Tropospheric ozone from OMI and plans for Sentinel 4

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Introduction

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- Retrieval scheme developed at RAL to infer ozone profiles, with tropospheric sensitivity, from nadir-uv spectrometers.
- Scheme selected to provide the nadir-uv-profile data for ESA's Climate Change Initiative (CCI) to generate multi-year data sets from GOME-1, GOME-2, SCIAMACHY and (recently) OMI
  - Re-processed versions of this data also to feed into Copernicus Climate Change service (C3S)
  - RAL running own near-real time processing of GOME-2
  - New OMI results considered sufficiently stable over time to submit to TOAR
- Scheme forms the basis for development of the ESA processor development for Sentinel 4 (GEO) & 5 (LEO)
- Algorithm development to cope with new demands / potential of S4 has taken place in parallel with development of the RAL scheme for OMI, leading to improvement / consolidation of the scheme
  - Will overview OMI results + scheme development for S4

Tropospheric ozone from uv sounders

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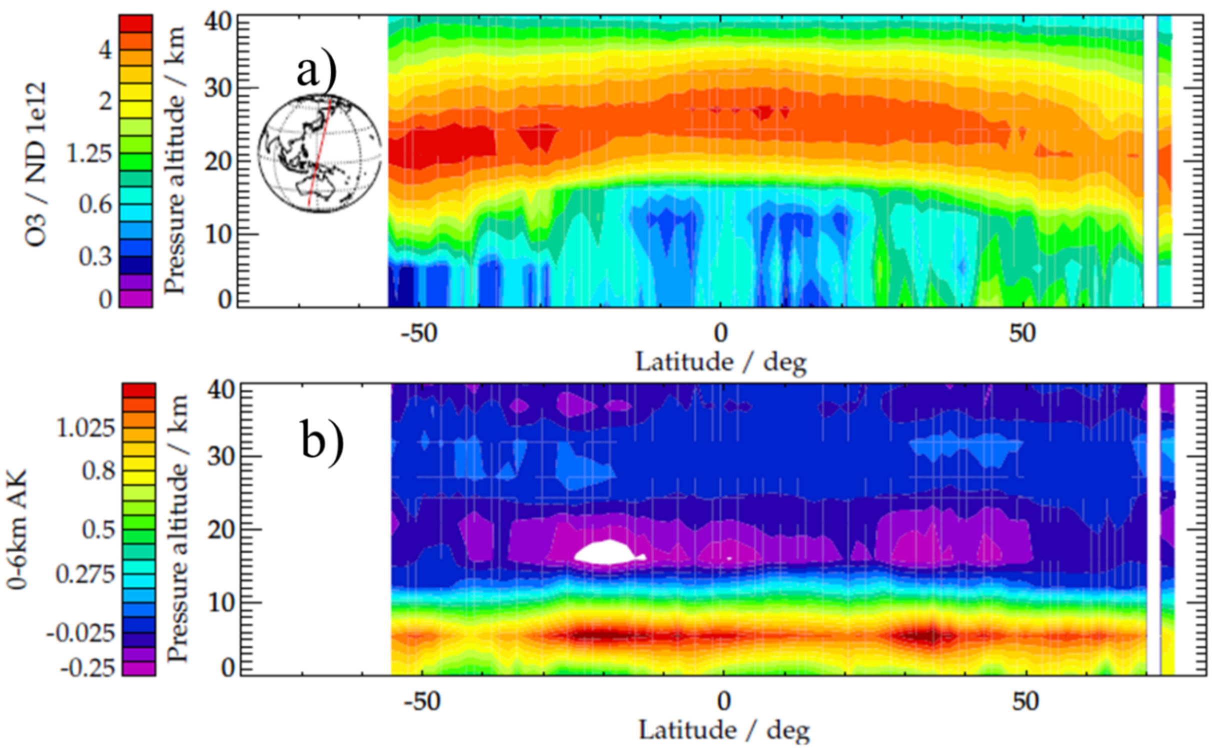
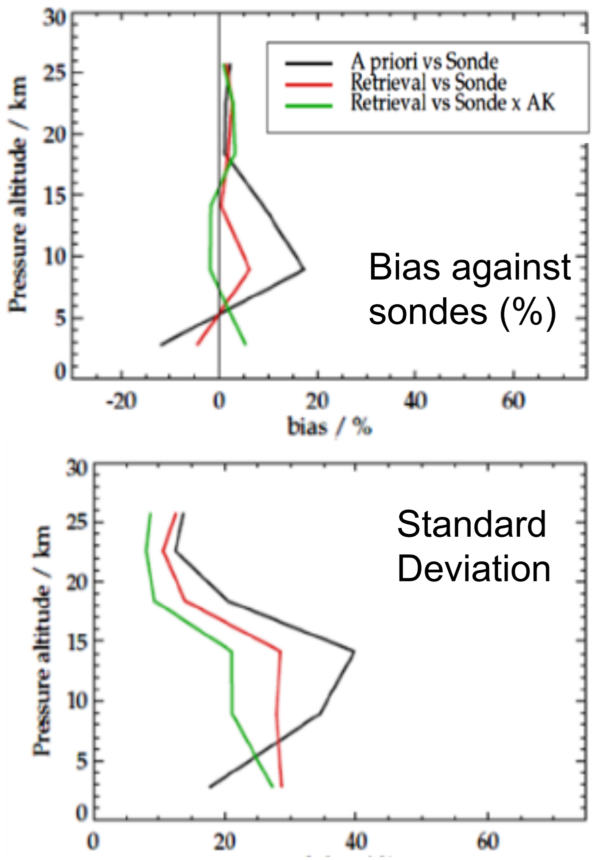
- Exploits wavelength dependence of ozone UV absorption in Hartley and Huggins bands to retrieve height-resolved information R.Munro *et al*, Nature (1998); G.Miles *et al.*, AMT (2015)
- Spectral fitting to <0.1% RMS precision in T-dependent Huggins bands extends information into troposphere

GOME-2A orbit Cross Section (25th Aug 2008)





Some details of OMI Scheme

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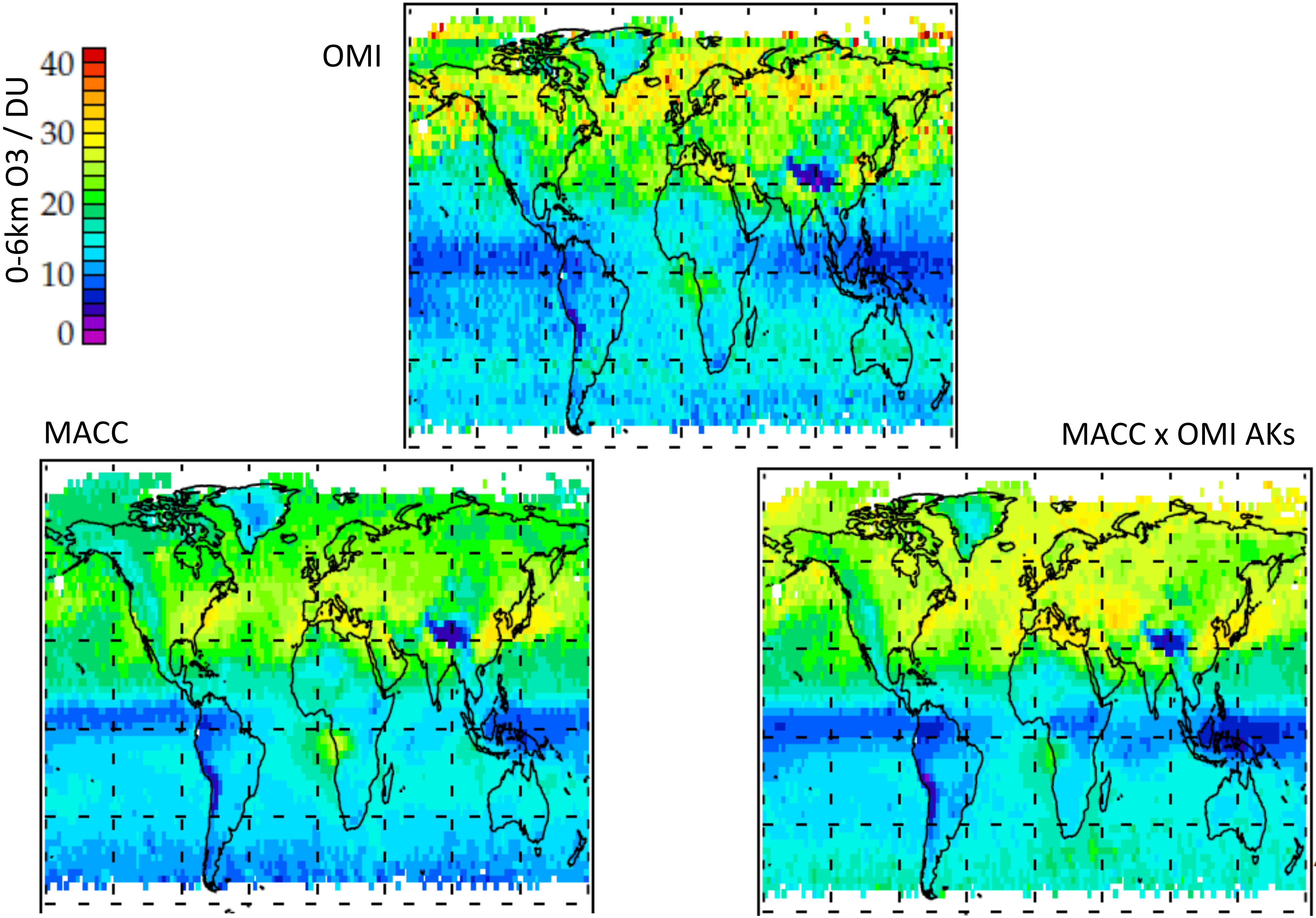
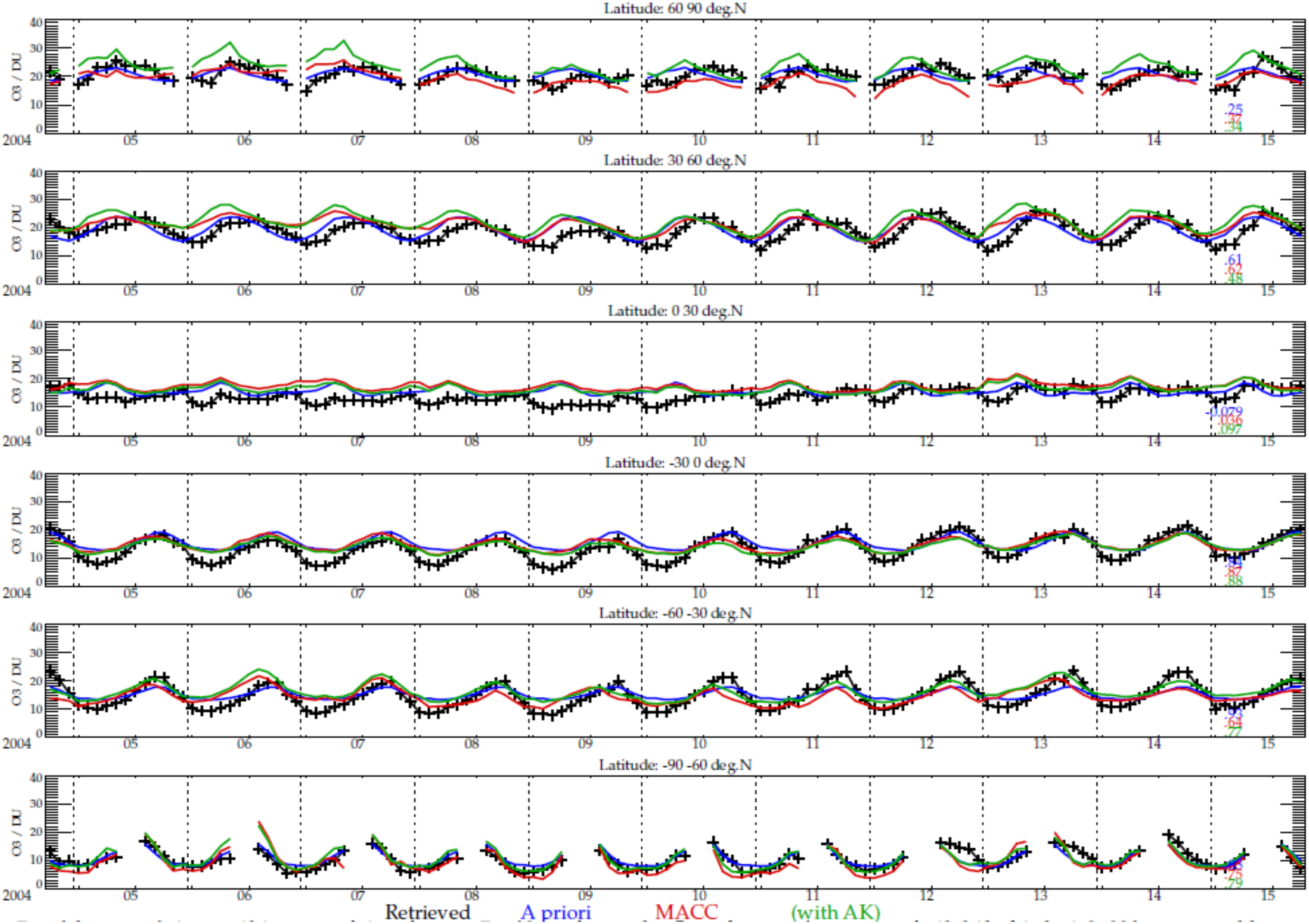
- Spectral range: 270-307nm from UV1; 321-338nm from UV2
- Joint fit of NO2, BrO, Formaldehyde, albedo, Ring scale factor, wavelength mis-registration, radiometric gain/offset parameters; cloud from operational L2.
- Modelling of Ring effect updated to better model effect on ozone absorption
- Uses Serdyuchenko cross-sections – after applying an optimised wavelength shift in Huggins range – these then lead to (slightly) better fit and bias in tropospheric ozone cf BMD
- So far we process at coarse spatial sampling due mainly to computational resource limits (but also to reduce noise)
  - UV2 pixels averaged 2x4 across-along track to approx 50x50km resolution.
  - UV1 averaged to match this
- Uses fixed solar referenced spectrum (median Nov 2004)
- Spectral response from fitting super-Gaussian to solar reference spectrum (varies x-track, constant with time)

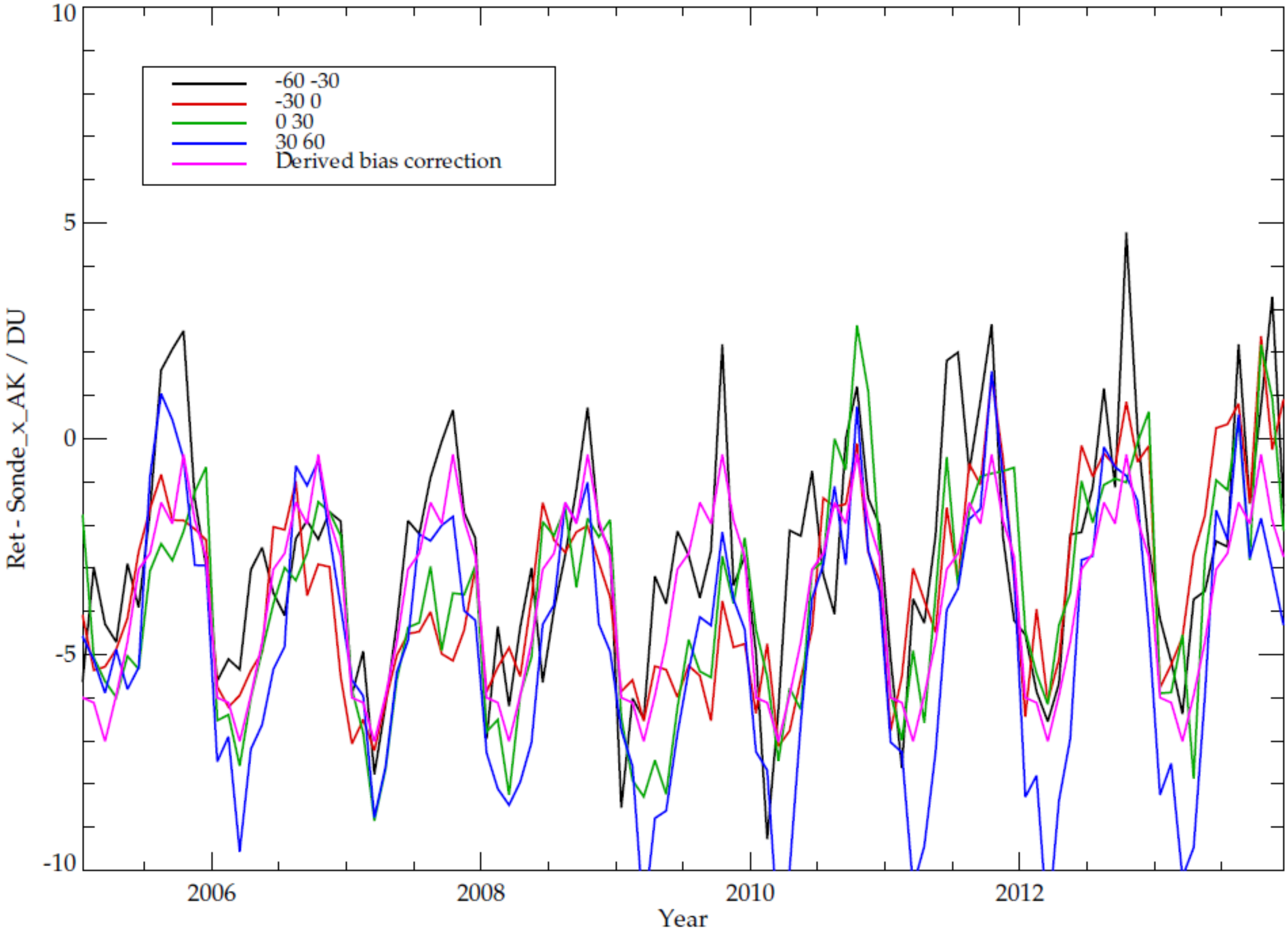
OMI / MACC re-analysis comparison Aug 2008



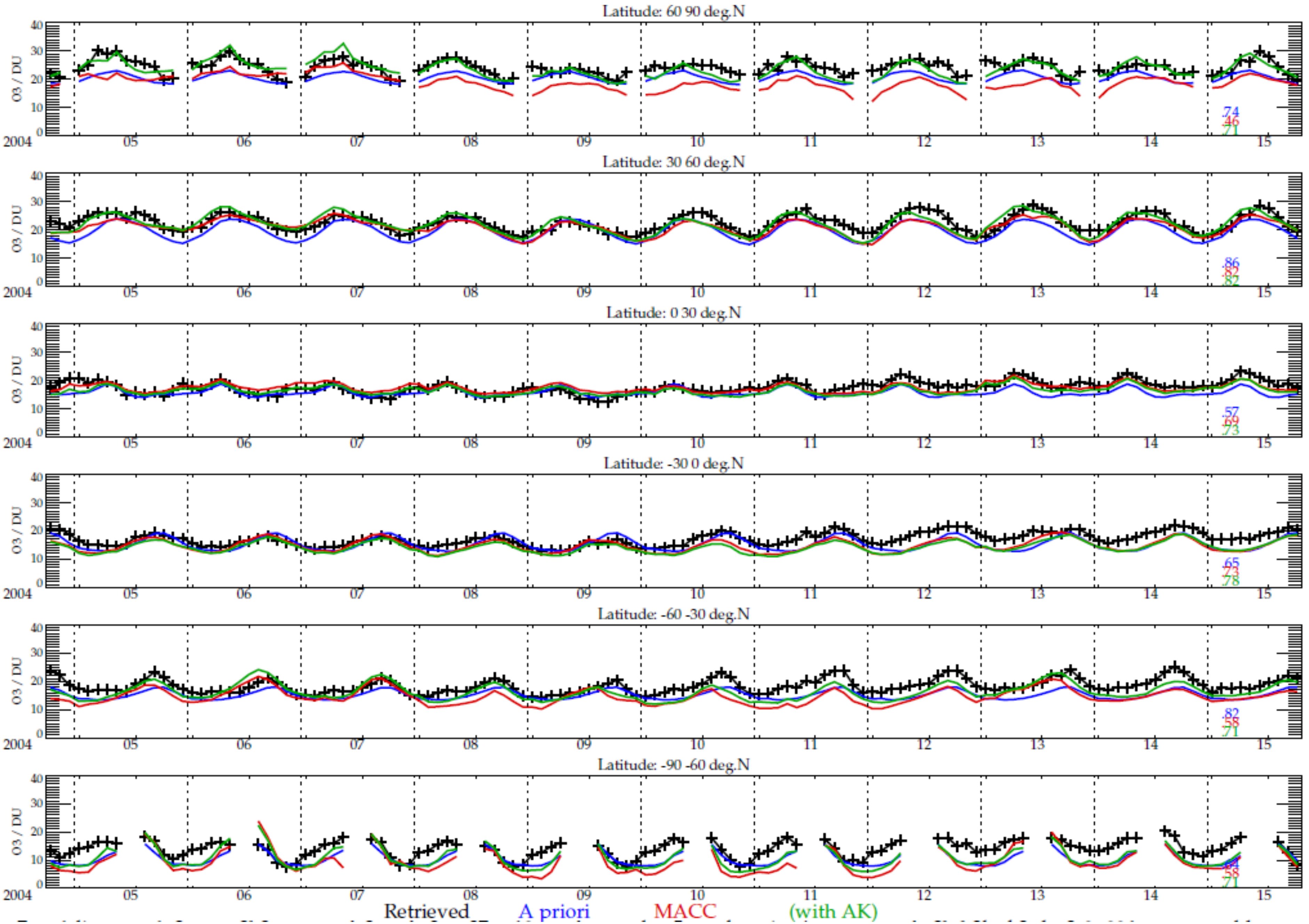
OMI time-series 0-6km OMI vs MACC



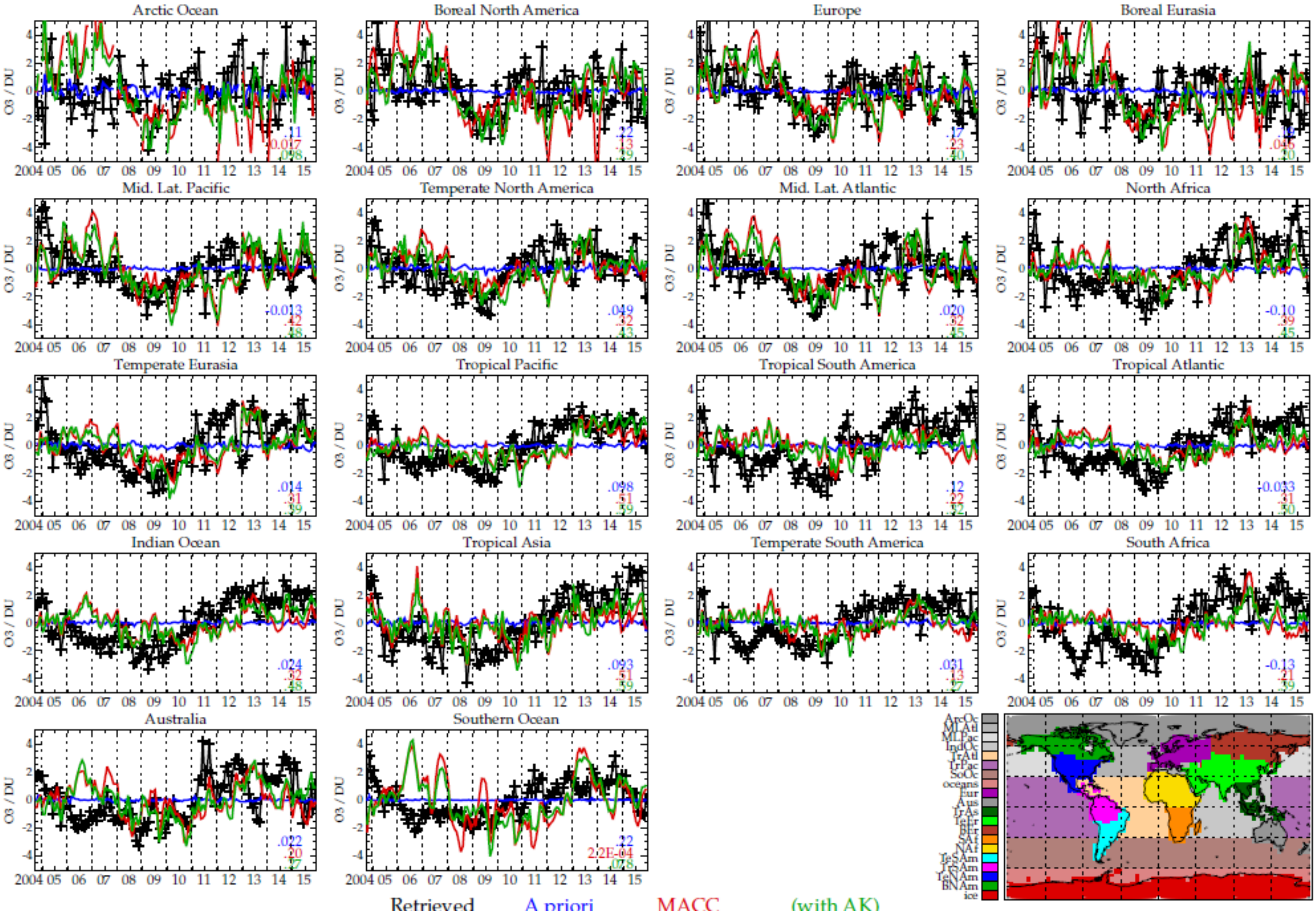
Global, monthly bias correction for OMI from sondes



OMI 0-6km column after monthly/global sonde correction



OMI 0-6km column anomaly from multi-annual, monthly mean



Future: Tropospheric Ozone from Sentinel 4

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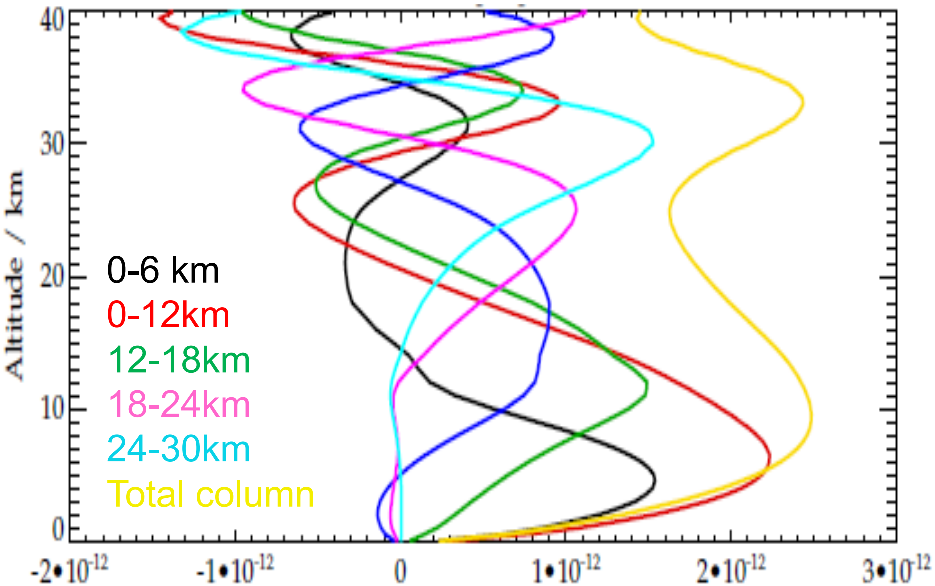
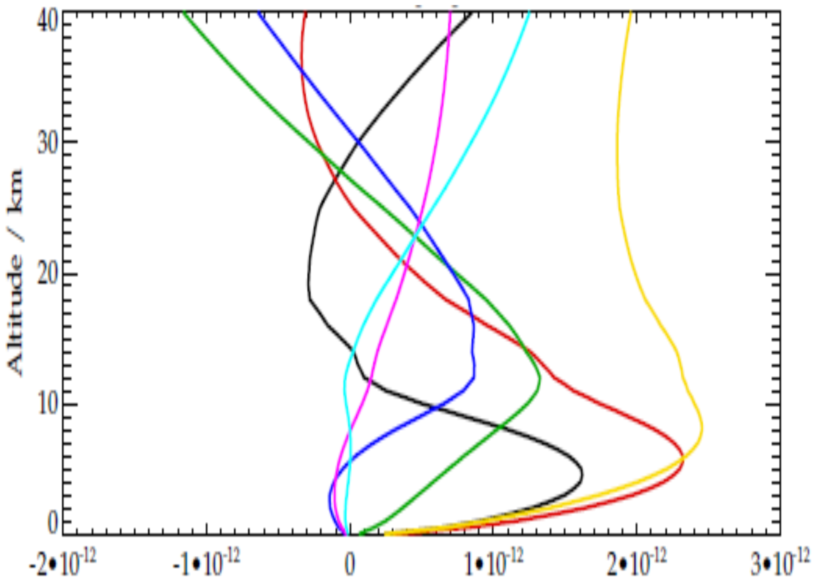
- S4 has no measurements of Hartley band below 305nm, which provides stratospheric profile information in all previous sensors
- Basis for S4 scheme to deliver tropospheric ozone without this spectral range being established via ESA S4 L2 processor development, so far document in ATBD v1.6

S5 simulation (270nm+)
Profile degrees of freedom: 6.5
0-6km column uncertainty: 30%
0-12km uncertainty: 11%
Averaging kernels



S4 simulation (305nm+)
Ozone DFS: 2.74
0-6km column uncertainty: 30%
0-12km uncertainty: 15%
Averaging kernels



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S4 O_3 information vs Spectral coverage

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0-6km ESD / %

	Co-add 1		Co-add 4	
	1000% gain error	1% gain error	1000% gain error	1% gain error
322 - 335 nm	49.6	48.4	34.7	34.3
317 - 335 nm	39.5	38.0	27.0	26.7
312 - 335 nm	36.5	34.1	25.7	25.2
312 - 340 nm	36.0	33.5	25.6	25.1
305 - 344 nm	33.9	29.9	23.7	22.7
301 - 344 nm	33.2	28.2	23.0	21.7

DoFS

	Co-add 1		Co-add 4	
	1000% gain error	1% gain error	1000% gain error	1% gain error
322 - 335 nm	1.63	1.64	1.99	1.99
317 - 335 nm	2.00	2.01	2.50	2.50
312 - 335 nm	2.49	2.53	2.87	2.87
312 - 340 nm	2.60	2.62	2.92	2.93
305 - 344 nm	3.23	3.27	3.79	3.80
301 - 344 nm	3.72	3.78	4.17	4.18

- Little benefit for tropospheric ozone from using broad-band absorption features (cf increased sensitivity to calibration errors)
- Extending coverage below 317 nm adds little information, esp when co-adding to $21x21km^2$ resolution – 317nm-335 coverage is current baseline
- Extra degree of freedom available in stratosphere if coverage extended towards 300nm (but fitting such broad range would be very challenging)

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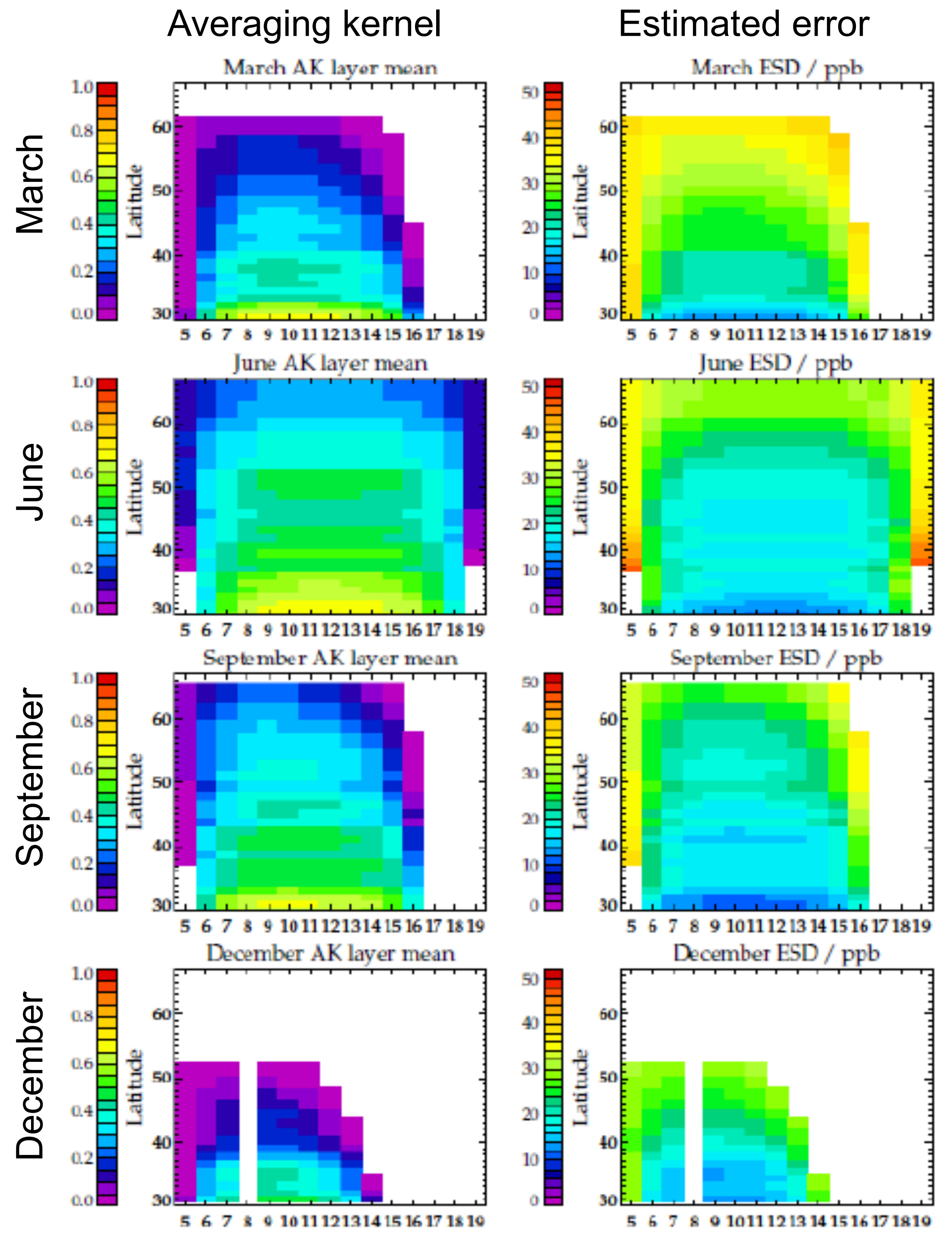
S4 O_3 information vs time of day + month

- Simulated performance at 0 longitude, as function of time of day + latitude for 4 months.
- Sensitivity to troposphere is much reduced in winter
- Sensitivity to ozone over low cloud can be slightly better



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Optimisation of forward model

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- Retrieval scheme runs on-line multiple scattering calculations (using LIDORT) – very computationally demanding
- Plan to adopt "PCFM" approach to reduce number of wavelengths at which these calculations are needed
- Also need to
  - ensure basic calculations are sufficiently accurate
    - NB complications from polarisation and Ring effect
  - reduce complexity of individual calculations:
    - Consider (low-stream) Rayleigh only atmosphere and deal with cloud + aerosol via fitted effective albedo + parametisation of cloud obscuration via AMF profiles
- The assumptions tested via tests on synthetic data based on realistic modelling including cloud + aerosol + full-Ring effect

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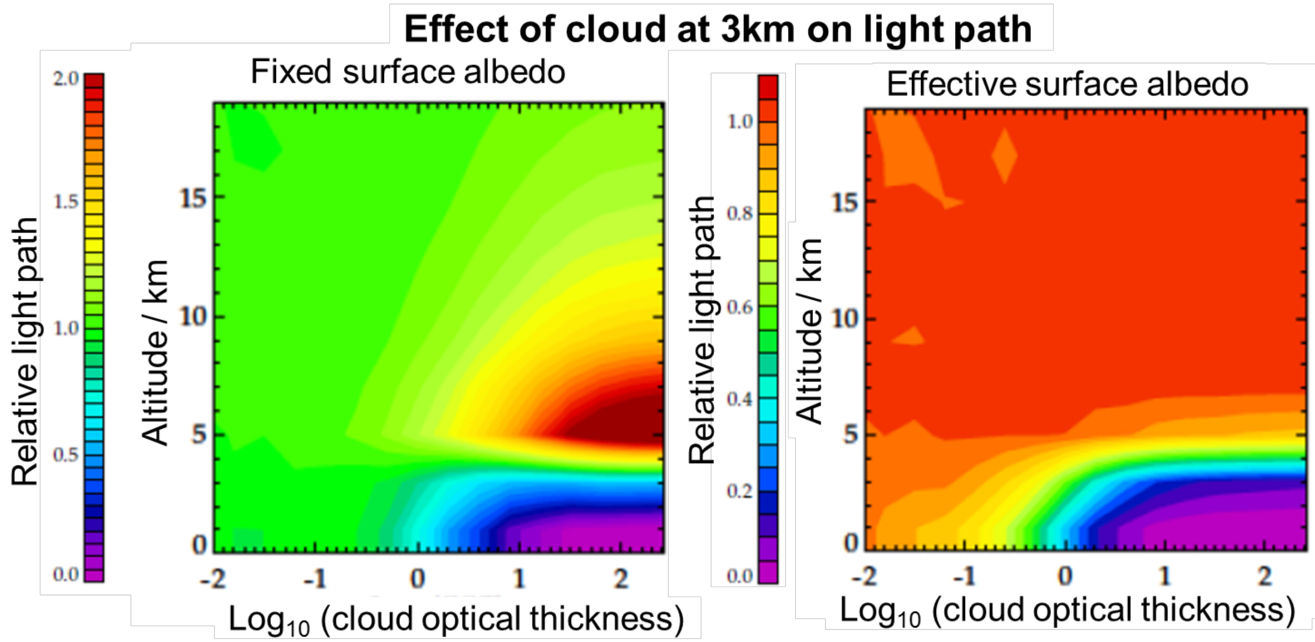
Modelling cloud

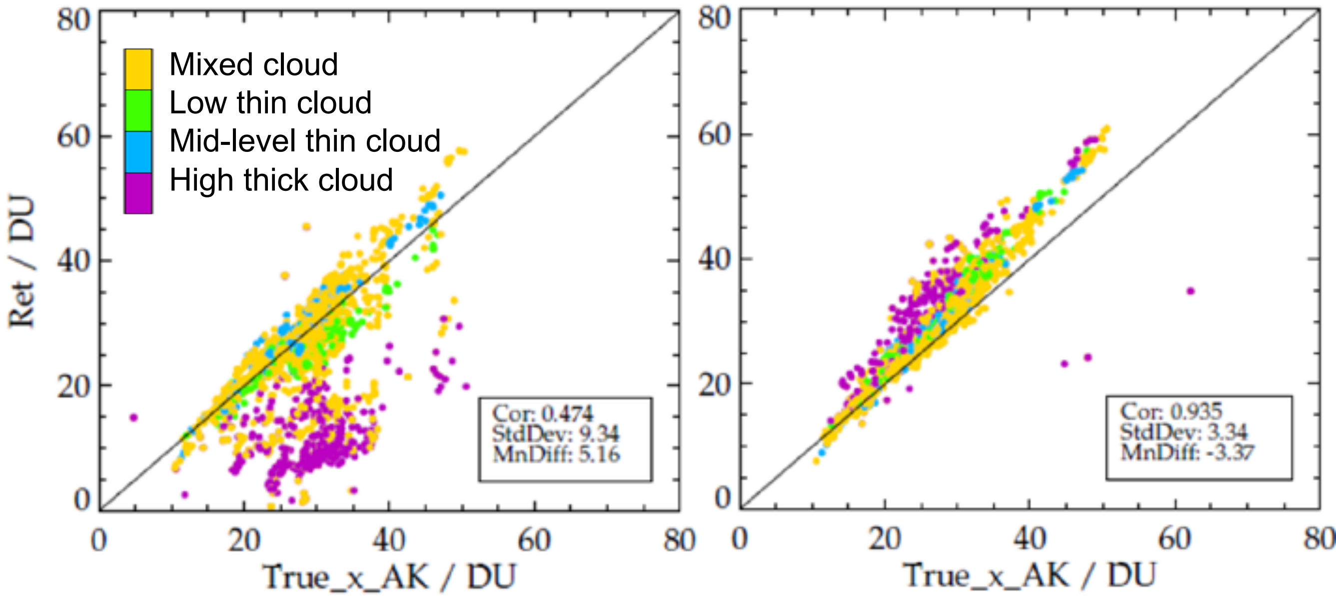
Cloud modelled via effective surface reflectance + AMF profile to characterise cloud obscuration



Tested by application to S4 L1 verification test data – independently generated by MPIC using SCIATRAN

Cloud modelled only via effective surface albedo

Cloud modelled using cloud AMFs



Impact of aerosol

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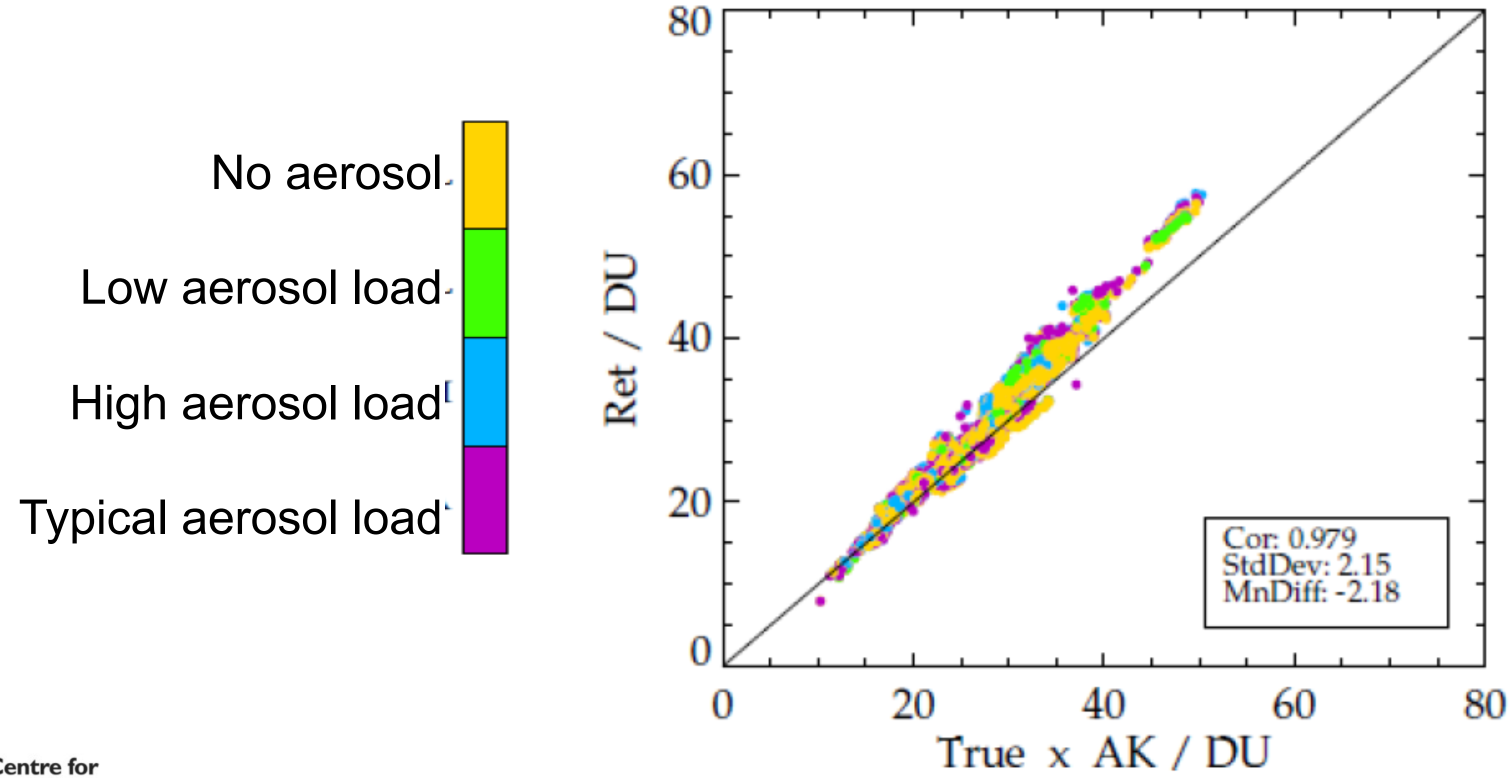
- Aerosol neglected in retrieval model (expected to be accomodated via cloud model and fitting of polynomial “gain”)
- Impact tested via independent verification data which included varying aerosol load (and BRDF variability)



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Modelling Ring effect

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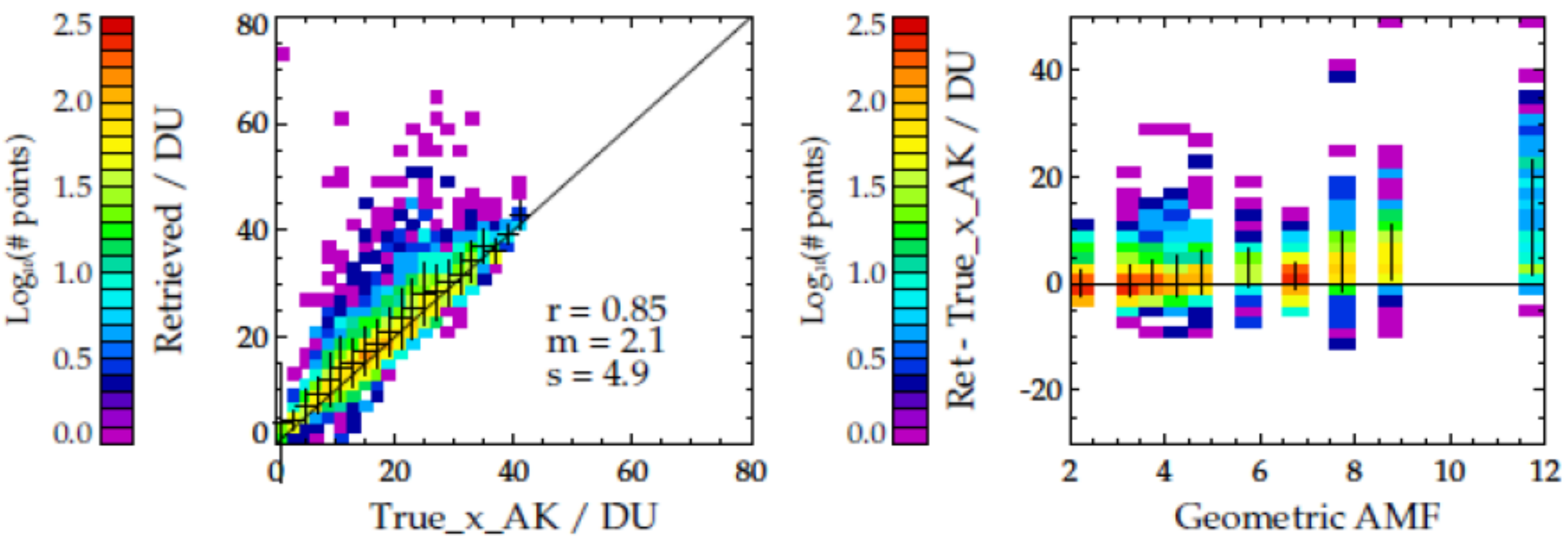
- Ring effect: "filling-in" of solar + terrestrial absorption by inellastic rotational Raman scattering (RRS) by air – too complex to fully simulate "on-line"
- Adopted approach based on convolving radiance contributions from each layer in atmosphere by Raman line spectrum (using source function from LIDORT)
- Amplitude of predicted filling-in scaled by retrieved parameter to deal with suppression of Ring effect in presence of high cloud
- Approach tested using LIDORT-RRS applied to 4000 scenarios spanning variations in atmospheric/surface conditions + solar/view geometry.



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Summary

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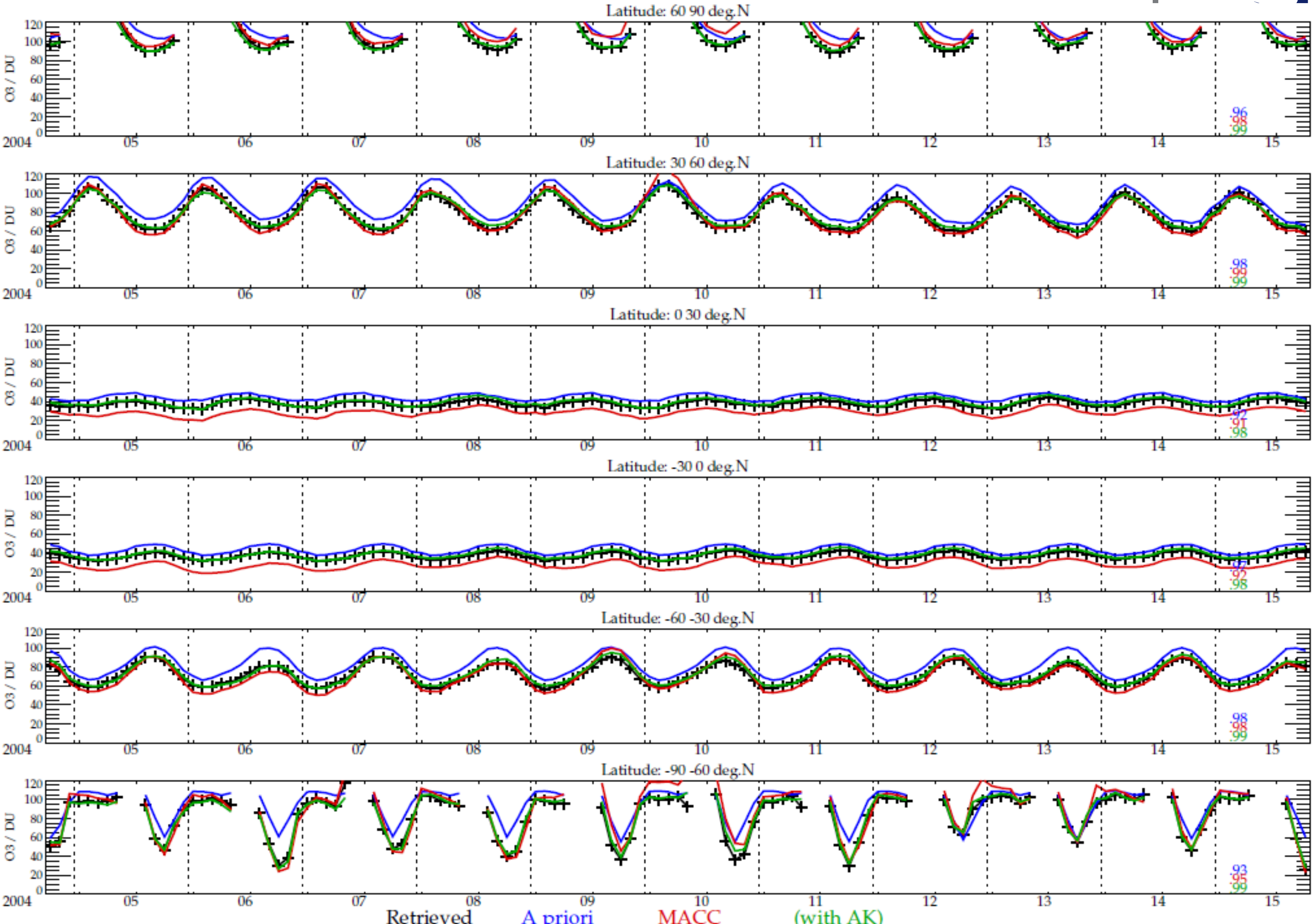
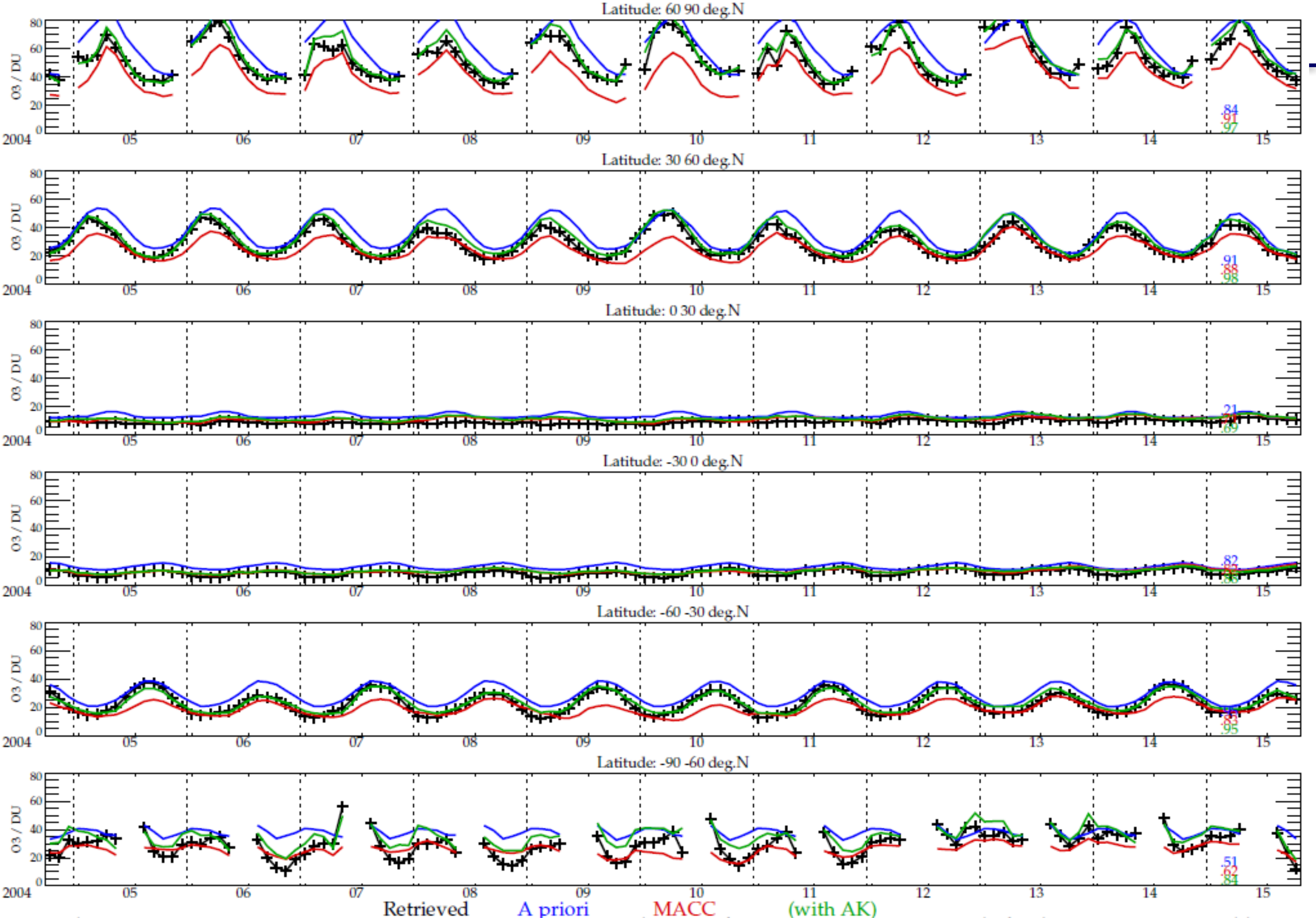
- Global ozone (1995-2015) data sets including tropospheric ozone being produced for ESA CCI using RAL scheme
- So far most stable data-set is OMI, leading to submission to TOAR
  - Other datasets being re-processed with improved algorithm, addressing instrument specific biases
- Scheme being adapted to be used as basis for Sentinels 4 + 5 via ESA projects
- S4 algorithm should deliver trop. ozone meeting 25-40% required uncertainty, though vertical sensitivity is limited and varies with time of day and season
- Through retrieval simulations , including independently generated spectra, various aspects of the forward modelling in the retrieval have been consolidated + confirm sufficient for purpose
  - Allow simplifications of FM which (in conjunction with PCFM approach) should allow significant computational speed improvements; this is to be test in next phase of algorithm development
- Performance depends on good instrument calibration + stability; in particular trop. ozone very sensitive to knowledge of spectral response, particularly in case of spectral misregistration radiance/irradiance

OMI time-series 12-21km vs MACC

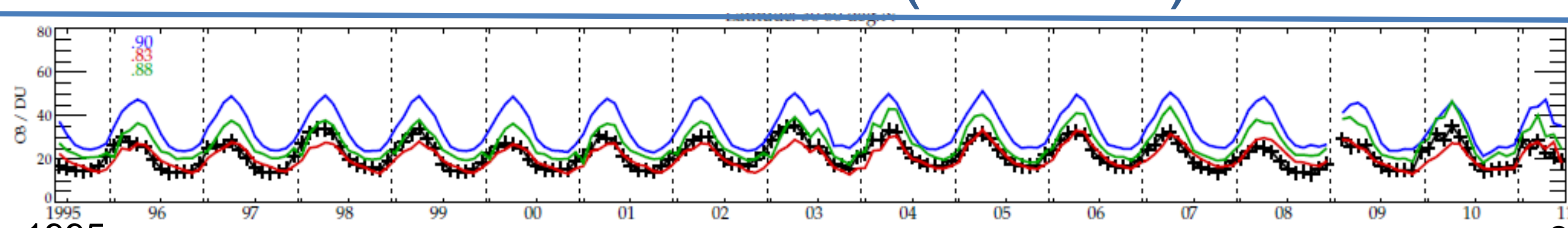


OMI time-series 6-12km vs MACC



CCI v1 Time-series of ozone (30-60N) from 1995-2013

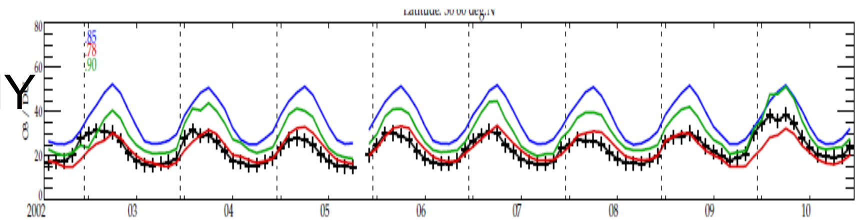
6-12 km column



GOME-1

1995 2011

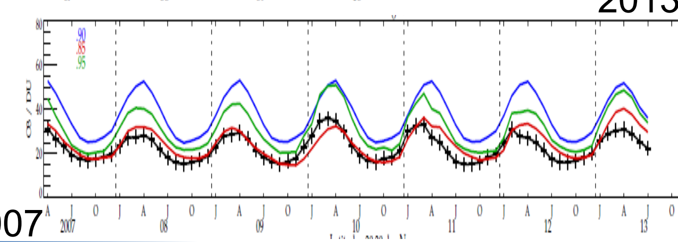
SCIACHY



2002 2013

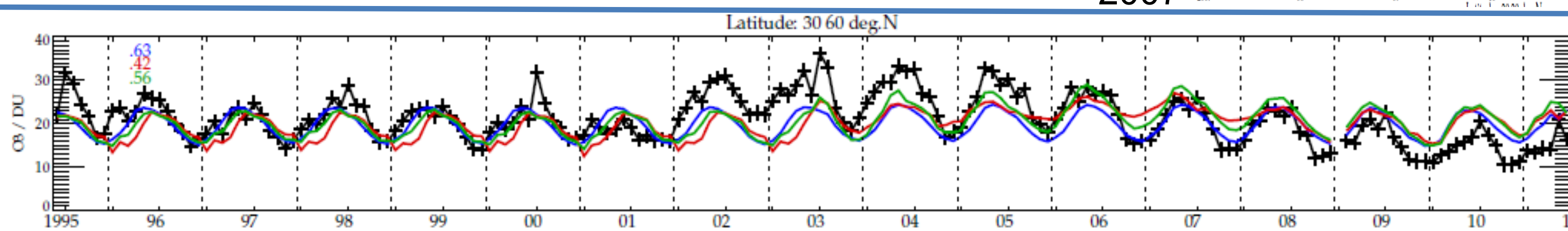
Retrieval
A priori
MACC reanalysis/NRT
MACC + AK

GOME-2



2007

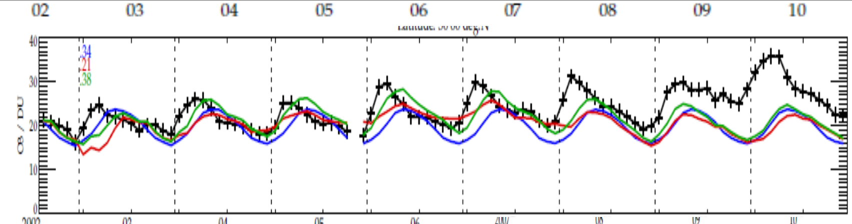
0-6 km column



GOME-1

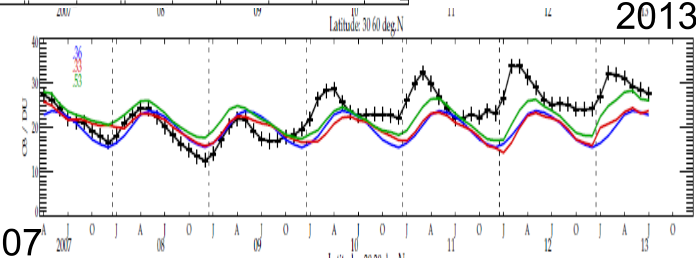
1995 2011

SCIAMACHY



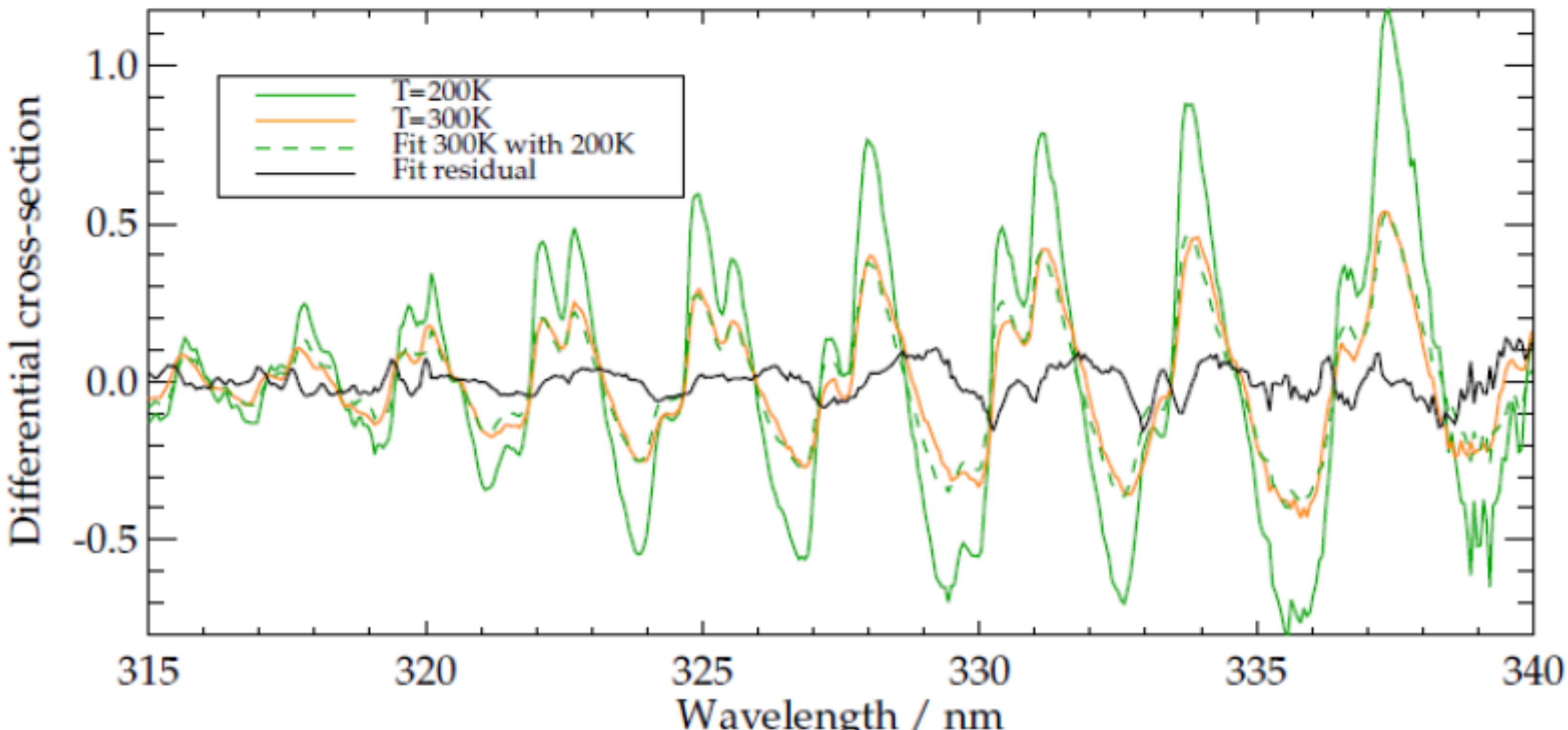
2002 2013

GOME-2



2007

More accurate account for instrumental artefacts to produce consistent times series from GOME-1, SCIA, GOME-2 being developed for next version



T=200K
T=300K
Fit 300K with 200K
Fit residual
Differential cross-section
1.0
0.5
0.0
-0.5
315
320
325
330
335
340
Wavelength / nm

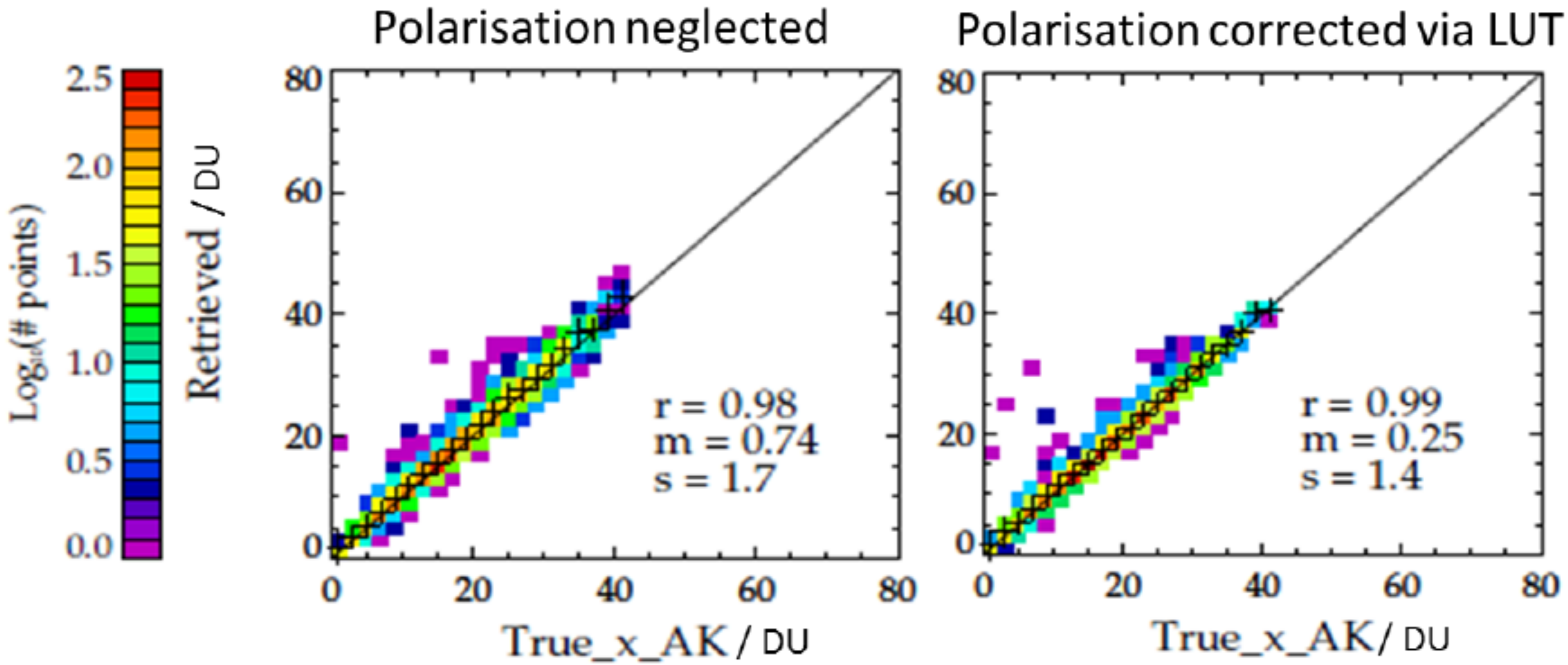


Figure 5-5: Assessment of retrieval errors caused by neglecting polarisation. Each panel is a scatter-density plot in which the colour of each cell indicates the number of individual points within its area. The left-hand panel shows the retrieved tropospheric ozone column when neglecting polarisation in the RTM, compared to the ideal retrieval ("True_x_AK"), computed applying averaging kernels to the true profile as discussed in section 5.7. The caption indicates the correlation coefficient (r), mean difference (m) and the standard deviation about the mean difference. The right-hand panel compares retrievals which are carried out using the polarisation correction LUT from the heritage scheme. Vertical black lines in the plot indicate the standard deviation of all points in a given column).