Brewer and Dobson ozone retrieval and uncertainty sources

Alberto Redondas

REG(ULL) Spanish State Meteorological Agency / La Laguna University

April 15, 2015

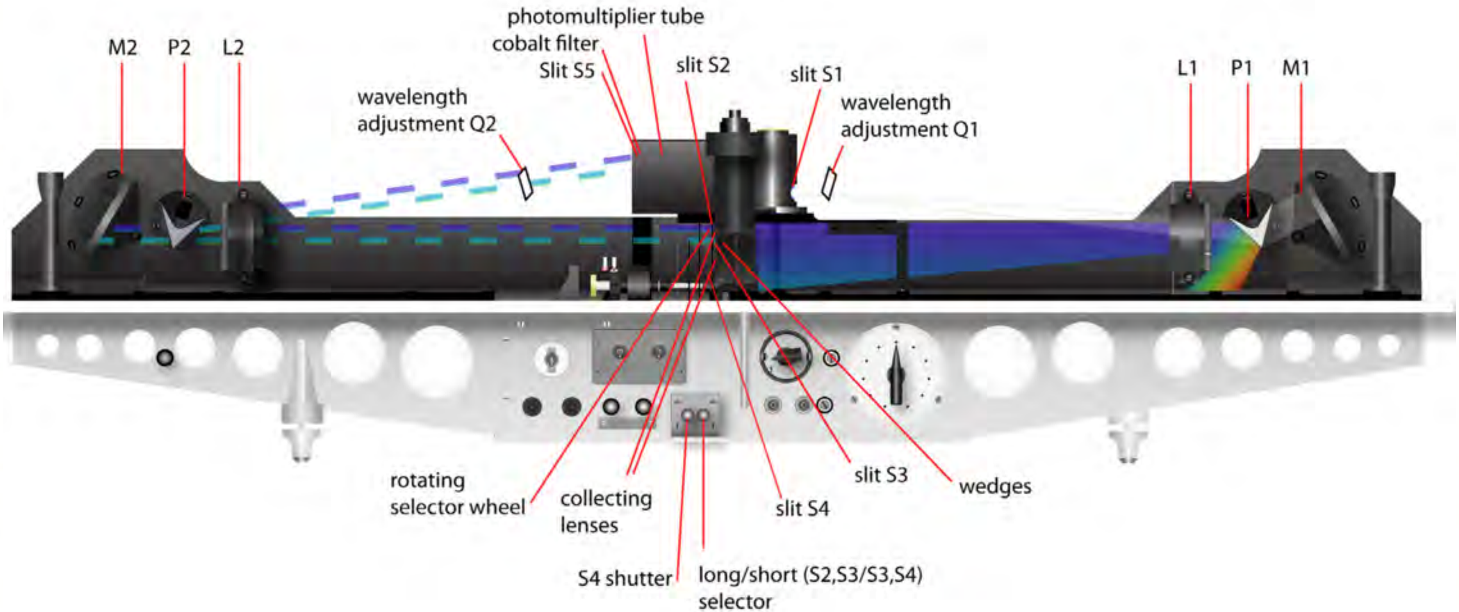
Introduction

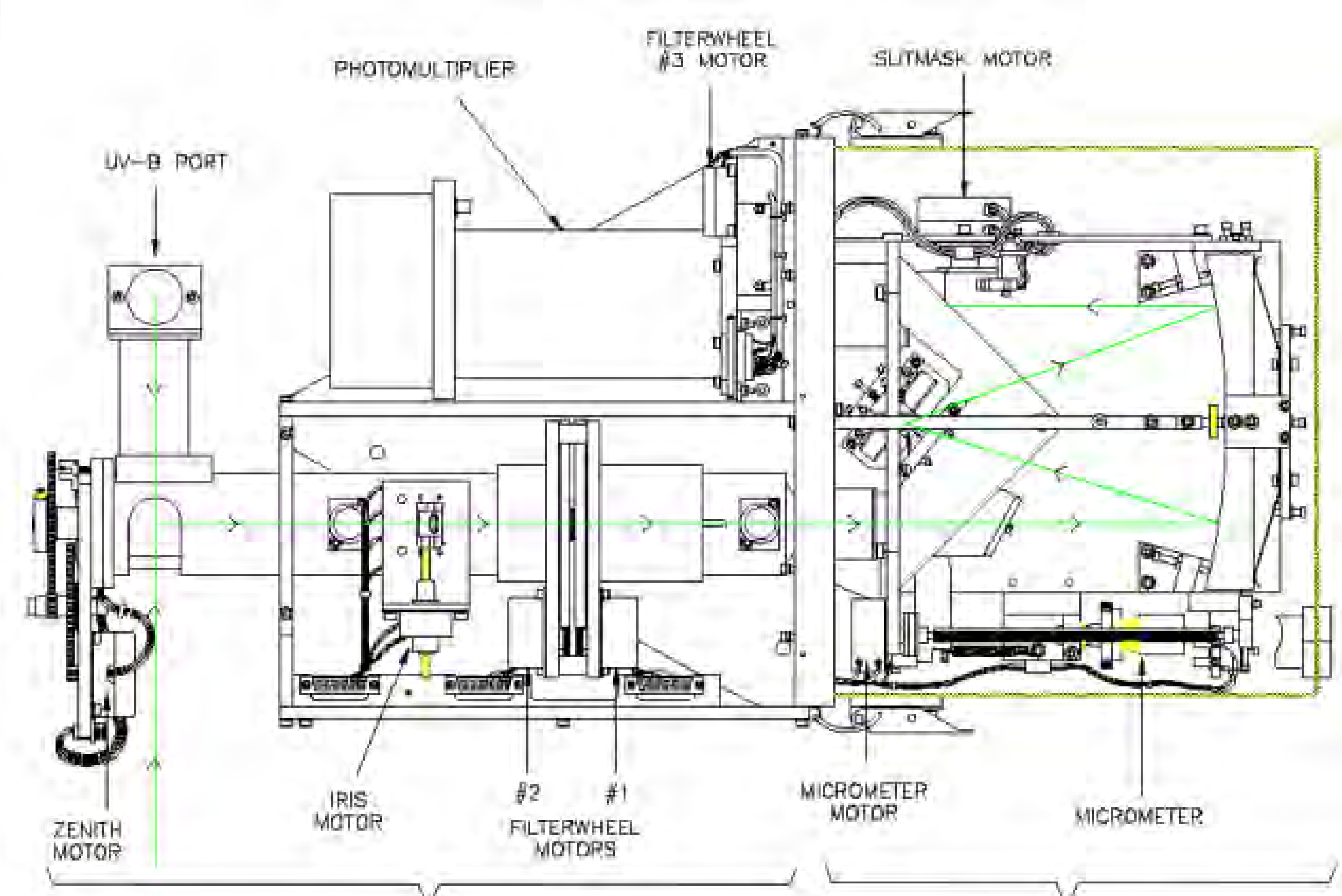
- The primary ground-based instruments used to report total column ozone (TOC) are Brewer and Dobson Spectrometers, in separate networks. These instruments make measurements of the UV irradiances, and through a well-defined process a TOC value is produced. Inherent in the algorithm is the use of a laboratory determined cross-section data set.
- The routine measurement of TOC started in the mid-1920s with a prototype of the Dobson instrument. A world-wide network grew up after the instrument re-design in 1947 and the International Geophysical Year in 1957.
- The Brewer Ozone Spectrometer was developed in Canada during the 1970s, and a commercial, automated version became available in the early 1980s.
- As observing organizations purchased these instruments and placed them in service alongside the Dobson instrument for long term measurements, the **seasonal and offset differences** in the results became evident.
- The Initial differences of 4% were removed with the adoption of Bass & Paur absorption coefficients. As measurements continued, a seasonal and offset difference was still evident

Introduction

- Measurements by both types of instruments are based on sun photometry and the TO3 is derived from the absorption of solar light in the Huggins band.
- The Dobson spectrophotometer is based on the measurements of the ratios of two wavelength pairs, while the Brewer spectrophotometer measures photoncounts at 5 wavelengths allowing the simultaneous measurement of ozone and of SO_2 column amount.
- For the separation of the wavelengths the Dobson instruments use 2 and the Brewer 5 slits.
- The field of view is 8º for Dobson and 3º for Brewer instruments.
- Dobson instruments have two prisms to separate the respective wavelengths, while Brewer instruments use one or two dispersive elements (holographic gratings).
- The Dobson assumes all the instrument have the same wavelengths and slits where the Brewer instruments are slightly different from instrument to instrument and determined during calibration.

Introduction




FILTERWHEEL
#3 MOTOR
PHOTOMULTIPLIER
SLITMASK MOTOR
UV-B PORT
ZENITH
MOTOR
IRIS
MOTOR
#2
#1
FILTERWHEEL
MOTORS
MICROMETER
MOTOR
MICROMETER

Dobson & Brewer Algorithm

The Dobson and Brewer ozone spectrophotometers measure solar direct irradiances at selected UV wavelengths. The ozone calculation in Dobson and Brewer can be summarized by this expression

$$X = \frac{N - B}{A\mu} \tag{1}$$

Where N is a linear combination of the logarithm of the measured spectral direct irradiances, extra-terrestrial (I_o) and ground (textbfI) at selected n wavelengths.

$$N = \sum_{i}^{n} w_i \log(\frac{I_i}{I{o_i}}) \tag{2}$$

A are the ozone absorption coefficient or Differential Cross Section (DXS) and B the Rayleigh coefficient, which are linear combinations of the ozone absorption (α) and Rayleigh molecular scattering (β), respectively, at corresponding wavelengths.

$$A = \sum_{i=1}^{n} w_i \alpha_i \tag{3}$$

$$B = \nu \frac{p}{p_o} \sum_{i=1}^{n} w_i \beta_i \tag{4}$$

All the instruments have a certain bandpass or slit function, the measured irradiances I , α_i and β_i are the convolution of the instrument slit function (S) with the corresponding cross sections (xs) or spectral irradiances.

$$\alpha_i = \frac{\int \sigma(\lambda)\, S_i(\lambda, \lambda')\, d\lambda}{\int S_i(\lambda, \lambda') d\lambda} \tag{5}$$

$$\int S_i(\lambda, \lambda') d\lambda = 1 \tag{6}$$

Finally the airmass is defined on the standard algorithm:

$$\mu_x = \sec\left\{\arcsin\left[\frac{R}{R+h_x}\cdot\sin(\theta)\right]\right\} \tag{7}$$

R : Earth Radius (6370km)

h_x : is the effective height set to $h_{sca} = 5km$ and $h_{O3} = 22km$)

θ : Solar zenith angle

$$\mu_x = \sec\left\{\arcsin\left[\frac{R}{R+h_x}\cdot\sin(\theta)\right]\right\} \tag{8}$$

$$\tag{9}$$

Calibration Constants

I_o : Extraterrestrial constant: Langley or transferred

$B, A,$: Are calculated and depend of the wavelength calibration

I : Solar irradiance are measured and depend of the instrumental calibration

μ : Are calculated

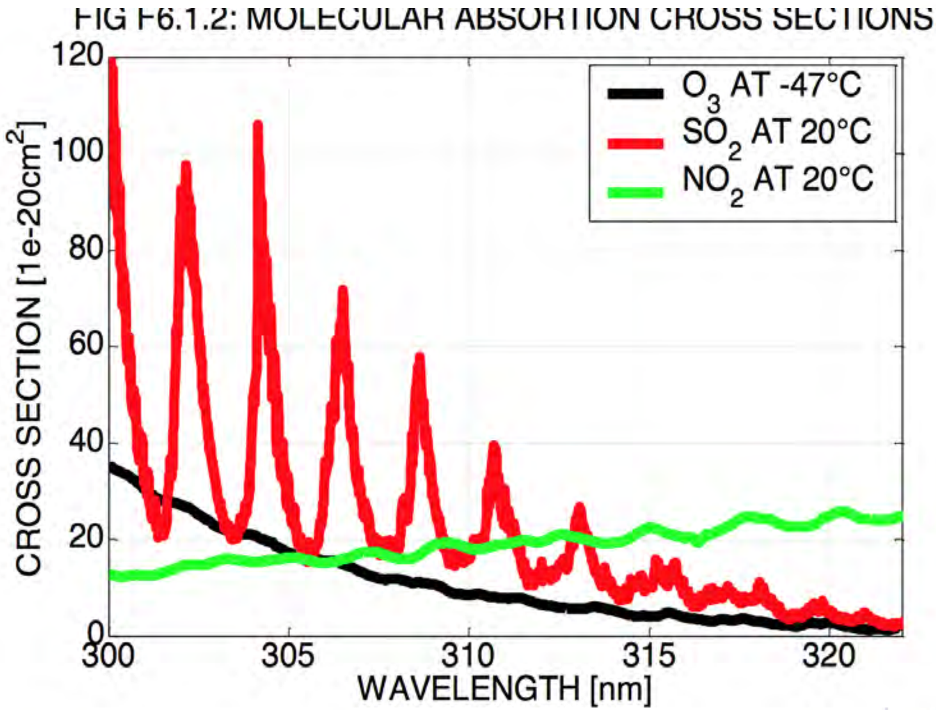
Table 1: Wavelengths and weighting coefficients used in the Dobson and Brewer operative algorithms.

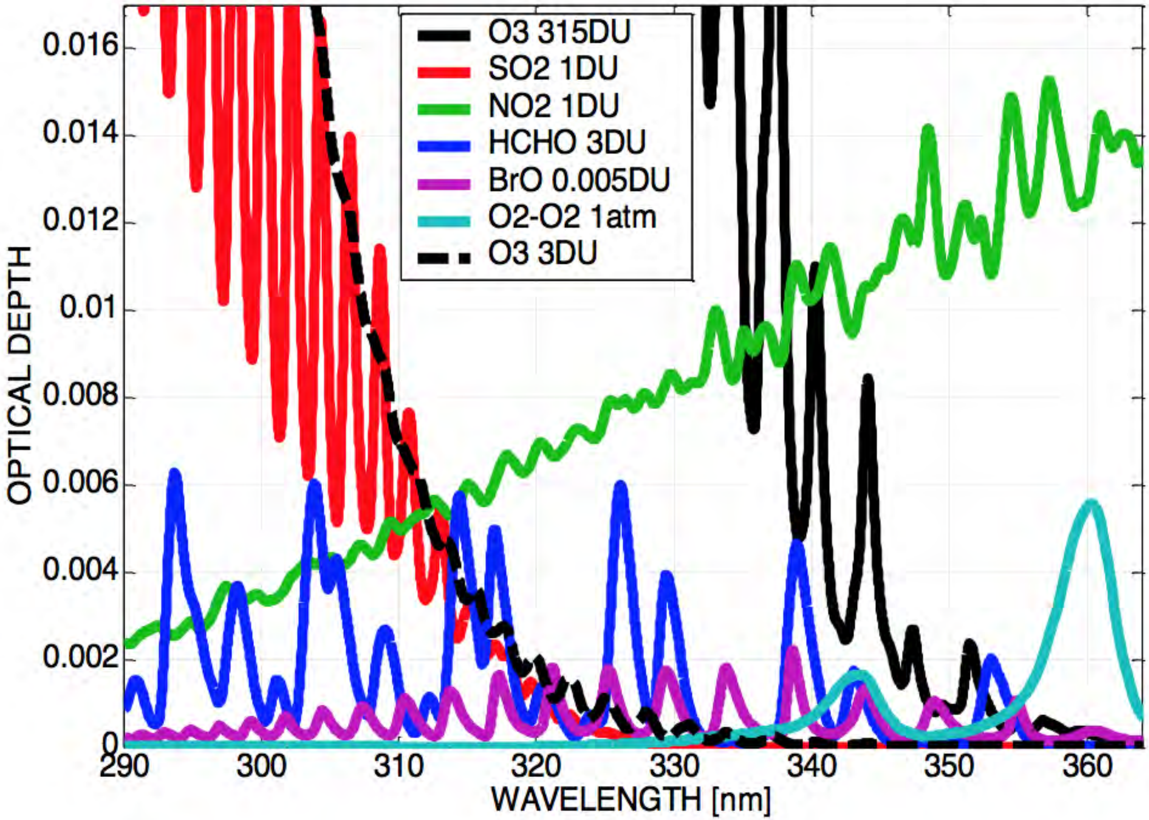
Brw slits	W	SD	FWHM	SD	w_i	Dobson slits	W	F	w_i
0	303.001				0	A1	305.5	0.9	1
2	306.301	0.014	0.548	0.016	0	C1	311.5	0.9	0
3	310.051	0.014	0.539	0.015	1	D1	317.5	0.9	1
4	313.501	0.015	0.555	0.012	−0.5	A2	325.0	2.9	−1
5	316.801	0.017	0.545	0.012	−2.2	C2	332.4	2.9	0
6	320.002	0.019	0.538	0.012	1.7	D2	339.9	2.9	−1

Algorithm asumptions

- Diffuse radiation is not considered $I_{measured} = I_{direct} + I_{diffuse}$
- Slits are parametrized, (no wings , no out-bands)
- Temperature in ozone cross section is set to constant value. (-44C / -45C Brewer)
- Height in the ozone layer is constant in Brewer /latitude dependent in Dobson.
- Rayleigh molecular scattering are fixed for all instruments (Bates 1984)
- Absorber profile is considered a delta at h effective.
- Additional absorbers are not considered ($SO_2, NO_2, HCLO$)
-

- XS are comparable but not the optical depth : $O_3 \approx 100 - 600 DU$, $SO_2 \approx 0 - 20 DU$, $NO_2 \approx 0 - 3 DU$.
- Brewer algorithm account for SO_2 but not Dobson.

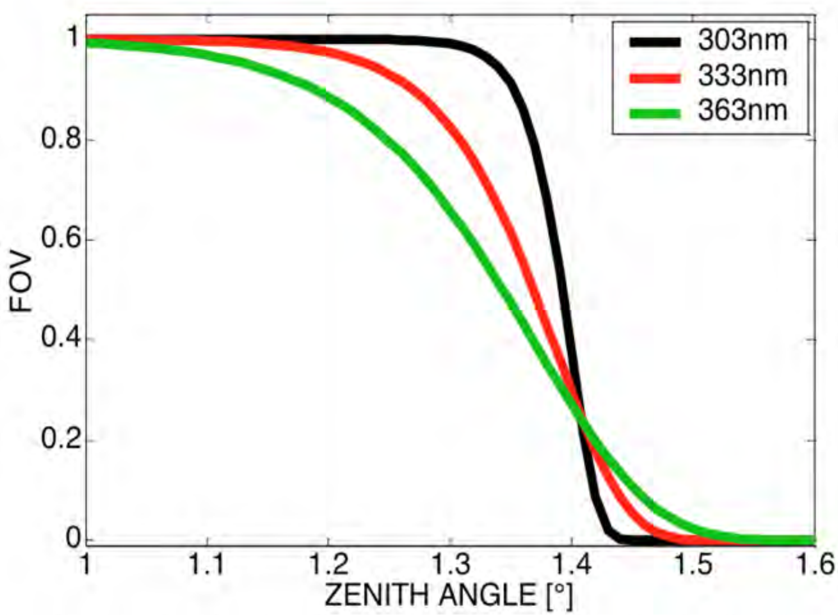




O3 315DU
SO2 1DU
NO2 1DU
HCHO 3DU
BrO 0.005DU
O2-O2 1atm
O3 3DU
OPTICAL DEPTH
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
290
300
310
320
330
340
350
360
WAVELENGTH [nm]

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] Arola et al [2004]).



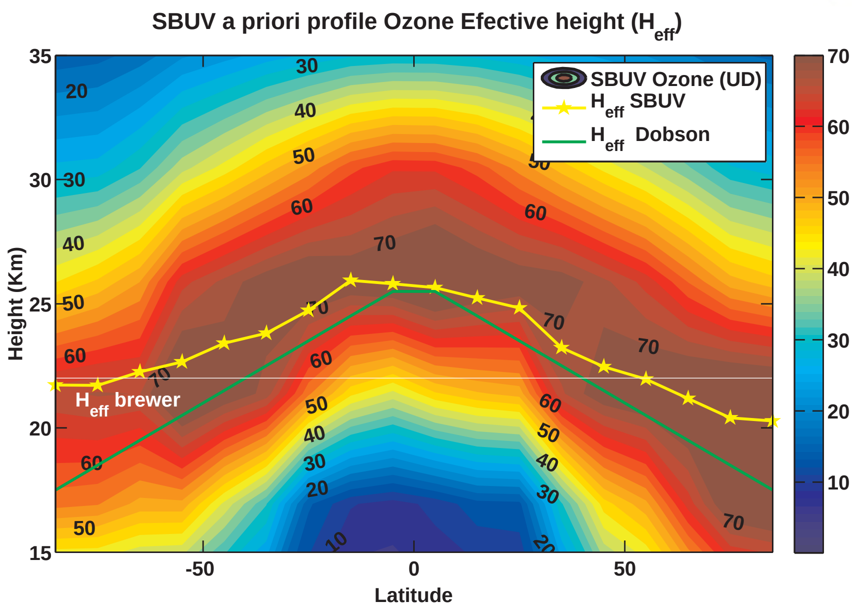
Ozone effective heigth

- We can define the effective height

$$h_{O_3} = \frac{\int_{Det}^{ToA} n_{O3}(h) \cdot h \cdot dh}{\int_{Det}^{ToA} n_{O3}(h) \cdot dh}$$

.

- Dobson mostly account for the observer variation but not Brewer.



Ozone cross section asumptions

The temperature dependence of the cross section is not considered (common temperature is assumed)

- Effective Temeperature

$$Teff_{O_3} = \frac{\int_{Det}^{ToA} n_{O3}(h) T(h) \cdot dh}{\int_{Det}^{ToA} n_{O3}(h) \cdot dh}$$

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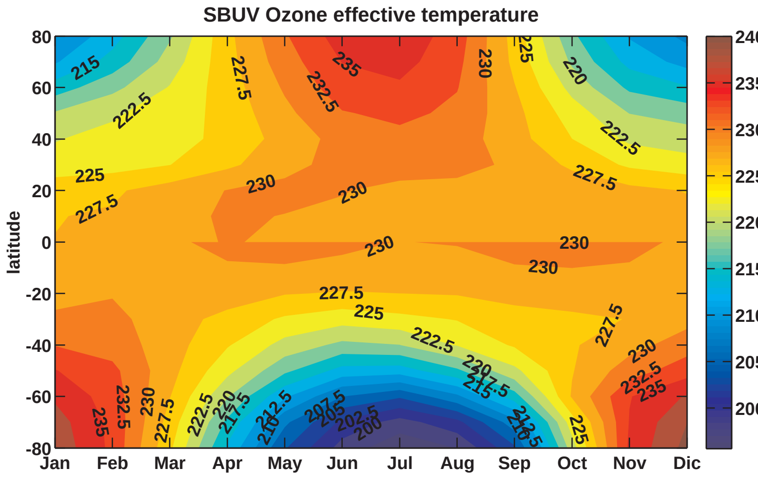
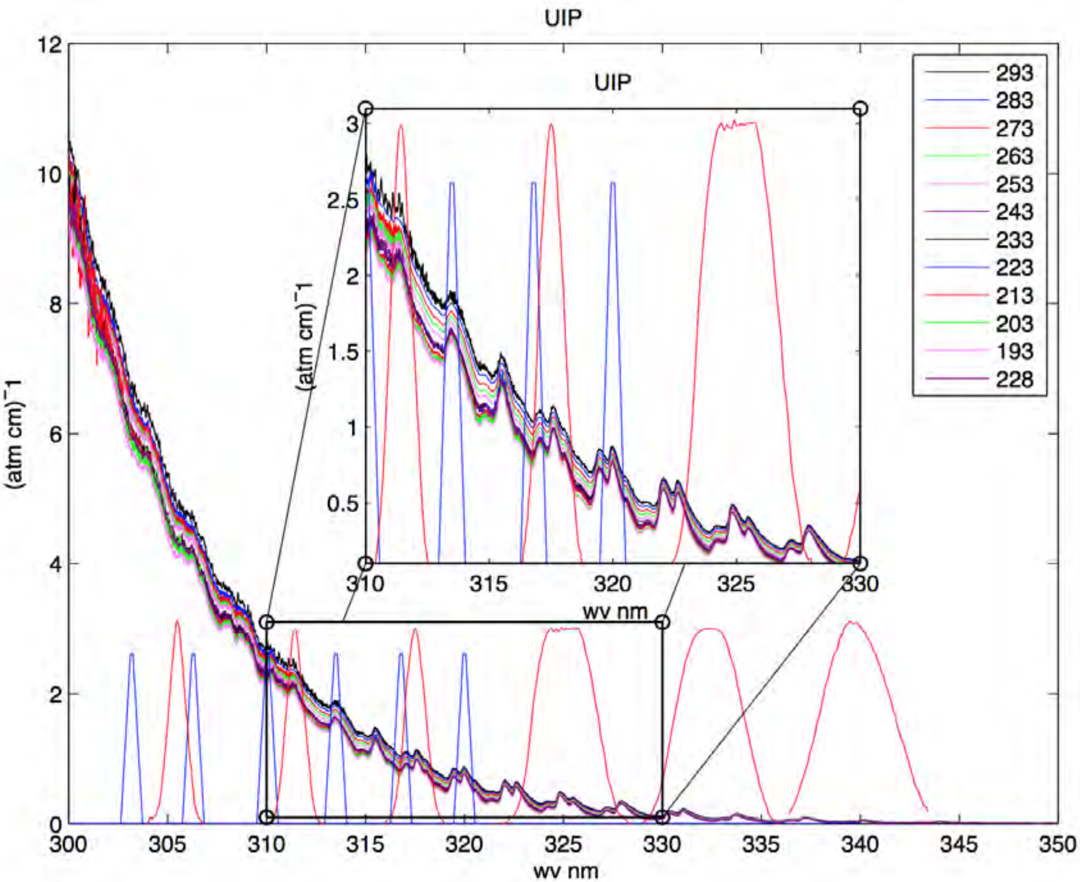
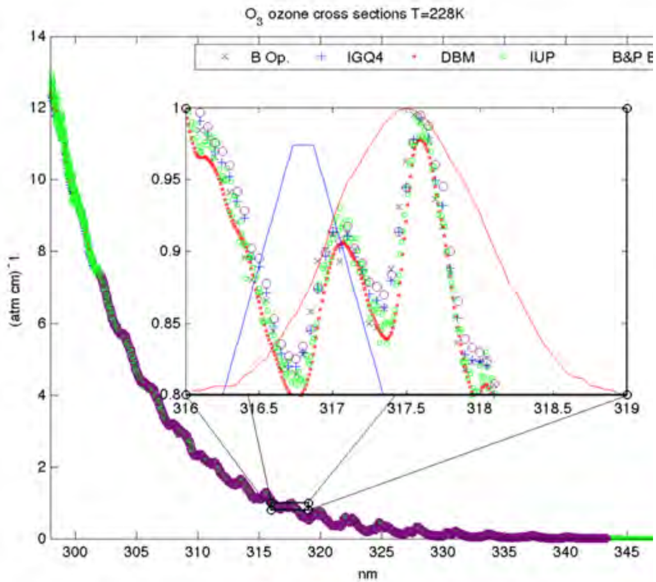


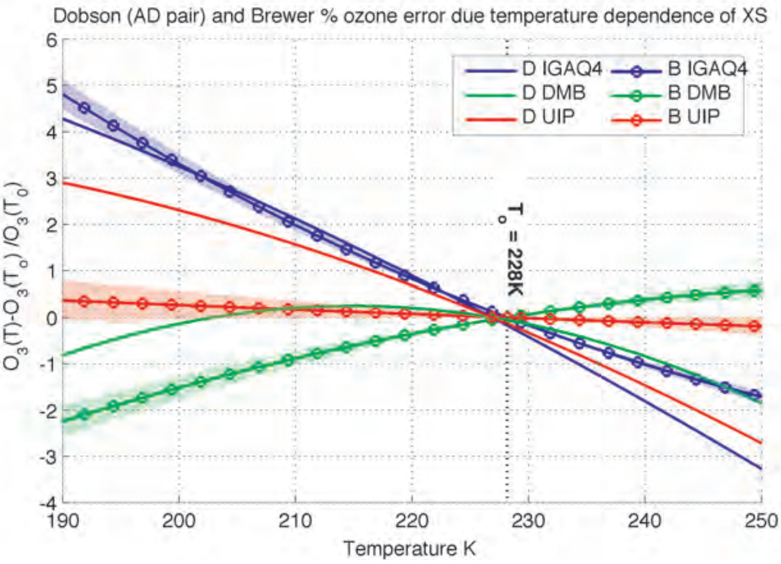
Ozone cross section asumptions

The temperature dependence of the ozone cross section is not considered.

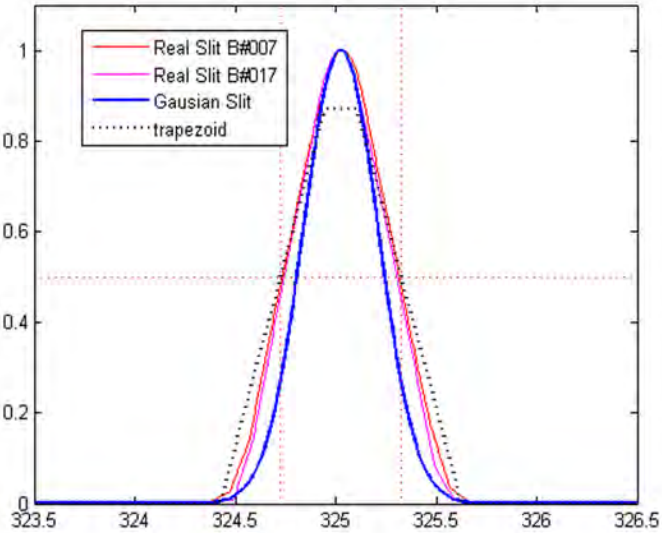


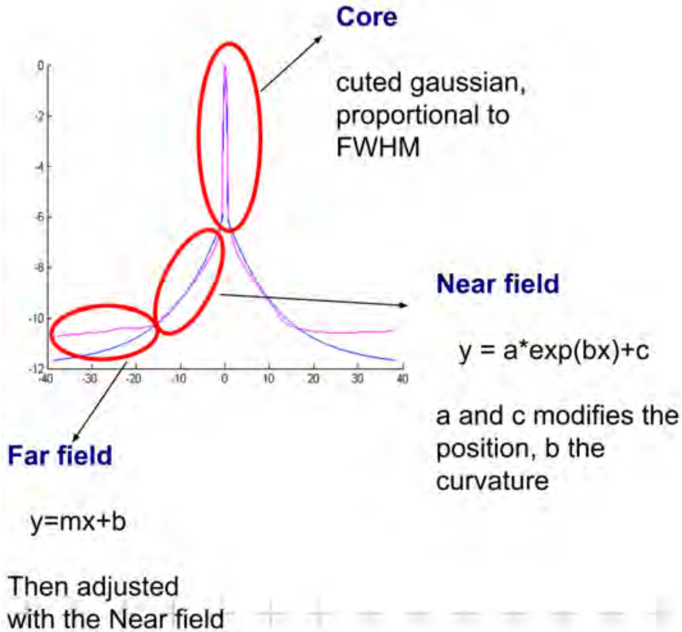
Different cross sections gives signifiant different scales and shows different temperature dependences





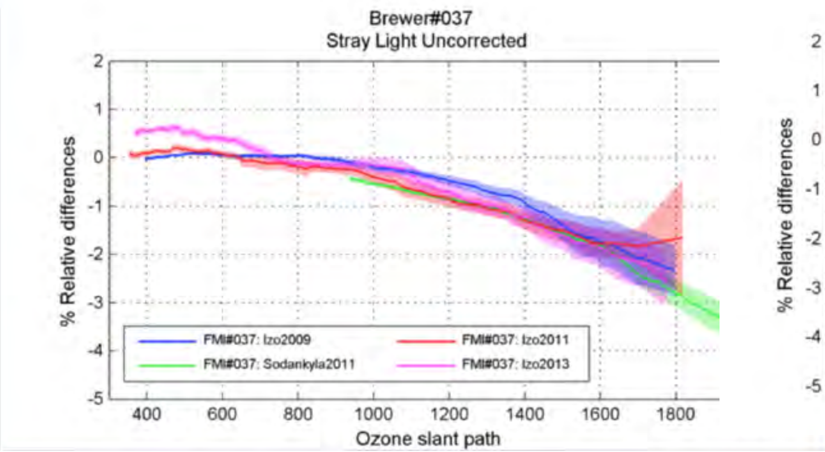
Slits are parametrized on the Brewer, trapezoidal with central wavelength and FWHM set for every instrument and every slit. For Dobson only reference instrument is available.

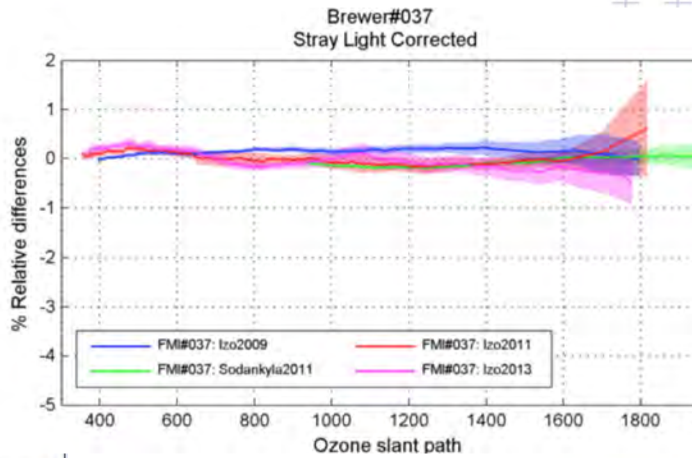




Stray Light

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.
An empirical correction were developed and can be transferred from calibrations and a model who use out of band measurements are also available.





Calibration transfer

Two methods of calibration has ben used : Two parameters calibration until year 2000 and one Parameter calibration after that.
Analysis of the errors due calibration transfer are not done yet.

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ETC=  Median   (MS9(inst)-   OSC(ref) * O3abs(inst)*10)
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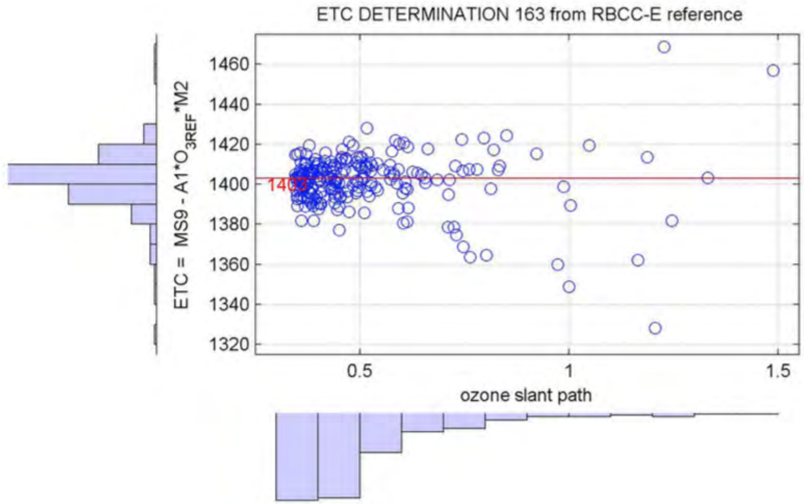
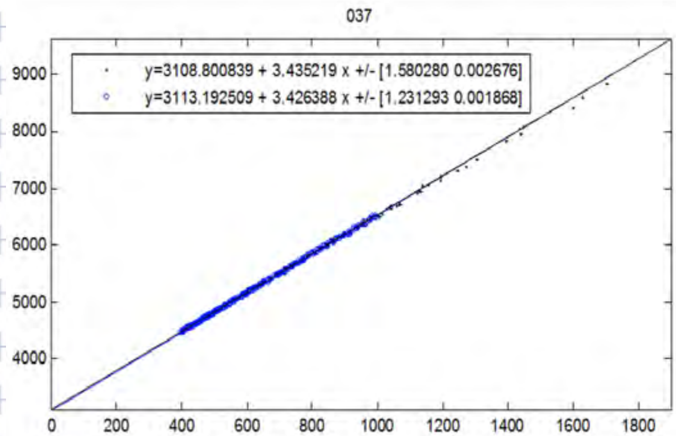
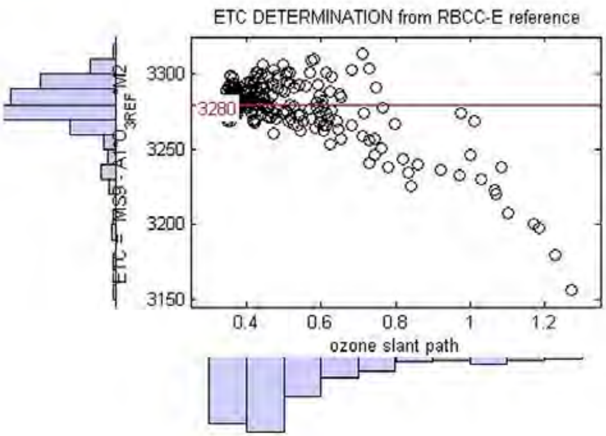


Two methods of calibration has ben used on Brewer : Two parameters calibration until year 2000 and one Parameter calibration after that.





Radiometric Calibration

Var	Abs uncertainty .	Rel u.	Remarks
q	$0.144^{\circ}{=}2.5$e-3rad		Registration time uncertainty of 30s
λ_i	0.006-0.023nm	$<0.007\%$	Independent value for all slits.
λ_i	0.01nm	0.00%	Slits are totally correlated
$\Delta fwhm$	0.004-0.019nm	0.64-3.24%	Independent value for all slits
R_c		4%	Estimated, slits are totally correlated
R_i		0.30%	For lab-calibration
R_i		0%-0.3%	Estimated Langley-calibration
ϵ_i	50s-1		Relative uncertainty depends on count

Brewer Operative Modes

	Ozone	**UV**
grating	Fixed at O3 position	Rotating
slit	6 quasi simultaneous	#1 and #5
FOV	$\approx 2^{\circ} - 3^{\circ}$	2π
Filter att.	ND automatic	ND fixed
Temperature	From Lamp ratios	Not implemented
Measurement	Relative (Ratios)	Absolute
Calibration	TravellingLangley	Lamp
QA/QC	Travelling RBCC-E	Travelling (QASUME)

Brewer Data Reduction

$$F_{oi} = \frac{2 \cdot (R_{ri} - R_{dark})}{Cy \cdot IT} \; countsseg$$

R_i : PMT readings

R_{dark} : Dark counts (slit #1)

Cy : Number of cycles (20 for DS) .

IT : Integration time (IT=0.1147 s) .

- The ozone measurement is done in "dynamic" mode, with a delay of the slit of dh=14ms.
- The measurement is done from slit 0 to 6 and backwards (2*IT/ slit)
- The PMT works in Photo Counting Mode

Brewer Data Reduction

$$f \equiv Count\ Rates\ , F = \log(f)$$

$$F_i = F_i + Af_{Filter\#} + CT_i * (Temp)$$

$$R6 = \sum_{i=1}^{4} w_i F_i$$

$$Af(\lambda) = Af + \lambda \Delta Af + ..$$

$$R6 = \sum_{i=1}^{4} w_i F + Af \sum_{i}^{4} wi + \Delta Af \sum_{i=1}^{4} w_i \lambda_i + Temp * \sum_{i=1}^{4} w_i CT_i$$

$R6$: Ozone Ratio.

Af : Filter attenuation

CT_i : Temperature coeffiicient slit i .

Brewer Data Reduction: Dead Time

Dead Time is a measure of how long the photo counting circuit is "dead", cannot count a second incoming photon. A Poison distribution is assumed for the probability P(k) of k incoming photons within a time τ.
The ratio of "detected" over true is approximated by

$$R = \frac{P(k=1)}{P(k \geq 1)} = \frac{\mu \cdot e^{-\mu}}{1 - e^{-\mu}} \approx e^{-\mu}$$

If N_M are measured photons and N_T are the "true"

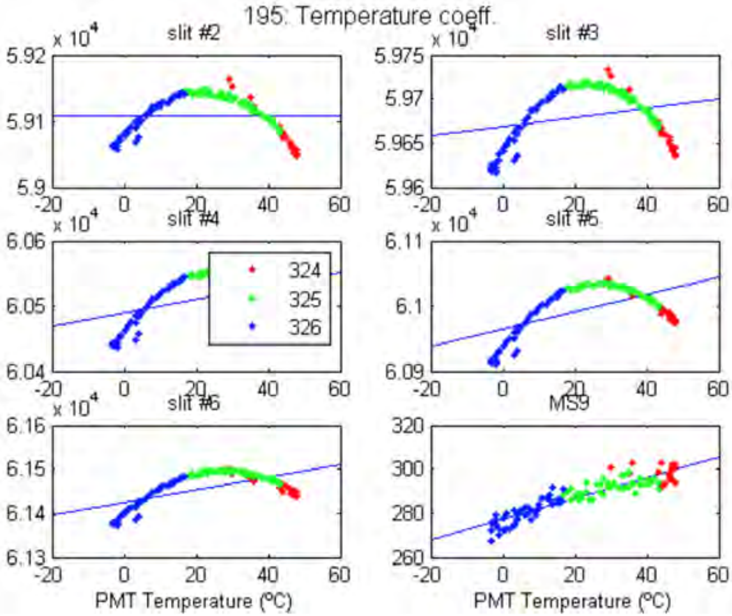
$$N_M = N_T \cdot R = N_T \cdot e^{-\mu} = N_T \cdot e^{-N_T \cdot \tau}$$

The Brewer software use this approximation for the correction and calculation of τ, assuming as a first guest $N_M = N_T$and iterating 9 times

$$N_T^{j+1} = N_M \cdot e^{N_T^j \cdot \tau}$$

- Dark count has no DT
- DT approximation .
- DT calculation (N3/N5)

- Method 1: Using internal lamp : Intensity changes not related with temperature
- Method 2: Climate Chamber (K&Z) frequent Hysteresis effect.
- During calibration campaings can only be checked



The Brewer software use only one number for the attenuation of the filter (neutral), but this number do not affect to the ozone calculation. As the measurement is done with an unique filter and the way the weights are defined $\sum_{i=1}^{4} w_i = 0$, the ozone ratio is not affected.
In a real instrument the attenuation is not neutral an can be considered linear, the condition $\sum_{i=1}^{4} w_i \lambda_i \approx 0$ is only an approximation and we see the efect of the filter on the ozone calculation.
This error can be easily corrected assuming the spectral dependence of the filter and correct for that.

$$R6(f\#) = R6 + \Delta A f \sum_{i=1}^{4} w_i \lambda_i$$

Direct Model (Brewer/Dobson)

$$F_{DIR} = F_0 \cdot \exp\left[-\mu \cdot \tau\right] \quad (10)$$

F_{DIR} : Direct sun irradiance (at wavelength λ).

F_0 : Extraterrestrial irradiance corrected for Sun-Earth distance.

τ : Total vertical extinction optical depth.

μ : Air mass factors

$$\mu \cdot \tau = \mu_{O_3} \cdot \tau_{O_3} + \mu_{SCA} \cdot \tau_{SCA} + \mu_{AER} \cdot \tau_{AER} + \mu_{SO_2} \cdot \tau_{SO_2} + \mu_{REST} \cdot \tau_{REST}$$

O_3, SO_2, SCA : O_3 and SO_2 absorption, Molecular scattering

AER, REST : Aerosol extinction and everything else. . . (NO2, HCHO, . . .)

$$\ln I_{DIR} = \ln I_0 - \mu_{O3} \cdot \tau*_{O3} \cdot \Omega_{O3} - \mu_{SCA} \cdot \tau_{SCA} - \ldots$$

$$\mu_{AER} \cdot \tau_{AER} - \mu_{SO2} \cdot \tau*_{SO2} \cdot \Omega_{SO2} - \mu_{REST} \cdot \tau*_{REST} \cdot \Omega_{REST}$$

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

Ω_x : Total Column for gas x

$\tau*_x$: Optical Depth for 1DU.

Direct Model (Brewer/Dobson

$$\Omega_{O_3} = \frac{\ln I_{DIR} - \ln I_0 - \mu_{SCA} \cdot \frac{p}{p_o} \cdot \tau_{SCA} - \mu_{aer} \cdot \tau_{aer} - \mu_{SO_2} \cdot \tau^*_{SO_2} \cdot \Omega_{SO_2} - \mu_x \cdot \tau^*_x \cdot \Omega_x}{\mu_{O_3} \cdot \tau * O_3}$$

p : Station pressure

p_o : Standard pressure

$$\mu_x = \sec\left\{\arcsin\left[\frac{R}{R + h_x} \cdot \sin(\theta)\right]\right\}$$

R : Earth Radius

h_x : Effective height abs x.

θ : Solar zenith angle

Direct Model (Brewer/Dobson

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

Parameter	Source	
P1-P2	μ_x	$h_{O_3} = 22km, h_{SCA} = 5km,$
P3-P5	μ_x	$h_{AER} = 2km, h_{SO_2} = 2km, h_{REST} = 2km$
P6	lnF_o	Assume obtained by Langley extrapolations at high mountair
P7	lnF_{DIR}	Measured corrected count rates (ISL, ASL!)
P8	$\tau^*_{O_3}$	Use Bass Paur [1985] cross sections, $(Teff_{O_3} = -45^\circ C)$
P9	τ^*_{SCA}	Use Bodhaine et al. [1999], standard pressure
P10	τ^*_{aer}	Assume Angstrom behavior
P11	$\tau^*_{SO_2}$	Use Vandaele et al. [1994] cross sections and $\Omega_{SO_2} = 1DU$
P12	τ^*_{REST}	$\Omega_{NO_2} = 0.7DU and \Omega_{HCLO} = 1DU$ and ... (=urban polluted)

Direct Model (Independent Variables)

I	Var		Remark
V1	θ	0.12° (0.01°)	Assume 30s registration time uncertainty (
V2	RAD	4%	Radiometric calibration (all slits)
V3	RADIND	0%	Radiometric calibration for each slit, I-inde
V4	F noise	Figure	Photon count noise, I-independent
V5	$\Delta\lambda$	0.01nm (0.004nm)	Wavelength shift, (directly after Hg-test)
V6	$Teff_{O_3}$	20° (5°, 1°)	Effective Temp. O_3 temperature (5° climat
V7	P/P0	1% (0.1%)	Surface pressure (if measured)
V8	τ_{340}	0.75 (0.04)	AOD at 340nm (if measured)
V9	α_{340}	0.7 (0.1)	Angstrom parameter at 340nm (if measure
V10	Ω_{SO_2}	100%	Total SO2 column
V11	Ω_{REST}	100%	Total column of other gases (mainly NO2)
V12	h_{O3}	5km (2km, 0.5km)	Eff O3 height (2km climatology, 0.5km son
V13	h_{SCA}	0.2km	Effective scattering height
V14	h_{AER}	4km	Effective aerosol height
V15	h_{SO_2}	10km	Effective SO2 height
V16	h_{REST}	10km	Effective height of other gases

$$\Omega_{O_3} = \frac{\ln I_{DIR} - \ln I_0 - \mu_{SCA} \cdot \frac{p}{p_o} \cdot \tau_{SCA} - \mu_{aer} \cdot \tau_{aer} - \mu_{SO_2} \cdot \tau^*_{SO_2} \cdot \Omega_{SO_2} - \mu_x \cdot \tau^*_x \cdot \Omega_x}{\mu_{O_3} \cdot \tau * O_3}$$

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

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

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

Direct Model (Brewer #171 results)

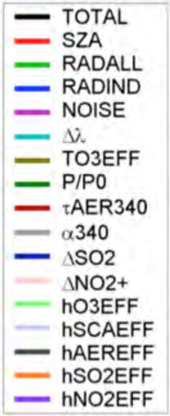
Total ozone from single wavelength

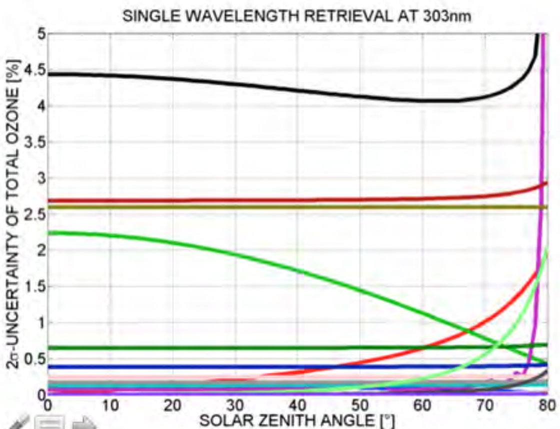
Small improvement

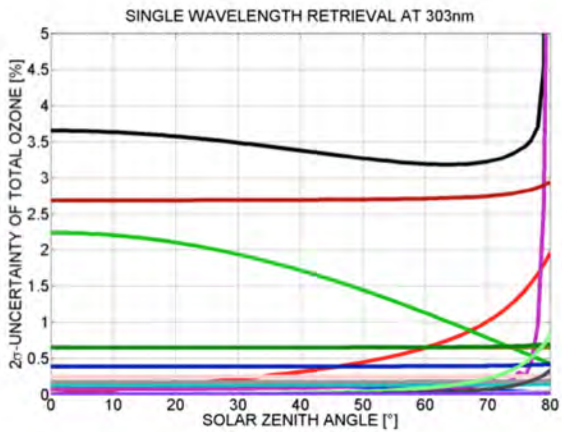
→ Down to ~4% uncertainty

Problems: AOD, noise, absolute radiometric calibration

→ Use more wavelengths







Direct Model (Brewer #171 results)

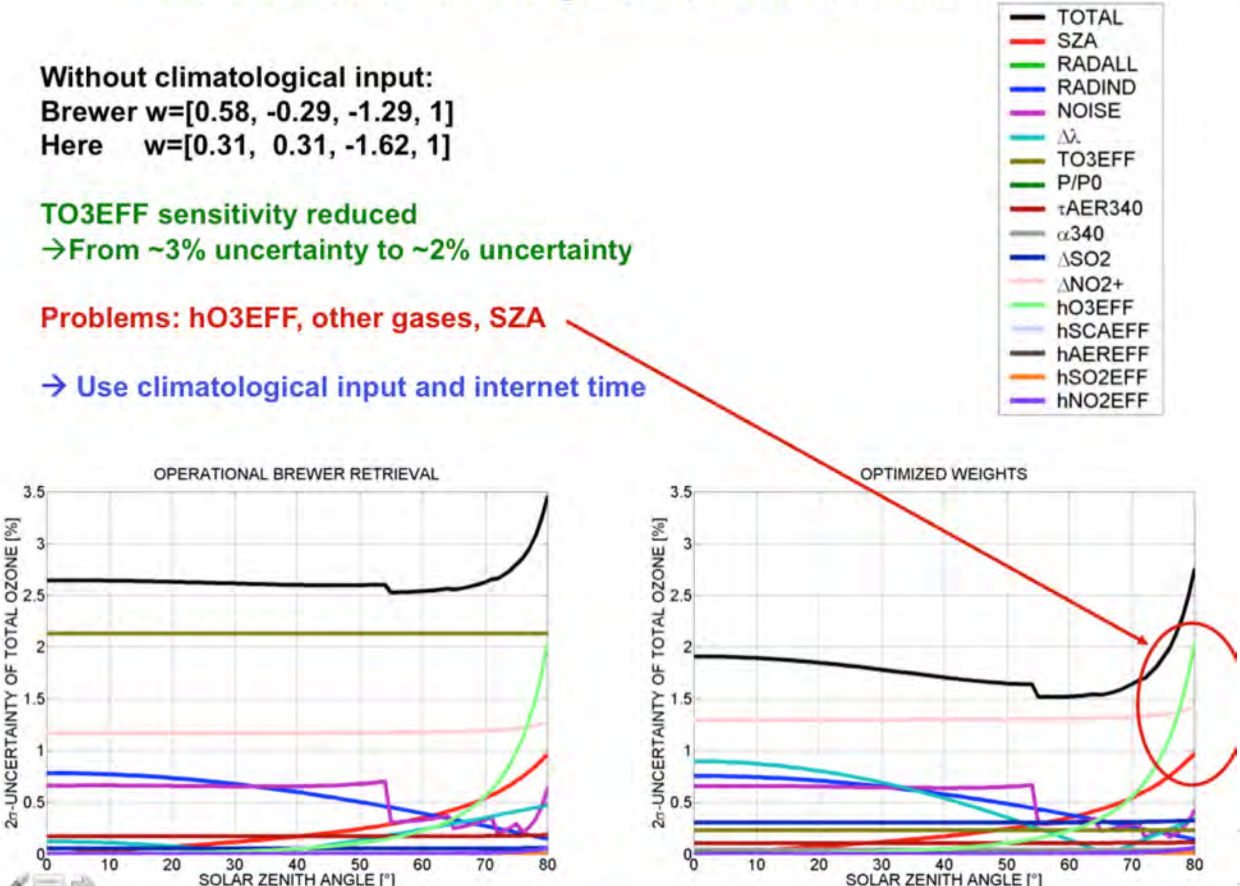
Total ozone from 4 wavelengths 310, 313, 317, 320nm

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



Direct Model (Brewer #171 results)

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

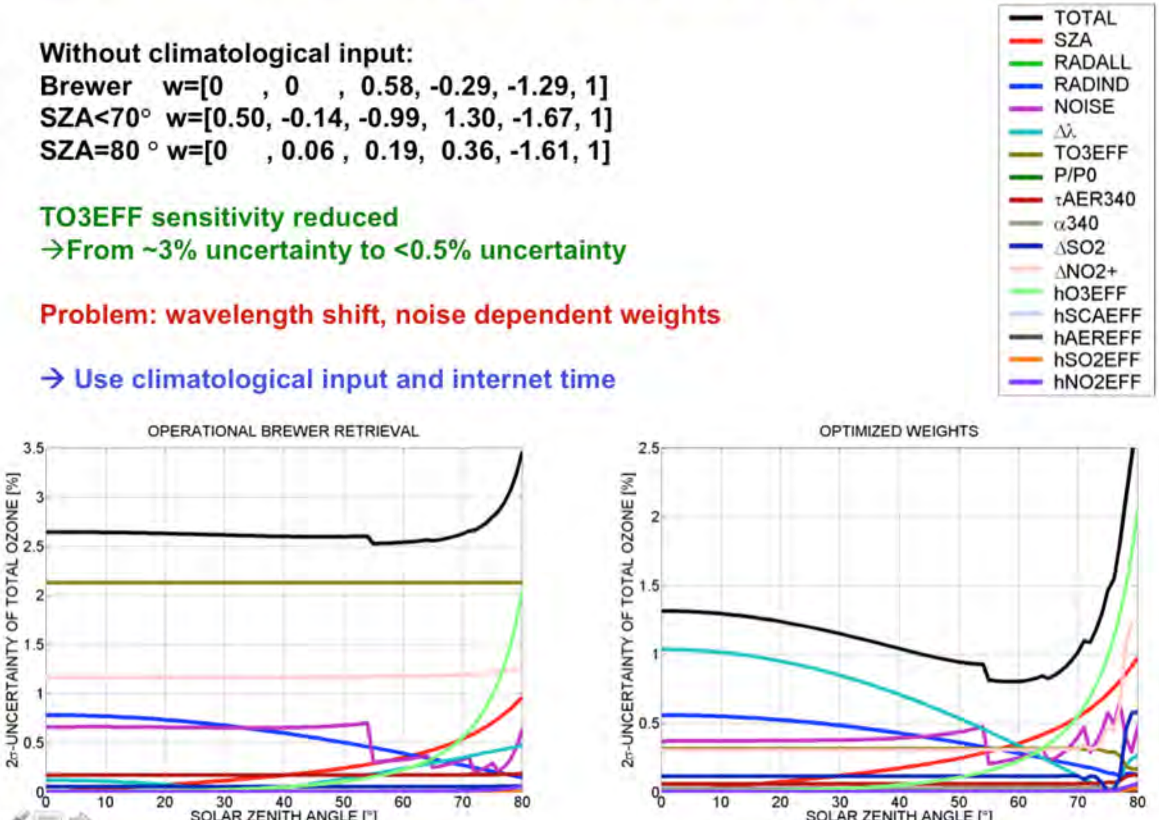
Without climatological input:

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



Future works

- Radiometric calibration need to be revised.
- Wavelength calibration
- Langley and Calibration transfer errors has to be addresed.
- Stray Light
- EUBREWNET database can be used to get the error parameters several instruments.