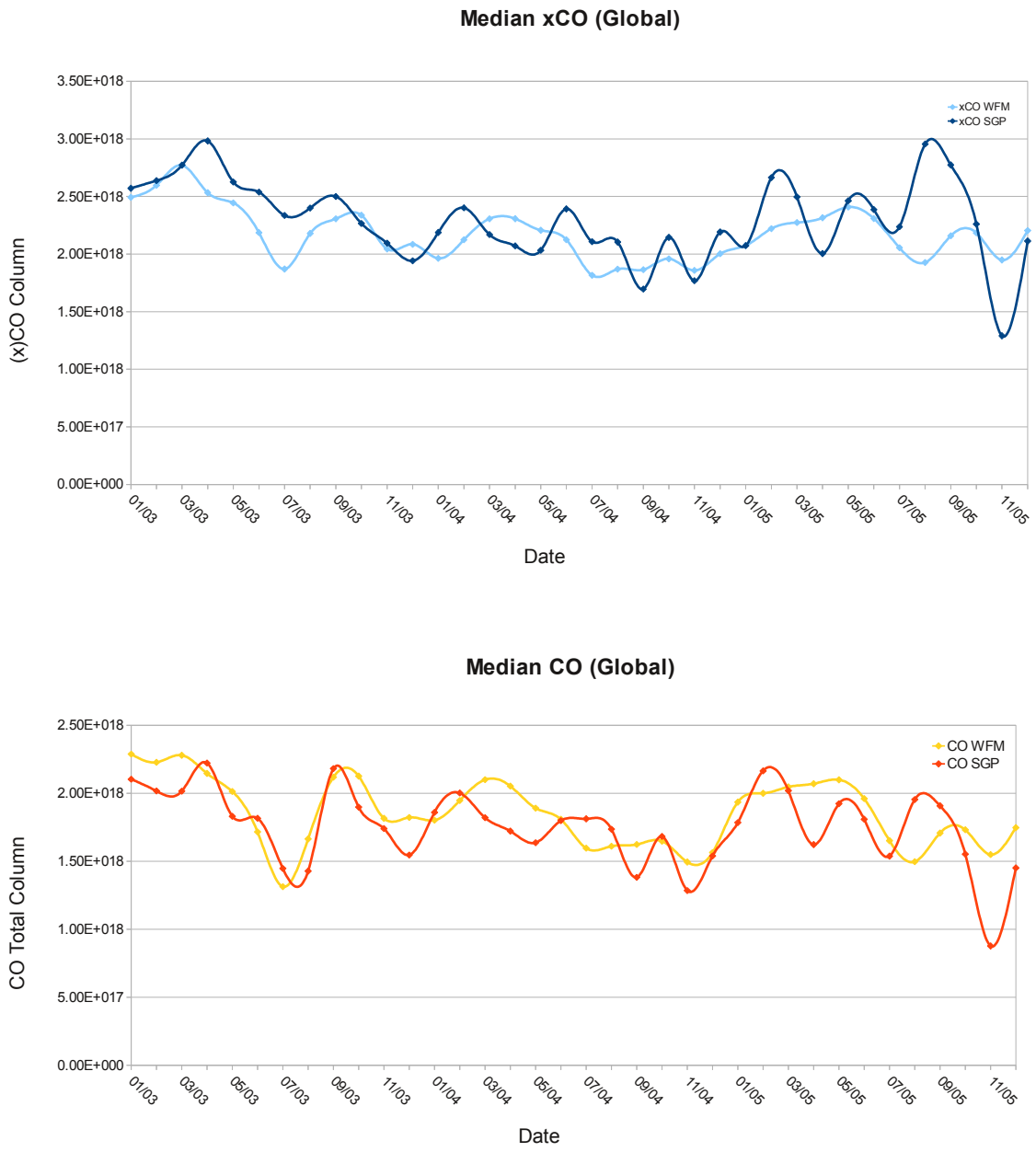


Figure 5.9: *Global median of xCO (top) and CO (bottom) as a function of time for SGP (darker colours) and WFMD (lighter colours).*

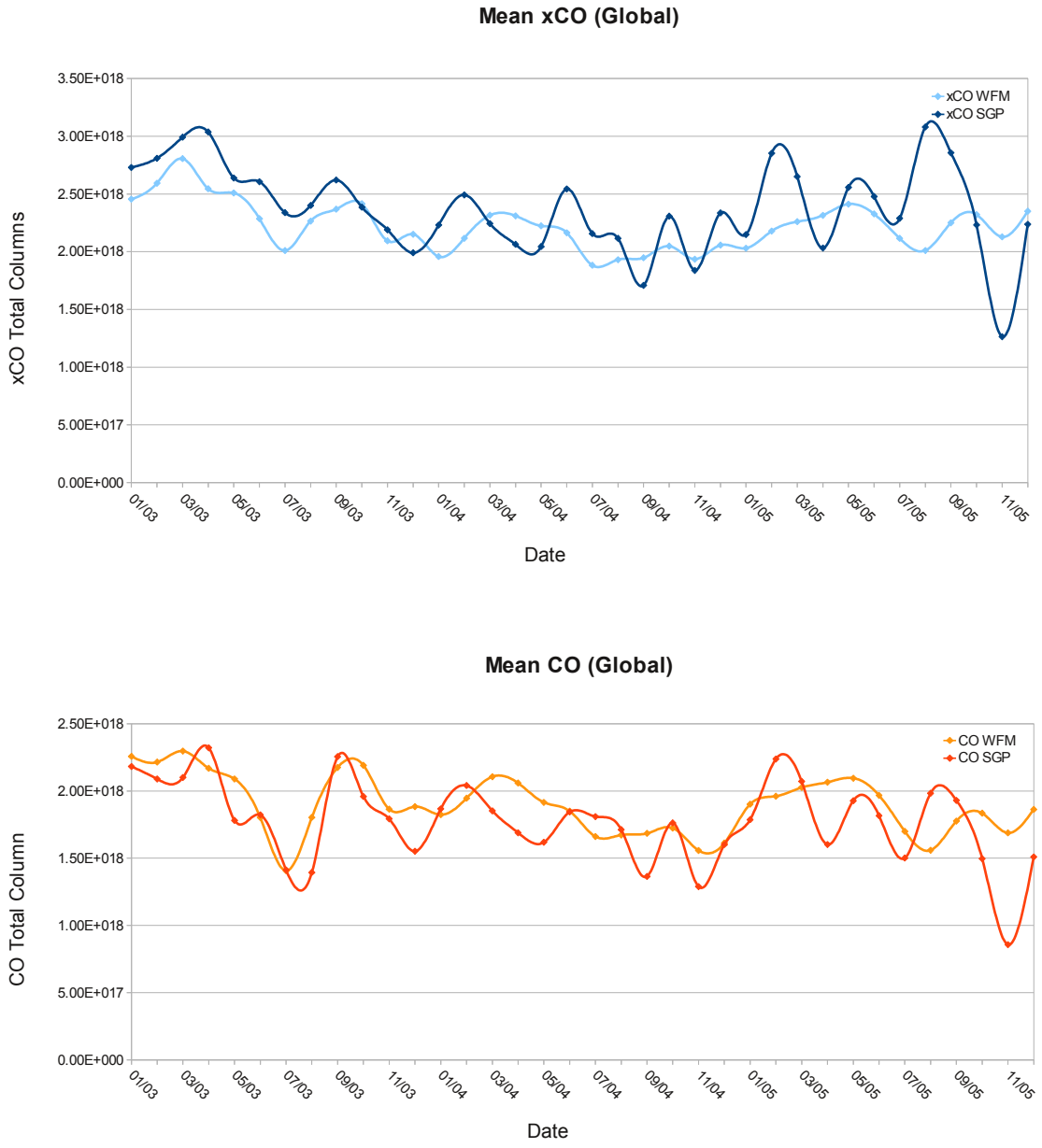


Figure 5.10: *Same as Figure 5.9 for the mean.*

5.3.5 Results discussion

The SGP CO products in Sec. 5.3.2 and 5.3.3 look in general good with some exceptions. The SGP CO global distributions show realistic local patterns, e.g. high VCD values at the Sahel region on February, high VCD values at central Africa bellow the equator on September or permanently high VCDs at South Eastern Asia. Seasonal variability is clearly seen. Biomass burnings are mostly responsible for the high concentrations at the Sahel region in Africa. The high CO concentrations at South Eastern Asia have mostly an anthropogenic origin. The PDFs of the data do not show anomalies (e.g. they are not

Poisson-like distributions). The XCO PDFs are systematically broader than those of VCD_CO, since in the former two fit parameters are involved (α_{CO} and α_{CH4}) instead of only one (α_{CO}) as in case of VCD_CO.

In April 2003 a bump in the right wing of the histogram is clearly discernible. The reason behind this bump can be better understood from the time series and the density series plots: The VCD values are too high during the second week of April 2003. This is likely to be caused by one or more bad spectral pixels included in the fit. The gap of data during the first week of April 2003 (see time series) is due to the non-convergence of the algorithm, rather than due to missing level0 data (as is the case during, e.g., decontamination periods). As before, the most likely reason is the inclusion of some bad pixel in the fit. In April 2004 there is another unexpected gap in the SGP CO product (see time series). As in case of April 2003, some bad pixels are thought to cause the retrieval algorithm to not converge. The other gaps in the data are also present in other SCIAMACHY scientific products (WFMD, IMLM).

In Sec. 5.3.2 and 5.3.3, only results of the months February, April and September are presented. The rest of the months were also processed with the operational processor and similar plots were produced. In Sec. 5.3.4, statistics of all months of the years 2003, 2004 and 2005 are shown. For comparison purposes, statistics of the retrieval algorithms WFMD and IMLM are also included.

Closer comparisons with independent measurements and/or SCIAMACHY scientific products (i.e. WFMD, IMLM, IMAP-DOAS) should determine the overall quality of the SGP CO products.

5.3.6 Disclaimer

The SGP v5.02 CO products are intended to be used as time-averaged products. Although single observations will be provided, they have large errors and they should not be used individually.

The main difference between versions 5.01 and v5.02 of SGP CO is the incorporation --in the latter version - of a spectral correction to the SCIAMACHY channel 8 level1b spectra. This correction brought a significant improvement in terms of quality of the product. At the moment the correction takes into account a wavelength dependent, linear wavelength shift. Investigations have shown a small time variability of the wavelength shift. The effect on the CO retrieval (if any) is unclear at the moment. In the next version of the processor, a more sophisticated wavelength correction will be implemented.

An ice layer grows on top of SCIAMACHY's channel 8 and affects the observed spectra: It reduces the instrument transmission and modifies the instrument slit function. In order to remove the ice layer from the detector, several decontamination operations have been done during the mission lifetime. Consequently, the impact of the ice layer is time-dependent. Monitoring of the fit parameters have shown that the scaling factor of CH4 (α_{CH4}) correlates with the instrument transmission. The scaling factor of CO α_{CO} is less affected by the ice layer growth (and accordingly VCD_CO will also be less affected). Since the XCO product includes α_{CH4} as a proxy and α_{CO} does not show the same behaviour, it will also be affected by the ice layer. Making a regression of α_{CH4} against instrument transmission, the α_{CH4} dependency can be modelled and the XCO product accordingly corrected. This correction is, however, not included in the SGP v5.02 product and users should be aware of this effect.

There are periods where the bad and dead pixel mask did not filter out all damaged spectral pixels. As a consequence of this, the fit algorithm does not convergence or it provides low quality (biased) data.

Summarizing, the CO products may suffer of a time-dependent bias due to level1b issues and the growth of an ice layer on top of SCIAMACHY's channel 8.

Additionally, the presence of clouds also affects the quality (or even the reliability) of the SGP v5.02 CO. SGP v5.02 contains clouds and aerosol products, but they are retrieved at a different wavelength region and are provided at a different integration time. Cloud fraction, cloud top height and cloud optical depth are important for cloud screening criteria and they must be re-calculated for CO integration times. Since α_{CH4} is a proxy for cloud top height, the effects of clouds are partially accounted for in XCO retrievals, whereas special care should be taken in case of VCD_CO.

Recommendations for Filtering

Filtering of the data is crucial to get a good CO product. In first instance we recommend the same filtering as used in this investigation:

- Convergence reached (first bit of quality flag == True),
- Solar zenith angle less than 80° (second bit of quality flag == True),
- only observations over land,
- only observations with cloud fraction less than 20% (from SGP v5.02 dataset "clouds_aerosol"), and retrieval error of CO VCD less than 1.5E+18.

These filter rules might get refined after a validation took place.

6 Regression Tests

As usual for regression tests, a shellscript was used that runs through all Level 2 files and calls the TDE to compare test and reference products. The following MDS were compared:

1. CLOUD_AEROSOL
2. NAD_UV0_O3
3. NAD_UV1_NO2
4. NAD_UV3_BRO
5. NAD_UV5_SO2
6. NAD_UV6_OCLO
7. NAD_UV7_SO2
8. NAD_UV8_H2O
9. NAD_IR3_CO
10. LIM_UV0_O3
11. LIM_UV1_NO2
12. LIM_UV3_BRO
13. LIM_CLOUDS

The output of the script was

Product	Cloud&Aerosol	NAD_UV0_O3	NAD_UV1_NO2	NAD_UV3_BrO	NAD_UV5_SO2	NAD UV6_OCLO	NAD_UV7_SO2	NAD_UV8_H2O	NAD_IR3_CO	LIM_UV0_O3	LIM_UV1_NO2	LIM_UV3_BRO	LIM_CLOUDS
SCI_OL__2PNPDE20051214_024739_000062162043_00218_19811_1262.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031027_113618_000059772021_00095_08666_0114.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031030_082053_000059742021_00136_08707_0167.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031108_065742_000059342021_00264_08835_0354.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031111_052250_000059662021_00306_08877_0413.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031113_005833_000059662021_00332_08903_0457.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031113_174436_000059662021_00342_08913_0472.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031123_191039_000059832021_00486_09057_0843.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031128_163232_000059612022_00055_09127_0799.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031201_131645_000059832022_00096_09168_0861.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031203_002955_000059612022_00117_09189_0899.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031207_114757_000059822022_00181_09253_1147.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031211_094209_000059612022_00237_09309_1114.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031213_065709_000060262022_00264_09336_1146.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20031217_031011_000060272022_00319_09391_1331.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20040115_194539_000059612023_00243_09816_1790.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2POLRA20040127_182730_000060002023_00414_09987_2025.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20020802_093420_000057082008_00151_02209_6028.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20020810_051658_000059332008_00263_02321_6224.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20020922_211146_000059542009_00387_02946_5191.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20021021_155758_000059312010_00298_03358_0195.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20021031_172353_000060152010_00442_03502_1460.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20030117_163251_000059612013_00055_04618_1553.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20030121_124504_000059822013_00110_04673_1532.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20030131_054818_000059382013_00249_04812_0261.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0
SCI_OL__2PPLRA20030409_115325_000059792015_00224_05789_0622.N1	0	0	0	0	**1**	0	**1**	0	**1**	0	0	0	0

Product	Cloud&Aerosol	NAD_UV0_O3	NAD_UV1_NO2	NAD_UV3_BrO	NAD_UV5_SO2	NADUV6_OCLO	NAD_UV7_SO2	NAD_UV8_H2O	NAD_IR3_CO	LIM_UV0_O3	LIM_UV1_NO2	LIM_UV3_BRO	LIM_CLOUDS
SCI_OL__2PPLRA20040309_112444_000059692025_00009_10584_0235.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20040310_091242_000059332025_00022_10597_0260.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20040504_052223_000060032026_00306_11382_1287.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20040722_190912_000056432028_00443_12521_0516.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20040917_040756_000059922030_00248_13328_1494.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20041003_090641_000059522030_00480_13560_1718.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20041118_214525_000060282032_00144_14226_2590.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20050115_093838_000059912033_00466_15049_3832.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20050307_161743_000059952035_00198_15783_4886.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20050523_141702_000059962037_00297_16884_6790.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20050710_191429_000057092038_00486_17574_0119.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20050913_100425_000060032040_00409_18499_1289.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060213_163755_000059392045_00098_20693_1073.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060428_193304_000060232047_00157_21754_2226.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060606_090800_000056942048_00208_22306_2834.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_012219_000056942048_00232_22330_2935.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_030255_000057342048_00233_22331_2937.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_044331_000056952048_00234_22332_2939.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_062406_000057342048_00235_22333_2941.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_080442_000056942048_00236_22334_2863.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_094518_000057342048_00237_22335_2864.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_112554_000056942048_00238_22336_2865.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_130630_000057342048_00239_22337_2866.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_144705_000056952048_00240_22338_2867.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_162741_000057342048_00241_22339_2868.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_180817_000056952048_00242_22340_2869.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_194853_000057342048_00243_22341_2870.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_212929_000056942048_00244_22342_2871.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060608_231005_000057342048_00245_22343_2872.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_013340_000056952048_00318_22416_2955.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_031416_000057352048_00319_22417_2956.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_045452_000056952048_00320_22418_2957.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_063528_000057352048_00321_22419_2958.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_081604_000056952048_00322_22420_2959.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_095640_000057352048_00323_22421_2960.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_113716_000056952048_00324_22422_2961.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_131751_000057352048_00325_22423_2962.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_145827_000056952048_00326_22424_2963.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_163903_000057352048_00327_22425_2964.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_181939_000056952048_00328_22426_2965.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_200015_000057352048_00329_22427_2966.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_214051_000056952048_00330_22428_2967.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060614_232127_000057352048_00331_22429_2968.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_010646_000059902050_00146_23246_0835.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_024721_000060042050_00147_23247_0836.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_042759_000059902050_00148_23248_0837.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_060834_000060042050_00149_23249_0838.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_074912_000059902050_00150_23250_0839.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_092947_000060042050_00151_23251_0840.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_111024_000059902050_00152_23252_0841.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_125059_000060042050_00153_23253_0842.N1	0	0	0	0	1	0	1	0	1	0	0	0	0

Product	Cloud&Aerosol	NAD_UV0_O3	NAD_UV1_NO2	NAD_UV3_BrO	NAD_UV5_SO2	NADUV6_OCLO	NAD_UV7_SO2	NAD_UV8_H2O	NAD_IR3_CO	LIM_UV0_O3	LIM_UV1_NO2	LIM_UV3_BRO	LIM_CLOUDS
SCI_OL__2PPLRA20060811_143137_000059902050_00154_23254_0843.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_161212_000060042050_00155_23255_0844.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_175250_000059902050_00156_23256_0845.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_193325_000060042050_00157_23257_0846.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060811_211402_000059902050_00158_23258_0847.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20060819_015541_000060042050_00261_23361_0954.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_030746_000059972052_00047_24149_1706.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_044906_000059482052_00048_24150_1707.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_062859_000059962052_00049_24151_1708.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_081019_000059482052_00050_24152_1709.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_095012_000059962052_00051_24153_1710.N1	**0**	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_113132_000059482052_00052_24154_1711.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_131124_000059962052_00053_24155_1712.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_145245_000059482052_00054_24156_1713.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_163237_000059972052_00055_24157_1714.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_181358_000059482052_00056_24158_1715.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_195350_000059962052_00057_24159_1716.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061013_213511_000059482052_00058_24160_1717.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061027_141120_000060242052_00254_24356_1924.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061202_184137_000059912053_00271_24874_0000.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_003228_000060022053_00389_24992_3150.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_021315_000059912053_00390_24993_3152.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_035340_000060032053_00391_24994_3154.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_053427_000059912053_00392_24995_5760.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_071452_000060022053_00393_24996_4469.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_085540_000059912053_00394_24997_4657.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_103605_000060022053_00395_24998_4778.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_121652_000059912053_00396_24999_4902.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_135717_000060032053_00397_25000_5000.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_153804_000059912053_00398_25001_5034.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_171829_000060032053_00399_25002_5136.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_185916_000059912053_00400_25003_5236.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20061211_203941_000060022053_00401_25004_5761.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20070103_165509_000059912054_00227_25331_3320.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20070109_120441_000059922054_00310_25414_6224.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20070303_174059_000059862056_00070_26176_2621.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20070320_034214_000059912056_00305_26411_7214.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20070515_175210_000056972058_00113_27221_4648.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20070715_173353_000057522059_00485_28094_3011.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20070915_182114_000059922061_00371_28982_8151.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20071115_180453_000059602063_00242_29855_3284.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20071223_180949_000059922064_00285_30399_1787.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20080221_182435_000059592066_00142_31258_5349.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20080420_172928_000060232067_00485_32102_4119.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20080619_174750_000056972069_00342_32961_9057.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PPLRA20080817_164920_000060042071_00184_33805_5238.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030110_201324_000060152012_00458_04520_0605.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030124_193330_000059612013_00157_04720_0740.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030127_093541_000059382013_00194_04757_0777.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030201_115858_000060212013_00267_04830_0312.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030204_034212_000059772013_00305_04868_0063.N1	0	0	0	0	1	0	1	0	1	0	0	0	0

Product	Cloud&Aerosol	NAD_UV0_O3	NAD_UV1_NO2	NAD_UV3_BrO	NAD_UV5_SO2	NADUV6_OCLO	NAD_UV7_SO2	NAD_UV8_H2O	NAD_IR3_CO	LIM_UV0_O3	LIM_UV1_NO2	LIM_UV3_BRO	LIM_CLOUDS
SCI_OL__2PSLRA20030210_021227_000059772013_00390_04953_0135.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030213_003742_000060092013_00432_04995_0171.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030215_162052_000059662013_00470_05033_0209.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030223_152900_000059832014_00083_05147_0324.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030227_114155_000060062014_00138_05202_0379.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030303_075437_000060172014_00193_05257_0513.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030308_033623_000059702014_00262_05326_0824.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030311_102423_000059332014_00309_05373_0868.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030314_020647_000060172014_00347_05411_0498.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030319_010920_000059732014_00418_05482_0778.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030329_192131_000059682015_00071_05636_0850.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030401_160721_000059352015_00112_05677_0853.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030413_094713_000059792015_00280_05845_1186.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030414_091529_000059792015_00294_05859_1212.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030422_064249_000059902015_00407_05972_0559.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030426_025607_000059862015_00462_06027_0616.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030508_000258_000056592016_00131_06197_0848.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030515_012255_000056852016_00232_06298_1194.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030526_204328_000056472016_00401_06467_1178.N1	0	0	0	0	1	0	1	0	0	0	0	0	0
SCI_OL__2PSLRA20030526_222404_000056792016_00402_06468_1276.N1	0	0	0	0	1	0	1	0	0	0	0	0	0
SCI_OL__2PSLRA20030529_122606_000056472016_00439_06505_1222.N1	0	0	0	0	1	0	1	0	0	0	0	0	0
SCI_OL__2PSLRA20030531_130323_000056782016_00468_06534_1361.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030604_041422_000056782017_00019_06586_1316.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030608_135157_000056462017_00082_06649_1429.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030608_171309_000056462017_00084_06651_1433.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030614_204544_000056462017_00172_06739_1552.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030619_194811_000056802017_00243_06810_0044.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030624_185041_000056502017_00314_06881_0122.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030628_132301_000056522017_00368_06935_0180.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030702_111635_000056542017_00424_06991_0249.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030708_094735_000056902018_00008_07076_0363.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030710_070348_000056592018_00035_07103_0392.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030717_032244_000056972018_00133_07201_0511.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030723_015356_000056692018_00218_07286_0827.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030730_232204_000057082018_00331_07399_0831.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030805_151059_000056802018_00412_07480_0931.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030807_090605_000057132018_00437_07505_0964.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030830_033631_000059802019_00262_07831_1438.N1	0	0	0	0	1	0	1	0	0	0	0	0	0
SCI_OL__2PSLRA20030830_083809_000060042019_00265_07834_1443.N1	0	0	0	0	1	0	1	0	0	0	0	0	0
SCI_OL__2PSLRA20030902_202746_000059642019_00315_07884_1506.N1	0	0	0	0	1	0	1	0	0	0	0	0	0
SCI_OL__2PSLRA20030903_163503_000059652019_00327_07896_1522.N1	0	0	0	0	1	0	1	0	0	0	0	0	0
SCI_OL__2PSLRA20030910_111410_000059362019_00424_07993_1648.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030916_080347_000059752020_00007_08077_1758.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030922_045448_000059312020_00091_08161_1876.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20030927_021533_000059742020_00161_08231_2086.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20031004_001602_000058872020_00260_08330_2108.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20031008_231804_000059342020_00331_08401_2218.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20031010_103030_000059712020_00352_08422_2244.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20031012_074712_000059342020_00379_08449_2294.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20031014_164626_000060182020_00413_08483_2468.N1	0	0	0	0	1	0	1	0	1	0	0	0	0
SCI_OL__2PSLRA20031021_144611_000059742021_00011_08582_2486.N1	0	0	0	0	1	0	1	0	1	0	0	0	0

Each row shows the name of the Level 2 file followed by the return codes of TDE for the 13 MDS. TDE return code 0 means that the test succeeded. Code 1 is returned if differences occurred. This can either be differences in corresponding values, or differences in record start times (which do not implicate differences in corresponding values). Return code 255 denotes an input error (did not appear in this test). Except for the 5th product (NAD_UV5_SO2), the 7th (NAD_UV7_SO2) and the 9th product (NAD_IR3_CO) all TDE return codes are 0. This means that for all unchanged products the regression tests succeeded. Note that the OClO product do not show any changes, because the fix of the polynomial degree was already incorporated in the reference version 5.2.

7 Summary

In this document the changes resulting from the validation are summarised and the new retrieval results are presented. Significant improvement for the Nadir retrieval of

- OClO slant columns
- SO_2 total columns
- CO total columns

have been achieved. A complete regression test was made to ensure that the changed algorithms do not degrade the quality of the algorithms that were successfully validated. In addition to the new retrieval results, recommendations for the Level 2 product disclaimer are given.

Based on this TN, the SQWG will decide on the start of re-processing with the new processor version.