Investigation of the optical and instrumental artifacts in the Brewer Umkehr ozone profile retrieval.

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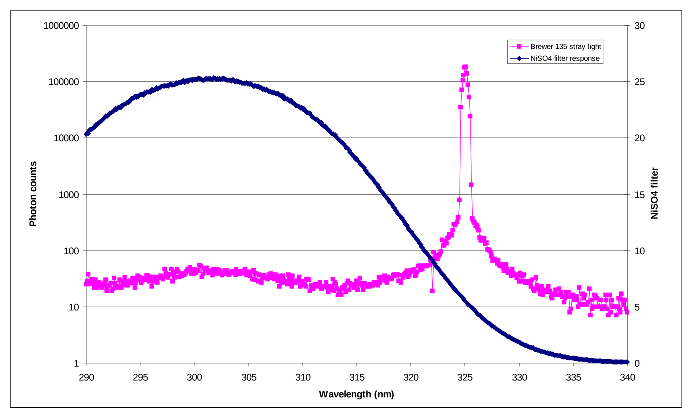
Problem: The Brewer response to the spectral zenith sky radiance must be accurately characterized, including polarization efficiency by the internal components and stray light effects.

Methods: R-T simulations of the zenith sky radiation based on the measured ozone and temperature profiles. Sensitivity analysis are done for various optical parameters to study their impact on the Brewer Umkehr measurements and retrieved ozone profiles.



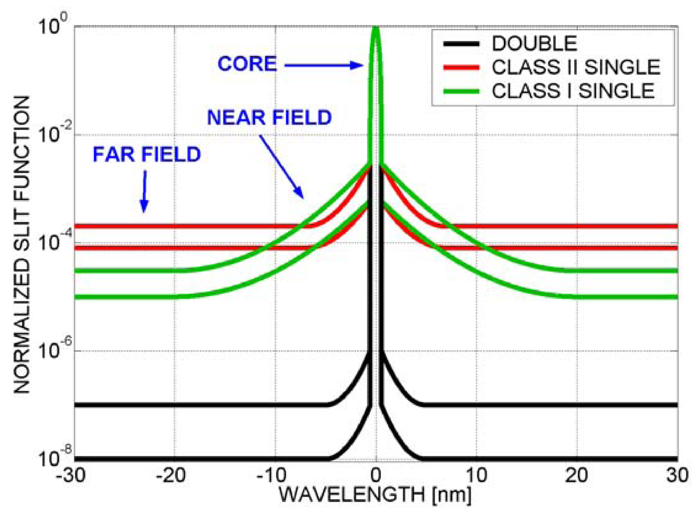


***Figure 1. (top).** The stray light of Brewer 135 was measured using a Helium-Cadmium laser, lasing at 325.029 nm. The laser intensity was measured on slit 1 of the Brewer's slit mask. The spectral responsivity of the Brewer's $NiSO_4$ or nickel sulfate filter (dark blue) is plotted along with the stray light measurement (pink). **(bottom)** Examples of a Brewer slit functions for double and two single Brewers. The far, near fields and core are indicated, and the errors bars are provided (figure of A. Cede, NASA/Goddard, private communication).*

Description of Umkehr measurements

The Brewer intensities in zenith sky view can be represented by the following equation (A. Cede, private communications):

$$N(O_3,\lambda_i,\theta) = 100 * \log_{10}[\int_0^\infty I(O_3,\lambda',\theta) * S(\lambda_i - \lambda') * T(\lambda') d\lambda']$$

Where

- *$N(O_3, \lambda_i, \theta)$* Umkehr N-value
- λ_i Center wavelength at slit i and fixed grating position
- O_3 Total ozone column
- *Θ* Solar zenith angle
- *$I(O_3, \lambda', \theta)$* Zenith intensity at wavelength λ', depends on other atmospheric parameters (e.g. aerosols), polarization included
- $T(\lambda')$ Spectral sensitivity of optical system (transmission characteristics of filters ($NiSO_4$ response), grating, PMT (photomultiplier tube), etc.)
- *$S(\lambda_i - \lambda')$* Slit function.

C-pair N-value is difference between 326 and 310 nm

Case study.

- A set of simulations are performed to analyze Umkehr measurements taken by several Brewers during an intensive campaign on September 20th, 2007 at the Table Mountain facilities.
- Vertical profiles of measured ozone concentrations from NOAA/ESRL ozone soundings below 10hPa pressure level and satellite (Aura Microwave Limb Sounder, MLS) above 10 hPa are combined.
- Simulated spectra are convolved for every spectral channel with a bandpass function analytically defined as follows:

a. the center is a trapezoid as assumed by J. Kerr (triangle cut at 87% of its height);
b. the "shoulders" are described by power function
c. the wings are set to $5 \cdot 10^{-5}$ level of light rejection

Table. Reference profile setting for model simulation of Brewer measurements in Boulder, CO on September 20th, 2007.

Parameter	Value
Altitude	1689 m asl
Surface albedo	0.03
Pressure	826 mbar
Temperature profile	US76 standard atmosphere (NASA and USAF, 1976)
Aerosol profile	Shettle (1989)
Mixing layer heigh	1000 m (assumed)
Aerosol optical depth	0.07 at 413.5 nm from MFRSR (NOAA)
Rayleigh scattering	"Default", i.e. Bates (1984)
Ozone profile	Merged from ozone sondes and MLS
Total ozone	276 DU
Ozone cross sections	Bass and Paur (1985) from TOMRAD
Extraterrestrial spectrum	MHP, Egli et al. (2013)
Wavelength range and step	300–400 nm, 0.05 nm
Bandpass	Center wavelengths and FWHMs from dispersion test + straylight
$NiSO_4$ transmittance	Taken into account (measured by P. Disterhoft)
Air refraction	off

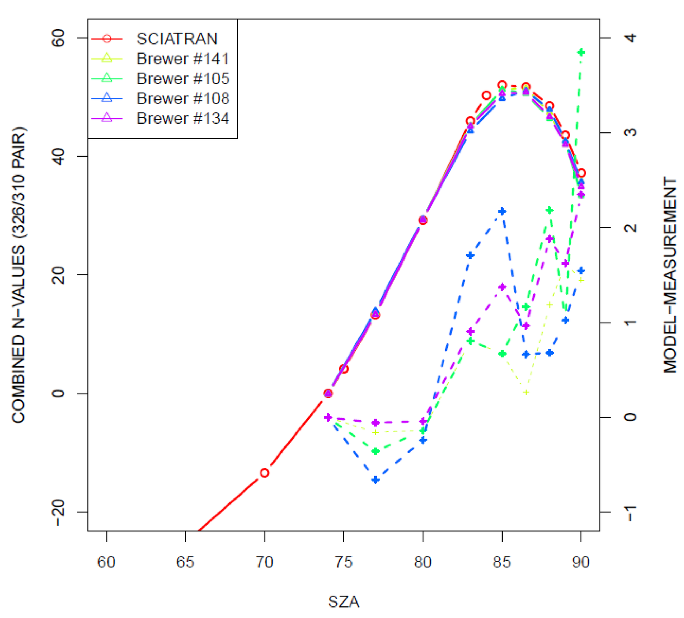
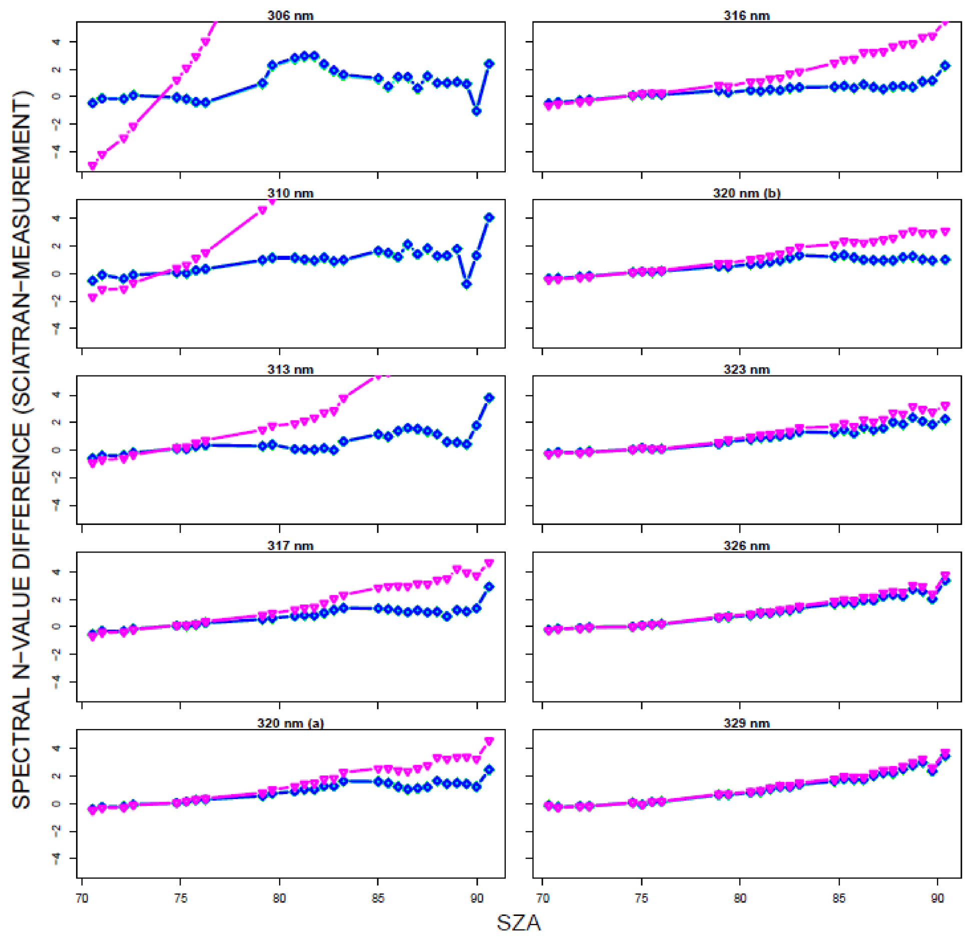


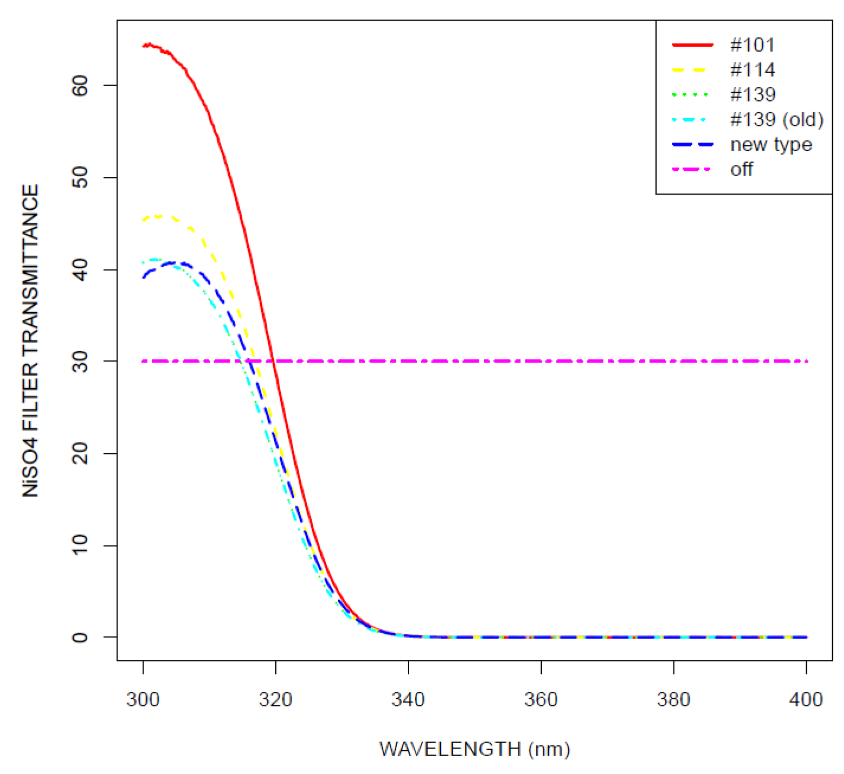
Figure 2. Solid lines: combined N-values (C-pair) from the model (reference simulation, Table 2) and several NOAA Brewer measurements. Dashed lines: differences between the simulated and measured N-values (right axis). The N-values were normalized at 74˚ SZA.

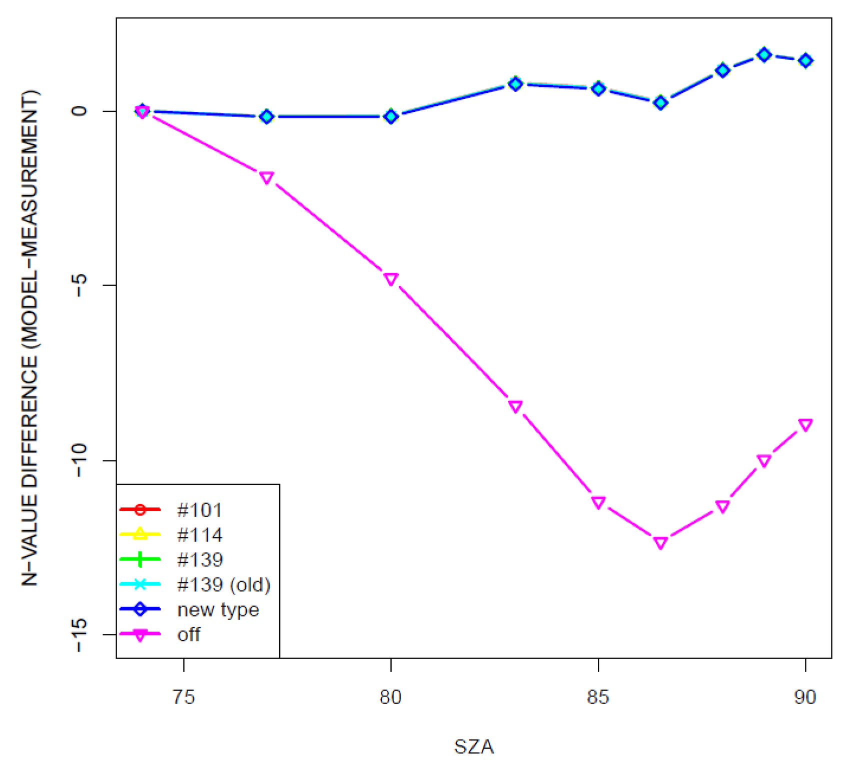


When the Brewer (except Mk III) is in the Ozone Mode, a UG-11/ **$NiSO_4$** filter prevents radiation above 325nm from passing through, thus reducing the visible Solar spectrum impact on Brewer measurements.

Figure 3 (left). Differences (log space) between radiances simulated by SCIATRAN (using different $NiSO_4$ transmittances – **plot to the right**) and measured by Brewer #141 for 10 spectral channels. The differences are normalized at 74˚ SZA. The results corresponding to the "real" filter functions are indistinguishable (blue and other colors), while the deviations when the $NiSO_4$ transmittance is neglected (purple) are very clear.

The figure to the far right demonstrates effect of simulation with $NiSO_4$ filter on the C-pair N-value, as function of SZA





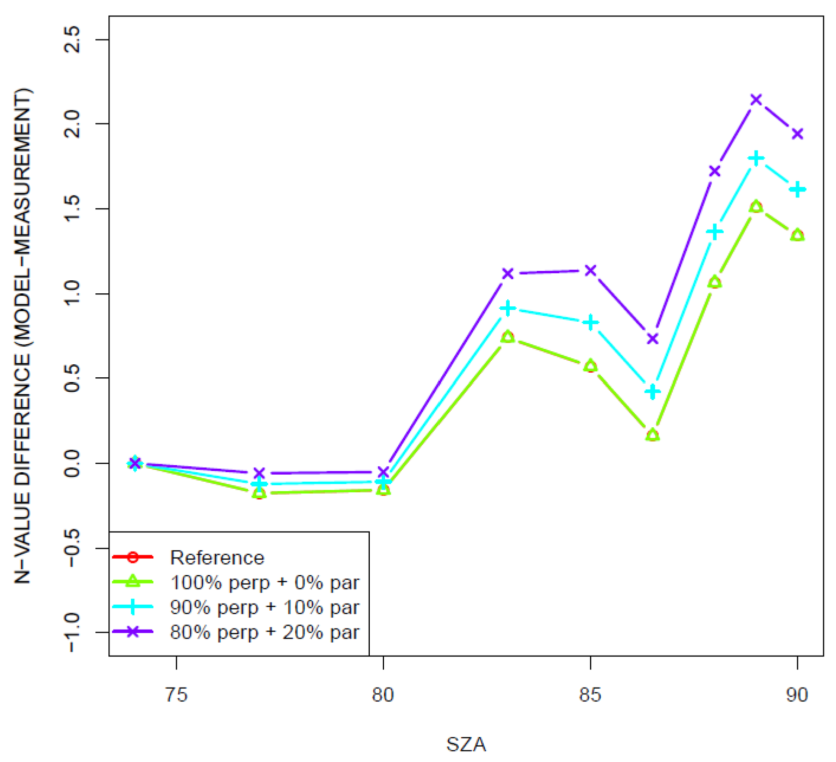


***Figure 4.** Effect of Brewer polarizing efficiencies on simulated N-values (C-pair) as compared to Brewer 141 measurements. The N-values were normalized at 74˚ SZA. The red and green curves cannot be easily distinguished.*

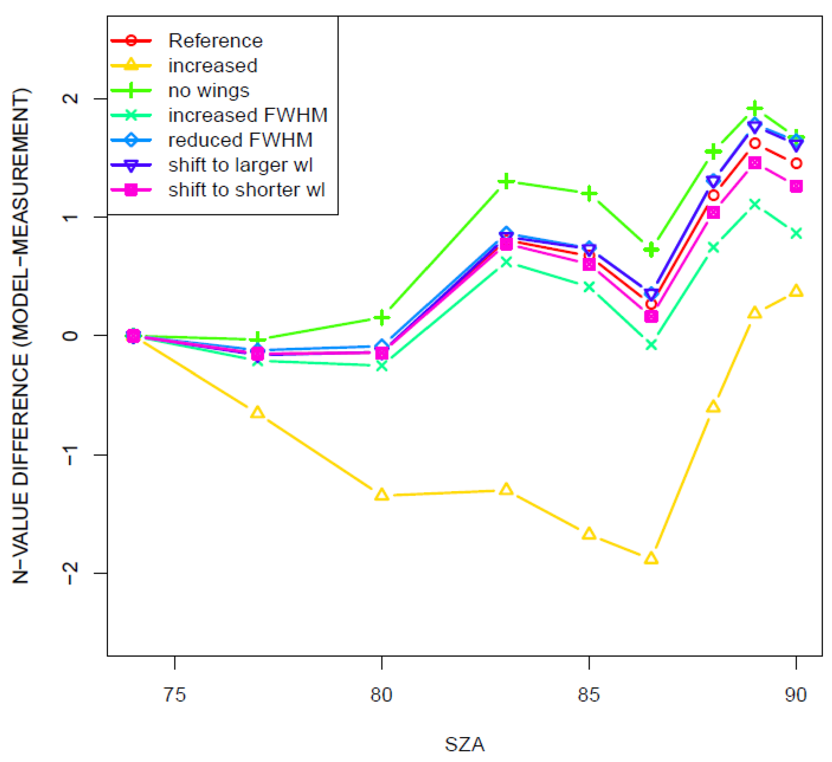


***Figure 5.** Effect of the band-pass on simulated N-values (C-pair) as compared to Brewer 141 measurements. The N-values were normalized at 74˚ SZA. The largest effect (yellow line) is due to increased level of the light in the wings.*

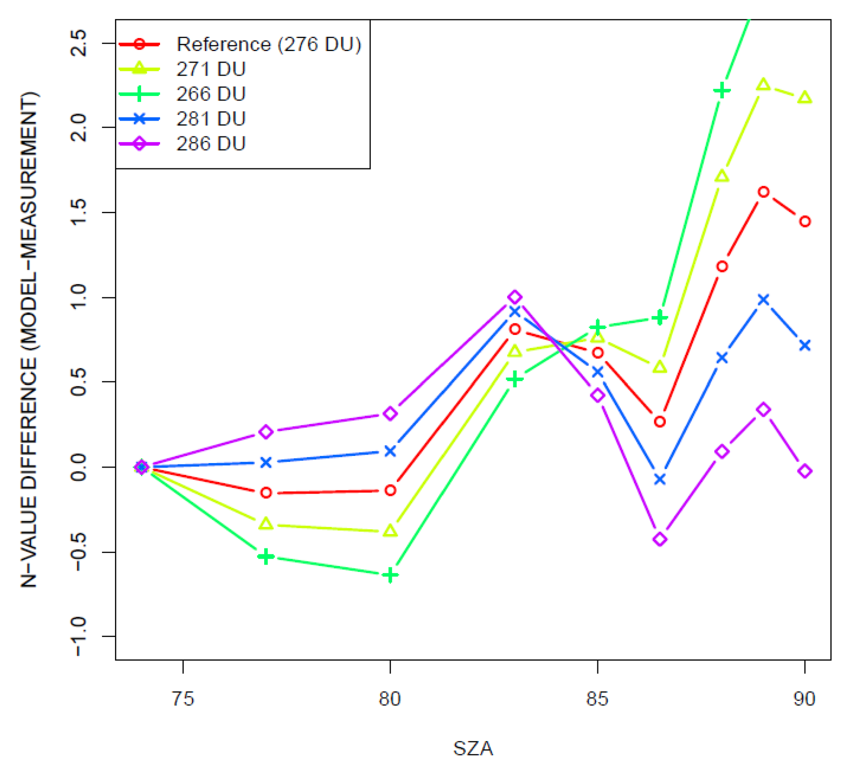


***Figure 6.** Differences between simulated (assuming different ozone columns) and measured N-values (C-pair). The N-values were normalized at 74˚ SZA.*

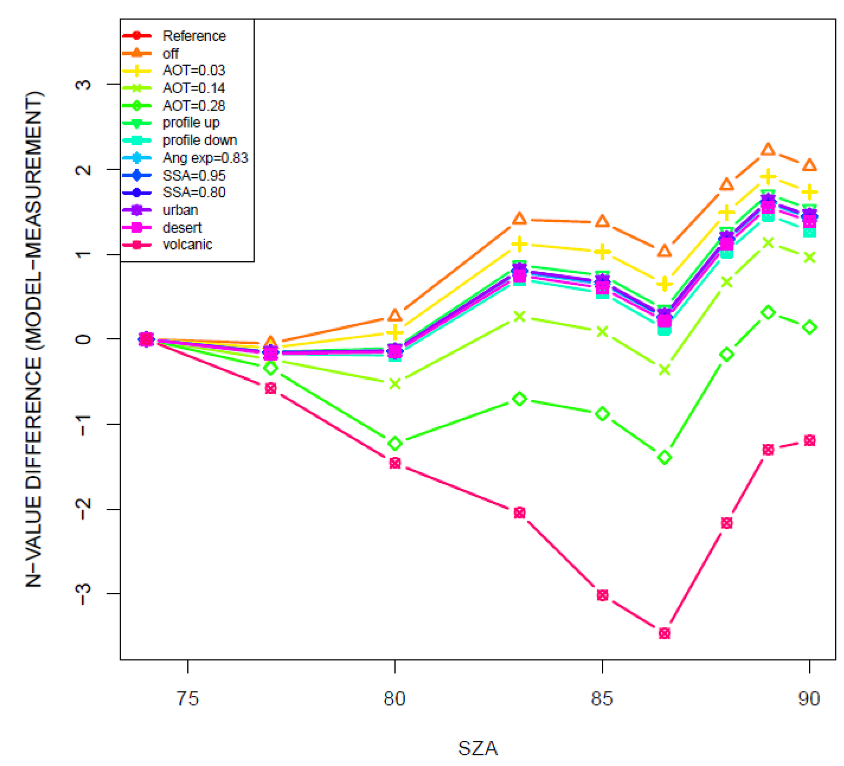


***Figure 7.** Differences between the simulated (different aerosol cases) and measured N-values (C-pair). Notice that the vertical scale was changed compared to previous simulations to completely fit the plots.*

Summary of Results

The most important results in this study address investigations of the Brewer and the retrieval of the O3 profile not previously possible. The impact of different effects on the O3 data product comprise:

1) The importance of the polarization efficiency in Umkehr ozone retrievals was inconclusive due to lack of full optical characterization of the Brewer. Further analyses are needed.
2) Effect of aerosols of different types and at different altitudes - significant effect
3) Ring effect – low impact (not shown in this poster)
4) $NiSO_4$ transmission characteristics showed low sensitivity to specifics of individual filters
5) Stray light variability in the shape of the slit and the level in wings - significant impact
6) Surface albedo sensitivity – small effect, except for snow on the ground
7) Refraction in simulations and calculation of SZAs for measurements – large uncertainty (not shown in this poster)

In conclusion, when using these results to improve characterization of the Brewer instruments, the quality of the vertical profile of O3 can be potentially implored significantly and support the long term assessment of changes in the vertical profile of O3. These are particularly important as stand alone data record and for the validation of space based O3 vertical profile measurements.

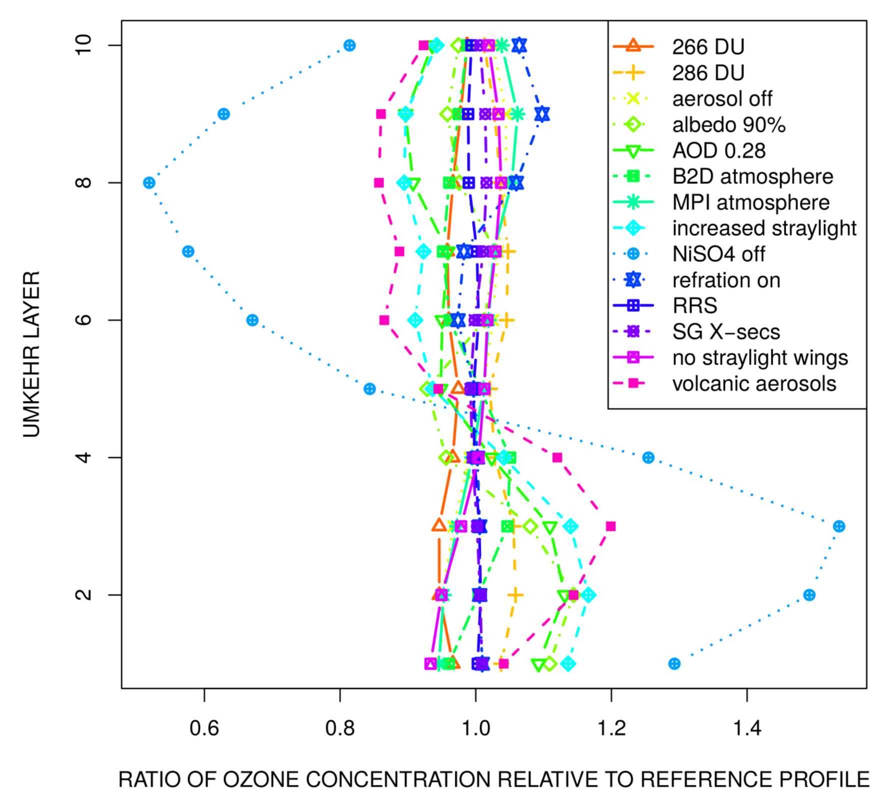


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Figure 8 (left). Impact of additional effects on retrieved ozone

reference = settings are described in the Table above.
266 DU/286 DU = ozone profile is normalized to 266/286 DU
Aerosol off = no aerosols used in simulation
Albedo 90% = surface albedo is set to 90 % (snow)
AOD 0.28 = aerosol (continental) from Shettle (1989), 0.28 optical depth
B2D atmosphere = 45˚ N profiles from 2D chemical-transport model of U. of Bremen (Sinnhuber et al. 2009)
MPI atmosphere =45˚ N profiles from 2D chemo-dynamical model developed at MPI Mainz (Brühl and Crutzen, 1993)
Increased stray light = stray light increased to by one order of magnitude
NiSO4 off = NiSO4 filter transmission function is not used
Refraction on = simulation with refraction scheme
RRS = simulation with atmospheric rotational Raman scattering effect
SG X-secs = ozone cross-section by Serdyuchenko et al. (2014);
No stray light = only core of the slit function is used in spectrum convolution
Volcanic aerosols = aerosols in stratosphere (extinction coefficient $1 \cdot 10^{-3}$ km^{-1} between 12 and 30 km altitude).