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Ozone profile retrieval from nadir TROPOMI measurements in the UV range

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S1 Sensitivity study: Correction of Ring effect and polarisation

To estimate the effectiveness of the Ring and polarisation correction in our retrieval, synthetic spectra with and without rotational Raman scattering (Ring effect) and polarisation were simulated. The TOPAS retrieval was then performed with Ring and polarisation correction switched off and applied to radiances with and without Ring/polarisation.

Figures S1 and S2 show the effect when polarisation and Ring effects are neglected in the retrieval. With polarisation, a larger scatter in the results is seen below 20 km. That is expected, since polarisation occurs mainly at longer wavelengths and these influence the ozone profiles near the ground. The Ring effect also impacts the lower part of the ozone profile up to about 35 km. If the Ring effect is ignored in the retrieval, very large deviations of more than 50% occur.

In the case that Ring/polarisation is not contained in the input radiances and is also not considered in the ozone profile retrieval (Figs. S3 and S4) the retrieval results do not show any differences in comparison to the results presented in Fig. 2 where the corrections are included. The conclusion can be drawn that both correction methods work well and are clearly required.

S2 Calibration correction: Using ozone profiles up to 80 km in the RTM of the retrieval

In the TOPAS retrieval profiles of ozone, pressure, and temperature up to 60 km are used in the radaitive transfer calculations. To assess the effect that this limit of the top-of-atmosphere altitude has on the calibration correction, the re-calibration spectra were reprocessed with an altitude grid up to 80 km for one orbit (5005) and one detector pixel row (correspnding to number 34 of the UV1 band). Figure S5 shows the calibration spectra obtained using different TOA altitudes in the RTM calcualtions. In UV1 and especially below 285 nm the differences between the RTM simulation and the MLS measurement strongly increases by limiting the altitude grid to 60 km (blue curve), which is due to the neglect of the Rayleigh scattering contribution from layers above 60 km. The re-calibration spectrum as used in TOPAS (blue) and reported in the paper is a combination of radiometric calibration and Rayleigh scattering correction. The advantage of a reduced altitude grid is a strong reduction in computation time.

The evaluation of one day of TROPOMI data was repeated using re-calibration spectra calculated with an RTM with layers up to 80 km. All TROPOMI across-track pixels with number 34 (UV1 counting) were reprocessed with the new re-calibration spectra and the resulting ozone profiles were compared to MLS and the previous retrieval results. The comparison is shown in Fig. S6: the ozone profile results from our standard retrieval in the top panels (A - C) and the new results in the bottom panels (D - F). The comparison to MLS (B and E) and MLS x AVK (C and F) shows slightly worse results for the new re-calibration spectra between 20 and 50 km. The positive bias above 50 km is due to the lower top of atmosphere in the retrieval, but the retrieval sensitivity for altitudes above 50 km is anyway reduced.

S3 Data: Ozonesonde and lidar measurements

The location, station name, and number of profiles of ozonesondes and lidars used for validation in this study are given in Table S1.

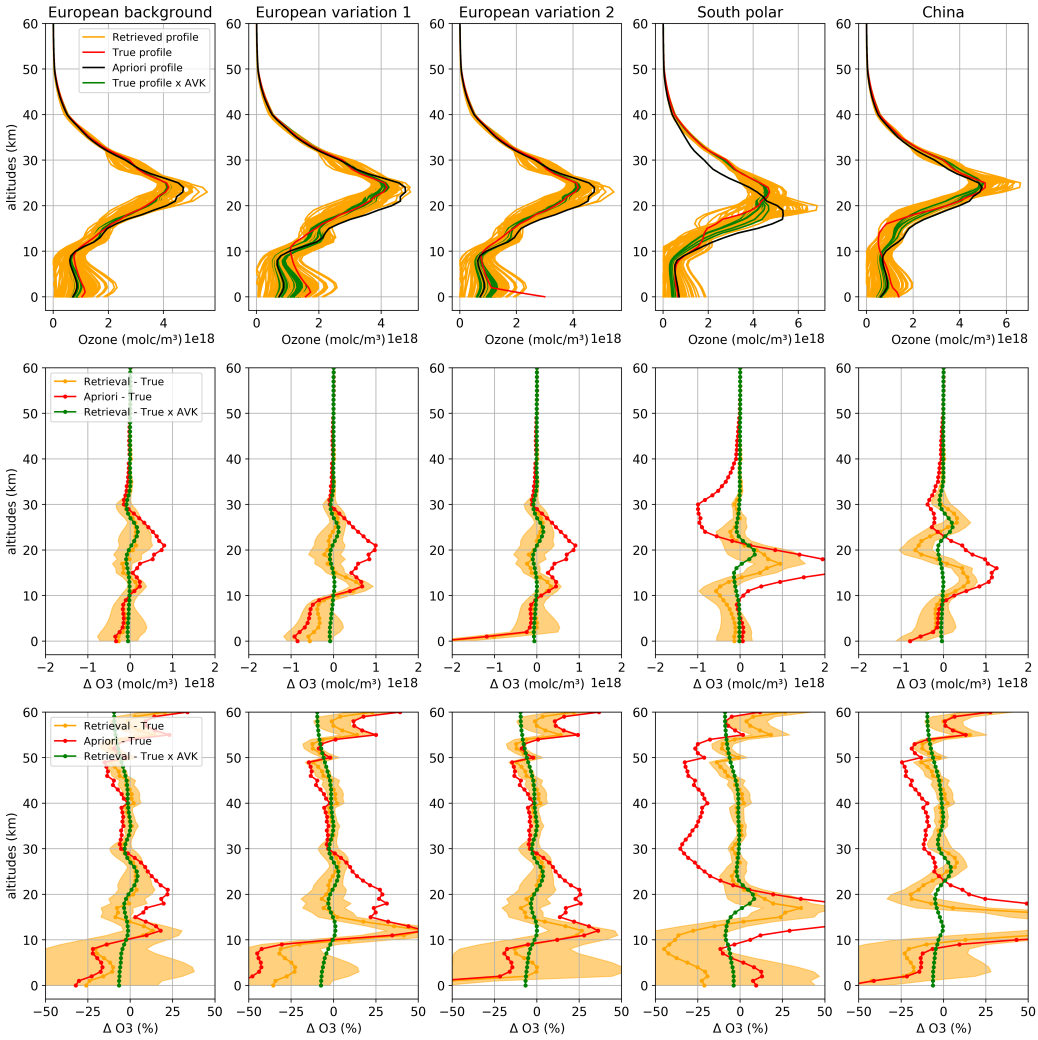

Figure S1: Ozone profile retrieval without polarisation correction for all geometry and albedo settings. The simulated radiance included polarisation.

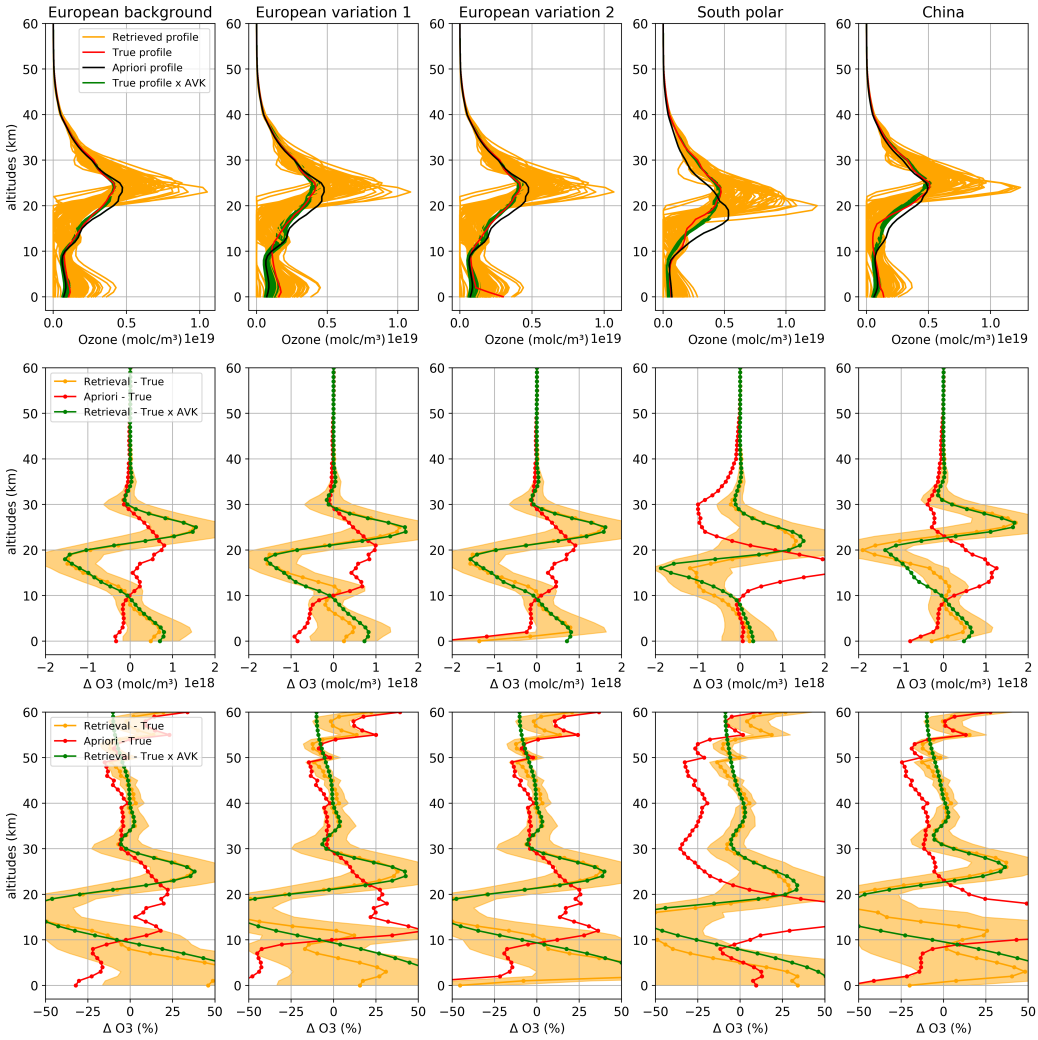

Figure S2: Ozone profile retrieval without Ring correction for all geometry and albedo settings. The simulated radiance include the Ring effect.

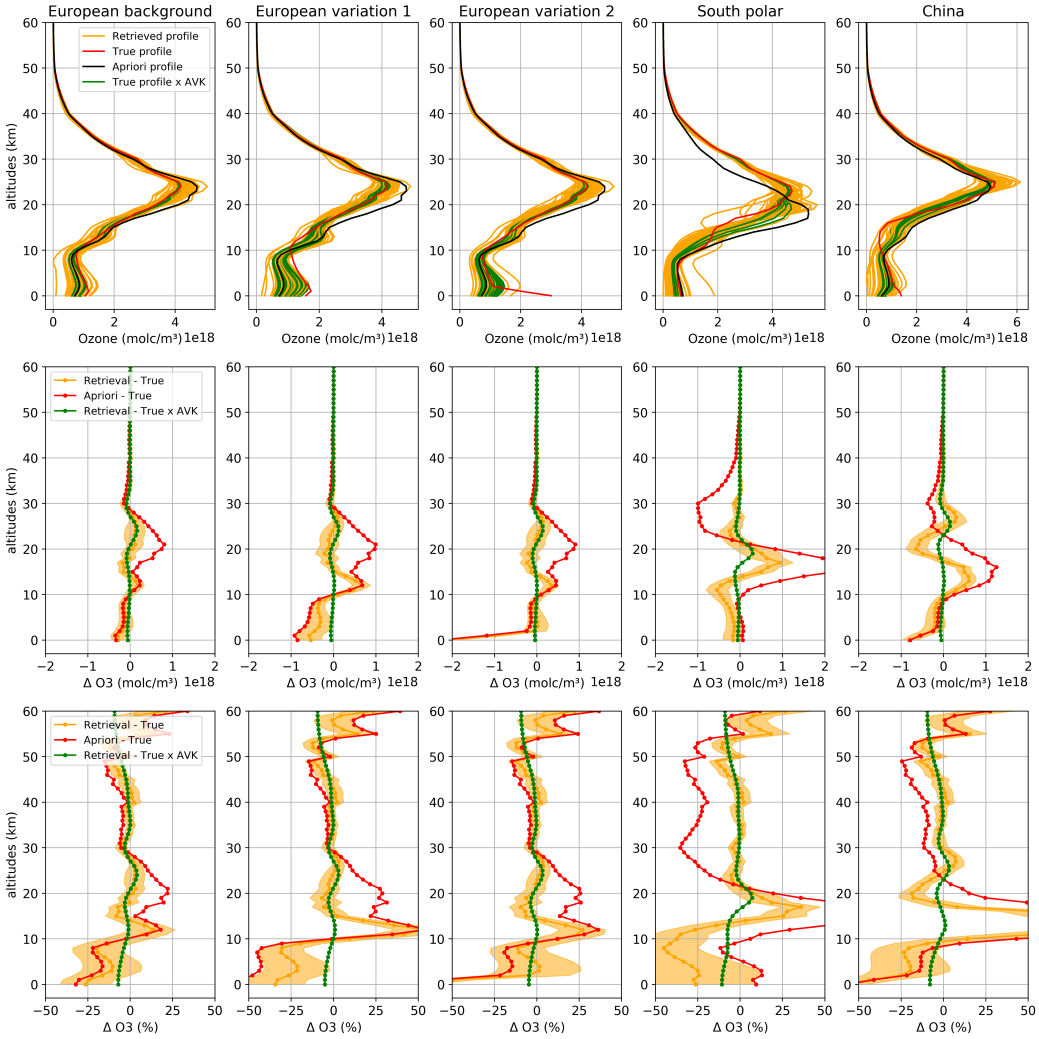

Figure S3: Same as S1, but the simulated input radiances were obtained without polarisation effects.

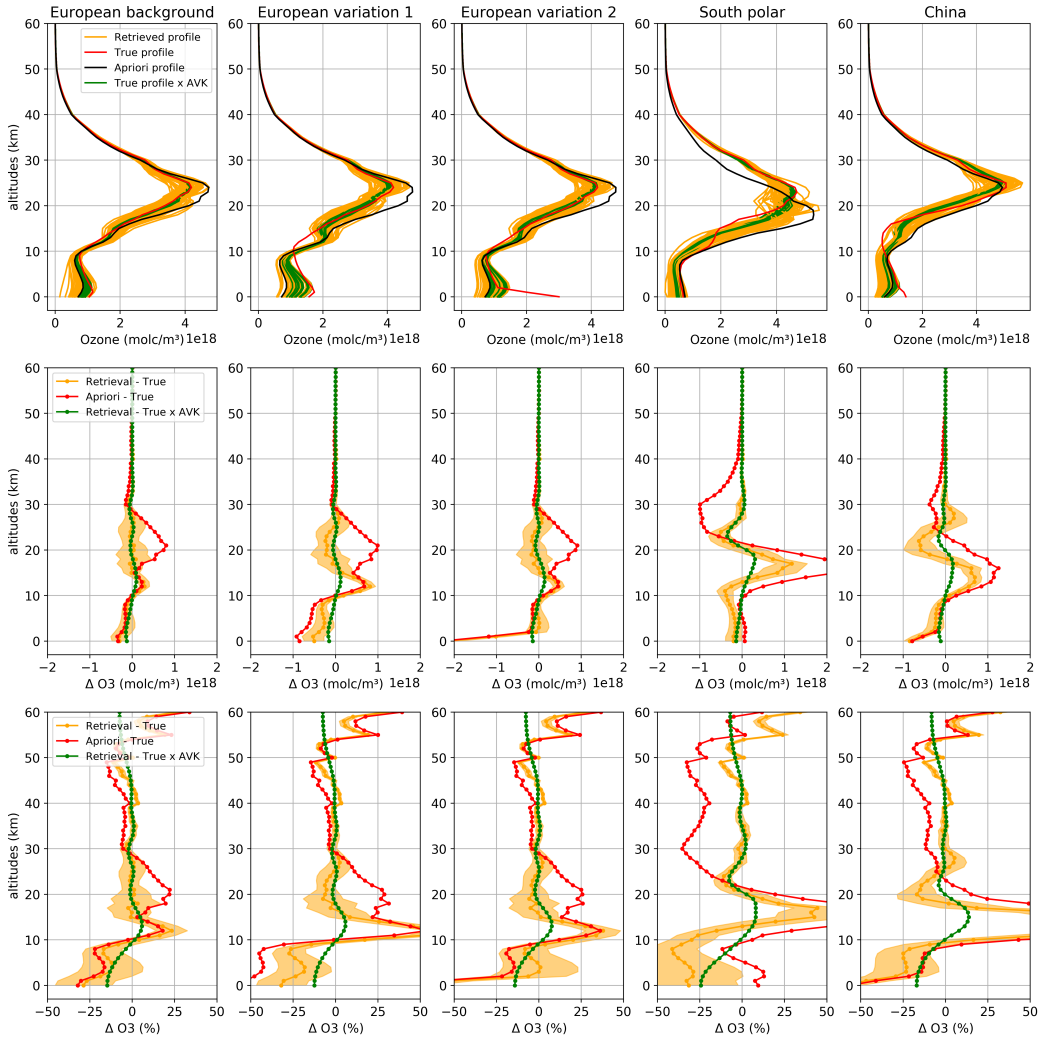

Figure S4: Same as S2, but the simulated input radiances do not include the Ring effect.

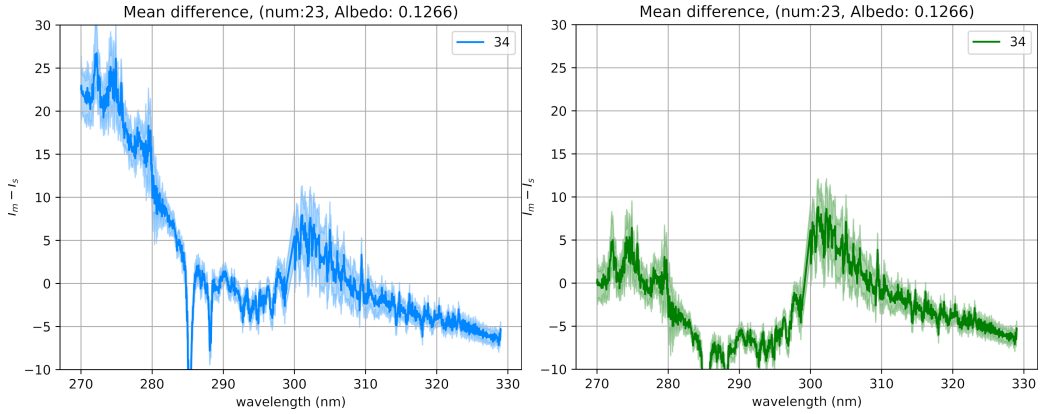

Figure S5: Example for re-calibration spectra calculated with a top of atmosphere at 60 km (right blue) and 80 km (left green) in the RTM for one orbit (5005) and detector pixel number 34.

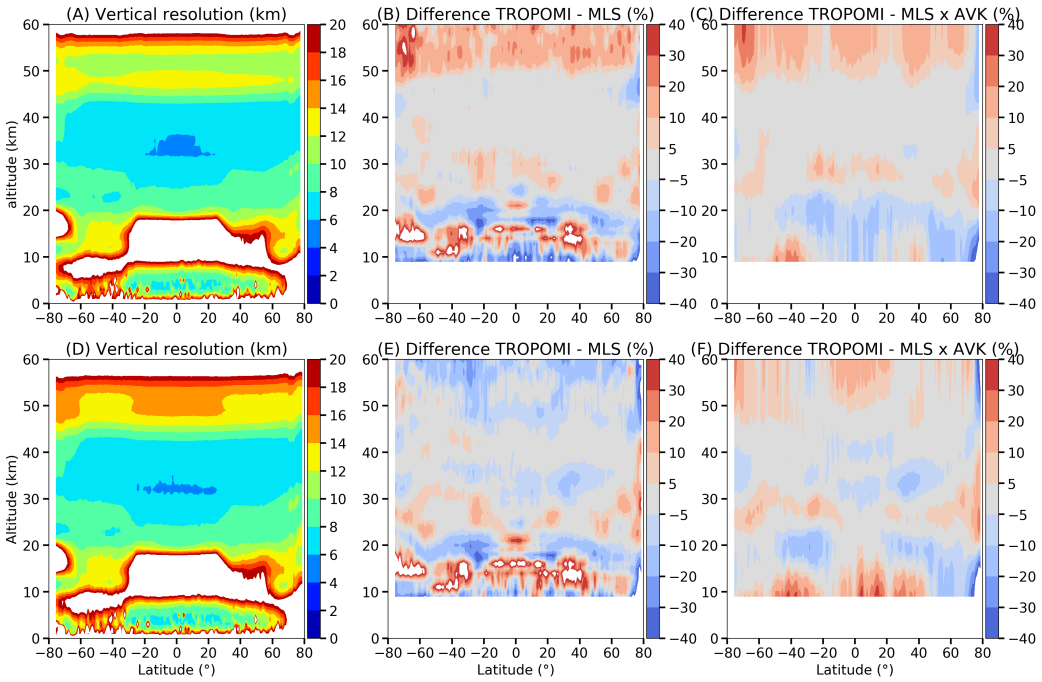

Figure S6: Comparison between original retrieval reported in the manuscript (top panels) and retrieval with the re-calibration spectrum calculated with RTM layers up to 80 km (lower panels). The retrieval was processed and zonally averaged only for across track pixel no 34 (UV1 counting) along the orbit from October 1, 2018.

Table S1: Ozonesonde and Lidar Stations

Ozonesonde station	Latitude	Longitude	nr. of profiles
King's Park	22.31	114.17	14
Alert	82.49	-62.34	1
Broadmeadows	-37.69	144.95	17
Churchill	58.74	-94.07	2
Davis	-68.58	77.97	3
De Bilt	52.1	5.18	17
Easter Island	-27.17	-109.42	3
Edmonton	53.54	-114.1	2
Eureka	79.98	-85.94	2
Goose Bay	53.31	-60.36	5
Hohenpeissenberg	47.8	11.0	29
Lauder	-45.04	169.68	9
Legionowo	52.41	20.96	15
Marambio	-64.23	-56.62	5
Macquarie Island	-54.5	158.94	8
Madrid	40.47	-3.58	15
Paramaribo	5.81	-55.21	2
Payerne	46.49	6.57	37
Pohang	36.03	129.38	7
Port Hardy	50.68	-127.38	2
Praha	50.0	14.44	8
Resolute	74.7	-94.96	2
Syowa	-69.01	39.58	4
Tateno (Tsukuba)	36.06	140.13	11
Uccle	50.8	4.35	19
Ushuaia	-54.85	-68.31	3
Valentia	51.93	-10.25	2
Yarmouth	43.87	-66.11	5
Hanoi, Vietnam	21.02	105.8	1
Hilo, HI	19.4	-155.4	6
Irene, South Africa	-25.9	28.2	1
Kuala Lumpur, Malaysia	2.73	101.7	1
Nairobi, Kenya	-1.3	36.8	6
Pago Pago, Am. Samoa	-14.2	-170.6	5
Paramaribo, Surinam	5.81	-55.21	3
Suva, Fiji	-18.1	178.4	4
Ozone lidar station	**Latitude**	**Longitude**	**Nr. of profiles**
Hohenpeissenberg	47.8	11.02	24
Lauder	-45.04	169.68	10
Maunaloa	19.54	-155.58	40
OHP	43.94	5.71	35
Tablemountain	34.4	-117.7	68