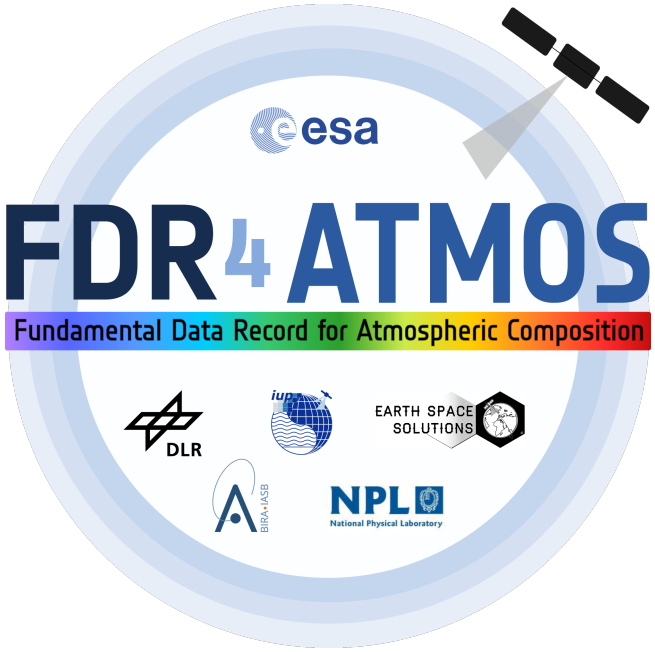
Level 2 Regression Test

FDR4ATMOS Task A

Issue 1

Deutsches Zentrum
für Luft- und Raumfahrt e.V.
in der Helmholtz-Gemeinschaft



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1 Introduction

1.1 Purpose and Scope of the Document

The project FDR4ATMOS (Fundamental Data Records in the domain of satellite Atmospheric Composition) has been initiated by the European Space Agency (ESA). In task A of the project the Level 0-1 processor for SCIAMACHY data is updated in order to correct an erroneous trend in the ozone total column.

In this document we describe the results of the regression testing for Level 2 data using version 7.0 as reference. The new Level 2 version 7.1 is based on the version 10 Level 1 products. Level 2 algorithms were not changed. As agreed in CCN1 to the original contract not only the total column of ozone, but all products were re-calculated [1]

1.2 Documents

1.2.1 Applicable Documents

[1] ESA. *CCN1 to Contract 4000128410/19/I-NS*.

1.2.2 References

[2] A. Keppens et al. *Multi-TASTE Phase F: Validation report SCIAMACHY SGP 7.00 Level-2 Data Products O3, NO2, CO, CH4, BrO and H2O*. Tech. rep. issue 1C. BIRA-IASB, Dec. 2019.

1.3 Abbreviations

ATBD	Algorithm Theoretical Base Document
FDR	Fundamental Data Record
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SoW	Statement of Work

2 Test Data and Test Procedure

2.1 Data Set

The level 2 processing is split in 240 parallel streams. The file lists for the streams are chronologically sorted, i.e. stream 1 processes data from the beginning of the mission and the last stream processes the last data of the mission. Each stream covers around 2 weeks of observations. In order to test if any regression has happened, we take the first 5 orbits of each stream. This gives us a maximum 1200 products that contains observations for each month, if all Level 1 files can be processed to Level 2.

The two processor versions use identical configurations. This was checked by comparing the configuration files stored in the Level 2 products.

2.2 Test Procedure

We will test the main parameter(s) for each product. In order to do this we first have to extract matching data for the previous processor version 7 and the new version 7.1. We do this as follows:

1. For each measurement data group in the Level 2 products extract all data and collect them in one file together with information on the original data product. The resulting file contain concatenated data for all variables. We do this separately for processor version 7 (reference) and the new version 7.1.
2. Calculate the absolute time of all measurements: The measurement groups in the product only contain the difference to a reference time that is stored once for each Level 2 product. The data for duplicate time stamps are removed to allow an unambiguous matching.
3. Using the absolute measurement times we combine the data in one data structure, where all parameters are saved and sorted according to the absolute measurement time. Missing data points for a given time are set to NaN.

The matching of data is performed with python `xarray`, which allows automatic matching along time and easy filtering.

In a first test we count the number of data points for both versions to check if we have a significant mismatch of data points. Note that we will have generally less data points for version 7.1., since the number of Level 1 products was smaller at the time of testing . The difference is currently under investigation. The comparison of the data is still valid, even after matching we usually have more than 10e5 data points distributed over the whole mission. Very large differences in data points will be investigated.

Using the collected data, we next perform a linear regression for the main parameters and calculate the relative difference in %:

$$RD = \frac{x_{new} - x_{ref}}{x_{ref}} * 100 \tag{1}$$

with

x_{new} Data from processor version 7.1

x_{ref} Data from processor version 7.0

For the linear regression we drop all data points that have no data for either V7.0 and V7.1. The results are documented in a table for selected parameters. The results of the linear regression and the *median* of the relative difference are shown in a table.

Since from the linear regression alone a regression cannot be excluded, we additionally show plots for the main parameter(s). These "standard" plots are the same for each parameter and are shown in a 2 x 2 grid:

Rolling mean of original value against index	Scatter plot with linear regression and 1-1 line
Mean relative difference resampled to a monthly time grid in %	Histogram of the percentage relative differences

For the relative difference of Limb data we show altitude resolved values with the relative difference encoded in a color map.

Notes:

- ➢ The original values are smoothed with a rolling mean and a window of 10000 points. This is done to make the larger development in time visible.
- ➢ The relative difference is given *in % of the reference value*

In case we deviate from the standard plot it will be mentioned in the figure caption. Unexpected results will be further analysed.

3 Nadir Products

3.1 Clouds

The following parameters are extracted:

- cloud_fraction
- cloud_optical_depth
- cloud_top_height

3.1.1 Data Set

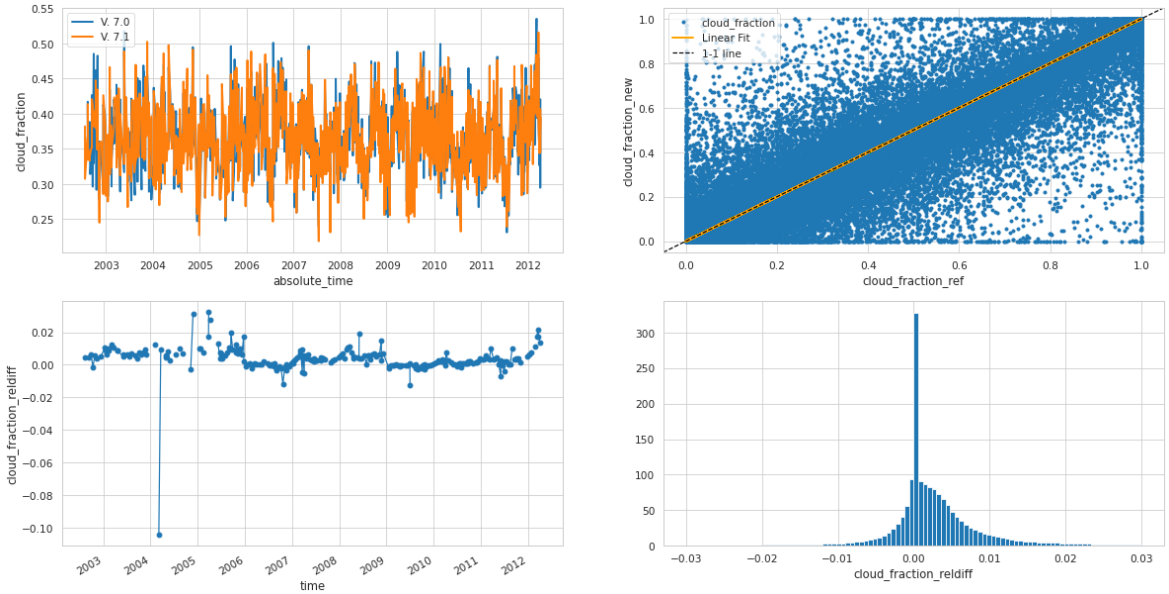
The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	12031800	1149
V. 7.1	11782380	1125

3.1.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]	*# AR
						D > 0% [% of total]*
cloud_fraction	10833800	0.9995 +- 9.507e-06	0.0001594 +- 4.531e-06	0.999	0.001467	78
cloud_optical_depth	8543659	0.9979 +- 1.951e-05	0.1011 +- 0.001292	0.9967	0	46
cloud_top_height	8543659	1.0021 +- 1.908e-05	-0.8026 +- 0.09668	0.9969	0	52

3.1.2.1 Cloud Fraction



3.1.2.2 Cloud Optical Depth

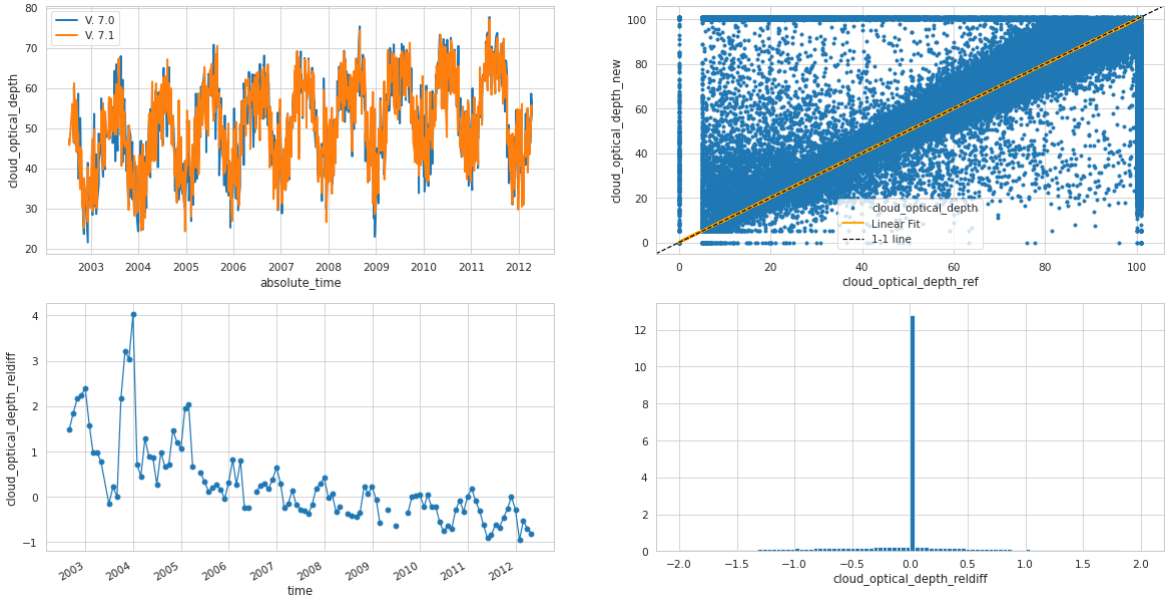


Figure 1: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences.*

The plot of the relative differences seems to indicate a trend and deviations of up to 4%. However, the linear regression, the median and the histogram shows that the overwhelming number of differences is 0.

3.1.2.3 Cloud Top Heights

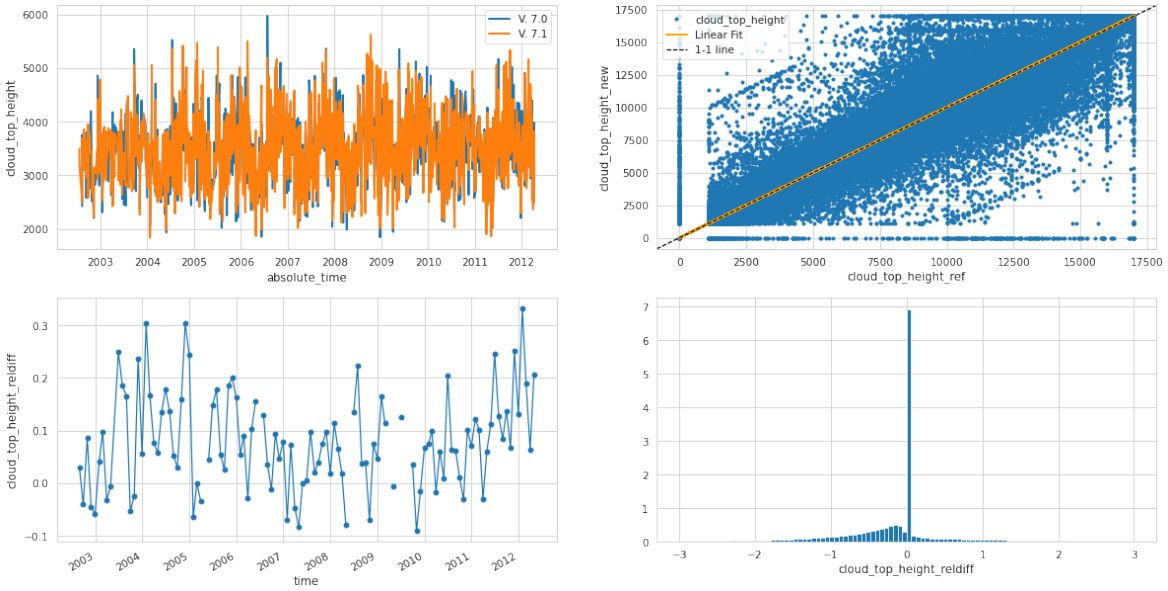


Figure 2: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences.*

3.2 Aerosols

The following parameters are extracted:

- absorbing_aerosol_indicator

3.2.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	12031800	1149
V. 7.1	11782380	1125

3.2.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
absorbing_aerosol_indicator	6440702	1.0208 +- 0.0001352	0.1218 +- 0.0001191	0.8985	17.13

3.2.2.1 Absorbing Aerosol Indicator

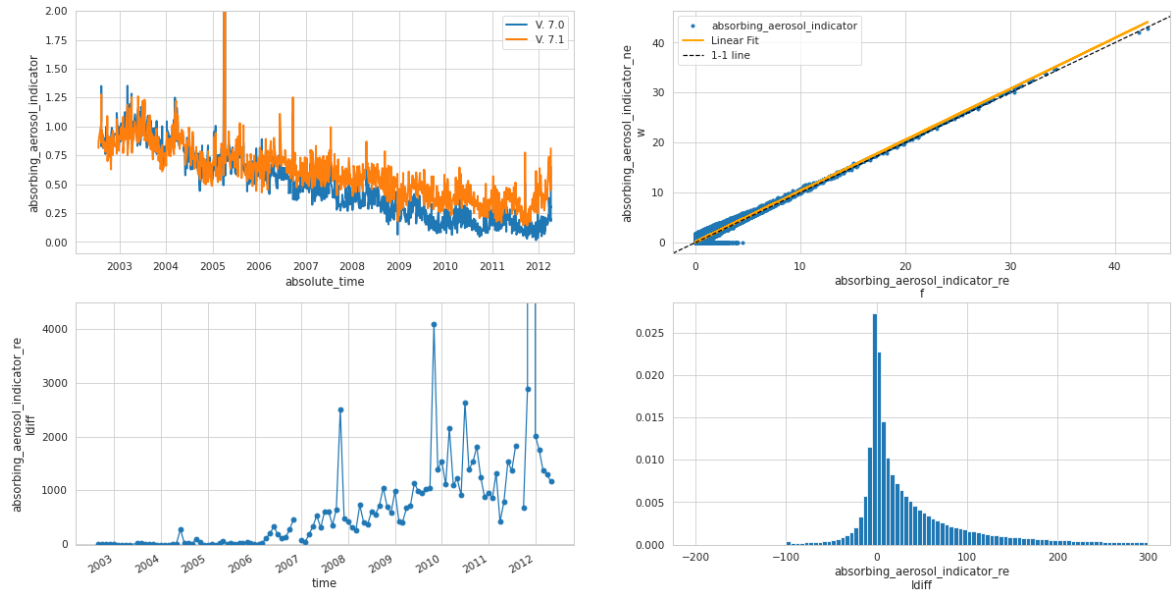


Figure 3: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences.*

3.2.3 Analysis

Fig. 4 shows the result of the last regression test. Shown are the median values for the AAI for each orbit of the verification data set. One can see that the version 6.01 started at higher values, then the values decrease until 2010, after which the values rise again. Version 7 had values near 0 from 2009 onwards. The new version restores at least part of the old behaviour: The values do not go to zero towards the end of the mission, but rise. The values are not directly comparable, since the previous test compares orbit medians for the verification set, while we show a rolling mean of more than 1000 orbits. From this comparison we can only conclude that a similar behaviour over time as in version 6.01 can be seen.

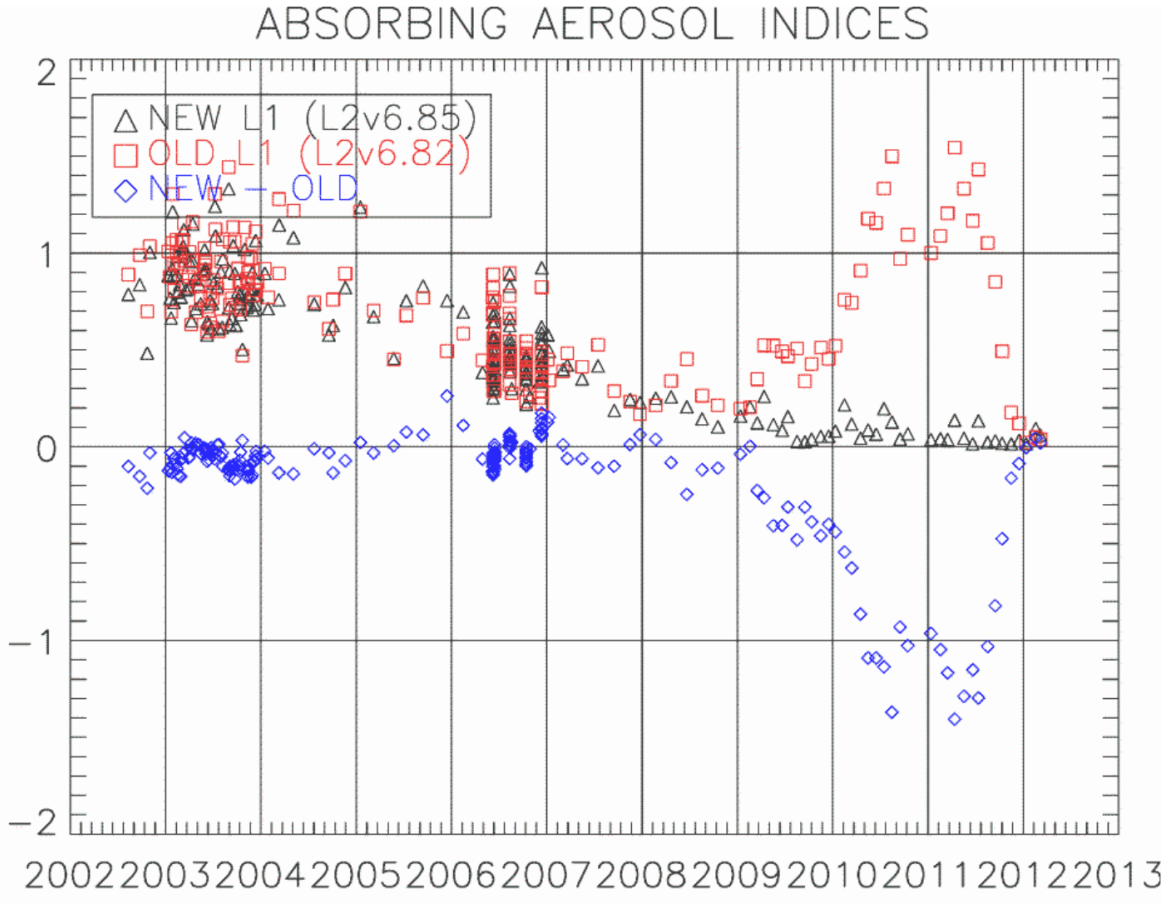


Figure 4: *Medians of AAI retrieved using L1v9 and L1v8 for each orbit as well as absolute differences between them as a function of time.*

3.3 Ozone

The following parameters are extracted:

- effective_slant_column_density
- vertical_column_density
- root_mean_square

3.3.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	5859357	1149
V. 7.1	5727038	1125

3.3.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
effective_slant_column_density	5250985	0.9987 +- 4.442e-06	2.445e+17 +- 1.254e+14	0.9999	0.8496
vertical_column_density	5250985	0.9940 +- 1.824e-05	1.216e+17 +- 1.435e+14	0.9982	0.8405
root_mean_square	5250985	0.9923 +- 4.517e-05	0.0002351 +- 1.188e-07	0.9892	9.042

3.3.2.1 Vertical Column Density

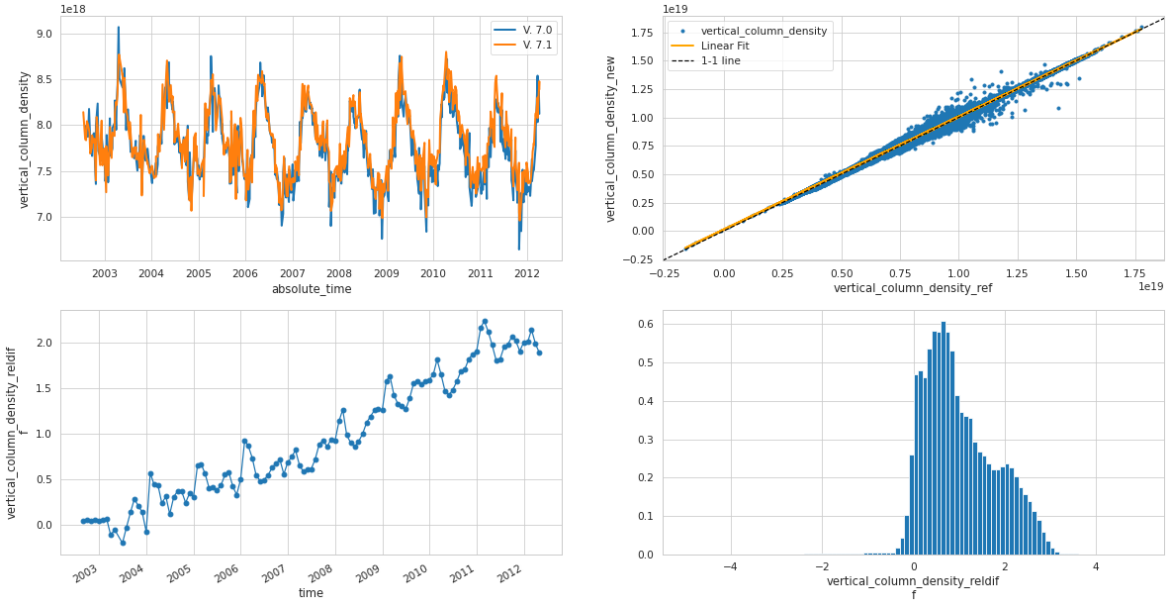


Figure 5: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.3.3 Analysis

The plot of the relative differences over time show that the values for the vertical column densities in version 7.1 are getting larger than the values for version 7.0 to reach around 2.5% at the end of the mission. Figure 6 shows the erroneous downward trend in version 7.0 vs the previous processor version: The version 7.0 values are getting too small over the mission. This trend is apparently corrected with version 7.1.

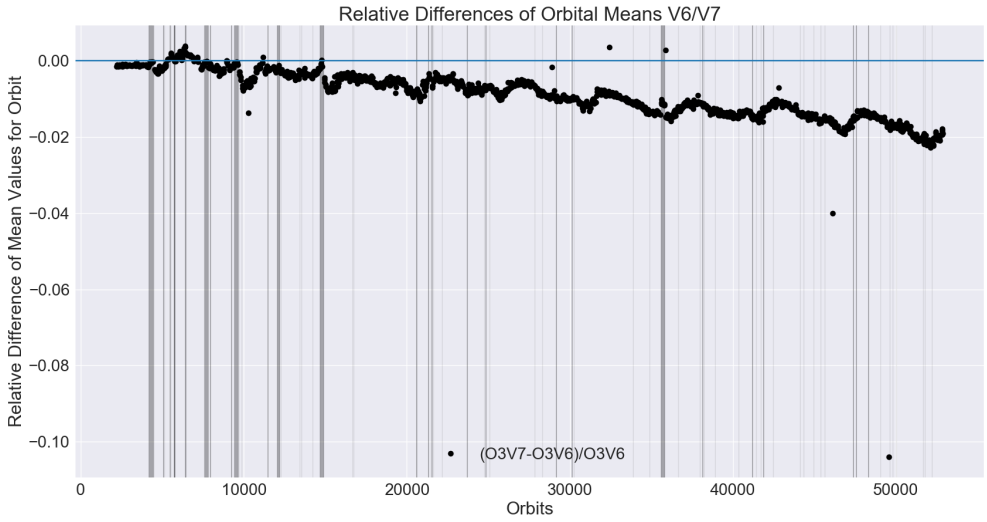


Figure 6: *Relative difference (v7 - V6.01)/V6.01 of total O_3 columns for the diagnostic data set. The values are not converted to percentages.*

We additionally made a comparison with Level V6 data that are still readily available at DLR (see Fig. 7 below). The comparison between V6 and V7 shows no clear trend, which is expected

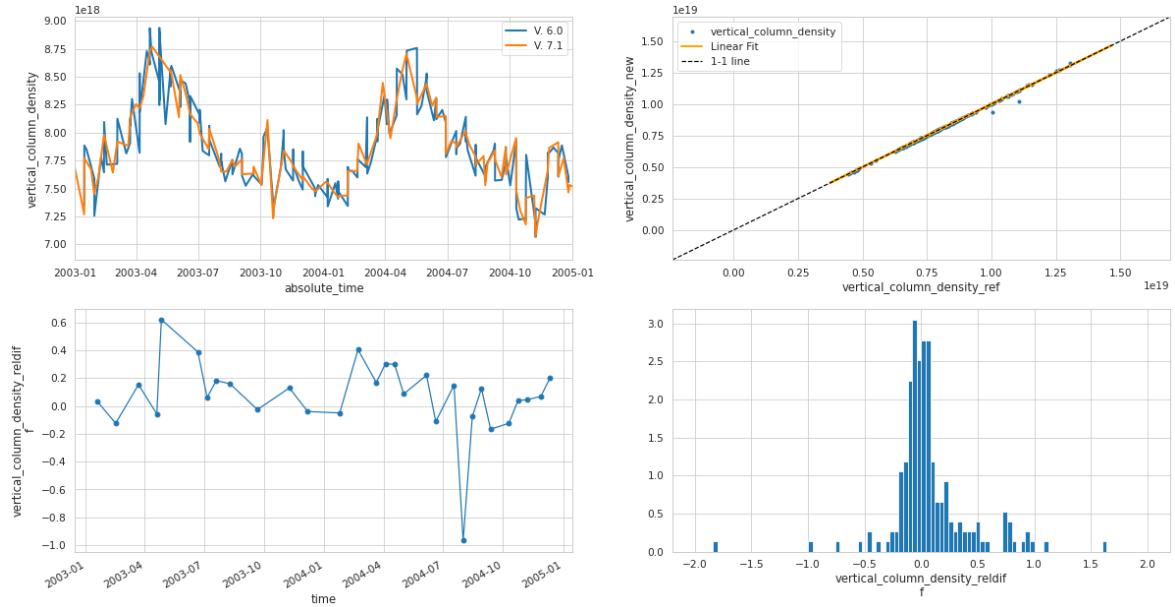


Figure 7: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

A validation of the new values will be done by BIRA

3.4 NO_2

The following parameters are extracted:

- slant_column_density
- total_vertical_column_density
- root_mean_square

3.4.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	10454632	1149
V. 7.1	10211412	1125

3.4.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
slant_column_density	9388365	0.9997 +- 1.118e-06	-2.544e+13 +- 2.012e+10	1	-0.04248
total_vertical_column_density	9388365	1.0004 +- 3.143e-06	-9.01e+12 +- 9.723e+09	0.9999	-0.04572
root_mean_square	9388365	1.0021 +- 2.492e-06	-1.149e-06 +- 1.992e-09	0.9999	0.004656

3.4.2.1 Vertical Column Density

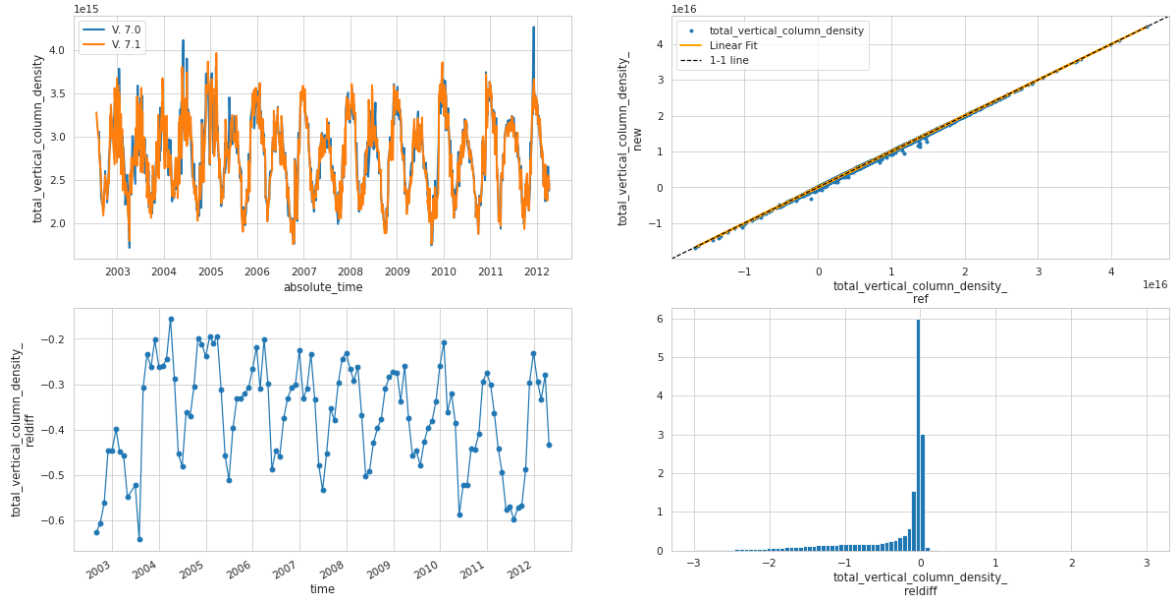


Figure 8: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.4.3 Analysis

V7.1 values are slightly lower (0.2 - 0.4%), but still within an acceptable range.

3.5 SO_2

The following parameters are extracted:

- slant_column_density
- vertical_column_density_anthropogenic
- vertical_column_density_error_anthropogenic
- vertical_column_density_volcanic
- vertical_column_density_error_volcanic
- root_mean_square

3.5.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	5331493	1148
V. 7.1	5234881	1124

3.5.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Med. R. Diff. [%]
slant_column_density	4785703	0.9851 +- 0.0001613	2.881e+15 +- 6.68e+12	0.8863	-1.339
vertical_column_density_anthropogenic	4785703	0.9859 +- 0.0001416	5.854e+15 +- 1.356e+13	0.9102	-1.339
vertical_column_density_error_anthropogenic	4785703	0.0011 +- 0.000171	11.5 +- 2.287	8.478e-06	0.006325
vertical_column_density_volcanic	4785703	0.9857 +- 0.000162	1.514e+15 +- 3.253e+12	0.8855	-1.339
vertical_column_density_error_volcanic	4785703	0.0011 +- 0.000171	11.5 +- 2.287	8.478e-06	0.006325
root_mean_square	4785703	0.9991 +- 2.778e-05	8.073e-06 +- 1.333e-07	0.9963	0.0007722

3.5.2.1 Slant Column Density

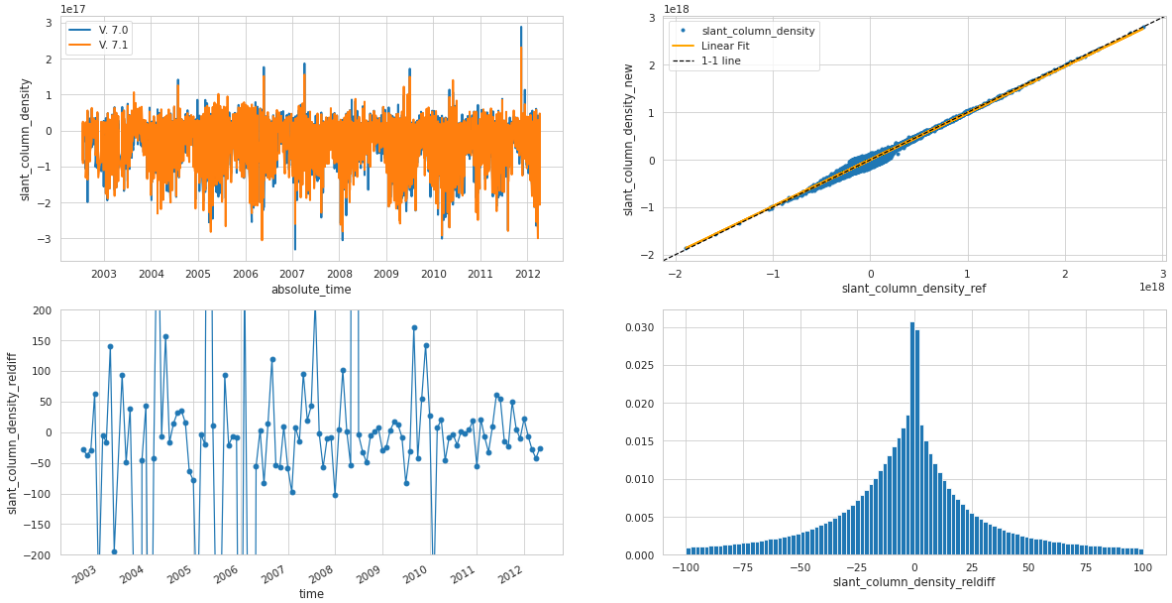


Figure 9: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.5.2.2 Anthropogenic vertical column density

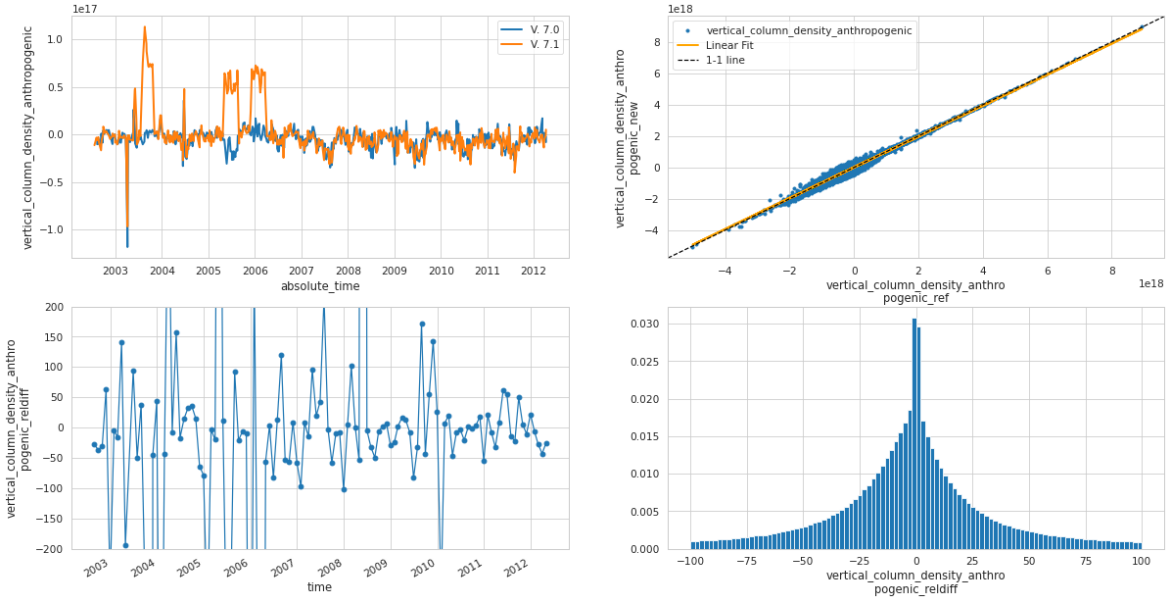


Figure 10: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.5.2.3 Error Anthropogenic vertical column density

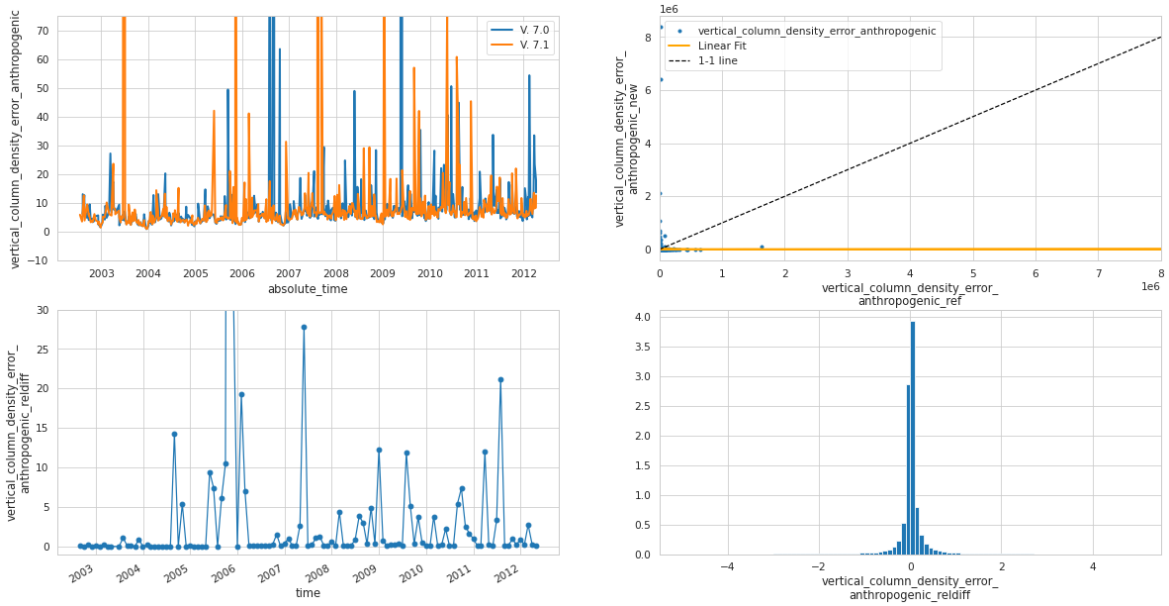


Figure 11: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.5.3 Analysis

The linear regression for the errors has a slope near 0. We recheck the linear regression after removal of outliers for

- ➢ vertical_column_density_error_anthropogenic
- ➢ vertical_column_density_error_volcanic

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density_error_anthropogenic	3896157	0.9987 +- 5.308e-05	0.003084 +- 7.501e-05	0.9891	0.005886
vertical_column_density_error_volcanic	3896157	0.9987 +- 5.308e-05	0.003084 +- 7.501e-05	0.9891	0.005886

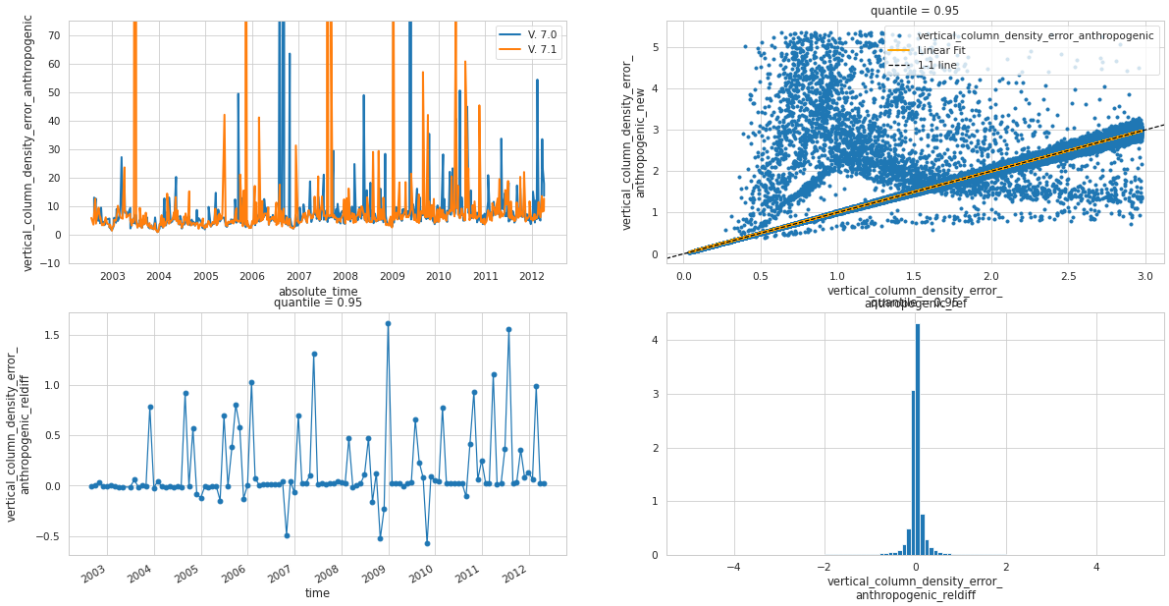


Figure 12: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences _*

After removing outliers using the 95th percentile the linear regression is near 1 for the VCD errors. The slopes for the linear regression for the vertical columns were already near one. A perfect slope of 1 cannot be expected, since the retrievals window is in the same spectral region as the one for O_3. The radiance in this region is changed in the new version in order to remove the ozone trend. Therefore we can also expect changes in the SO_2 values

3.6 HCHO

The following parameters are extracted:

- slant_column_density
- slant_column_density_error
- vertical_column_density
- vertical_column_density_error
- root_mean_square

3.6.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	4304079	1148
V. 7.1	4227850	1124

3.6.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
slant_column_density	3857787	0.9840 +- 0.0003339	2.654e+14 +- 6.396e+12	0.6924	-1.359
slant_column_density_error	3857787	0.0079 +- 0.001359	18.04 +- 2.839	8.831e-06	-0.4997
vertical_column_density	3857787	0.9937 +- 0.0002441	-5.793e+13 +- 3.694e+12	0.8111	-1.041
vertical_column_density_error	3857787	0.0018 +- 0.0004112	52.82 +- 7.035	5.072e-06	-0.3586
root_mean_square	3857787	0.9999 +- 6.687e-05	4.16e-06 +- 1.204e-07	0.983	0.0007299

The VCD errors show no correlation.

3.6.2.1 Slant Column Density

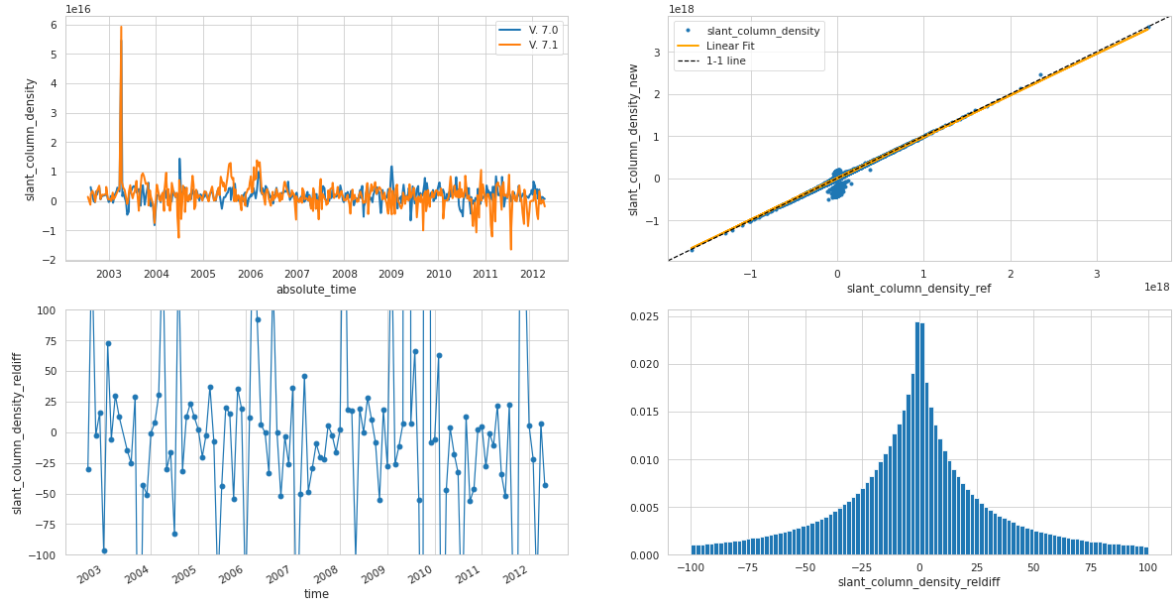


Figure 13: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.6.2.2 Vertical column density

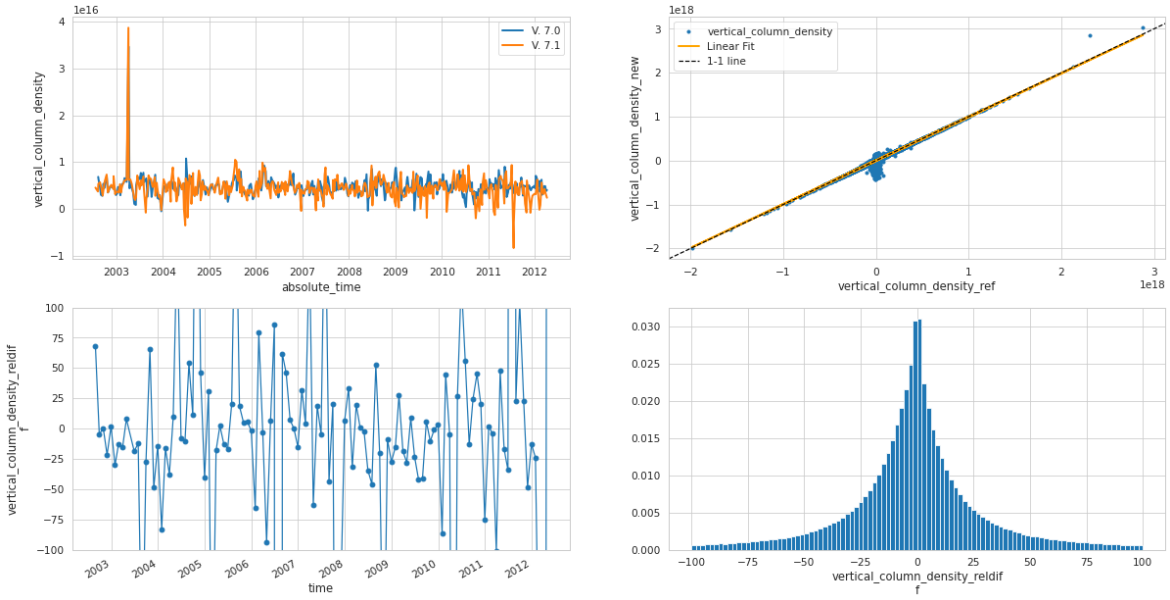


Figure 14: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.6.3 Analysis

The linear regression for the errors has a slope near 0. We recheck the linear regression after removal of outliers for

- vertical_column_density_error

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density_error	3481871	0.9305 +- 0.0003875	0.3544 +- 0.001841	0.6235	-0.2316

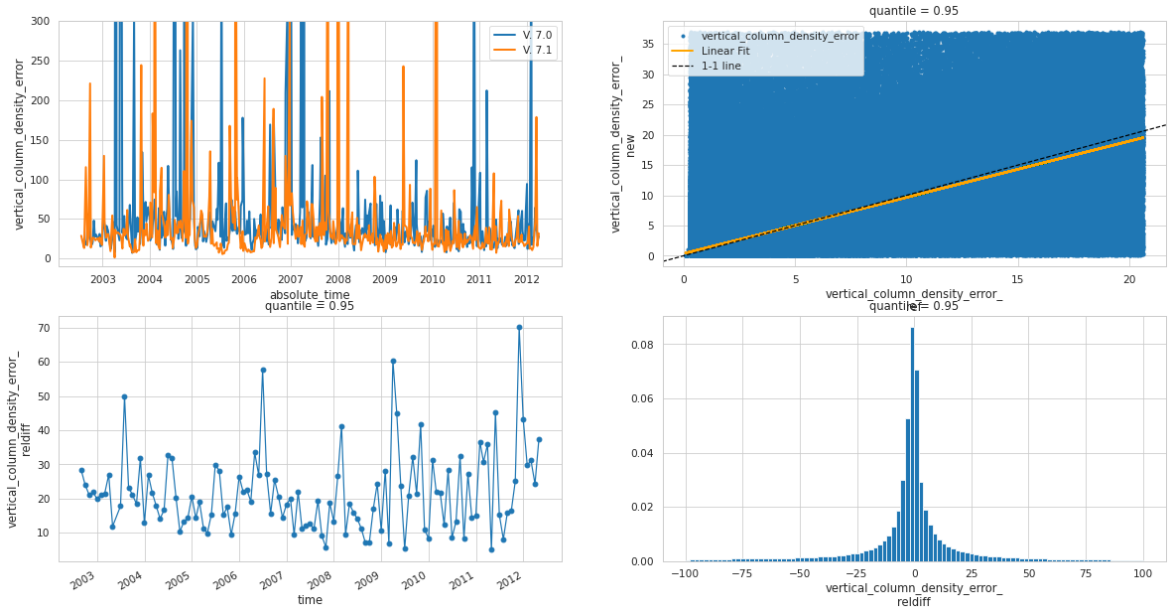


Figure 15: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

After removing outliers using the 95th percentile the linear regression is near 1 for the VCD errors. However, the R^2 value remains low, indicating a large number of outliers

3.7 BrO

The following parameters are extracted:

- slant_column_density
- slant_column_density_error
- total_vertical_column_density
- root_mean_square

3.7.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	5860054	1149
V. 7.1	5753327	1125

3.7.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
slant_column_density	5263012	1.0066 +- 0.0002044	-2.06e+12 +- 3.499e+10	0.8217	0.05628
slant_column_density_error	5263012	0.0540 +- 0.0004523	1.441 +- 0.2594	0.0027	-0.06318
total_vertical_column_density	3775024	1.0073 +- 0.0004424	-6.639e+11 +- 2.058e+10	0.5786	0.2894
root_mean_square	5263012	0.9980 +- 0.000108	1.14e-05 +- 2.754e-07	0.942	9.97e-06

3.7.2.1 Slant Column Density

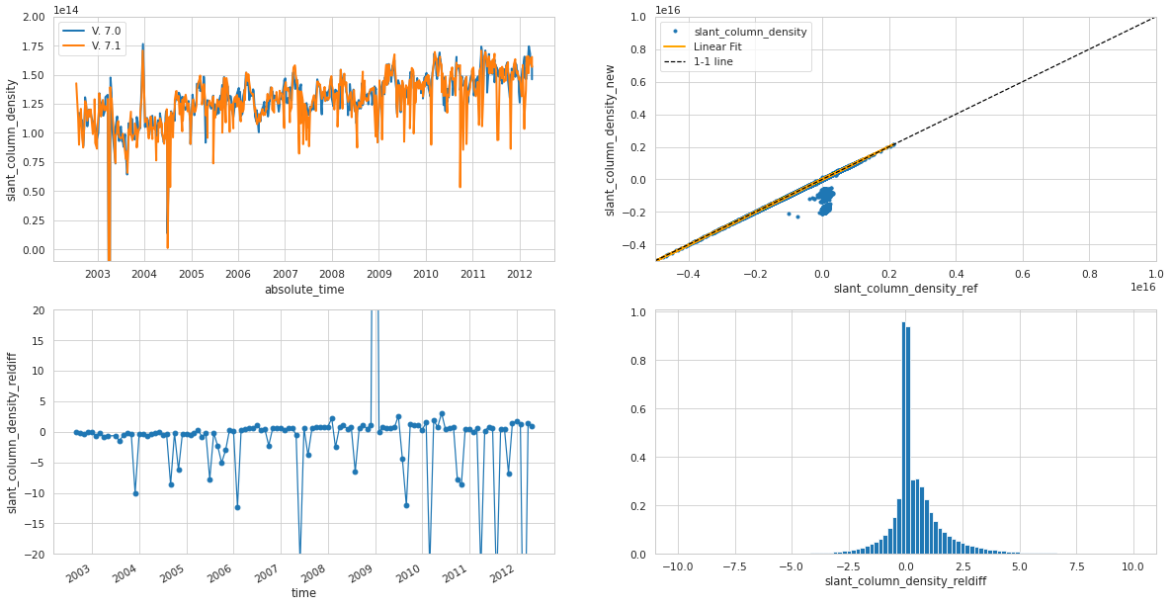


Figure 16: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.7.2.2 Vertical column density

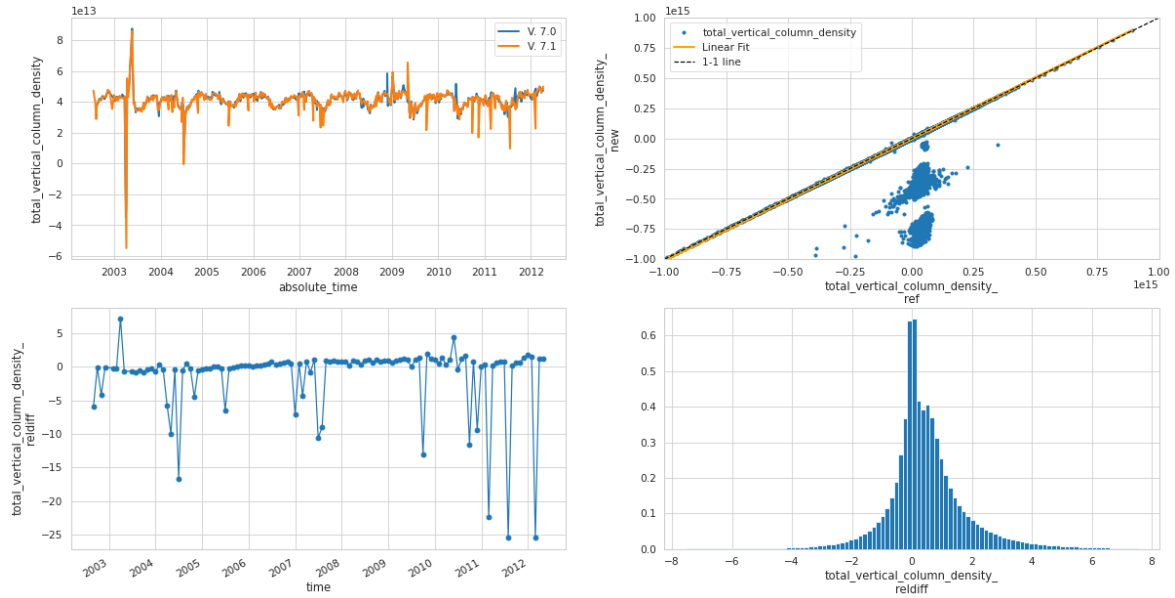


Figure 17: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences.*

3.7.3 Analysis

The linear regression for the errors has a slope near 0. We recheck the linear regression after removal of outliers for

➢ slant_column_density_error

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
slant_column_density_error	4750311	0.9921 +- 3.615e-05	0.001537 +- 2.313e-05	0.9937	-0.06016

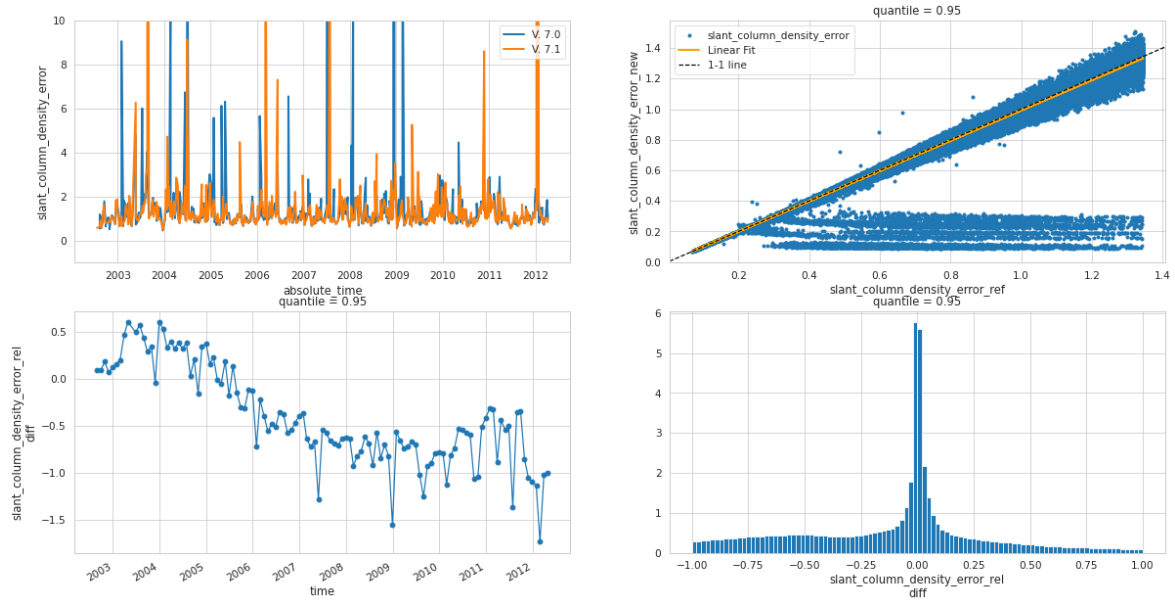


Figure 18: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

After removing outliers using the 95th percentile the linear regression is near 1 for the errors.

3.8 CHOCHO

The following parameters are extracted:

- slant_column_density
- slant_column_density_error
- vertical_column_density
- vertical_column_density_error
- root_mean_square

3.8.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	10424636	1149
V. 7.1	8273958	1124

We have significantly less values for version 7.1.

3.8.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
slant_column_density	7600732	0.4529 +- 0.0001864	-4.119e+13 +- 3.367e+11	0.4372	-23.71
slant_column_density_error	7600732	0.5318 +- 0.0007502	4.324 +- 0.6903	0.062	0
vertical_column_density	7600732	0.5144 +- 0.0001878	-1.542e+13 +- 1.454e+11	0.4967	-22.46
vertical_column_density_error	7600732	0.8613 +- 0.001864	3.383 +- 1.773	0.02732	0
root_mean_square	7600732	0.9989 +- 1.684e-05	8.991e-07 +- 8.062e-09	0.9978	0

The correlation for all values is low. For version 7.1 a significant number of values seem to be corrupt and cannot be plotted.

3.8.2.1 Slant Column Density

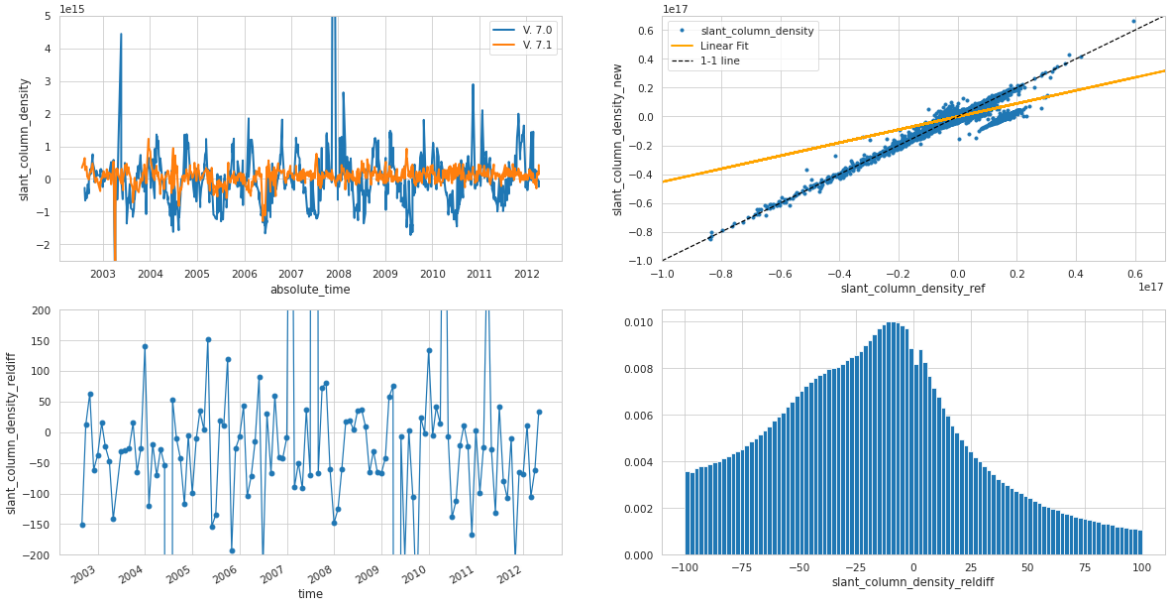


Figure 19: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.8.2.2 Vertical column density

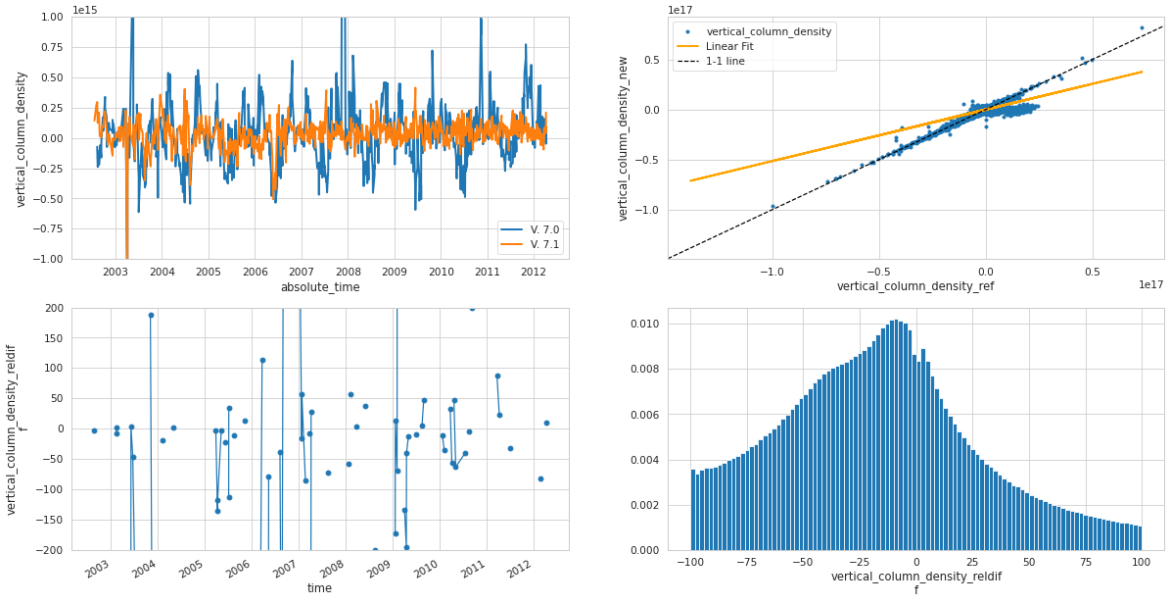


Figure 20: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.8.3 Analysis

The linear regression for the errors has a slope near 0.

- ➢ vertical_column_density
- ➢ vertical_column_density_error

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density	5706895	0.7010 +- 0.0002567	-6.333e+12 +- 8.721e+10	0.5666	-22.36
vertical_column_density_error	5706895	0.9334 +- 0.0003418	0.1548 +- 0.0004787	0.5666	0

The removal of outliers does not improve the correlation of the vertical column values. The values of the new version are still considerably lower than those of version 7.0.

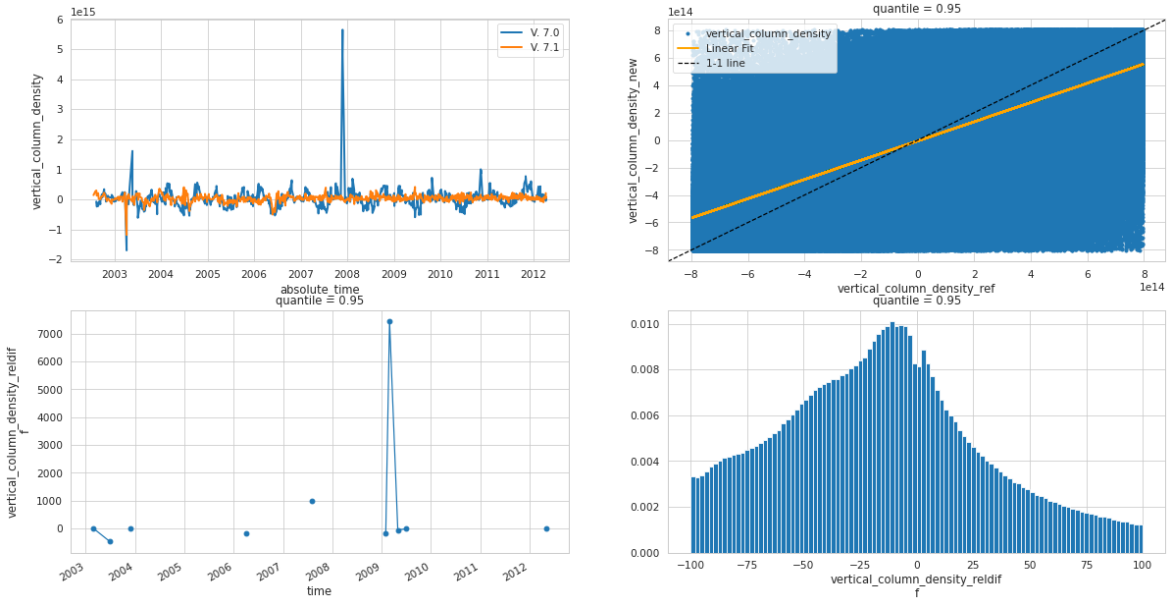


Figure 21: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.9 OCIO

The following parameters are extracted:

- slant_column_density
- slant_column_density_error
- root_mean_square

3.9.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	6035248	1149
V. 7.1	5924998	1125

3.9.2 Comparison

The following table shows the number of time matched records that have valid values and the results of a linear regression between selected variables:

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
slant_column_density	5421303	1.0002 +- 3.22e-05	5.832e+11 +- 2.082e+09	0.9944	-0.4359
slant_column_density_error	5421303	0.1128 +- 0.0004474	10.28 +- 1.064	0.01159	0.4105
root_mean_square	5421303	0.9987 +- 5.78e-05	5.337e-06 +- 1.152e-07	0.9822	-0.01279

3.9.2.1 Slant Column Density

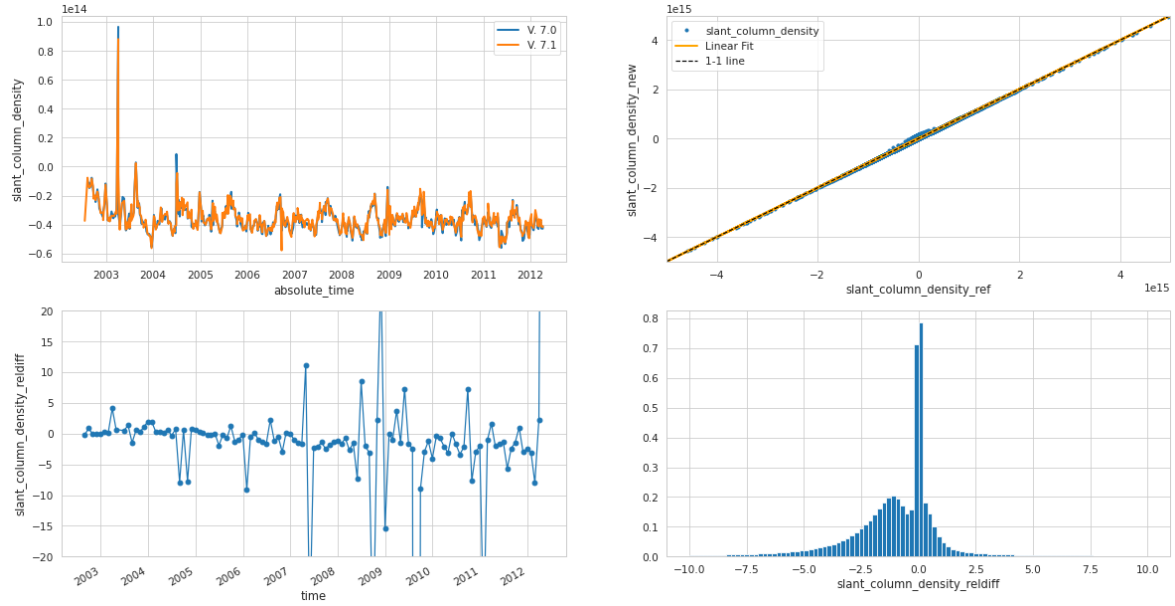


Figure 22: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.9.3 Analysis

The linear regression for the errors has a slope near 0, therefore we removed outliers and recalculated the linear regression

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
slant_column_density	703963	1.0017 +- 8.104e-05	4.788e+11 +- 7.729e+08	0.9954	-0.1048
slant_column_density_error	703963	1.0790 +- 0.0006468	-0.2383 +- 0.007973	0.7981	0.1049
root_mean_square	703963	0.9997 +- 2.607e-06	9.802e-08 +- 4.504e-09	1	-0.0126

After the removal outliers the correlation of the slant column errors is very good.

3.10 H_2O

The following parameters are extracted:

- ➢ vertical_column_density
- ➢ vertical_column_density_error
- ➢ root_mean_square

3.10.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	8839966	1149
V. 7.1	8653210	1125

3.10.2 Comparison

The following table shows the number of time matched records that have valid values and the results of a linear regression between selected variables:

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density	7955496	1.0000 +- 1.185e-07	2.411e+15 +- 6.798e+15	1	-0.0001036
vertical_column_density_error	7955496	1.0002 +- 1.912e-06	3.098e-06 +- 1.913e-07	1	0.0001449
root_mean_square	7955496	0.9998 +- 3.535e-06	1.628e-06 +- 1.88e-08	0.9999	2.642e-05

The two versions show near identical results

3.10.2.1 Vertical column density

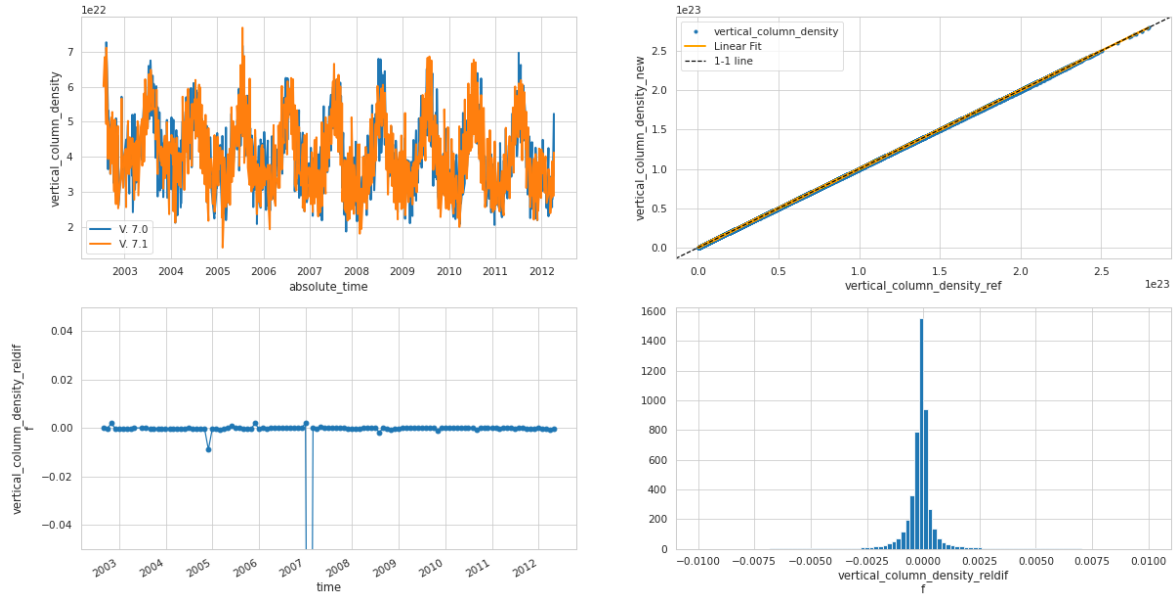


Figure 23: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.11 CH_4

The following parameters are extracted:

- ➢ vertical_column_density_ch4
- ➢ vertical_column_density_error_ch4
- ➢ vertical_column_density_xch4
- ➢ vertical_column_density_error_xch4
- ➢ vertical_column_density_flag

3.11.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	10805227	1149
V. 7.1	10583801	1125

3.11.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density_ch4	9731051	4.6115 +- 0.003509	-9.344e+19 +- 1.588e+17	0.1507	7.487
vertical_column_density_error_ch4	9731051	40.1787 +- 0.9213	1.195e+21 +- 4.788e+20	0.0001954	0.7807
vertical_column_density_xch4	9731051	0.0037 +- 0.008643	7.103e+19 +- 6.881e+18	1.863e-08	12.49
vertical_column_density_error_xch4	9731051	-0.0001 +- 0.114	-4.491e+24 +- 4.238e+24	2.578e-14	7.49

Flags:

Parameter	# matches	Slope	Intercept	R^2	# ARD > 0% [% of total]
vertical_column_density_flag	9731051	0.9303 +- 0.0001079	3668 +- 6.276	0.8842	18

3.11.2.1 Vertical Column Density CH_4

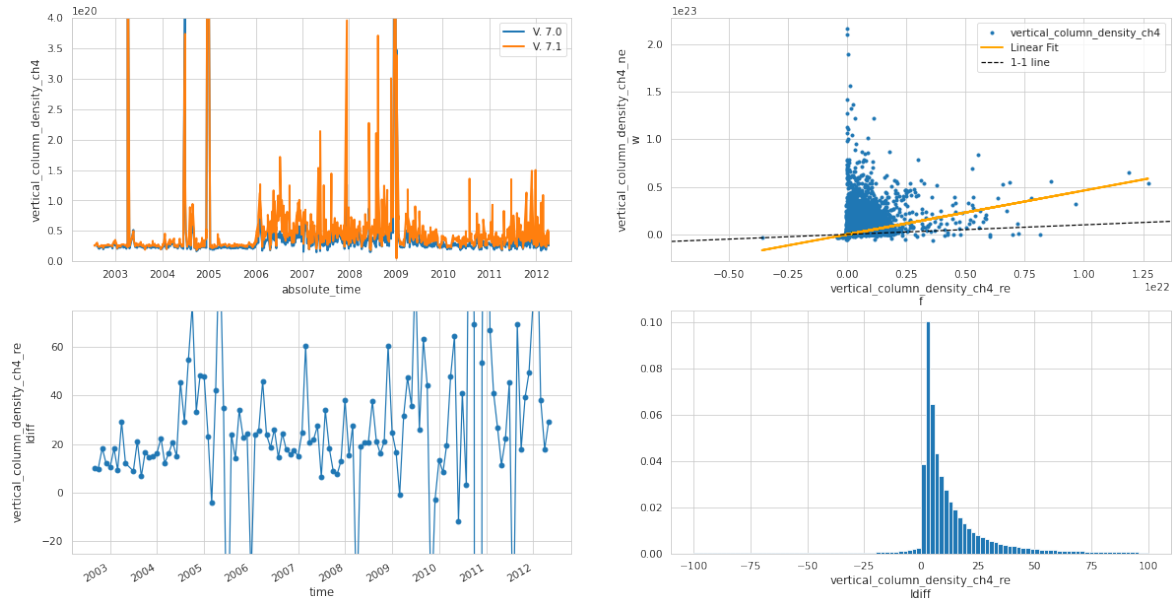


Figure 24: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.11.2.2 Vertical column density xCH_4

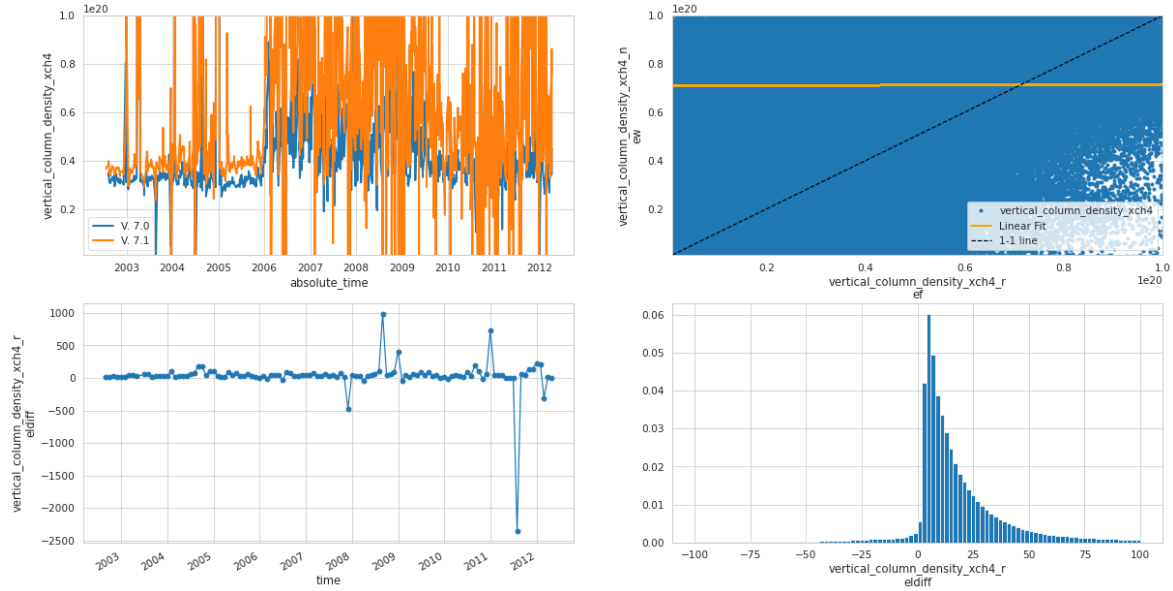


Figure 25: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.11.2.3 Vertical column density flag

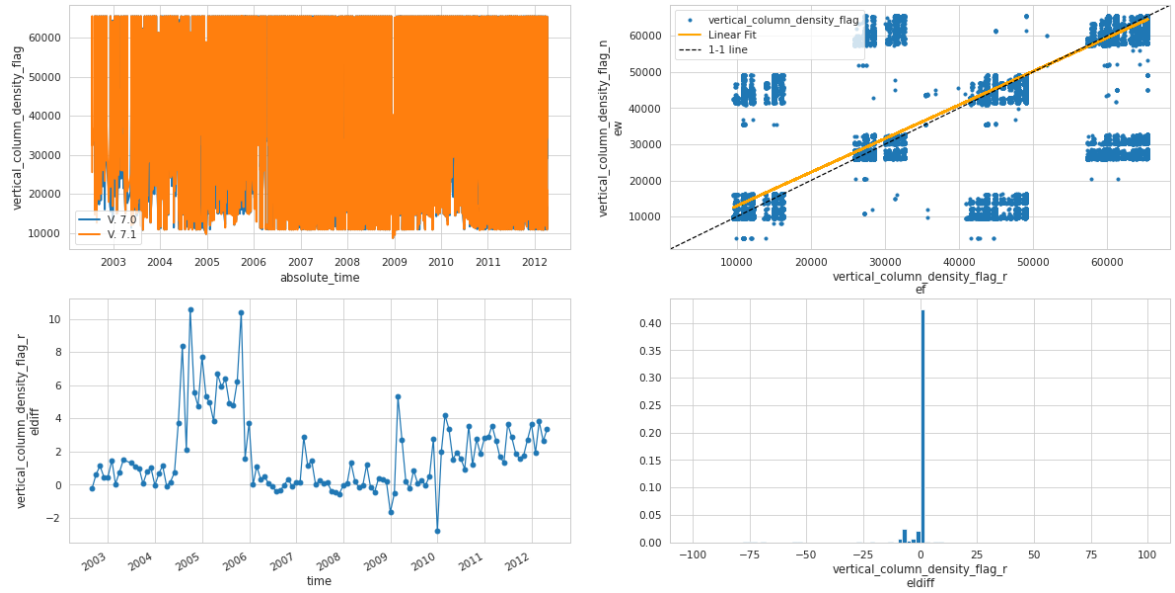


Figure 26: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

The calculation of the VCD flag, which should be used for filtering, is different in version 7.1. From a first look it seems that not all flag values are calculated, since the V7.1 values are capped at the top while the V7 values also have higher values (which is expected). This is maybe just an effect of the different values for the VCDs

3.11.3 Analysis

In order to check if the bad agreement between the processor versions is caused by individual outliers, we removed all data with values above the 95th quantile and repeated the calculation of the linear regresssion

- vertical_column_density_ch4
- vertical_column_density_xch4

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density_ch4	7912776	1.0025 +- 0.0001801	2.731e+18 +- 4.647e+15	0.7966	6.142
vertical_column_density_xch4	7912776	0.9613 +- 0.0002463	6.593e+18 +- 8.422e+15	0.6581	10.55

After removing outliers, the linear regression is fairly good, although the significance is a bit low, indicating a larger variance.

3.11.3.1 Vertical Column Density CH_4 (95% quantile)

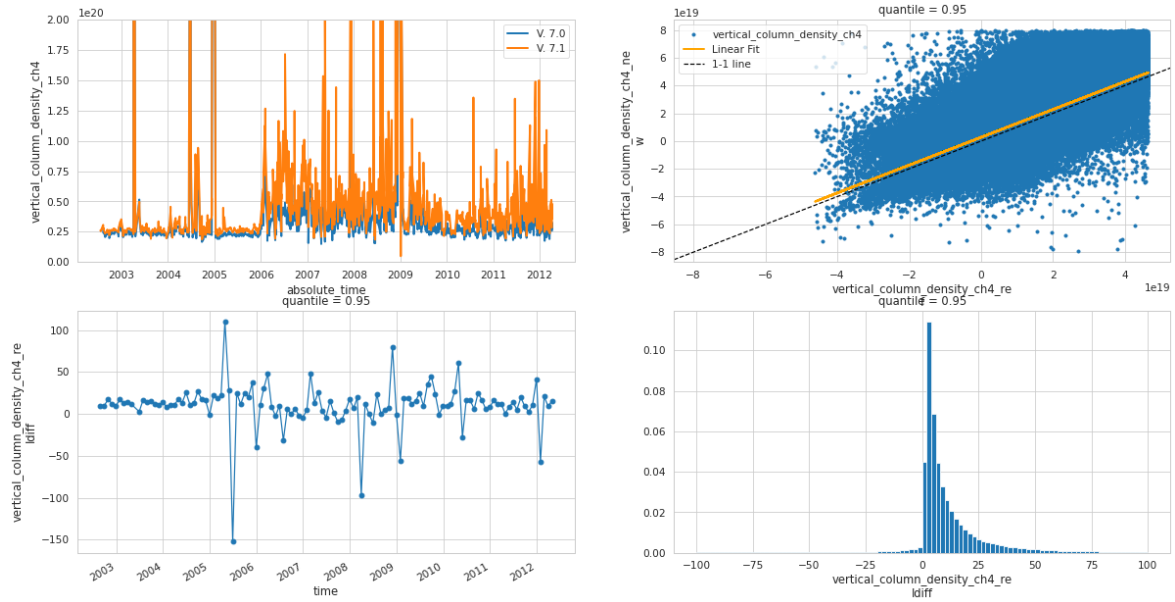


Figure 27: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.11.3.2 Vertical column density xCH_4 (95% quantile)

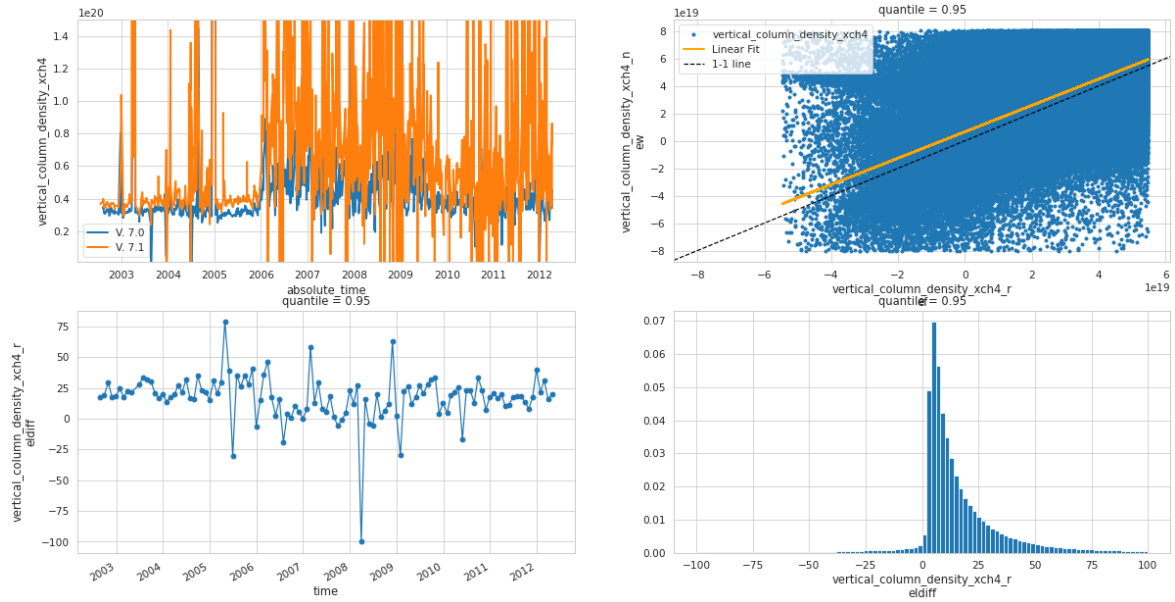


Figure 28: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

The vertical columns show an offset of around 25%. Therefore we did additional comparisons with the validated version 6.01 of CH4.

3.11.3.3 Comparison V6/V7.1 for CH4

A comparison with V6 data for CH_4 shows that the values are generally similar between the versions. Version 6 has more outliers than V7

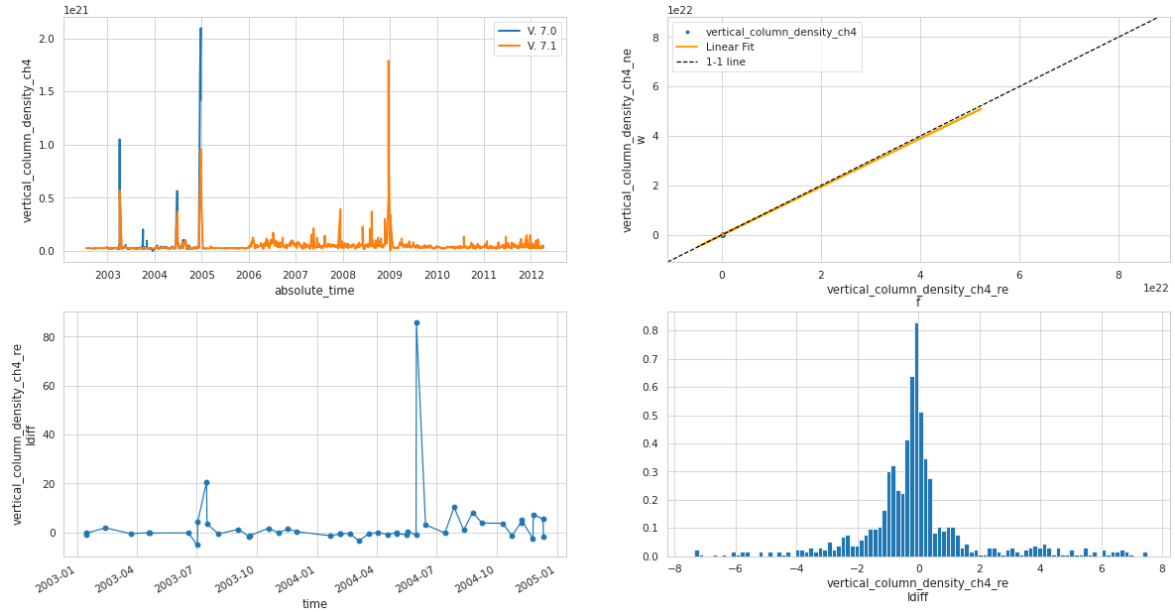


Figure 29: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.11.3.4 Comparison V6/V7.1 for xCH4

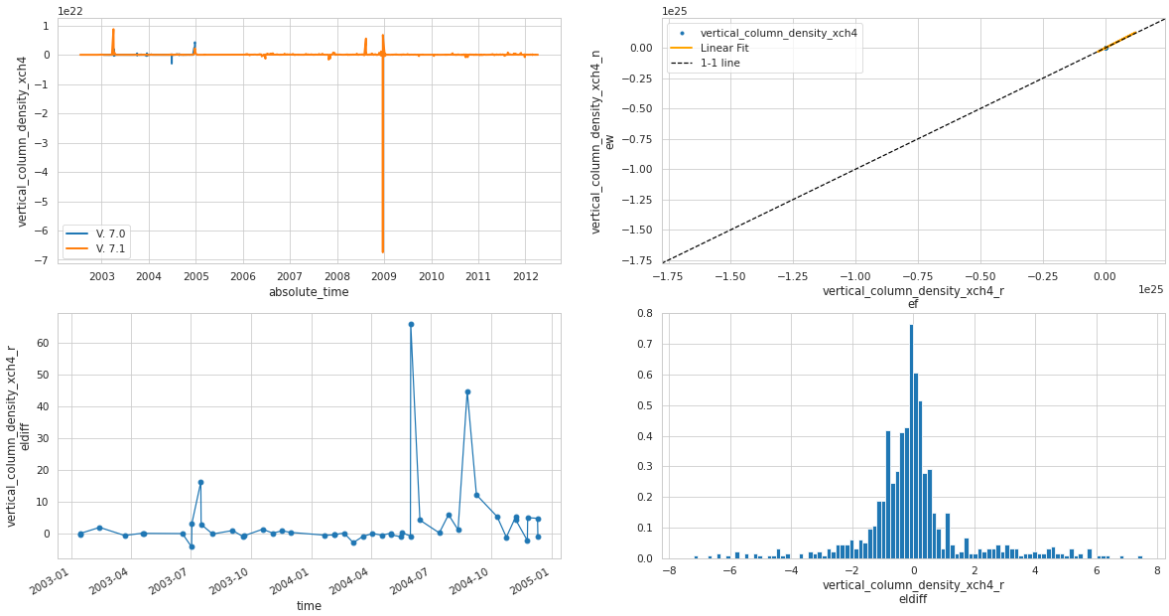


Figure 30: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

There is no systematic offset between the version 6 and version 7.1 data sets

3.12 CO

The following parameters are extracted:

- ➢ vertical_column_density_co
- ➢ vertical_column_density_error_co
- ➢ vertical_column_density_xco
- ➢ vertical_column_density_error_xco
- ➢ vertical_column_density_flag

3.12.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	2365153	1117
V. 7.1	2313334	1094

3.12.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density_co	2120872	0.6721 +- 0.0003975	9.344e+17 +- 1.402e+16	0.5741	-6.707
vertical_column_density_error_co	2120872	3.2245 +- 0.02083	4.858e+22 +- 5.369e+22	0.01117	-2.279
vertical_column_density_xco	2120872	0.0006 +- 0.0006166	8.553e+18 +- 2.21e+18	4.439e-07	-6.613
vertical_column_density_error_xco	2120872	0.0000 +- 0.0007389	7.45e+21 +- 3.672e+22	1.924e-09	-2.851

Flag comparison

Parameter	# matches	Slope	Intercept	R^2	# ARD > 0% [% of total]
vertical_column_density_flag	2120872	0.7763 +- 0.0004159	1.414e+04 +- 26.36	0.6216	16

3.12.2.1 Vertical Column Density CO

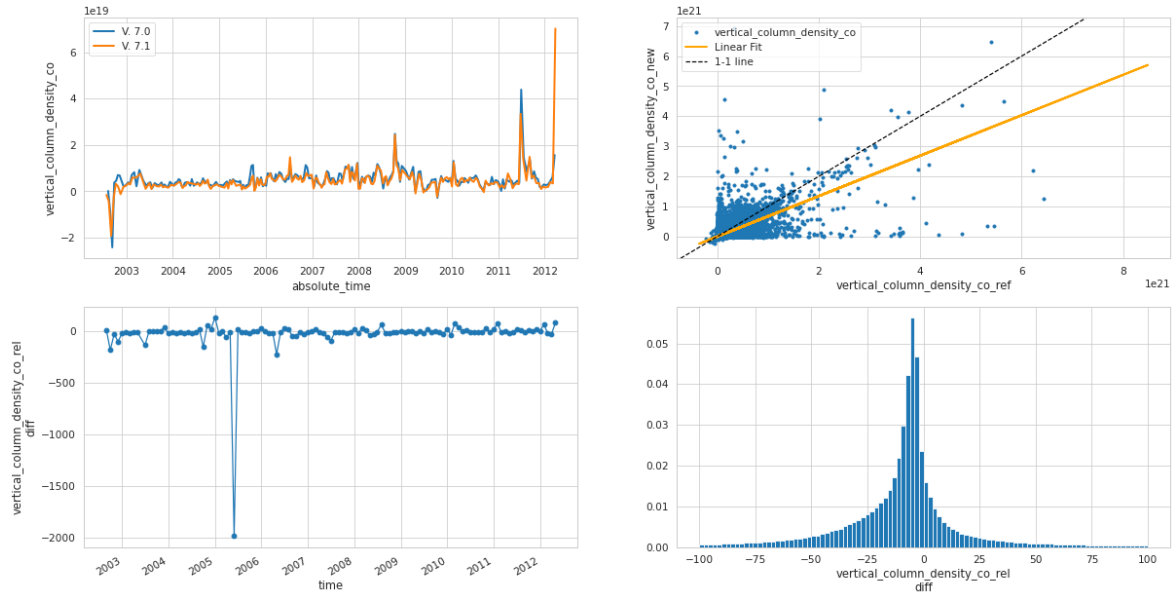


Figure 31: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.12.2.2 Vertical column density xCO

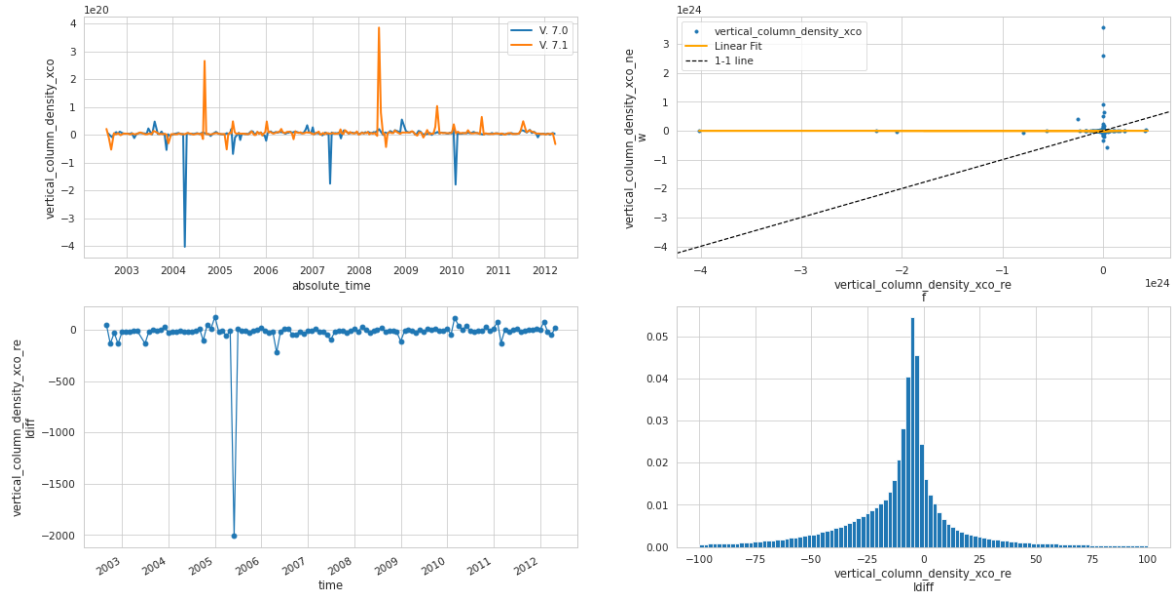


Figure 32: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.12.2.3 Vertical column density flag

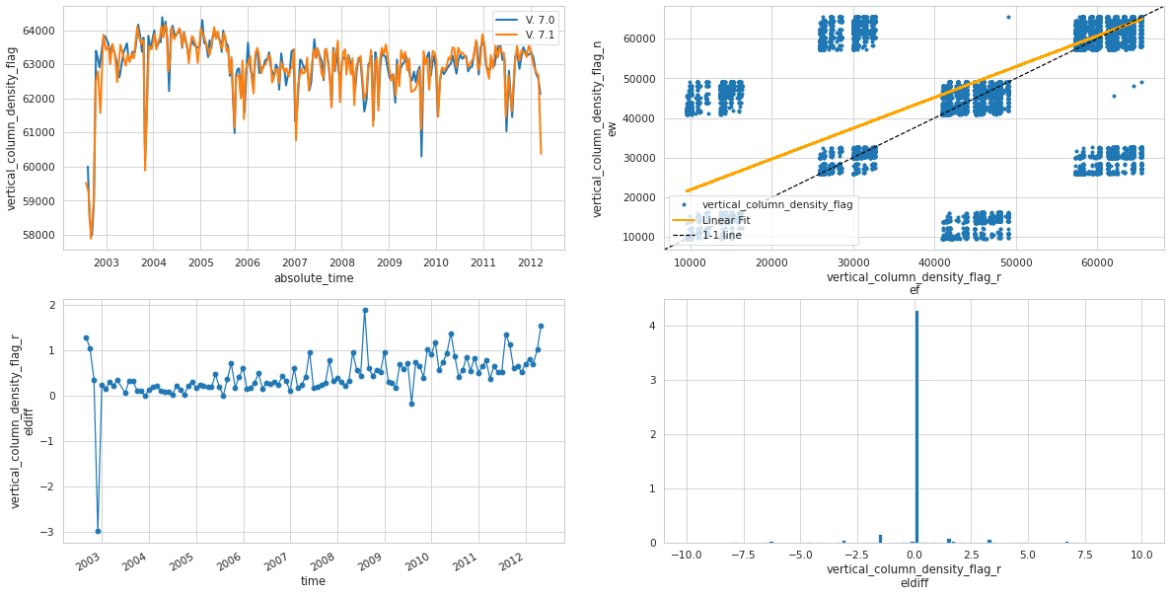


Figure 33: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

3.12.3 Analysis

3.12.3.1 Influence of outliers

The influence of outliers is checked below. We remove all values above the 95th quantile for the vertical column values of both versions separately and repeat the analysis. We also do the same for the error values

- ➢ vertical_column_density_co
- ➢ vertical_column_density_xco

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density_co	1676688	0.9635 +- 0.0002805	-2.643e+17 +- 8.003e+14	0.8756	-7.205
vertical_column_density_xco	1676688	0.9551 +- 0.0002721	-3.593e+17 +- 1.079e+15	0.8802	-7.1

The comparison for the CO values after removal of outliers in version 7 and 7.1 is shown in Fig. 34.

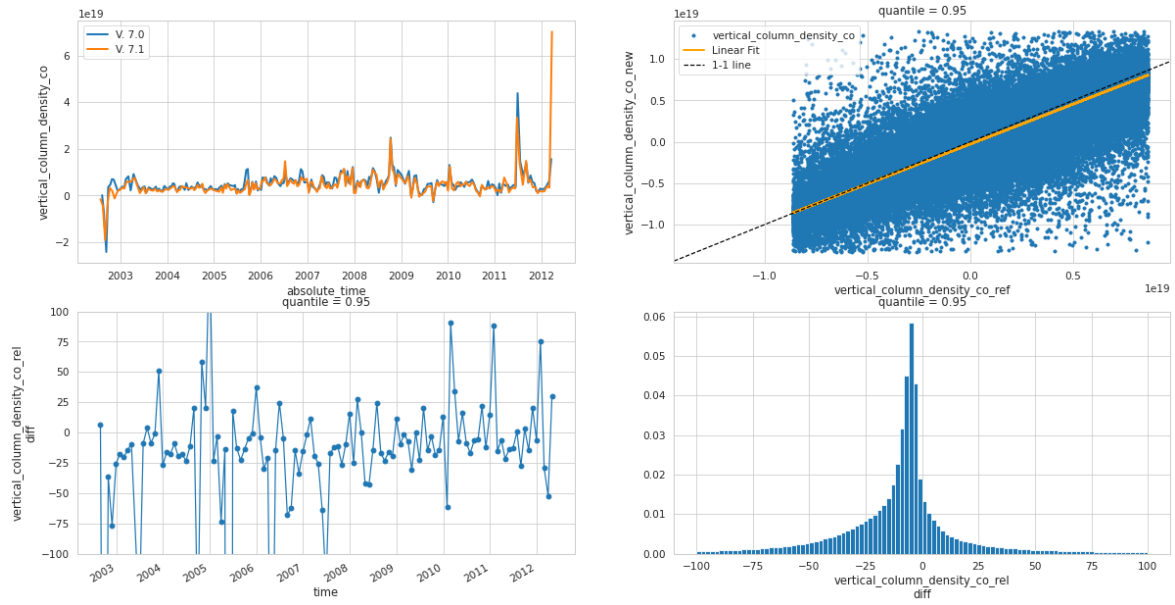


Figure 34: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

Fig. 35 shows the results for xCO after the removal of outliers.

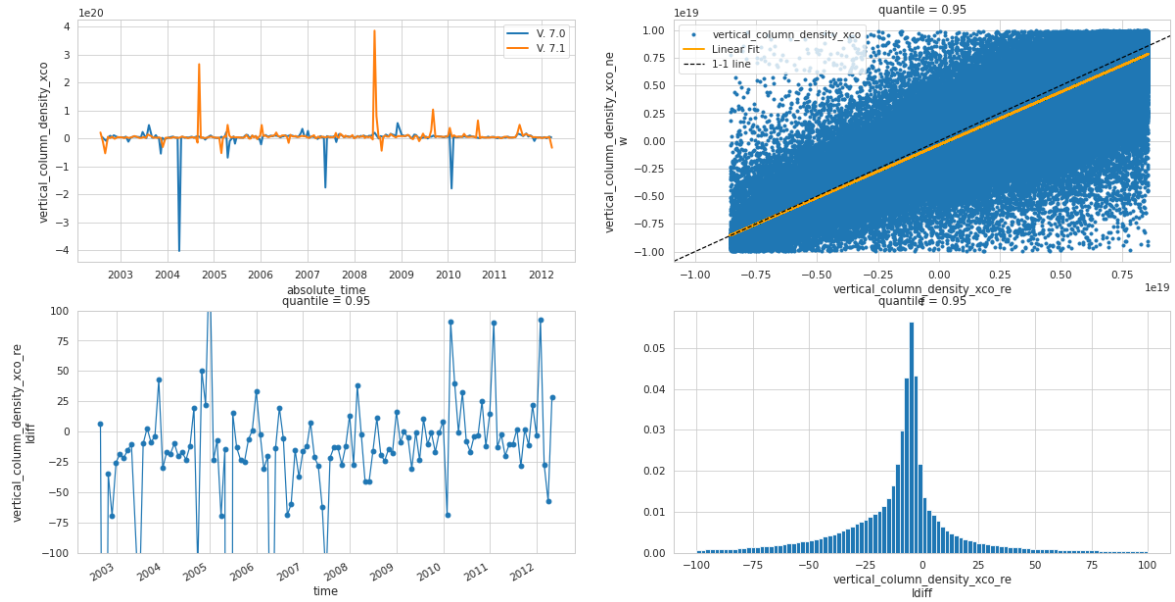


Figure 35: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

Errors:

- vertical_column_density_error_co
- vertical_column_density_error_xco

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
vertical_column_density_error_co	1725967	0.8751 +- 0.0002961	1.65e+17 +- 1.269e+15	0.8349	-1.684
vertical_column_density_error_xco	1725967	0.8741 +- 0.0003163	2.104e+17 +- 1.57e+15	0.8157	-2.184

Fig. 36 shows the error calculated for CO.

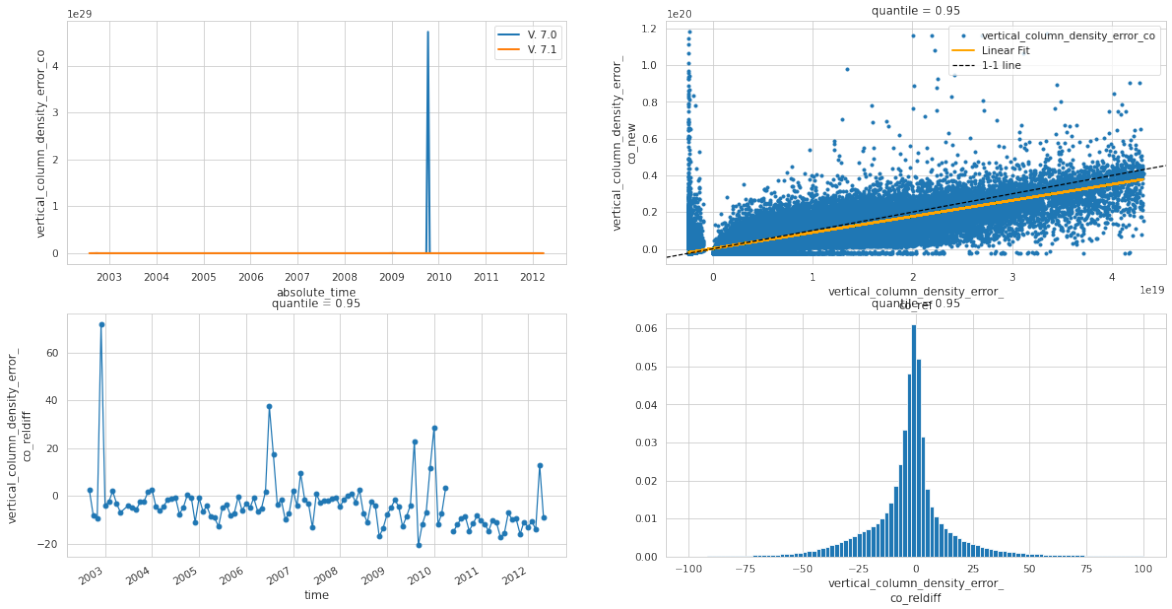


Figure 36: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

Removing the outliers improves the situation significantly, especially for the vertical columns. But the error values still do not agree completely and the CO values are systematically lower than in the previous version.

4 Limb Products

4.1 Limb Clouds

The following parameters are extracted:

- ice_cloud_flag
- ice_cloud_height
- noctilucent_cloud_flag
- noctilucent_cloud_height
- polar_stratospheric_cloud_flag
- polar_stratospheric_cloud_height
- water_cloud_flag
- water_cloud_height

4.1.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	102342	1105
V. 7.1	100252	1082

4.1.2 Comparison

The following table shows the number of time matched records that have valid values and the results of a linear regression between selected variables:

#+name limbcloud_linreg

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
ice_cloud_height	91424	0.9506 +- 0.001133	546.6 +- 11.24	0.885	-6.908e-05
noctilucent_cloud_height	91424	0.9988 +- 0.0001434	4.319 +- 3.539	0.9981	0
polar_stratospheric_cloud_height	91424	0.9980 +- 0.0002256	1.409 +- 0.6234	0.9953	-1.914e-05
water_cloud_height	91424	0.9990 +- 0.0001615	9.538 +- 1.612	0.9976	-7.106e-05

For flags the median difference does not make much sense as a test parameter. Therefore we calculated the percentage where the absolute difference is larger than 0:

Parameter	# matches	Slope	Intercept	R^2	# ARD > 0% [% of total]
ice_cloud_flag	91424	0.9074 +- 0.001233	0.08676 +- 0.0009975	0.8556	3.4
noctilucent_cloud_flag	91424	0.9990 +- 0.0001076	4.996e-05 +- 7.885e-05	0.9989	0.023
polar_stratospheric_cloud_flag	91424	0.9982 +- 0.0002423	8.975e-05 +- 3.836e-05	0.9946	0.013
water_cloud_flag	91424	0.9932 +- 0.0003741	0.008214 +- 0.0006485	0.9872	0.29

With the exception of the values for the ice cloud retrieval the agreement between the processor versions is very good. The differences for the ice clouds is a bit larger.

4.1.2.1 Ice cloud flag

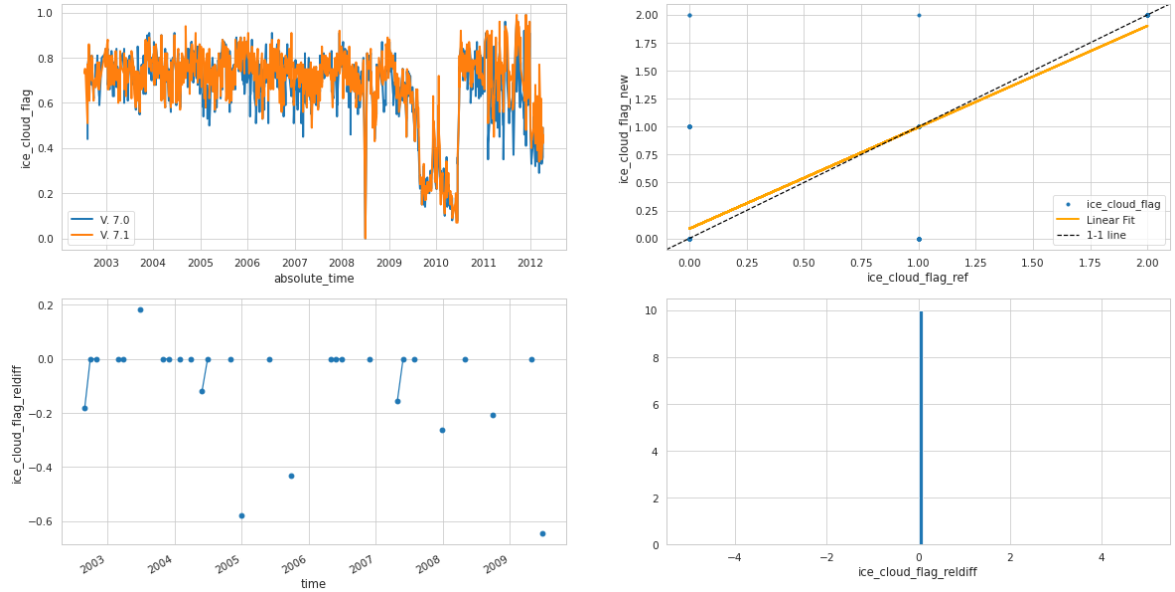


Figure 37: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.1.2.2 Ice cloud height

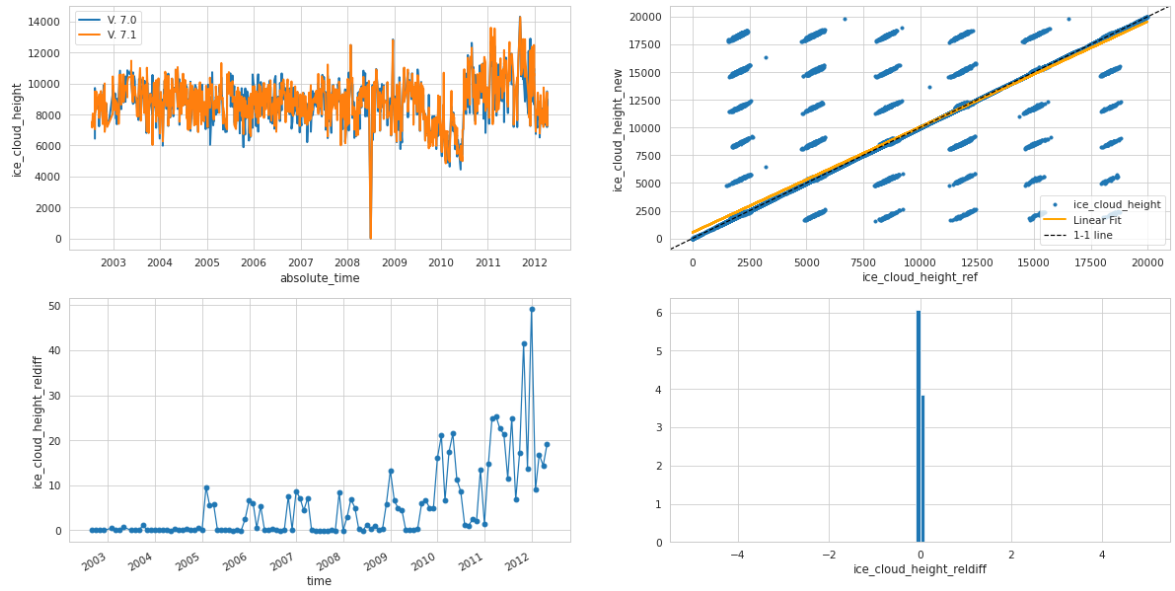


Figure 38: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.1.2.3 Noctilucent cloud flag

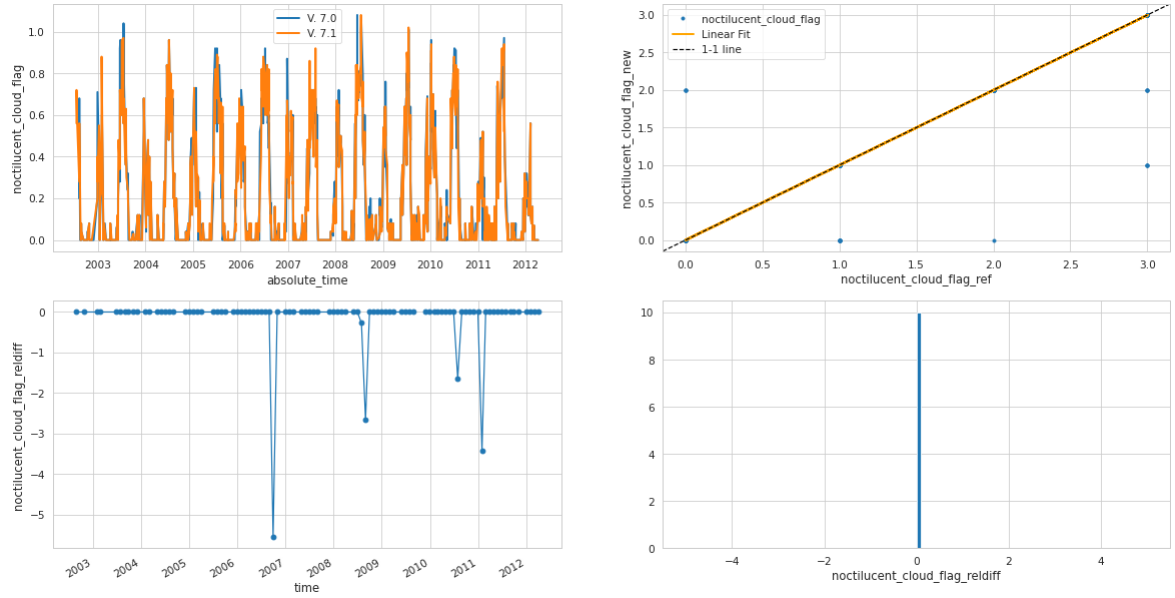


Figure 39: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.1.2.4 Noctilucent cloud height

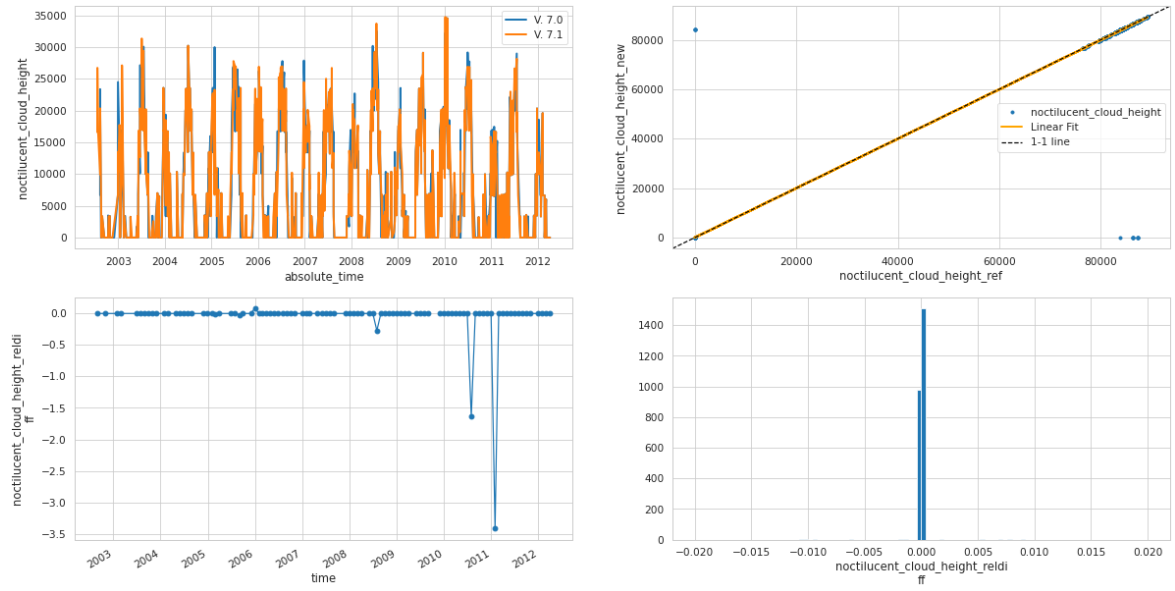


Figure 40: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.1.2.5 Polar_stratospheric_cloud_flag

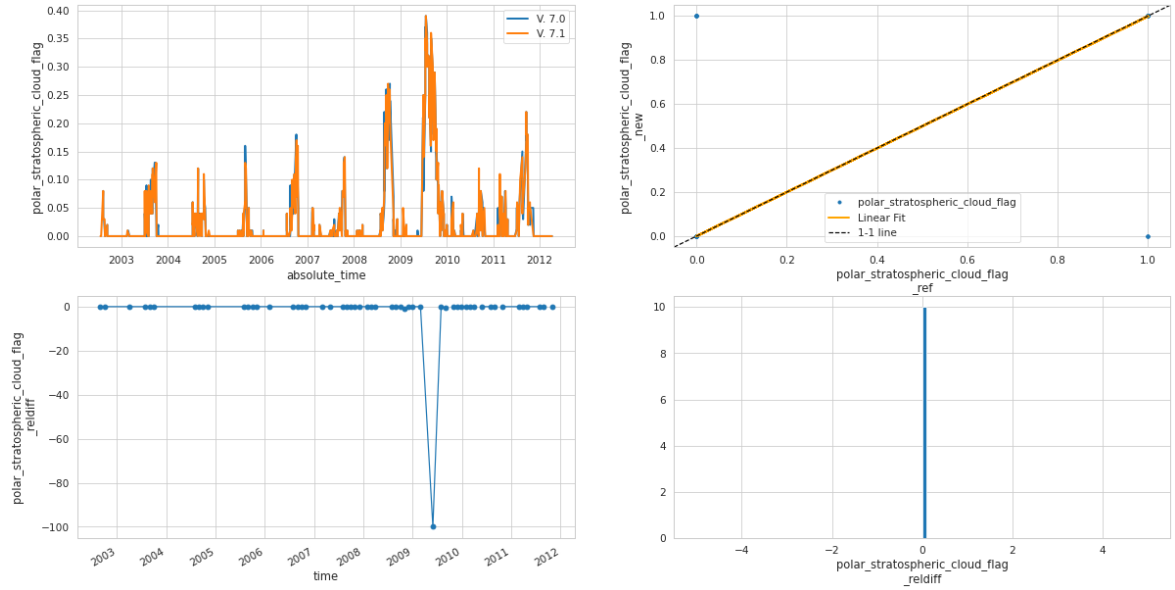


Figure 41: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.1.2.6 Polar stratospheric cloud_height

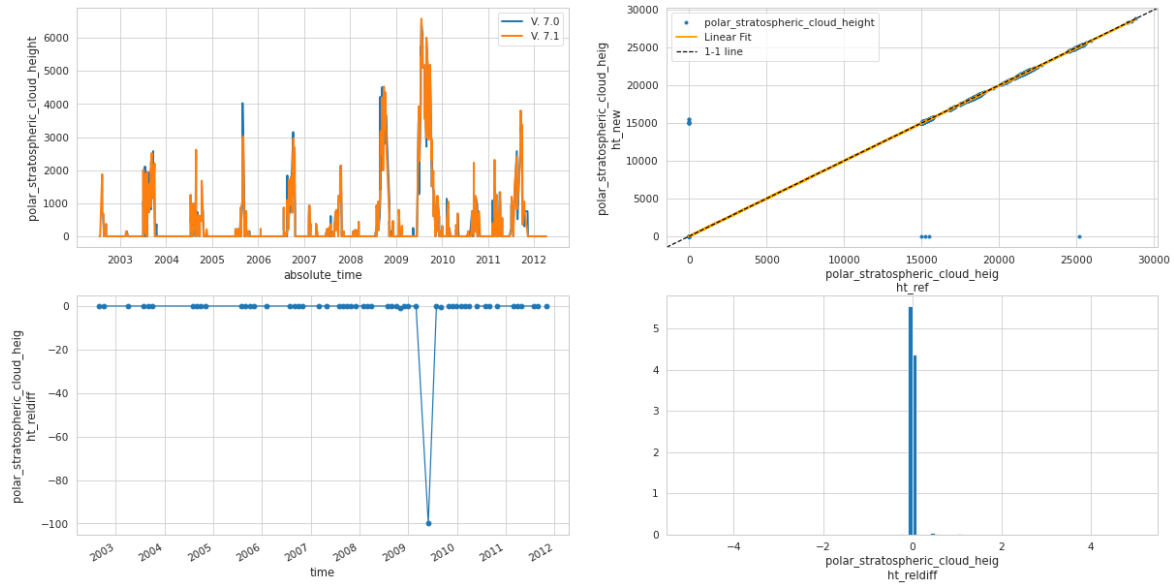


Figure 42: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.1.2.7 Water cloud flag

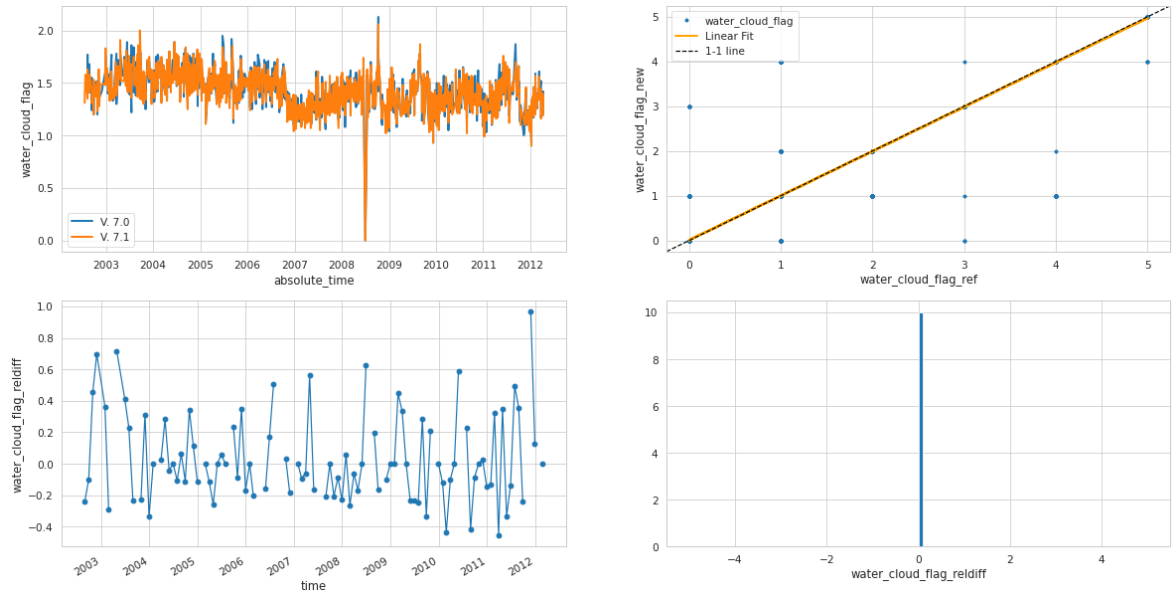


Figure 43: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.1.2.8 Water cloud height

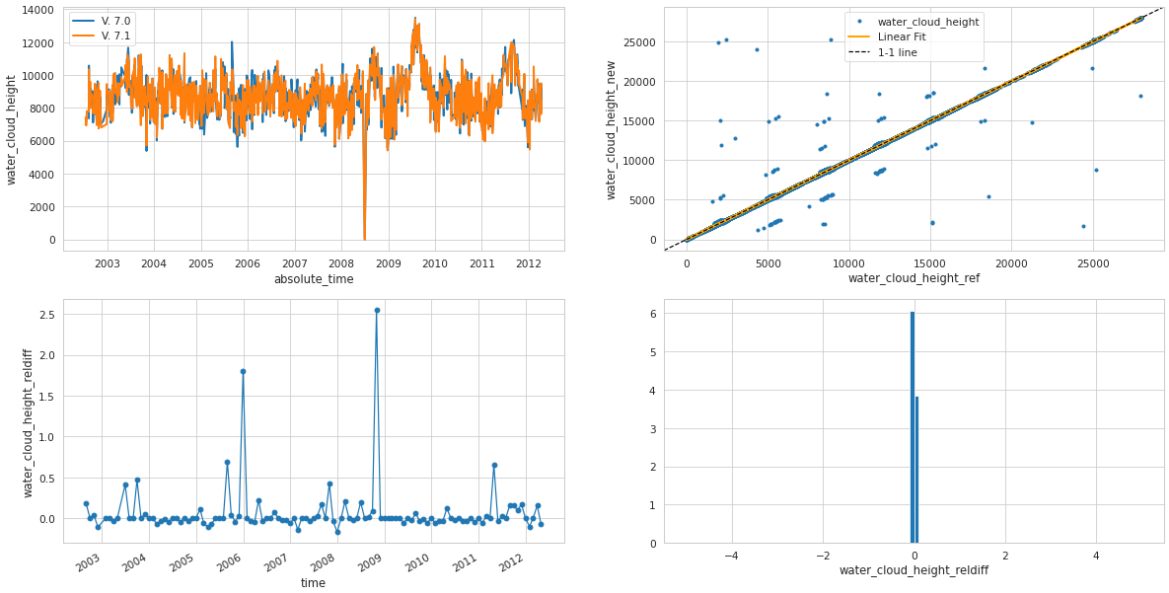


Figure 44: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.2 Ozone

The following parameters are extracted:

- number_density_retrieved

4.2.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	27045	1067
V. 7.1	26487	1045

4.2.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Med. R. Diff. [%]
number_density_retrieved	652448	0.9999 +- 4.628e-06	6.473e+07 +- 1.048e+07	1	0

The values of the 2 versions agree.

4.2.2.1 Number Density

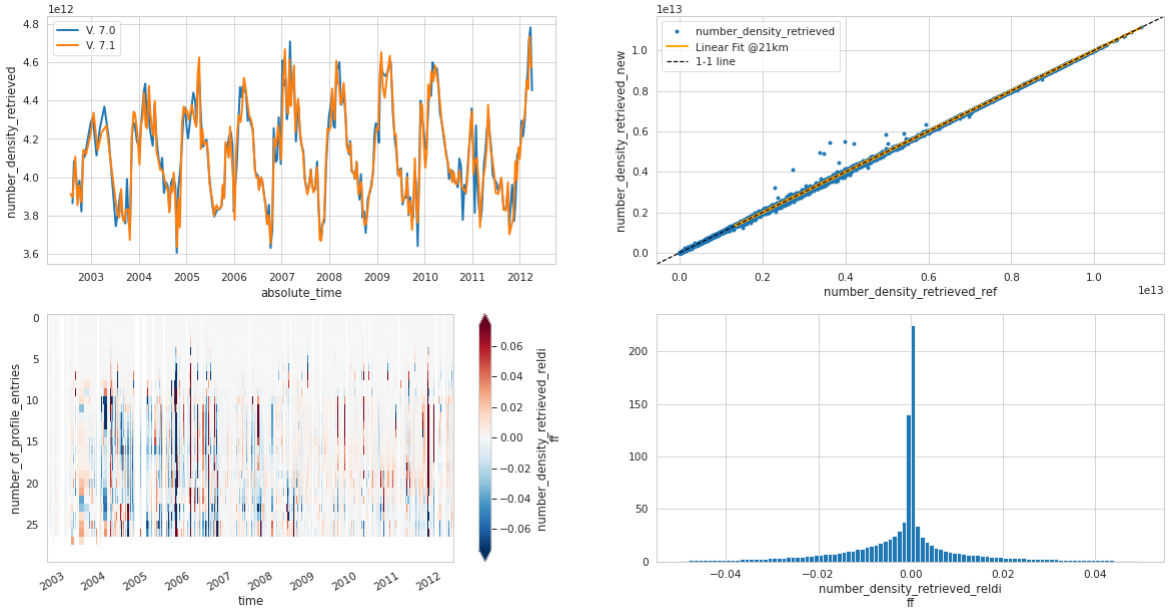


Figure 45: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.3 NO_2

The following parameters are extracted:

- number_density_retrieved

4.3.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	111336	1096
V. 7.1	108998	1073

4.3.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Med. R. Diff. [%]
number_density_retrieved	2669729	1.0000 +- 1.644e-06	7692 +- 1377	1	0

The values of the two versions agree.

4.3.2.1 Number Density

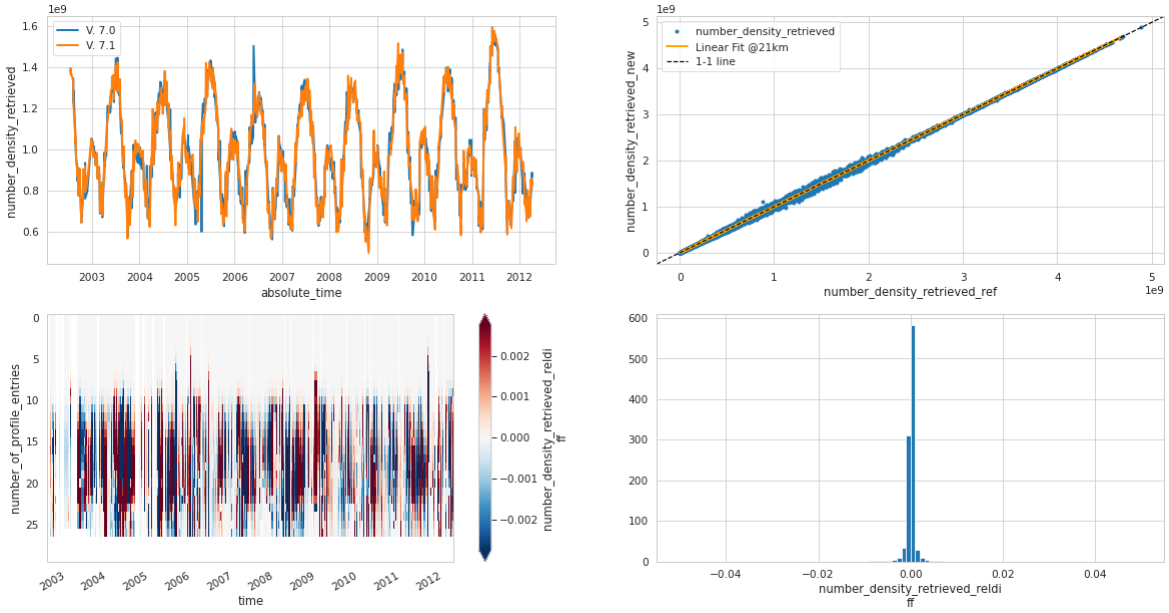


Figure 46: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

4.4 BrO

The following parameters are extracted:

- number_density_retrieved

4.4.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	99451	1054
V. 7.1	97379	1032

4.4.2 Comparison

Parameter	# matches	Slope	Intercept	R^2	Med. R. Diff. [%]
number_density_retrieved	2544896	0.9926 +- 6.812e-05	1.01e+04 +- 725	0.9882	-9.206e-06

The values of the versions agree.

4.4.2.1 Number Density

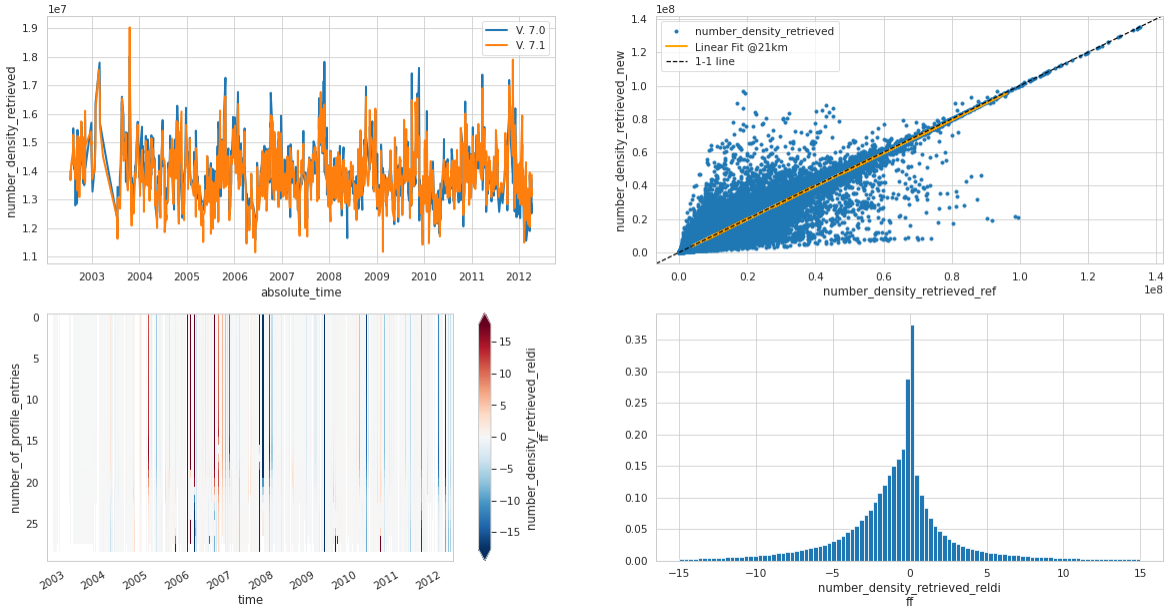


Figure 47: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

5 Tropospheric Products

5.1 NO2

The following parameters are extracted:

- ➢ tropospheric_slant_column_density
- ➢ tropospheric_vertical_column_density
- ➢ root_mean_square

5.1.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	10454632	1149
V. 7.1	10211412	1125

5.1.2 Comparison

The following table shows the number of time matched records that have valid values and the results of a linear regression between selected variables:

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
tropospheric_slant_column_density	2237842	0.9362 +- 0.0002681	1.347e+14 +- 5.26e+11	0.8449	-1.052
tropospheric_vertical_column_density	2237842	0.9866 +- 0.0001311	4.14e+13 +- 2.259e+11	0.962	-1.052
root_mean_square	9388365	1.0021 +- 2.492e-06	-1.149e-06 +- 1.992e-09	0.9999	0.004656

The agreement of the two values is good with the 7.1 values a bit larger than the version 7.0.

5.1.2.1 Tropospheric Vertical Column Density

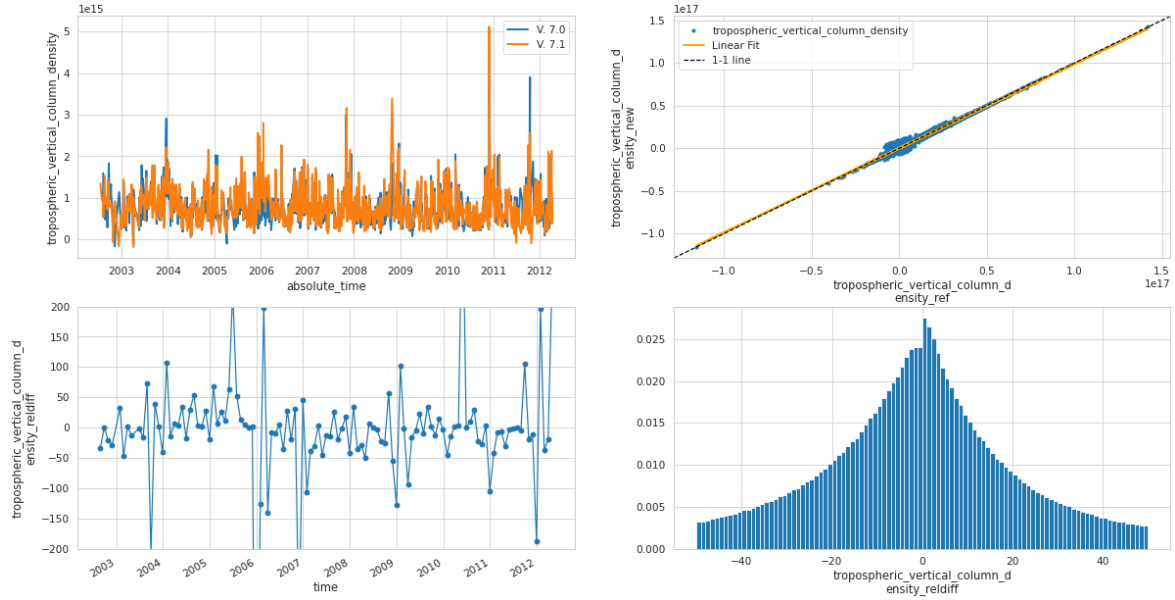


Figure 48: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

5.2 BrO

check The following parameters are extracted:

- ➢ tropospheric_slant_column_density
- ➢ tropospheric_vertical_column_density

5.2.1 Data Set

The total number of extracted test data is

Version	# Records	# orbits
V. 7.0	5860054	1149
V. 7.1	5753327	1125

5.2.2 Comparison

The following table shows the number of time matched records that have valid values and the results of a linear regression between selected variables:

Parameter	# matches	Slope	Intercept	R^2	Median R. Diff. [%]
tropospheric_slant_column_density	2460206	1.0034 +- 0.0004664	-1.622e+12 +- 3.694e+10	0.6529	-0.2996
tropospheric_vertical_column_density	2460206	1.0120 +- 0.0005511	-9.222e+11 +- 1.788e+10	0.5782	-0.2909

The values of the two versions agree.

5.2.2.1 Tropospheric Slant Column Density

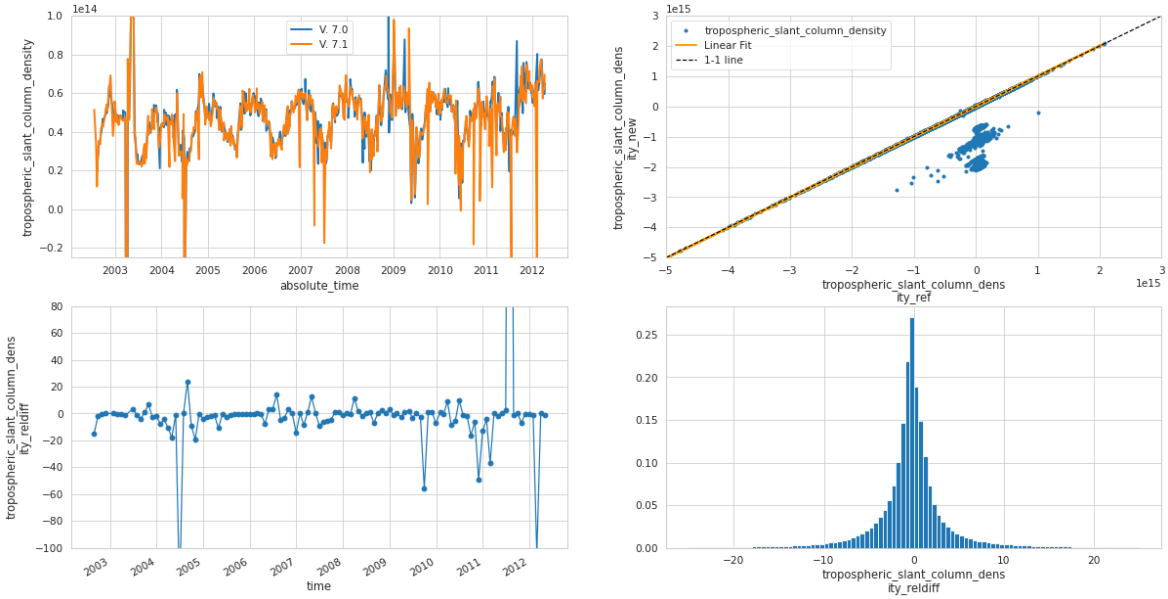


Figure 49: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

5.2.2.2 Tropospheric Vertical column density

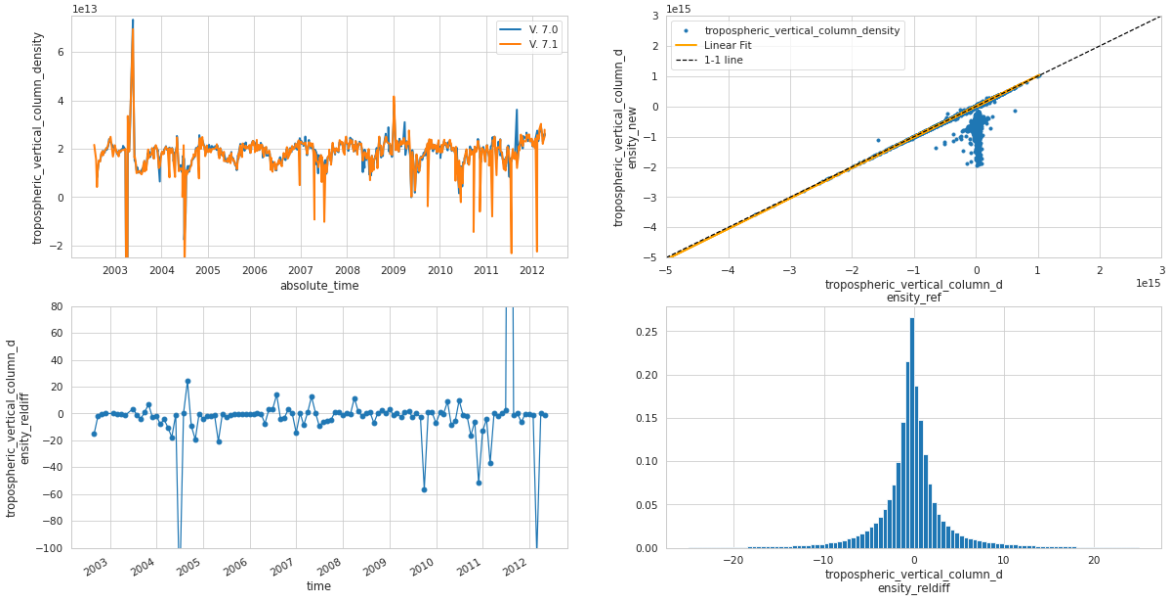


Figure 50: *From top left clockwise: Values for both processor versions, scatter plot, relative difference and histogram of relative differences*

6 Comparison of regression test results with validation

BIRA did a comparison between the deviations shown here and the typical error of retrievals for the species where validations results were available:

Product	**Regression test V7.01 - V7.0** (FDR4ATMOS_L2RegressionTest-FDR4ATA-TN-DLR-007, 19 Jan 2023)	**Ground-based validation V7.0** (TN-BIRA-IASB-MultiTASTE-Phase-F-SCIA-SGP7-Iss1_RevC, 18 Dec 2019)	**Conclusion expected quality V7.01**	**Release maturity**
Nadir O3	(vertical column density) - V7.01 is 0.8% larger than V7.0 (Table 3.3.2) - V7.01-V7.0 drift is +2. . . +2.5% over mission (Fig 5) - V7.01-V6 has no clear time dependence	Dedicated results for V7.1 in TN-BIRA-IASB-FDR4ATMOS-SCIA-SGP7.1-Iss1-revB (7 Dec 2022)	- Bias, dispersion, stability similar to V6. - Drift of V7.01 is even slightly reduced w.r.t. that of V6.	Good to go
Nadir NO2	(total vertical column density) - V7.01 is ~0.05% smaller than V7.0 (median) - Seasonal & long-term structure in V7.01 minus V7.0, with magnitude of ~0.3% (or ~8-10 x 1012 molec cm-2) (Fig 8)	- Bias & dispersion V7.0-GND range between 3-8 x 1014 molec cm-2 - This is 2 orders larger than results of regression test	Ground-based validation won't be able to distinguish V7.01 from V7.0; Differences are below typical measurement uncertainties.	Good to go
Nadir BrO	- Median difference less than 0.3% - Changes of 1-2% over mission lifetime	- Bias & dispersion V7.0-GND range between 10-15% - This is 1 order larger than results of regression test	Ground-based validation won't be able to distinguish V7.01 from V7.0	Good to go
Nadir H2O	- Relative differences are negligible (< 1e-4 %)	- Bias V7.0-GND ranges between 5-15% - Dispersion V7.0-GND ranges between 20-30% - Several orders larger than results of regression test	Ground-based validation won't be able to distinguish V7.01 from V7.0	Good to go
Nadir CH4	(VCD CH4) with Q95 filter (Sect 3.11.3) - Median value V7.01-V7.0 is +6%. - Time series show a range +10-20%. - Time series V7.01-V6 have no time structure.	- Median value monthly mean V7.0-FTIR is -35 to -10%. - Dispersion monthly mean is 5-15%.	Bias V7.01 wrt FTIR is expected to be smaller than that of V7.0	Likely good to go (with recommendations for outlier screening)
Nadir CO	(VCD CO) with Q95 filter (Sect 3.12.3) - Median value -7.2% - No clear structure in time series	- Median value monthly mean V7.0-FTIR is -20 to +45%. - Dispersion monthly mean is 10-30%.	Not clear whether bias of V7.01 wrt FTIR will be better. At least no change in time structure expected.	Possibly good to go (with recommendations for outlier screening)
Limb O3	- Median difference is 0% (all latitudes & altitudes) - The range of relative differences is just +-0.05%.	- Bias of V7.0 oscillates ~2% around V6 result. - Drift of V7.0 oscillates by 6-8%/dec, not seen for V6.	Ground-based validation won't be able to distinguish V7.01 from V7.0	Not recommended, due to complicated vertical pattern in drift.
Limb BrO	- Median relative difference is 0% - No clear structure in time series	(Analysis covers 15-27 km range) - Bias ranges between -50% and 0%. - Dispersion ranges between 25-50%.	Ground-based validation won't be able to distinguish V7.01 from V7.0	Good to go

7 Summary

The table below shows a summary of the results

Table 2: *Result of regression test results.*

Species	Spectral Range	Status	BIRA
Cloud Fraction	PMDs	OK	
Cloud Optical Thickness	753-775 nm (O2A)	OK	
Cloud Top Height	753-775 nm (O2A)	OK	
Absorbing Aerosol Indicator	340/380 nm	(OK), similar to 6.01	
Nadir SO2 (uses BG DB)	315-327 nm	OK	
Nadir O3	325-335 nm	OK	OK
Nadir HCHO (uses BG DB)	328.5-346 nm	(OK)	
Nadir BrO	336-351 nm	OK	OK
Nadir OClO	365-389 nm	OK	
Nadir NO2	426.5-451.5 nm	OK	
Nadir CHOCHO (uses BG DB)	435-457 nm	not OK	
Nadir H2O	688-799 nm	OK	OK
Nadir CH4	2324.4-2335.0 nm	OK	OK
Nadir CO	1557.2-1594.1 nm & 1628.9-1670.6 nm	(OK)	(OK)
Limb Clouds			
Noctilucent cloud height	265/291 nm	OK	
Polar stratospheric cloud height	750/1090 nm	OK	
Water cloud height	750/1090 nm	OK	
Ice cloud height	1550/1685 nm	systematic difference for groups of data	
Limb O3	283-310 nm & 520-590 nm	Results agree	Not OK
Limb BrO	337-357 nm	OK	OK
Limb NO2	420-470 nm	OK	
Trop. BrO (uses offset correction)	336-351 nm	OK, V7.1 has lower values around zero	
Trop. NO2 (uses L/N matching)	426.5-451.5 nm (N), 420-470 nm (L)	OK, values slightly lower than 7.0	

For most retrievals, the new version 7.1 has similar or even nearly identical values for the main results. The comparison shown here could not explain the differences in the CHOCHO retrieval. These retrieval was numerically unstable in previous versions. Version 7.1 apparently has corrupt values (and the number of values is significantly lower).

Additionally, some peculiarities can be seen in the comparison:

1. For the retrievals of SO_2, HCHO, OClO, CH_4, CO the error values can only be reconciled after removing outliers.
2. For the retrievals of HCHO, BrO and tropospheric NO_2 version 7.1 shows a cluster of values that is lower than in the previous version. These clusters are around zero and the retrieval is likely not reliable in that value range.
3. The values for Limb O_3 agree, but there are oscillations in the data that cannot be seen in the comparison with independent data (see [2]). Version 7.1 show no improvement in this respect. V.6 did not show this behaviour.