Brewer algorithm sensitivity analysis

A. Redondas
A. Cede

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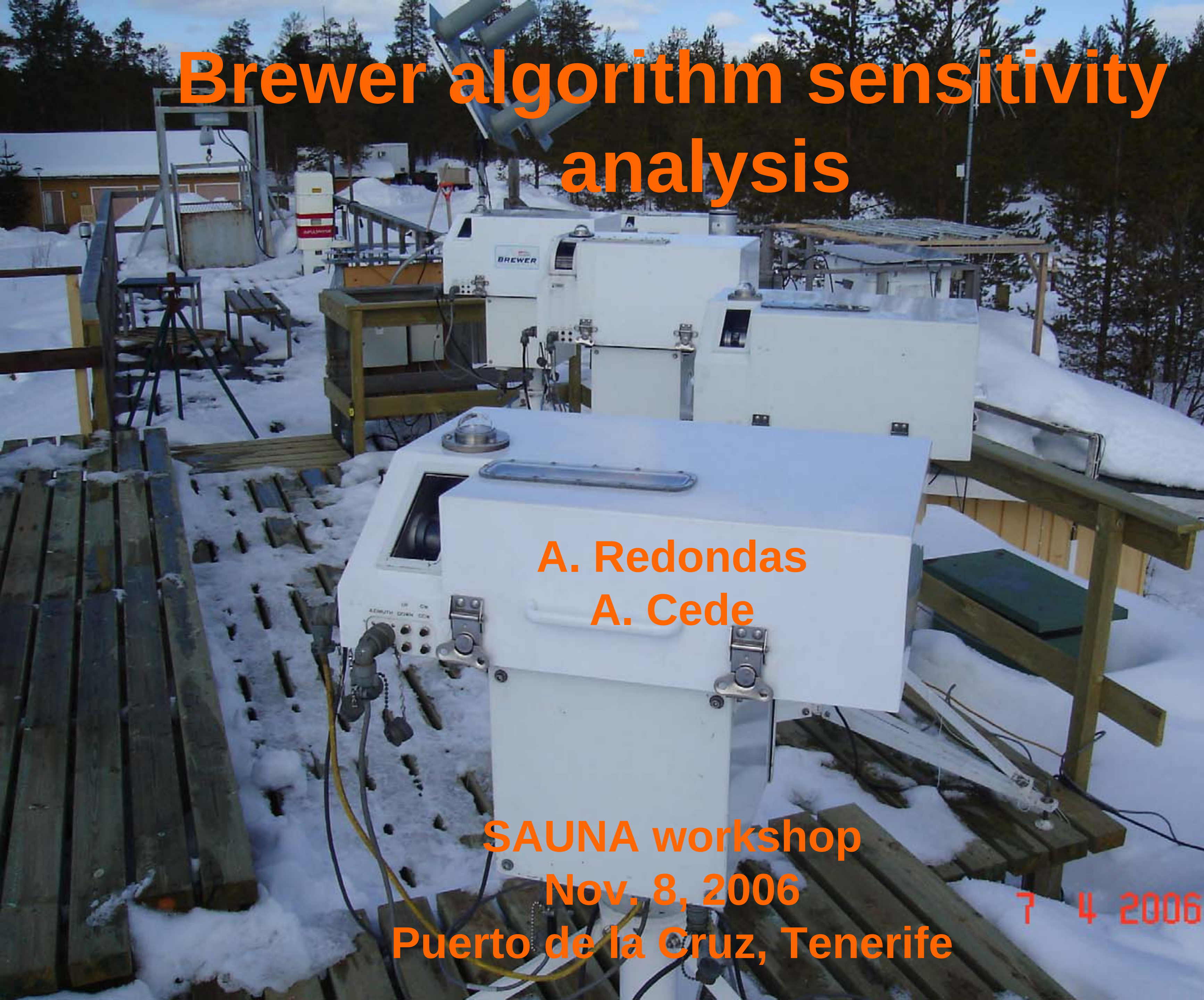


Brewer direct sun total ozone algorithm

Basic equation: $$F_{DIR} = F_0 \cdot \exp[-AMF \cdot \tau]$$

F_{DIR}	Direct sun irradiance (at wavelength λ)
F_0	Extraterrestrial irradiance corrected for Sun-Earth distance
τ	Total vertical extinction optical depth
AMF	Air mass factor = slant column over vertical column

$$AMF \cdot \tau = AMF_{O3} \cdot \tau_{O3} + AMF_{SCA} \cdot \tau_{SCA} + AMF_{AER} \cdot \tau_{AER} + AMF_{SO2} \cdot \tau_{SO2} + AMF_{REST} \cdot \tau_{REST}$$

O3, SO2, SCA	Ozone and SO_2 absorption, Molecular scattering
AER, REST	Aerosol extinction and everything else… (mainly NO_2, HCHO, …)

$$\tau_x = \Omega_x \cdot \tau^*_x$$

τ^*_x	Optical depth for 1DU
Ω_x	Total column of respective gas in DU

→ logarithm:

$$\ln F_{DIR} = \ln F_0 - AMF_{O3} \cdot \tau^*_{O3} \cdot \Omega_{O3} - AMF_{SCA} \cdot \tau_{SCA} - \ldots$$
$$AMF_{AER} \cdot \tau_{AER} - AMF_{SO2} \cdot \tau^*_{SO2} \cdot \Omega_{SO2} - AMF_{REST} \cdot \tau^*_{REST} \cdot \Omega_{REST}$$

Brewer direct sun total ozone algorithm

→ solve for Ω_{O3}

$$\Omega_{O3} = \frac{\ln F_0 - \ln F_{DIR} - AMF_{SCA} \cdot \frac{p}{p_0} \cdot \tau^*_{SCA} - AMF_{AER} \cdot \tau_{AER} - AMF_{SO2} \cdot \tau^*_{SO2} \cdot \Omega_{SO2} - AMF_{REST} \cdot \tau^*_{REST} \cdot \Omega_{REST}}{AMF_{O3} \cdot \tau^*_{O3}}$$

p_0	Standard surface air pressure at location
p	True surface air pressure at location

Air mass factor equation:

SZA	Solar zenith angle
R	Earth's radius (~6370km)
h_{xEFF}	Effective layer height of species x

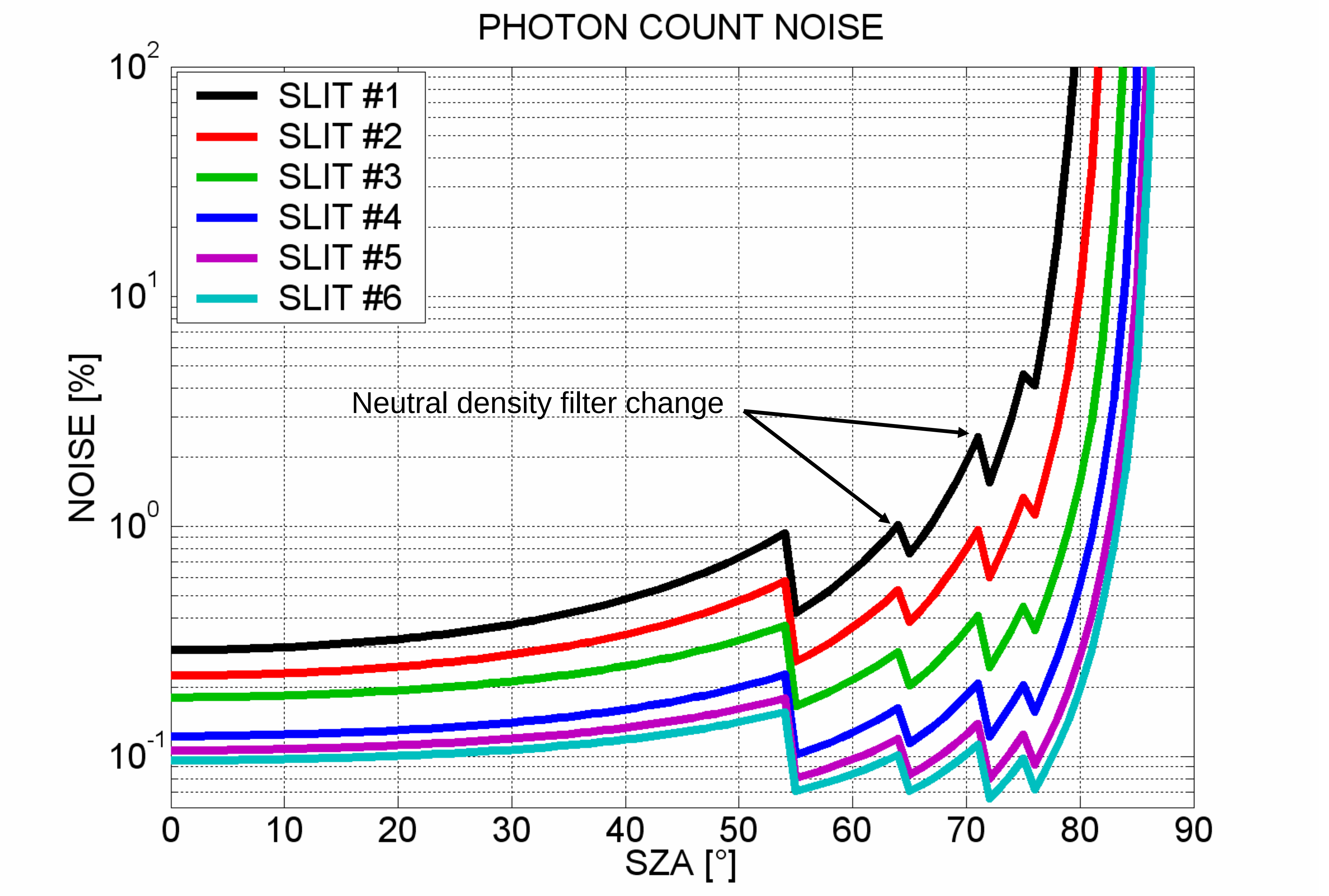
$$AMF_x \sim \sec\left\{\arcsin\left[\frac{R}{R + h_{xEFF}} \cdot \sin(SZA)\right]\right\}$$

	Parameter	Source
P1-P5	AMF_x	h_{O3EFF}=22km, h_{SCAEFF}=5km, h_{AEREFF}=2km, h_{SO2EFF}=2km, $h_{RESTEFF}$=2km
P6	$\ln F_0$	Assume obtained by Langley extrapolations at high mountain station
P7	$\ln F_{DIR}$	Measured corrected count rates (ISL, ASL!)
P8	τ^*_{O3}	Use Bass & Paur [1985] cross sections, $T_{O3EFFSTAN}$=-45°C
P9	τ_{SCA}	Use Bodhaine et al. [1999], standard pressure
P10	τ_{AER}	Assume Angstrom behavior
P11	τ_{SO2}	Use Vandaele et al. [1994] cross sections and Ω_{SO2}=1DU
P12	τ_{REST}	Use Ω_{NO2}=0.7DU and Ω_{HCHO}=1DU and … (=urban polluted)

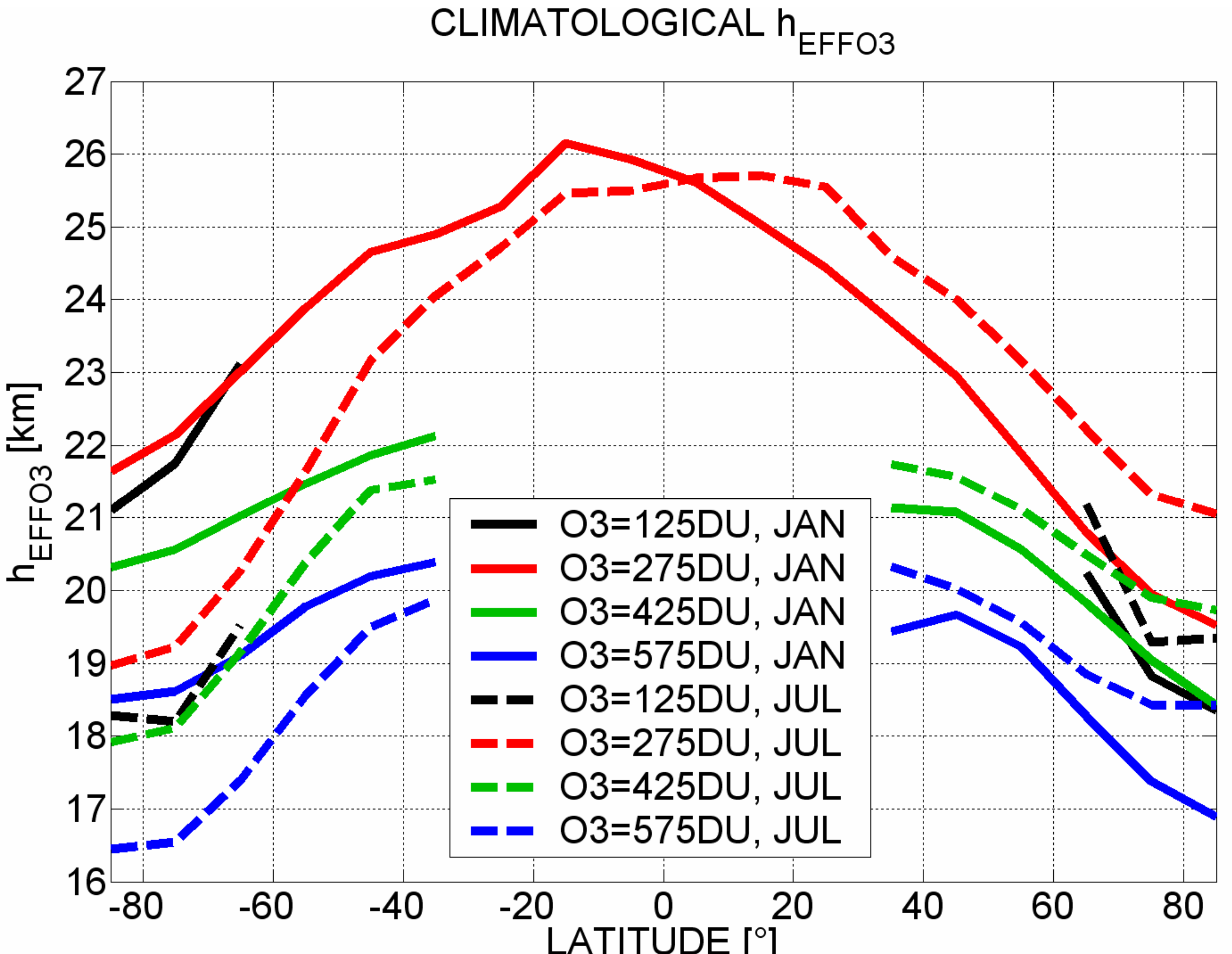
Independent variables

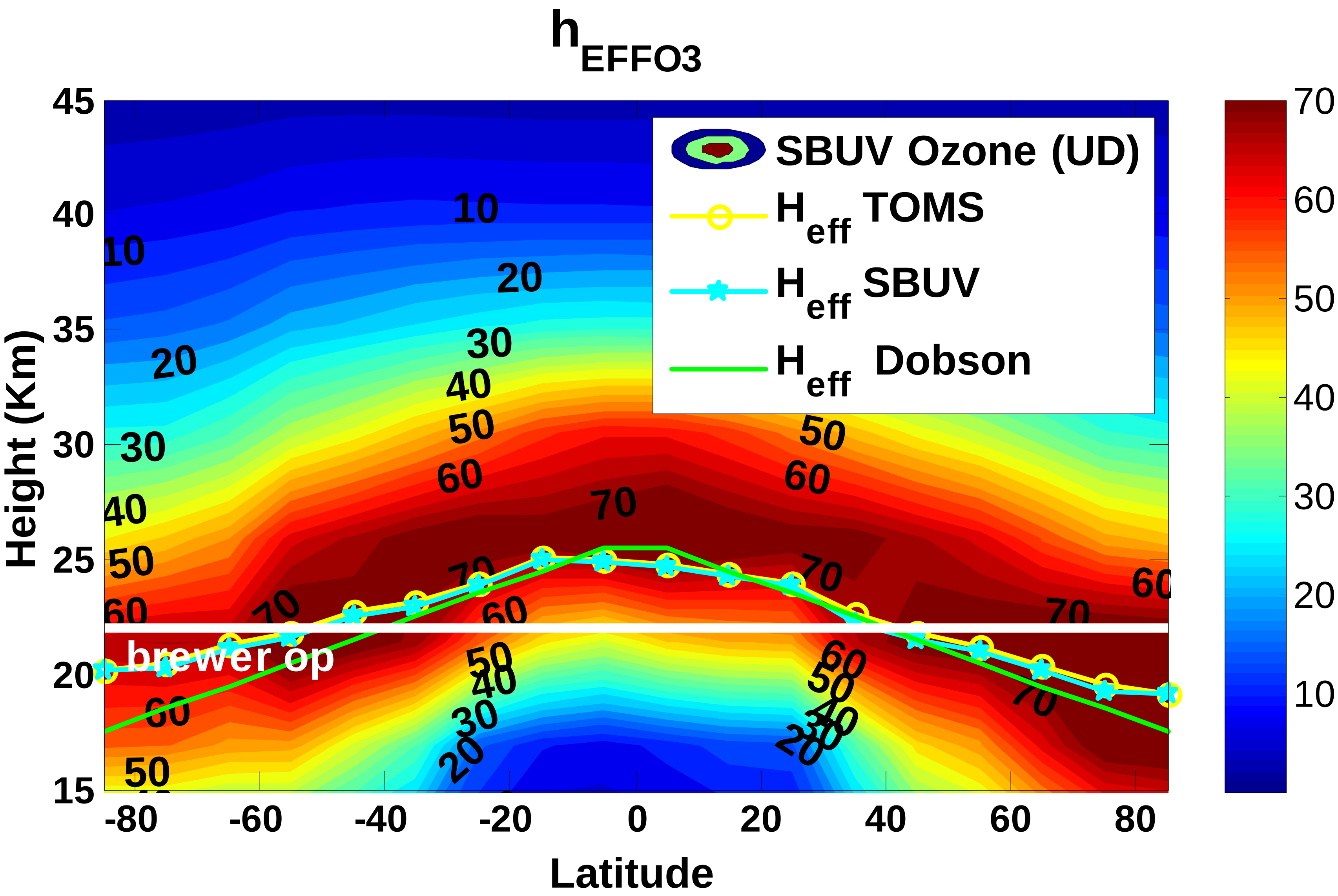
	Independent Variable	Estimated Uncertainty (2σ)	Remark
V1	SZA	0.12° (0.01°)	Assume 30s registration time uncertainty (1s)
V2	RAD_{ALL}	4%	Radiometric calibration, same for all λ
V3	RAD_{IND}	0.28, 0.15, 0.12, 0.08, 0.06, 0%	Radiometric calibration for each slit, λ-independent From “Ratio Langleys”
V4	NOISE	→ Figure	Photon count noise, λ-independent
V5	$\Delta\lambda$	0.01nm (0.004nm)	Wavelength shift, same for all λ (directly after Hg-test)
V6	T_{O3EFF}	20° (5°, 1°)	Eff. O_3 temperature (5° climatology, 1° sonde)
V7	P/P_0	1% (0.1%)	Surface pressure (if measured)
V8	τ_{AER340}	0.75 (0.04)	AOD at 340nm (if measured)
V9	α_{340}	0.7 (0.1)	Angstrom parameter at 340nm (if measured)
V10	Ω_{SO2}	100%	Total SO_2 column
V11	Ω_{REST}	100%	Total column of other gases (mainly NO_2)
V12	h_{O3EFF}	5km (2km, 0.5km)	Eff O_3 height (2km climatology, 0.5km sonde)
V13	h_{SCAEFF}	0.2km	Effective scattering height
V14	h_{AEREFF}	4km	Effective aerosol height
V15	h_{SO2EFF}	10km	Effective SO_2 height
V16	$h_{RESTEFF}$	10km	Effective height of other gases

Expanded noise at standard conditions



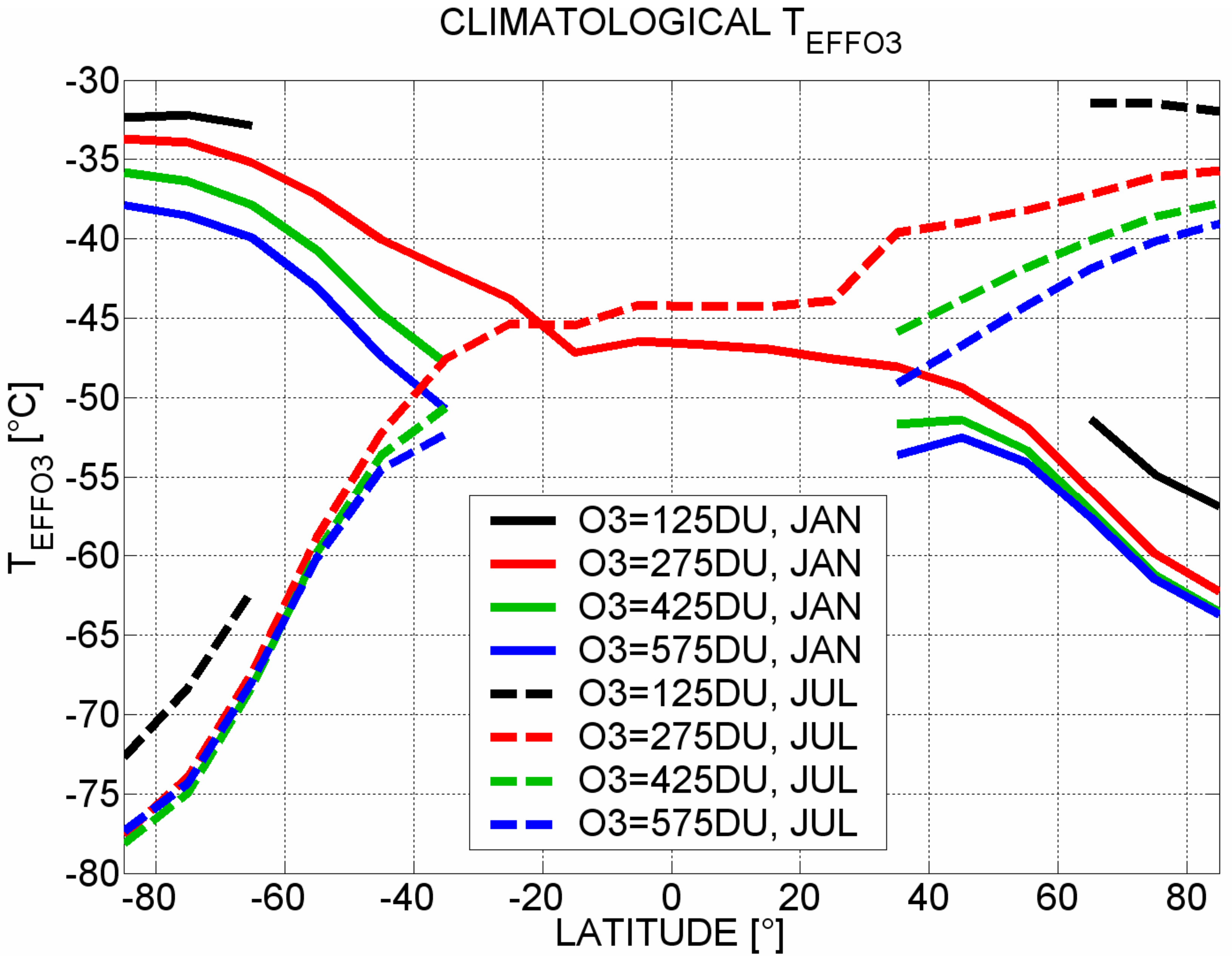
Variation of climatological hO3EFF





h_{EFFO3}
SBUV Ozone (UD)
H_{eff} TOMS
H_{eff} SBUV
H_{eff} Dobson
brewer op
Height (Km)
Latitude

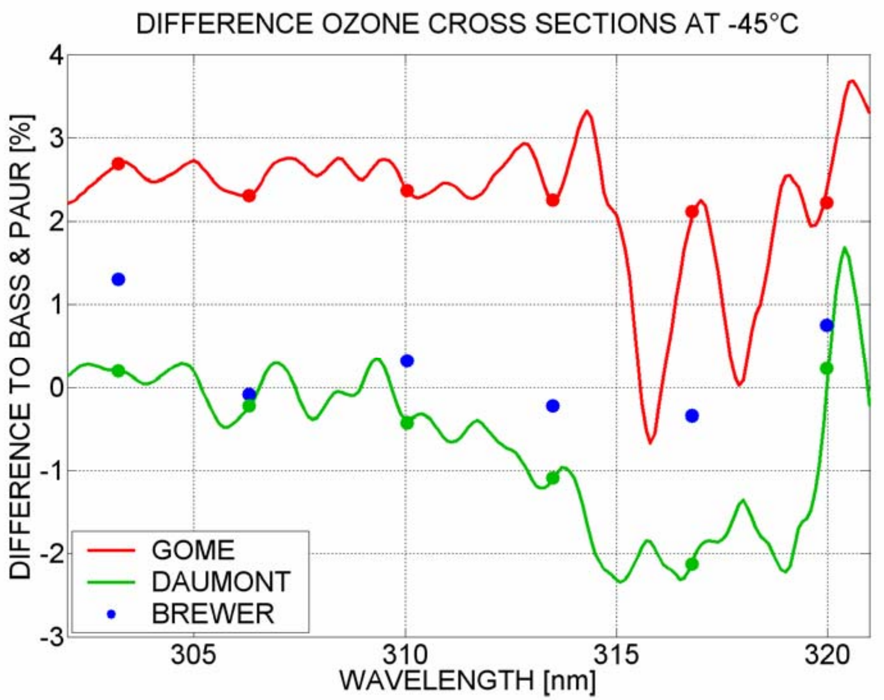
Variation of climatological TO3EFF

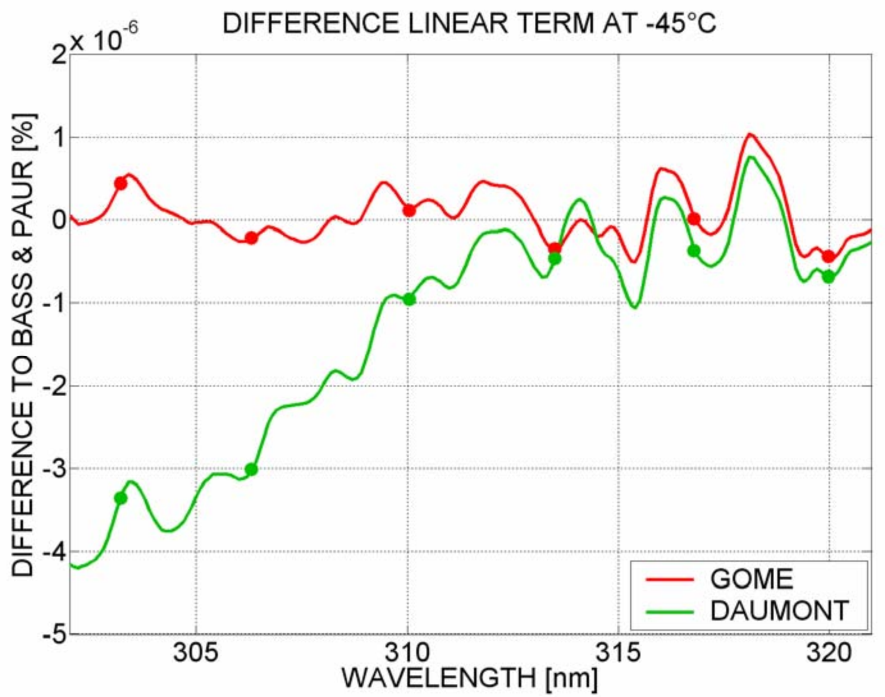


Ozone cross sections

$$\tau^*_{O3} = \tau^*_{O3} + \tau'^*_{O3} \cdot (T_{O3EFF} - T_{O3EFFSTAN}) + \tau''^*_{O3} \cdot (T_{O3EFF} - T_{O3EFFSTAN})^2 + \frac{\partial \tau^*_{O3}}{\partial \lambda} \cdot \Delta\lambda$$

τ^*_{O3}, τ'^*_{O3}, and τ''^*_{O3} are the 0, 1st, and 2nd order derivative of τ^*_{O3} with respect to temperature at $T_{O3EFFSTAN}$=-45°C, using actual Brewer wavelengths and slit functions.





Uncertainty estimation

$$\Omega_{O3} = \frac{\ln F_0 - \ln F_{DIR} - AMF_{SCA} \cdot \frac{p}{p_0} \cdot \tau *_{SCA} - AMF_{AER} \cdot \tau_{AER} - AMF_{SO2} \cdot \tau *_{SO2} \cdot \Omega_{SO2} - AMF_{REST} \cdot \tau *_{REST} \cdot \Omega_{REST}}{AMF_{O3} \cdot \tau *_{O3}}$$

$$\Omega_{O3} = \frac{P6 - P7 - P2 \cdot P9 - P3 \cdot P10 - P4 \cdot P11 - P5 \cdot P12}{P1 \cdot P8}$$

$$\sigma^2_{\Omega O3} = \sum_i \left(\frac{\partial \Omega_{O3}}{\partial Vi} \right)^2 \cdot \sigma^2_{Vi}$$

$$\frac{\partial \Omega_{O3}}{\partial Vi} = \sum_j \frac{\partial \Omega_{O3}}{\partial Pj} \cdot \frac{\partial Pj}{\partial Vi}$$

Assumes independent Vi

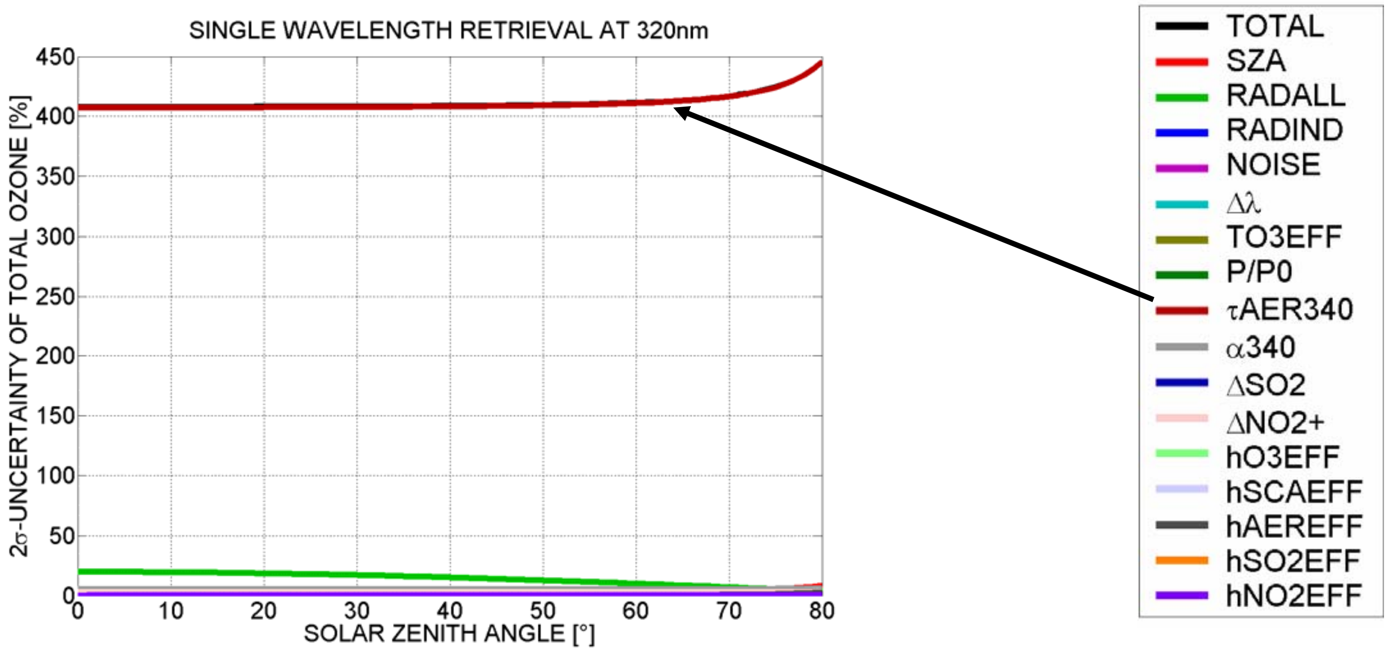
V3 and V4 are actually 6 variables each.

Total ozone from single wavelength

Retrieve total ozone from absolute measurement at 320nm

Aerosols kill you

→ Need AOD measurement?

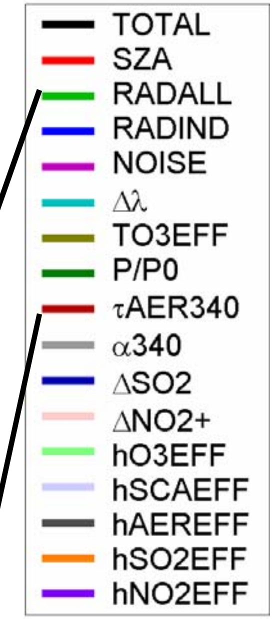


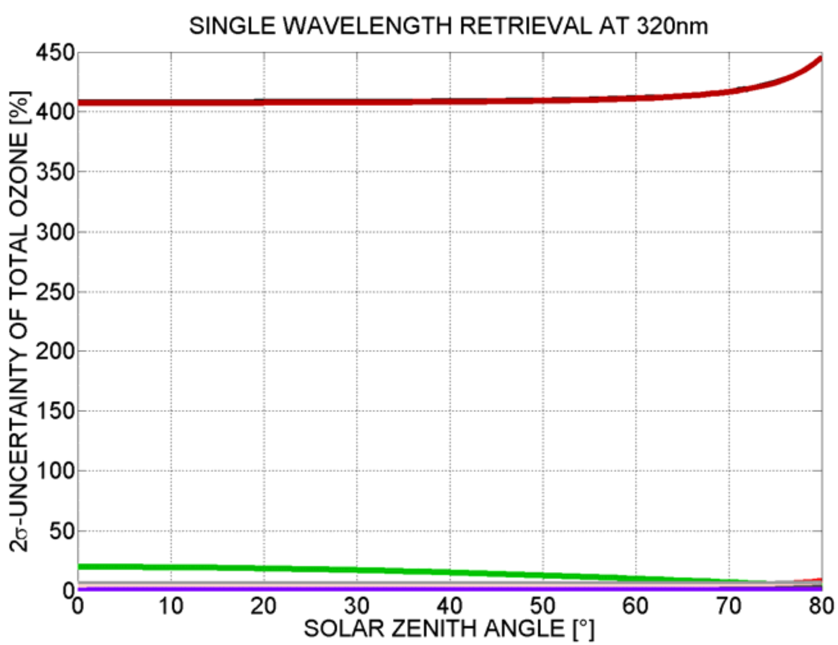
Total ozone from single wavelength

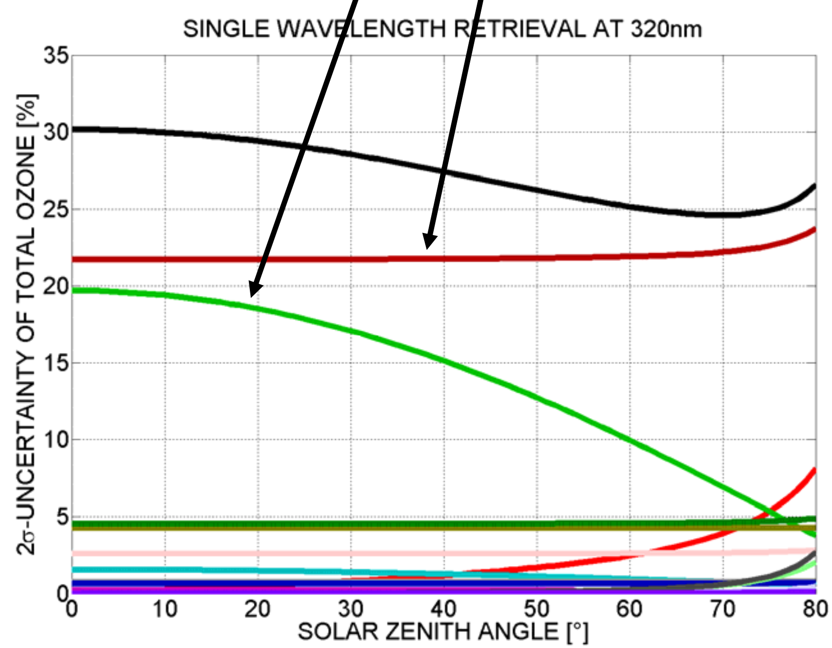
Retrieve total ozone from absolute measurement at 320nm and AOD from different input (e.g. at 340nm)

Aerosols and absolute radiometric calibration are still to dominant

→ Need wavelength with more ozone sensitivity?







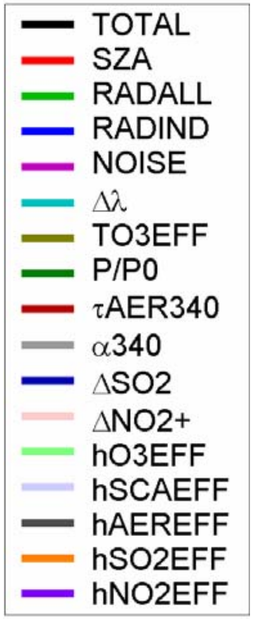
Total ozone from single wavelength

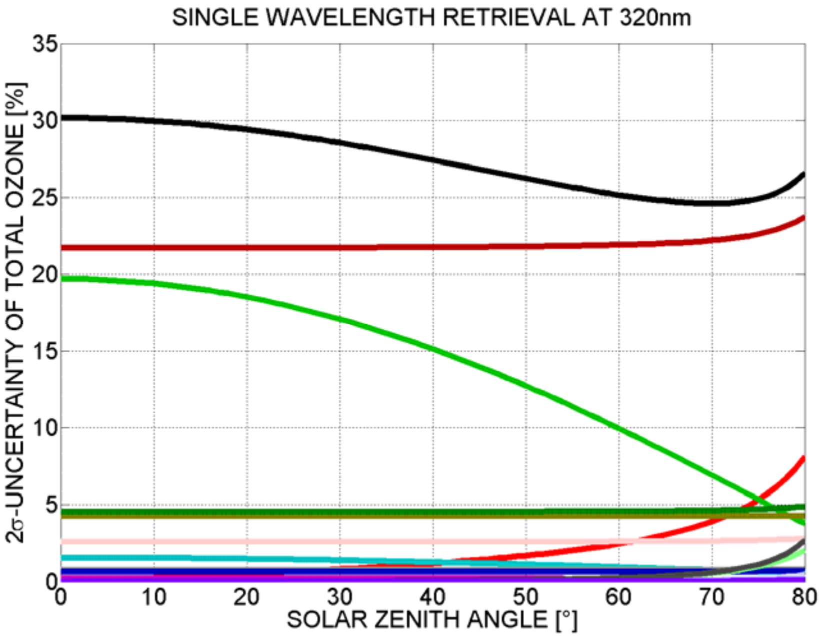
Retrieve total ozone from
absolute measurement at 303nm and using AOD at 340nm

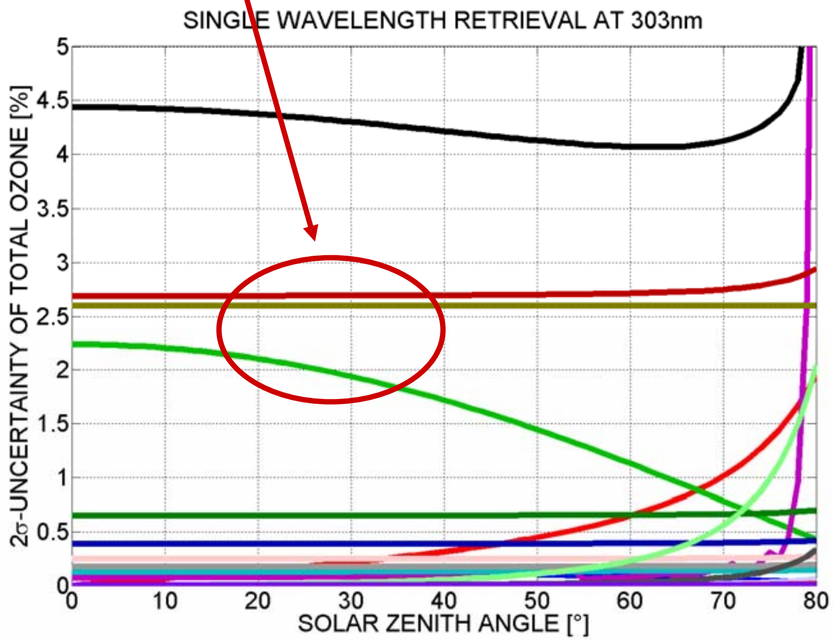
Already down to ~5% uncertainty

Problems: AOD, TO3EFF, noise, absolute radiometric calibration

→ Take TO3EFF and hO3EFF from climatology?







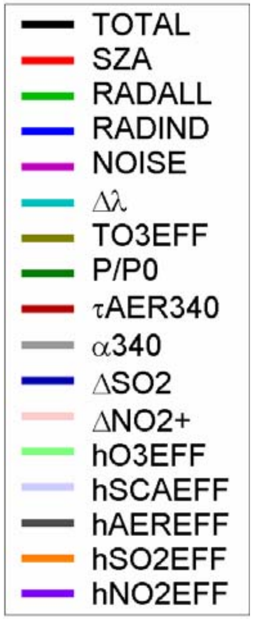
Total ozone from single wavelength

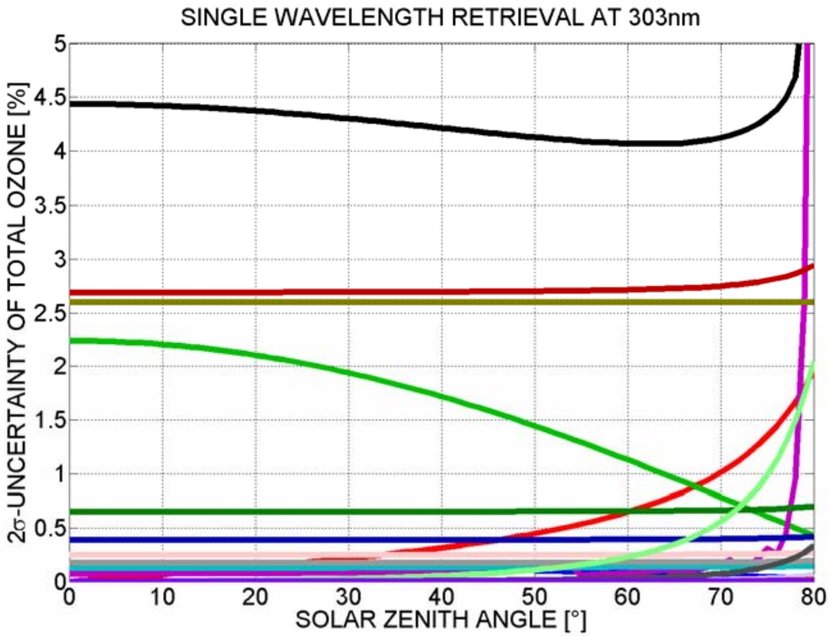
Small improvement

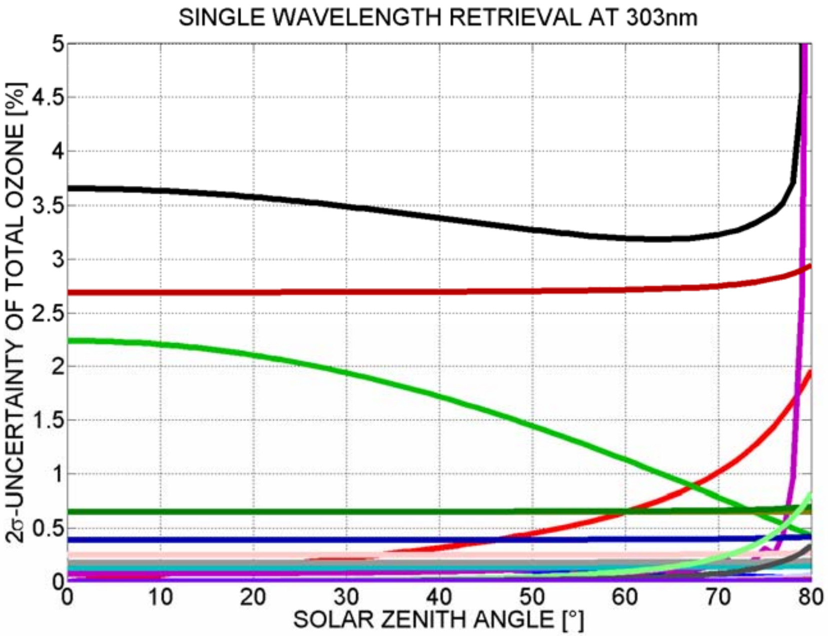
→ Down to ~4% uncertainty

Problems: AOD, noise, absolute radiometric calibration

→ Use more wavelengths







Total ozone from several wavelengths

$$\Omega_{O3} = \frac{\ln F_0 - \ln F_{DIR} - AMF_{SCA} \cdot \frac{p}{p_0} \cdot \tau^*_{SCA} - AMF_{AER} \cdot \tau_{AER} - AMF_{SO2} \cdot \tau^*_{SO2} \cdot \Omega_{SO2} - AMF_{REST} \cdot \tau^*_{REST} \cdot \Omega_{REST}}{AMF_{O3} \cdot \tau^*_{O3}}$$

$$\Omega_{O3} = \frac{\sum_\lambda w_\lambda \cdot \left[\ln F_{0\lambda} - \ln F_{DIR\lambda} - AMF_{SCA} \cdot \frac{p}{p_0} \cdot \tau^*_{SCA\lambda} - AMF_{AER} \cdot \tau_{AER\lambda} - AMF_{SO2} \cdot \tau^*_{SO2\lambda} \cdot \Omega_{SO2} - AMF_{REST} \cdot \tau^*_{REST\lambda} \cdot \Omega_{REST}\right]}{AMF_{O3} \cdot \sum_\lambda w_\lambda \cdot \tau^*_{O3\lambda}}$$

Weights of operational Brewer retrieval
w=[-1, 0.5, 2.2, -1.7]

Normalized with respect to slit #6
w=[0.58, -0.29, -1.29, 1]

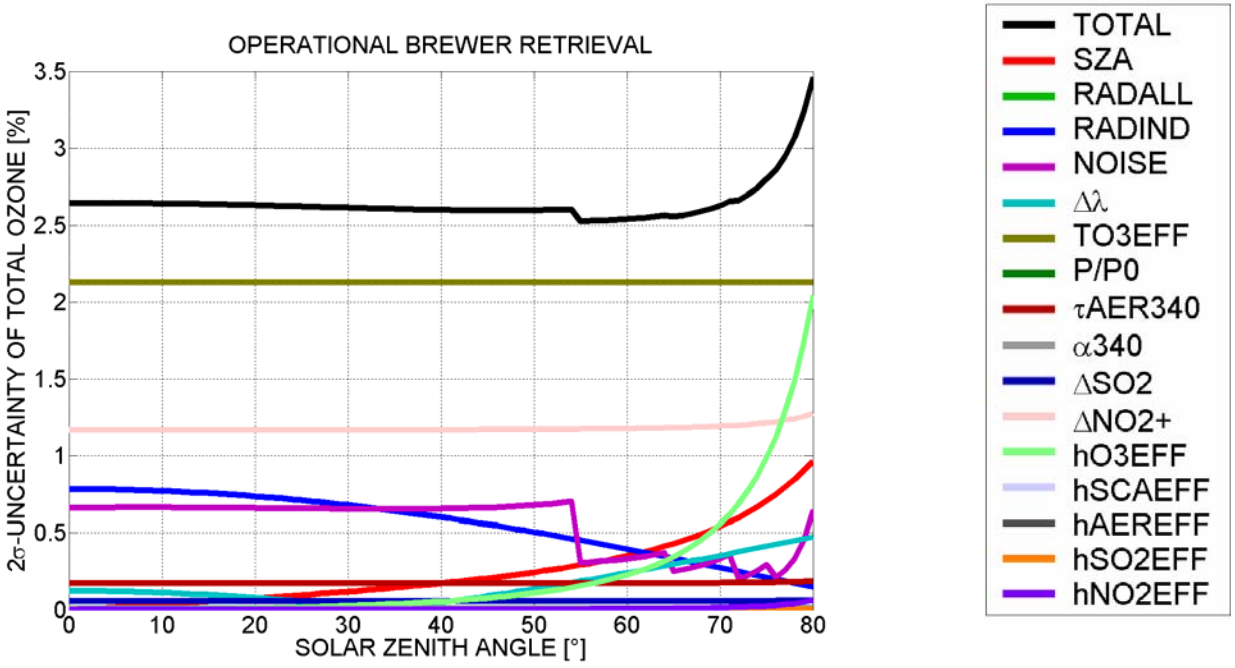
Total ozone from 4 wavelengths 310, 313, 317, 320nm

Operational Brewer retrieval (no AOD needed)
w=[0.58, -0.29, -1.29, 1]

Aerosol and absolute calibration problems disappear
→Down to ~3% uncertainty

Problems: TO3EFF, hO3EFF, other gases, SZA

→ Use climatological input and internet time



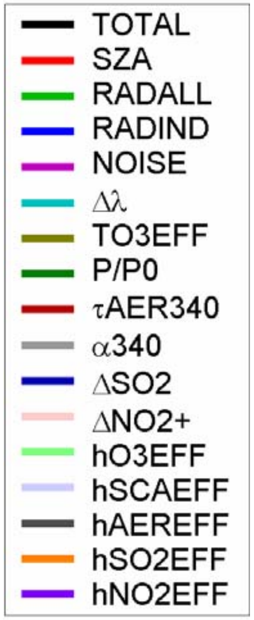
Total ozone from 4 wavelengths 310, 313, 317, 320nm

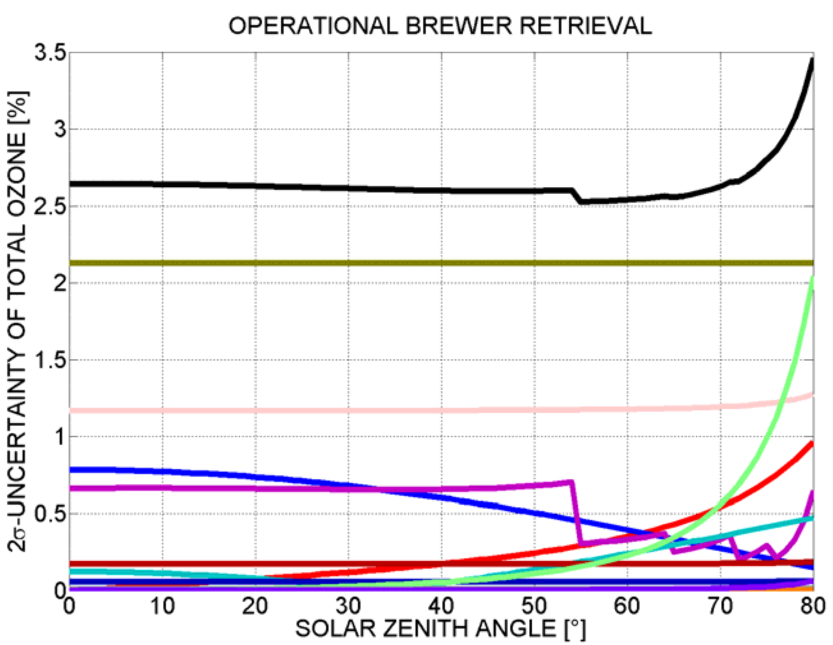
Operational Brewer retrieval & climatological input

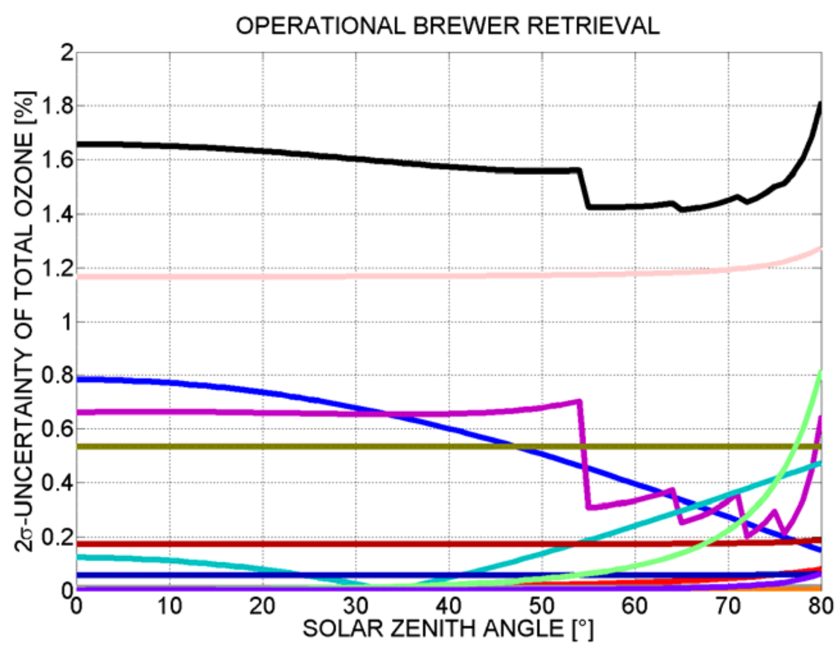
→Down to <2% uncertainty

Problem: other gases

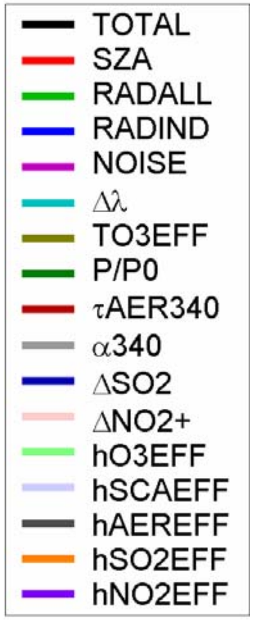
→ How about other weights?







Total ozone from 4 wavelengths 310, 313, 317, 320nm

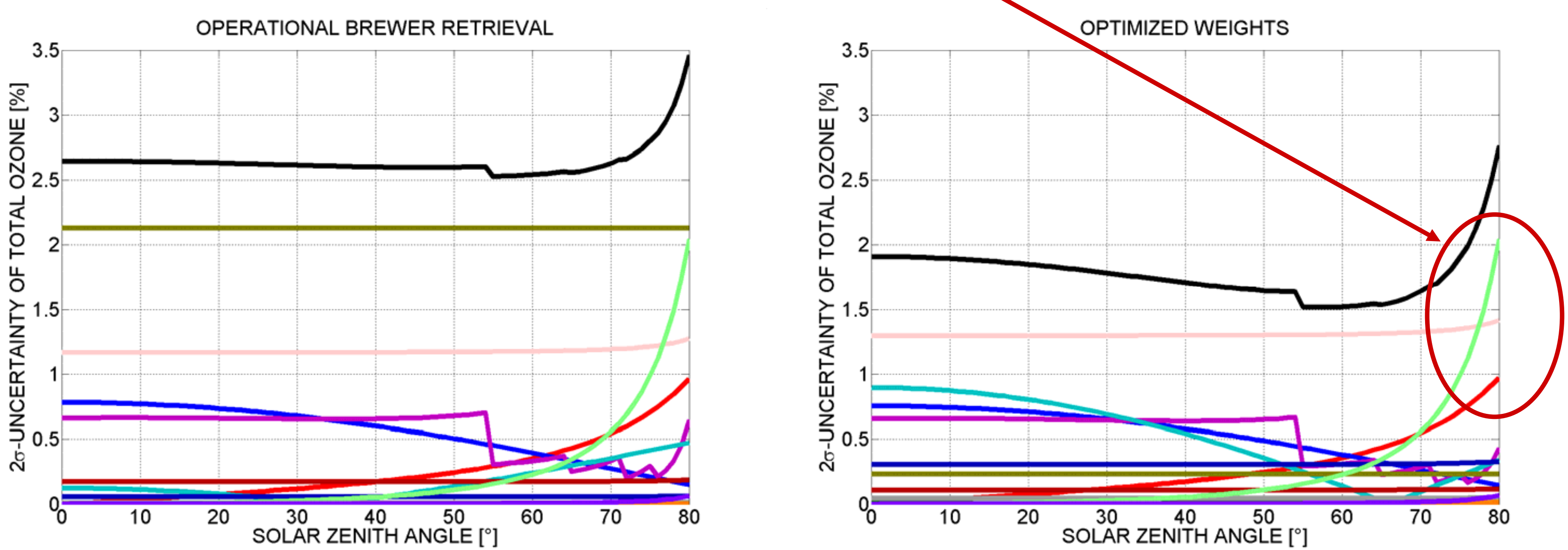


Without climatological input:
Brewer w=[0.58, -0.29, -1.29, 1]
Here w=[0.31, 0.31, -1.62, 1]

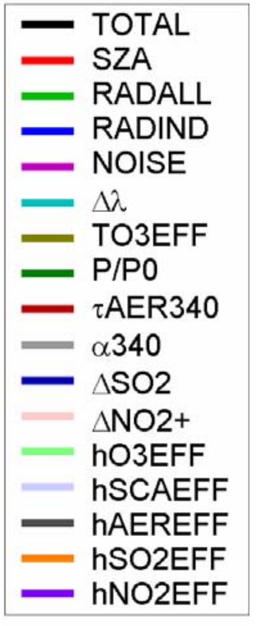
TO3EFF sensitivity reduced
→From ~3% uncertainty to ~2% uncertainty

Problems: hO3EFF, other gases, SZA

→ Use climatological input and internet time



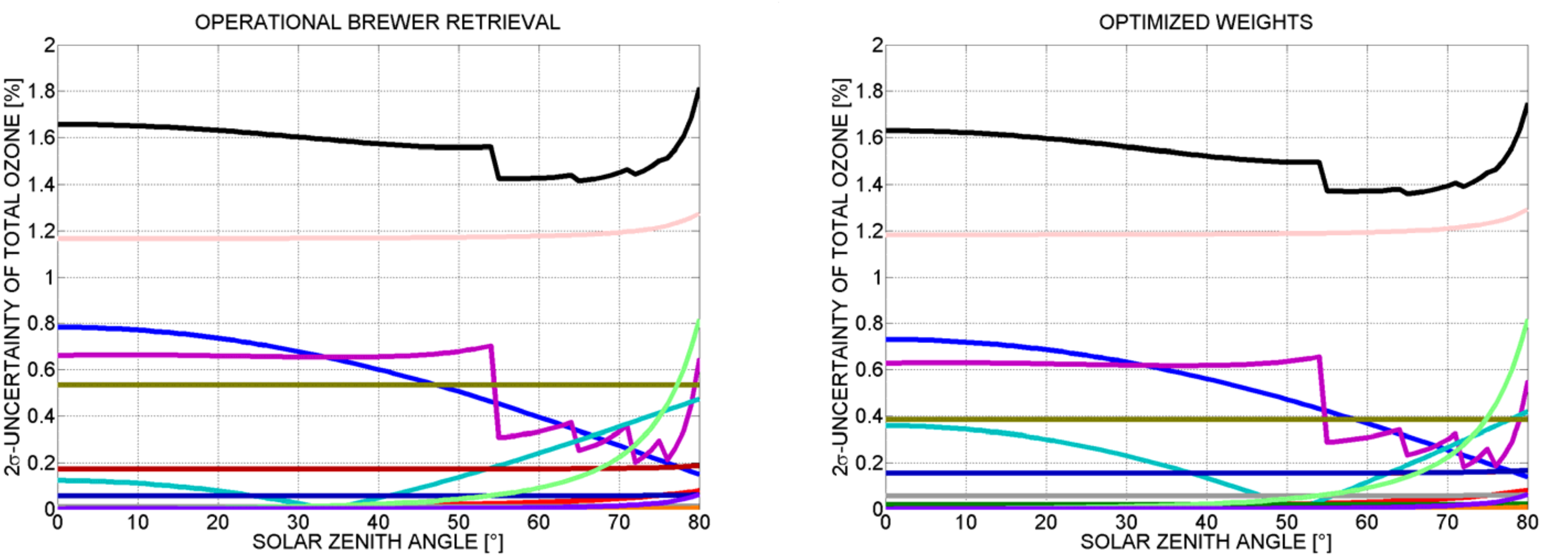
Total ozone from 4 wavelengths 310, 313, 317, 320nm



With climatological input:
Brewer w=[0.58, -0.29, -1.29, 1]
Here w=[0.51, -0.10, -1.41, 1]

Practically same weights and same result
→Brewer weights assume low uncertainty in TO3EFF and hO3EFF?

→ Why not use all 6 wavelengths?



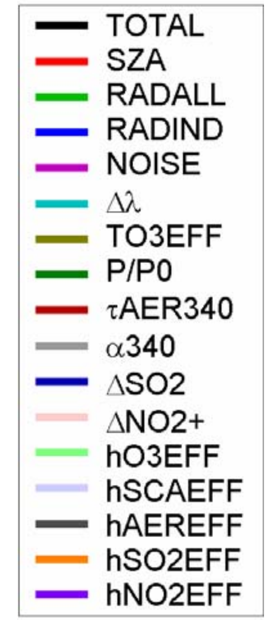
Total ozone from 6 wavelengths 303, 306, 310, 313, 317, 320nm

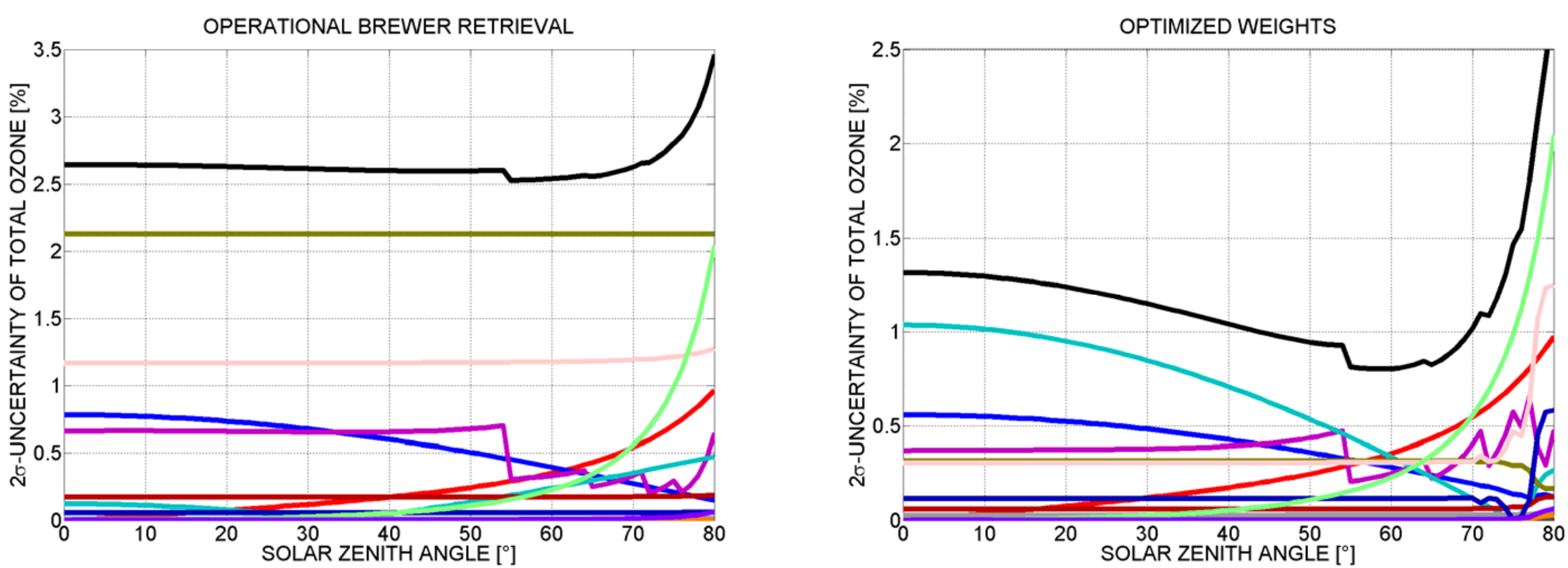
Without climatological input:
Brewer w=[0 , 0 , 0.58, -0.29, -1.29, 1]
SZA<70° w=[0.50, -0.14, -0.99, 1.30, -1.67, 1]
SZA=80 ° w=[0 , 0.06 , 0.19, 0.36, -1.61, 1]

TO3EFF sensitivity reduced
→From ~3% uncertainty to <0.5% uncertainty

Problem: wavelength shift, noise dependent weights

→ Use climatological input and internet time





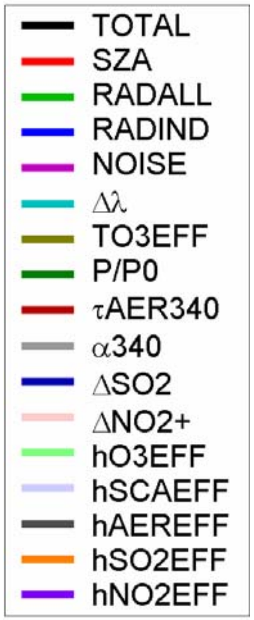
Total ozone from 6 wavelengths 303, 306, 310, 313, 317, 320nm

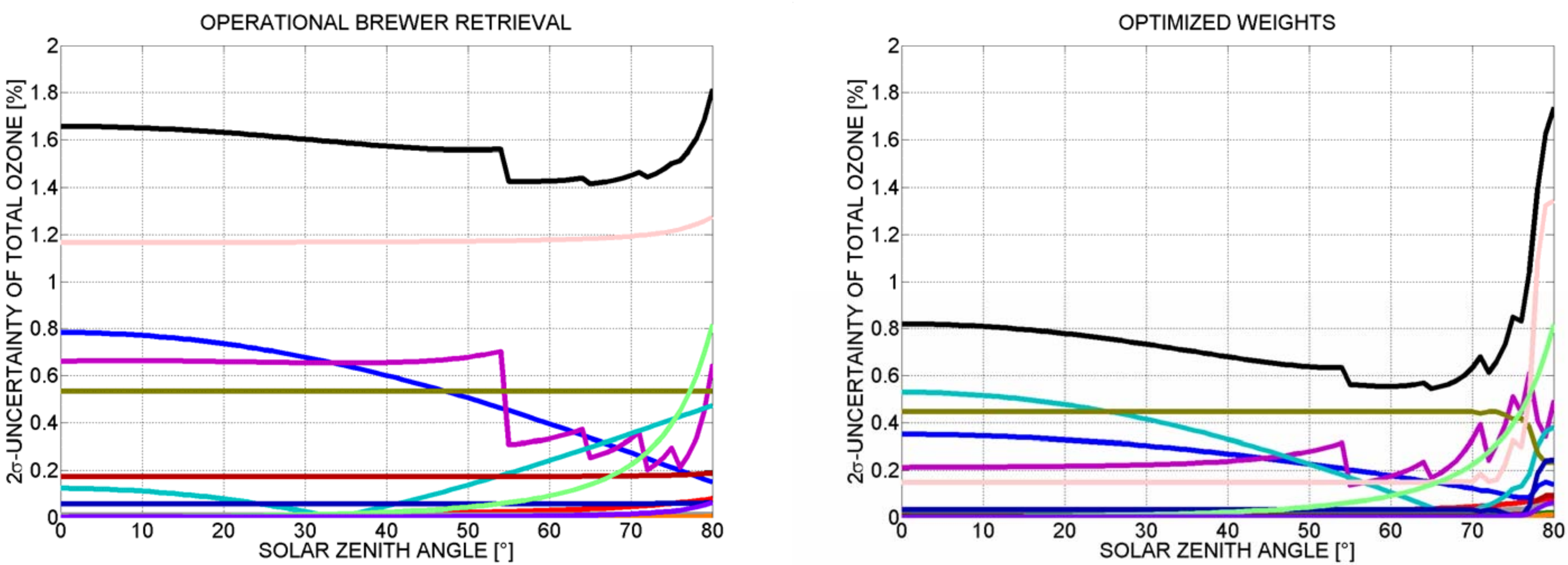
With climatological input:
Brewer w=[0 , 0 , 0.58, -0.29, -1.29, 1]
SZA<70° w=[0.48, 0.01, -0.49, -0.14, -0.86, 1]
SZA=80° w=[0 , 0 , 0.42, 0.09, -1.51, 1]

similar at SZA=80°

TO3EFF sensitivity reduced
→From ~1.7% uncertainty to ~1% uncertainty
→Wavelength shift sensitivity reduced

Problems: TO3EFF, wavelength shift, noise-dependent weights





Systematic errors

Systematic or statistical error: depends on time scale

Noise: purely statistical error

Instrument calibration: purely systematic error

TO3EFF:

→ Over the time of 1 day, the difference between the true TO3EFF and assumed TO3EFF (=-45°C) produces a systematic error.

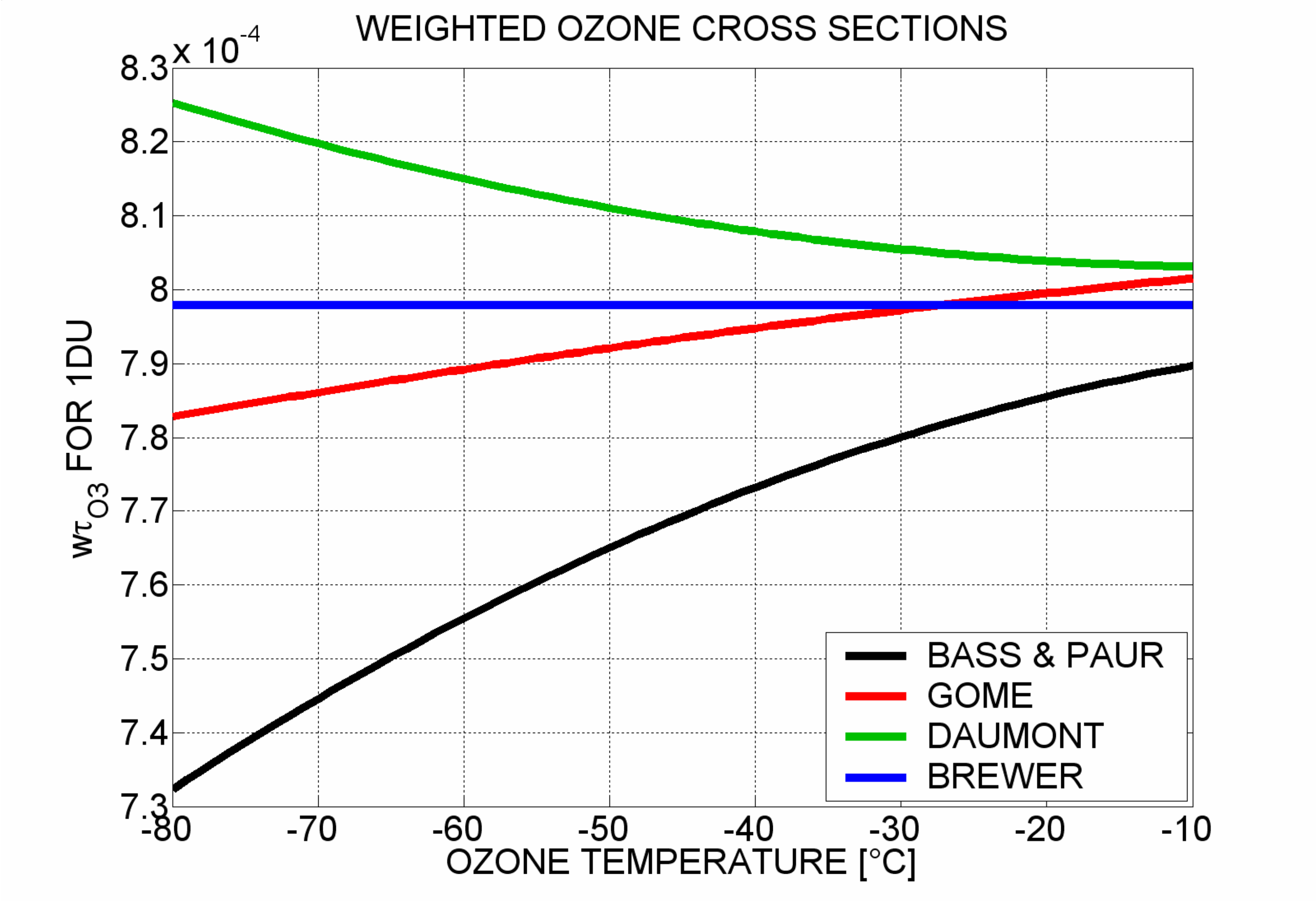
→ Over the time of 1 year, the TO3EFF-uncertainty has a systematic component (difference of yearly average TO3EFF at location to -45°C) and a statistical component (yearly variance of TO3EFF at location)

Systematic errors mostly depend on difference in atmospheric conditions between calibration period and measurement period

Here:
Assume characteristics of double Brewer #171 and a calibration from „Ratio-Langleys“ at standard conditions (300DU total ozone) with 1.6<AMF<3.

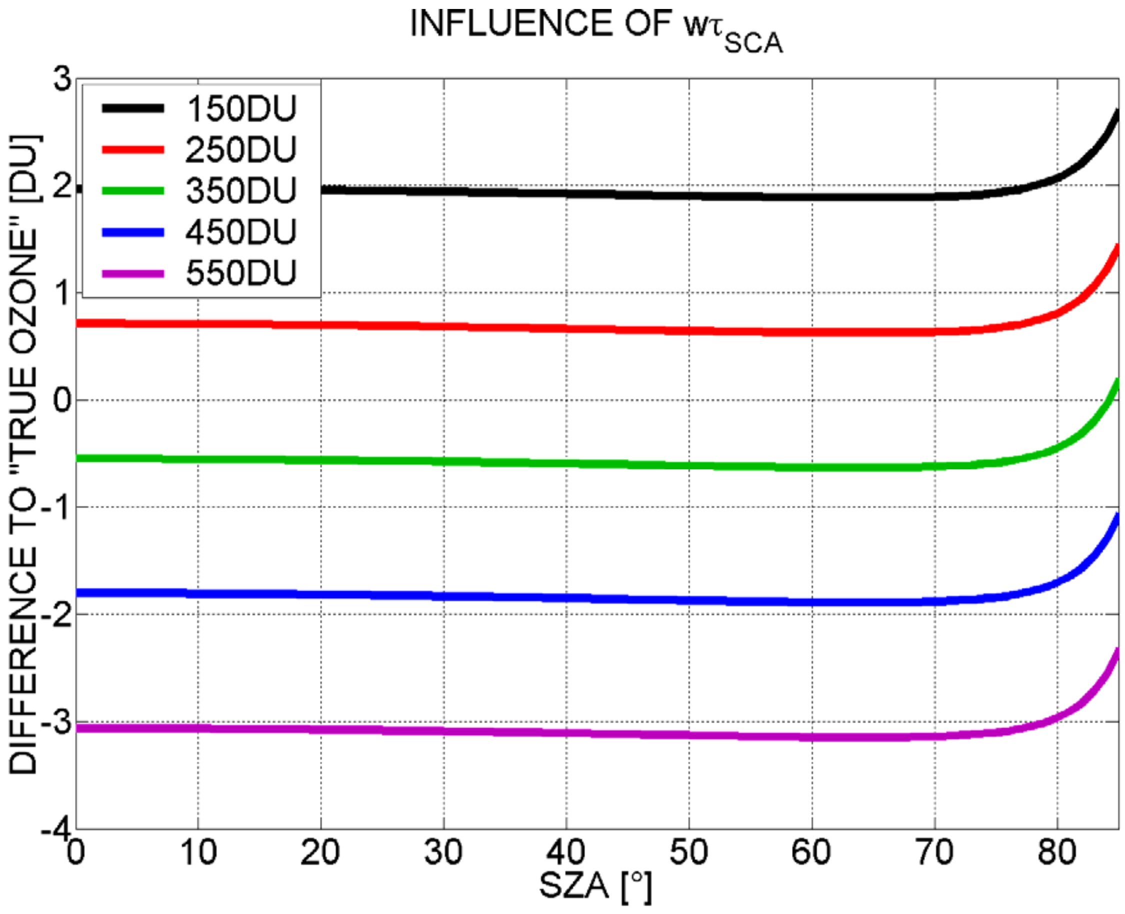
Weighted ozone cross sections

The operational $w\tau^*_{O3}$ for #171 is 7.97e-4 (blue line). Using other cross sections this differs significantly.



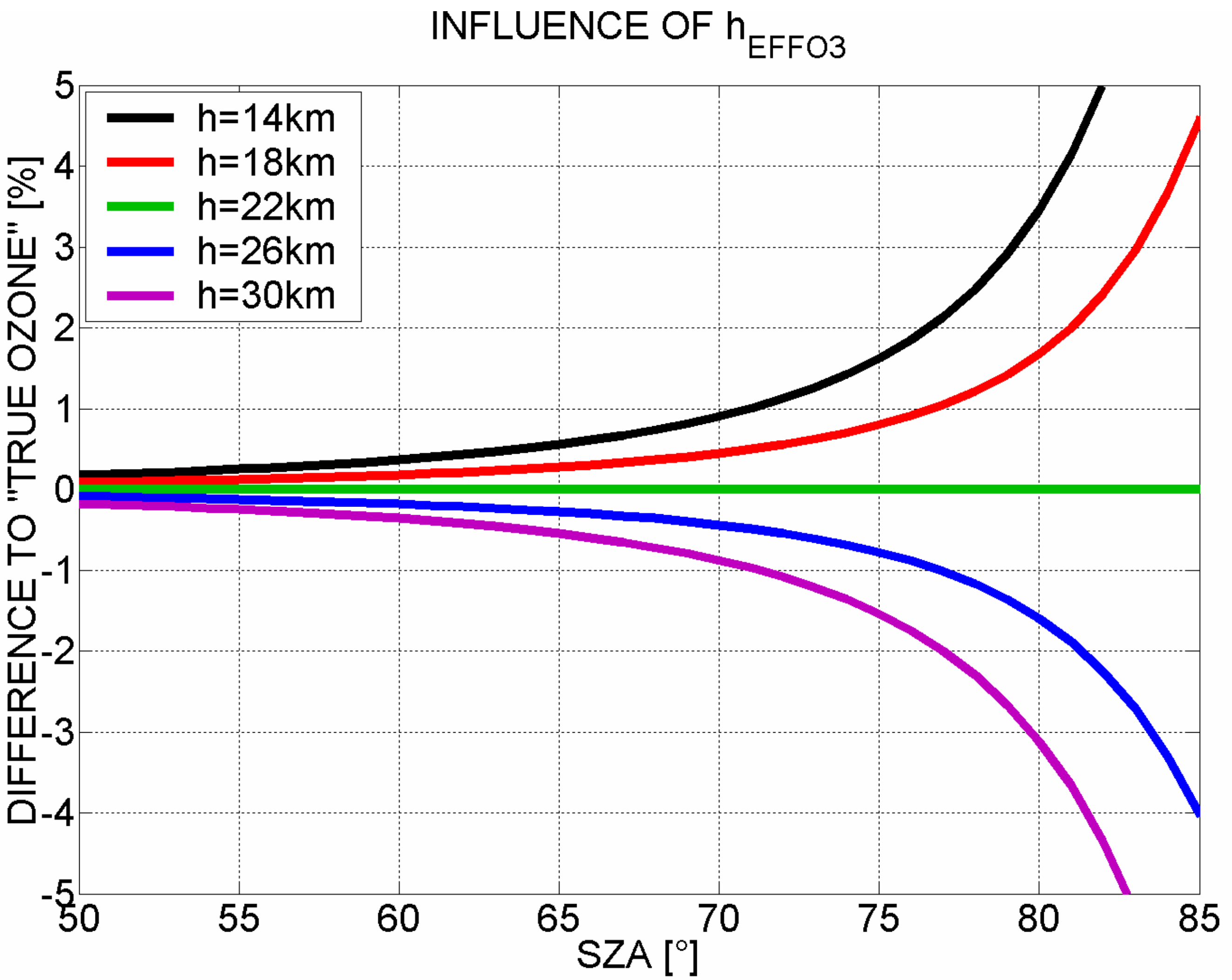
Weighted molecular cross section

The operational $w\tau^*_{SCA}$ for #171 is -2.3e-4. Using *Bodhaine et al.* we obtain $w\tau^*_{SCA}$=+27.0e-4. Replacing the former by the latter get systematic differences of –1.25DU per 100DU difference of the measured ozone to the “calibration ozone” (=300DU). Under this assumptions the retrieved ozone of #171 during SAUNA was between 1.1 and 2.6DU underestimated (the total column was between 400 and 500DU).



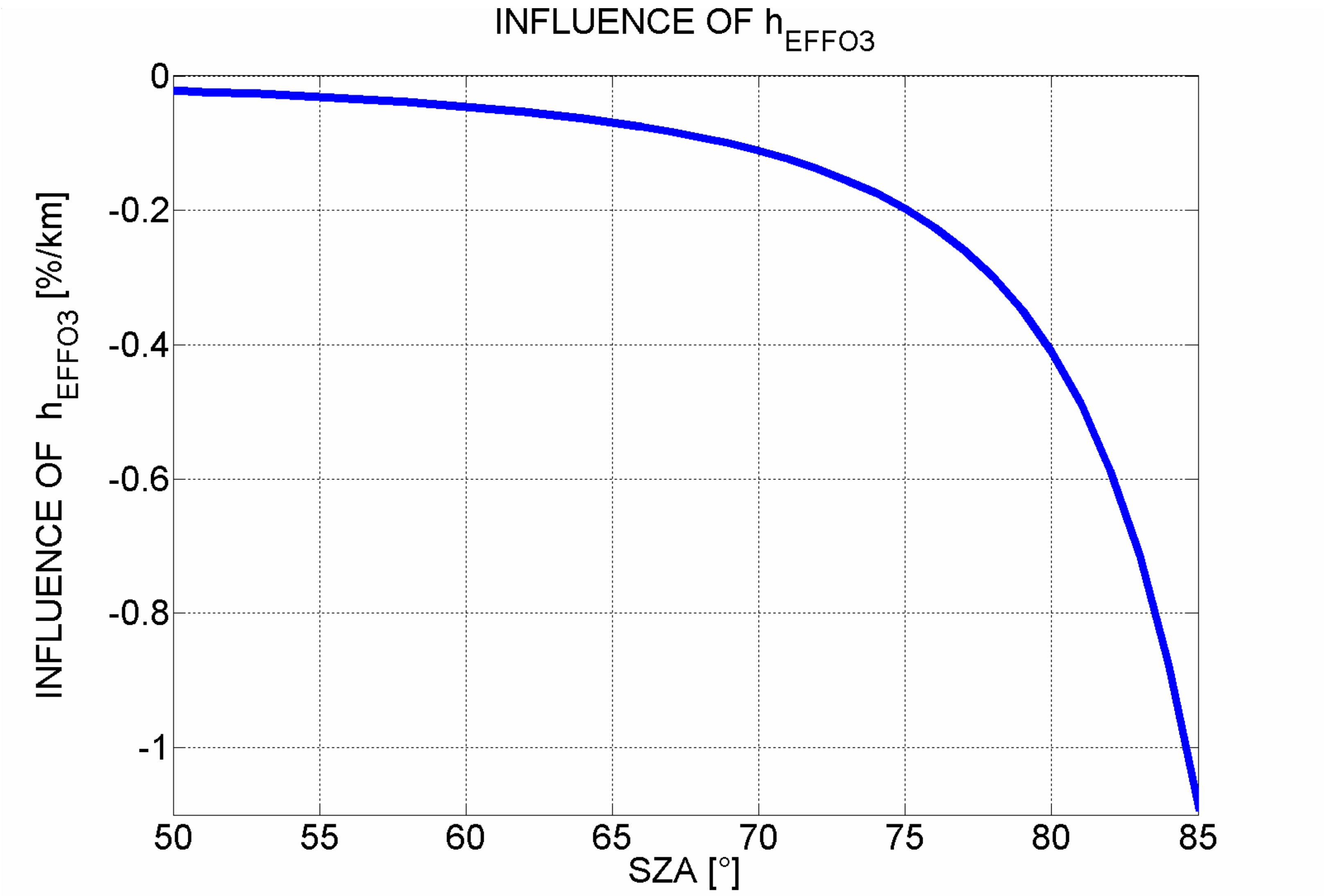
Effective ozone height

If the hO3EFF was 22km during the instrument calibration, then…
(during SAUNA hO3EF ranged from 18km to 20km)



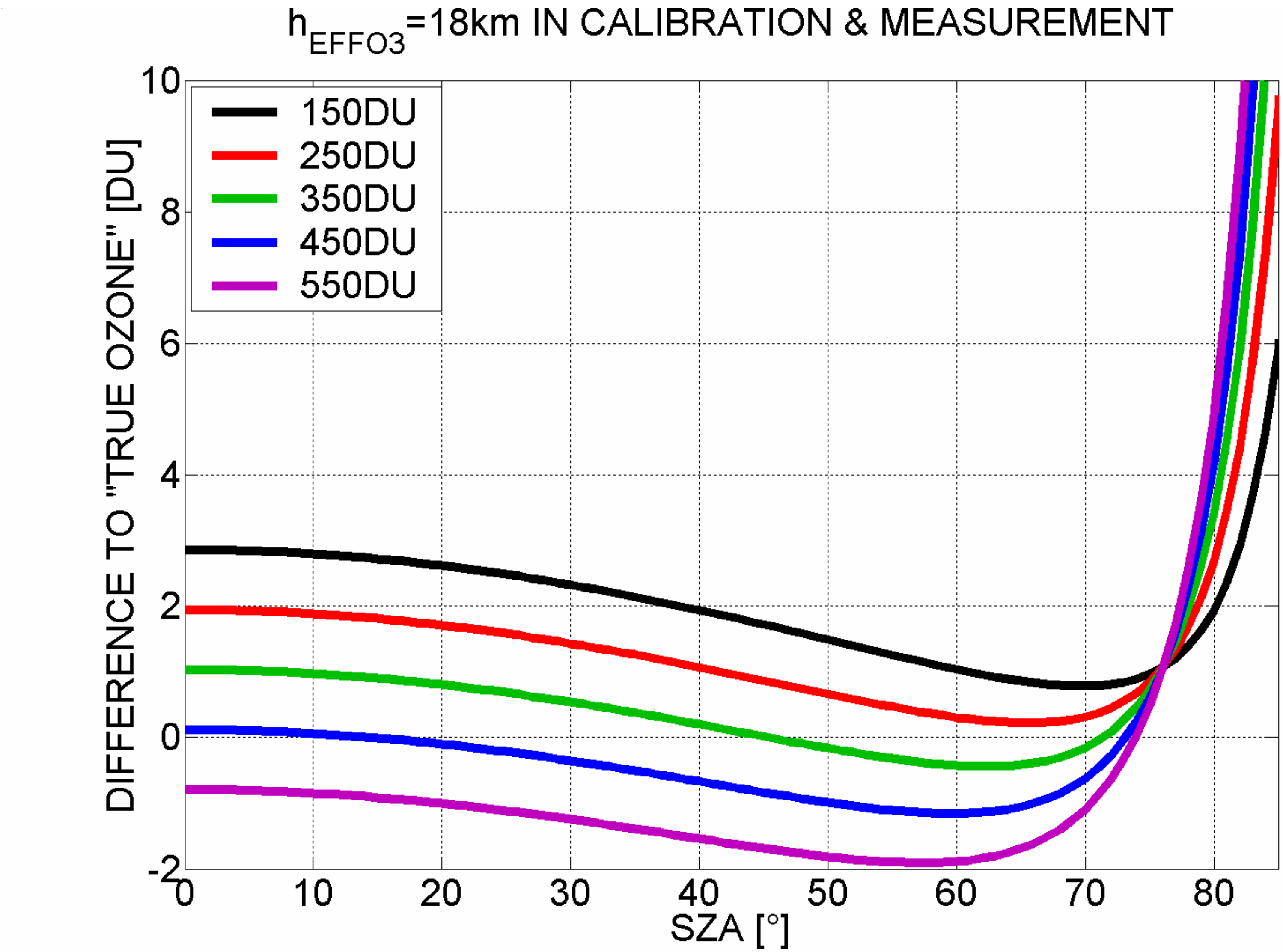
Effective ozone height

E.g. at SZA=80° the ozone is underestimated by 0.4% for each km that hO3EFF is higher than 22km.

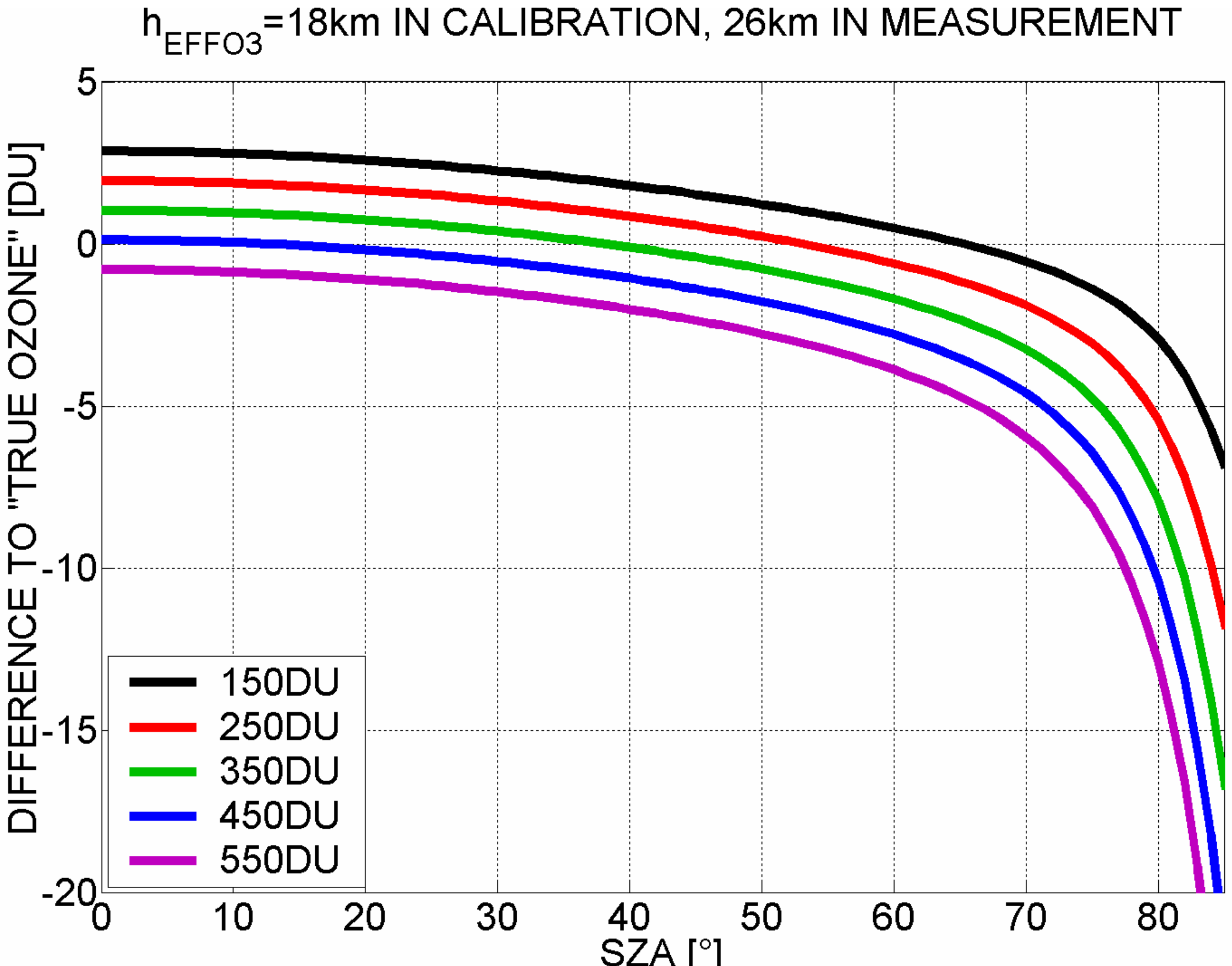


Effective ozone height

If hO3EFF was not 22km during the calibration, things get more difficult…

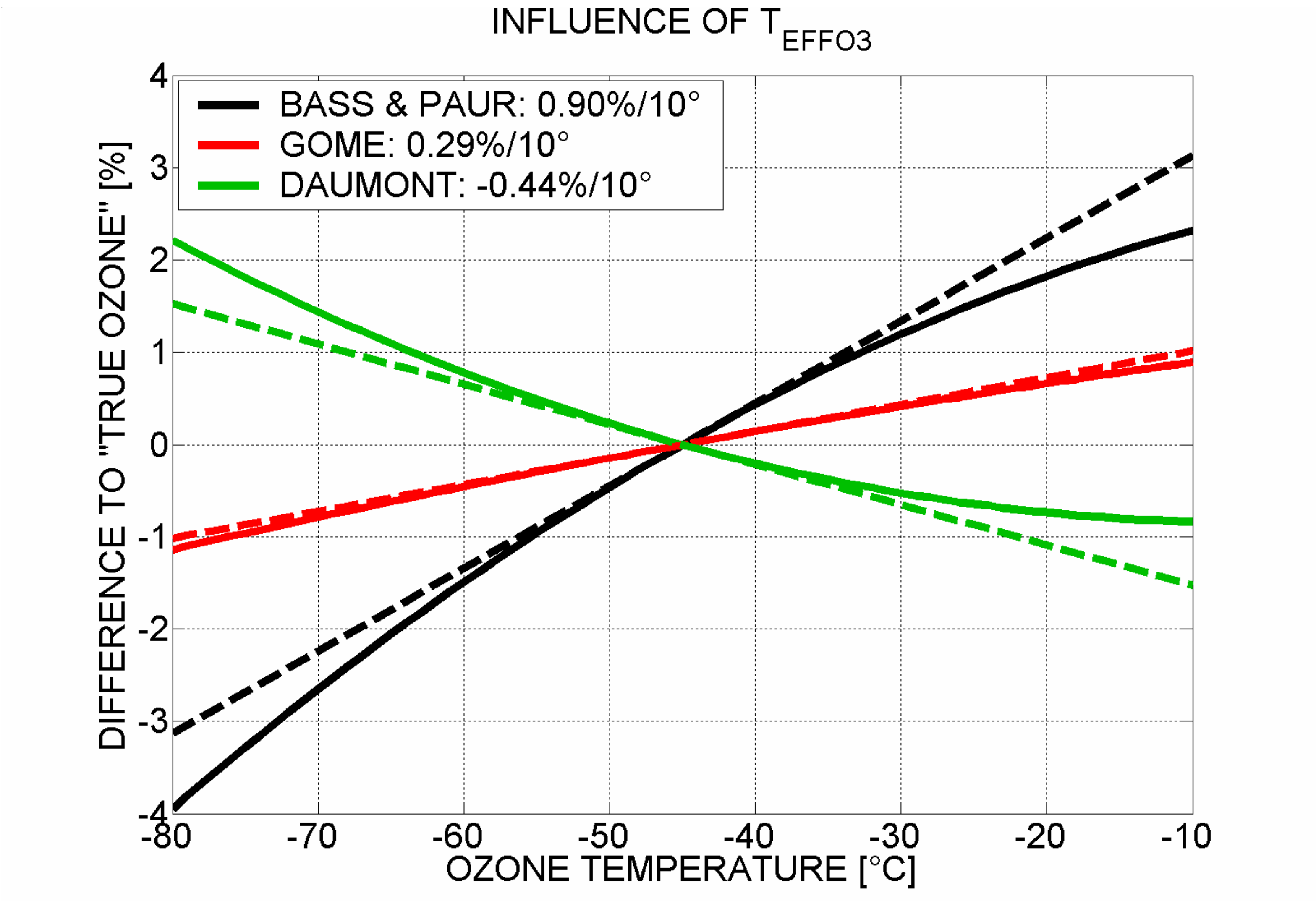


Effective ozone height



Effective ozone temperature

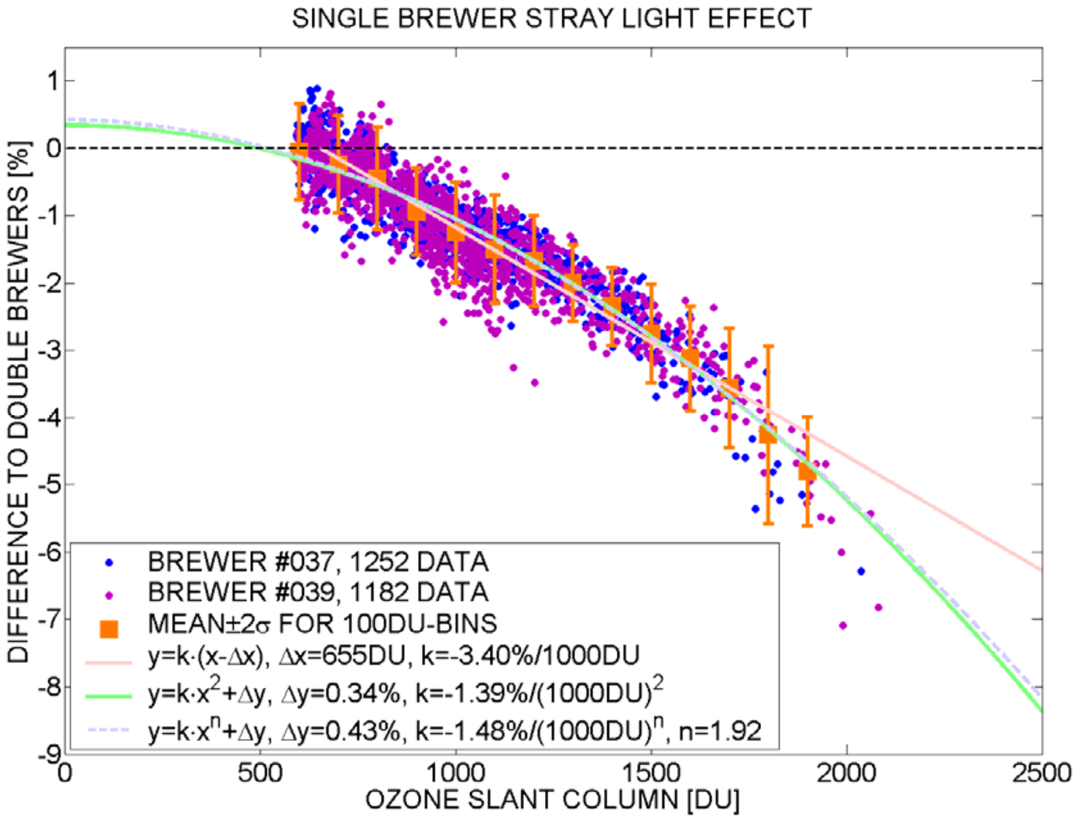
During SAUNA TO3EFF ranged from –56°C to –46°C



Instrumental stray light

Instrumental stray light (ISL):

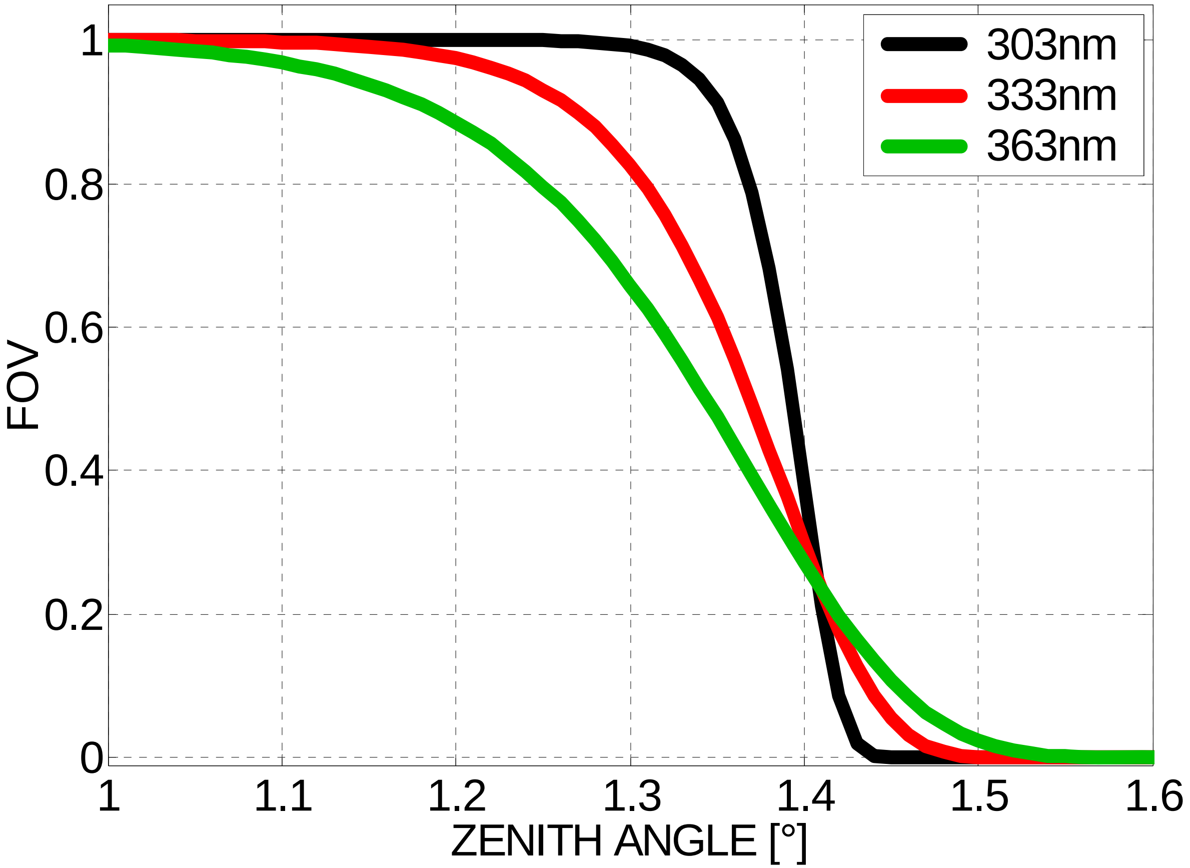
Due to not perfect slit function the measurements at one wavelength “leak” into those at other wavelengths. Since the stray light level of double Brewers is below 10^{-7} the ISL is negligible. For single Brewers (~$3x10^{-5}$) this is important.



Atmospheric scattered light

Atmospheric scattered light (ASL):

The Brewer's field of view (FOV) is about 2.7° full angle. Therefore a fraction of the diffuse radiance (circumsolar) is measured together with the direct irradiance. This signal-increase increases with the amount of scattering, i.e. mainly with SZA and aerosols. The net effect is an underestimation of the true ozone (see Bernhard et al. [2005]).



Summary systematic errors

Change in parameter	$O3_{MEAS}$-$O3_{TRUE}$=…	…for SAUNA
$w\tau^*_{SCA} \rightarrow w\tau^*_{SCA}$(Bodhaine)	-1.26×10^{-2} x $(\Omega_{O3}-\Omega_{O3CAL})$	-0.3 to –0.5%
$h_{EFFO3} \rightarrow h_{EFFO3}$+1km	<-0.2% @ SZA<75° -0.4% @ SZA=80°	-2km to -4km → +0.8 to +1.6% @ SZA=80°
$T_{EFFO3} \rightarrow T_{EFFO3}$+10°	+0.9% (Bass & Paur) +0.3% (GOME) -0.4% (Daumont)	-1 to -12°C → 0 to -0.9% 0 to -0.3% 0 to +0.4%
Different ozone cross sections		?
ASL		?
Total SAUNA	Use GOME-Temp-dep →	SZA<75°: -0.4 to +0.5% SZA=80°: 0.0 to +1.0%

Conclusions

- The optimal solution for the weights is usually a rather „smooth minimum“. Slightly different choices give nearly the same results.

- Using climatological data for TO3EFF and hO3Eff reduces the statistical uncertainty in the Brewer total ozone retrieval from ~3% to <2% (i.e sondes not needed)

-Using all 6 wavelengths reduces the uncertainty from ~1.6% to ~0.8% for SZA<75° (double Brewers only!).

- An empirical ISL-correction for single Brewers from SAUNA has been determined (ref next talk)

- The quantitative effect of ASL is not well known.

- To renew the Brewer algorithm using new parameters (e.g. other cross sections, different hO3EFF), the calibration data for each instrument are needed.

- Scattering cross sections should be calculated for each individual Brewer’s wavelengths and slit function.