Effect of the Ozone Cross section in Total Ozone in Dobson and Brewer Algorithms

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- 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.

- 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

Summary

1. We used five ozone cross section data sets : three B&P; Daumont, Malicet & Brion (DBM); and the new University of Bremen set (IUP).

2. The ozone absorption coefficients for Brewer and Dobson are calculated using the Brewer-Dobson operative method.

3. Dobson & Brewer Algorithms use a fixed temperature of the ozone layer, the error due this assumption is analyzed.

4. We apply these calculations to two existing dataset
   - Langley Calibration of Reference Instruments
   - Arosa Payern Brewer-Dobson and ozonesoundings record

Dobson & Brewer Algorithm

The Dobson and Brewer ozone spectrophotometer 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 (I) at selected n wavelengths, 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.

$$N = \sum_i^n w_i \log(\frac{I_i}{Io_i}), \quad A = \sum_{i=1}^n w_i \alpha_i \quad B = \nu \frac{p}{p_o} \sum_{i=1}^n w_i \beta_i$$

Where α_i and β_i are the convolution of the instrument slit function (S) with the corresponding cross sections (xs).

Calculation

- The ozone absorption coefficient is calculated using the Brewer operative method witch is the same that 'approximation method' used by Berhard for Dobson in 2005.

$$\alpha_i = \frac{\int \sigma(\lambda)\, S_i(\lambda, \lambda')\, d\lambda}{\int S_i(\lambda, \lambda') d\lambda} \qquad (2)$$

  - S is the instrument slit function for the corresponding wavelength
  - σ the ozone cross section at `Fixed` temperature, -46.3 C for Dobson Network and -45C for Brewer instruments

- The Dobson's assume that all the instrumets have the same slit function and wavelength center as reference instrument #083.

- Brewer network every instrument have a mesured slit and central wavelengths calculated during calibration.
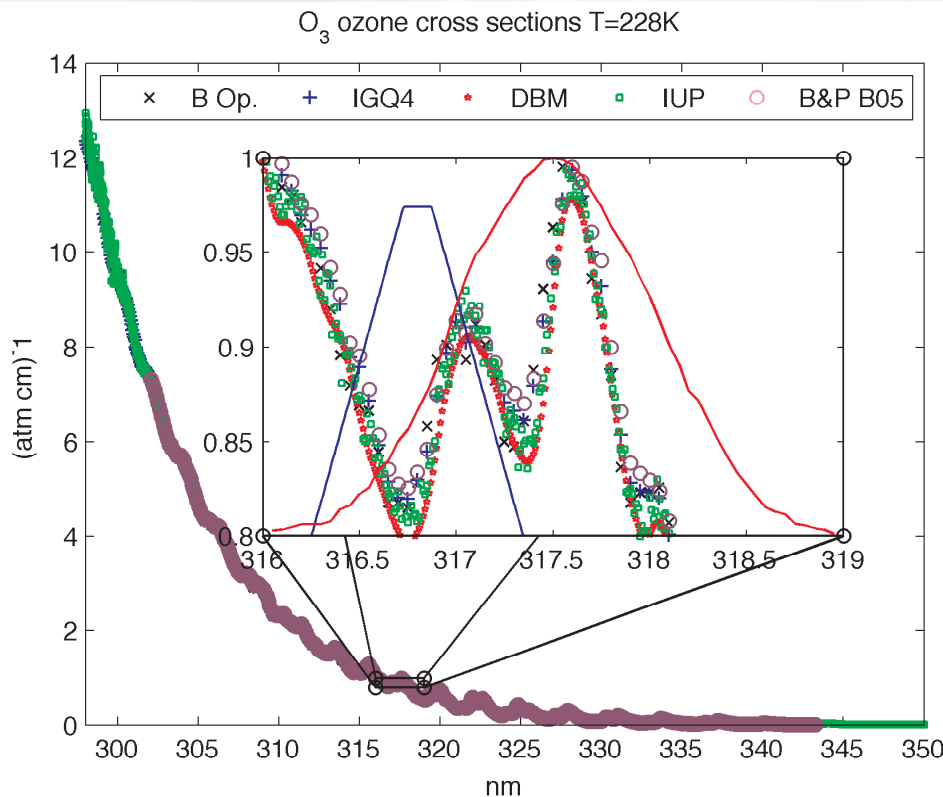
Figure 1 : Studied XS at 228K and slit functions of Brewer and Dobson

- Three Bass &Paur cross sections:
    - **Brewer Operative (BOp)** : Is the B&P at 228K without any adjustment. 'Not available at IGACO but at -Mainz Spectral Database-.
    - **IGACO B&P IGQ4**
        - Individual temperatures: Six individual temperatures. This files do not agree with B&P paper and do not include -45 C set. This dataset appears to be spectra at selected temperatures calculated from the polynomial fitted to the original data excluding 218K (Weber 2011),
        - **Quadratic coefficients on the file "Bp.par"** Used In this work to be consistent with the Komhyr determination of Bass & Paur on Dobson.
    - **Berhard 2005 (B05)**, B&P corrected by temperature dependence and extended with Molina & Molina cross section. Includes **dynamical** effects convolving the XS with temperature profile and ozone profile and top of the atmosphere solar spectrum.
- **Daumont, Brion & Malicet (DBM)**, Measured at 5 temperatures, including 228K also we use the quadratic fit for the temperature dependence studies. We also use the Liu 2007 quadratic fit excluded the 273°K set .
- **Serdychenco et all (IUP)**, The newly determined data set from Bremen University, Institute for e Enviromental Physics (IUP) are also available at IGACO with ten temperatures files and the quadratic fit **(IUPQ)**.
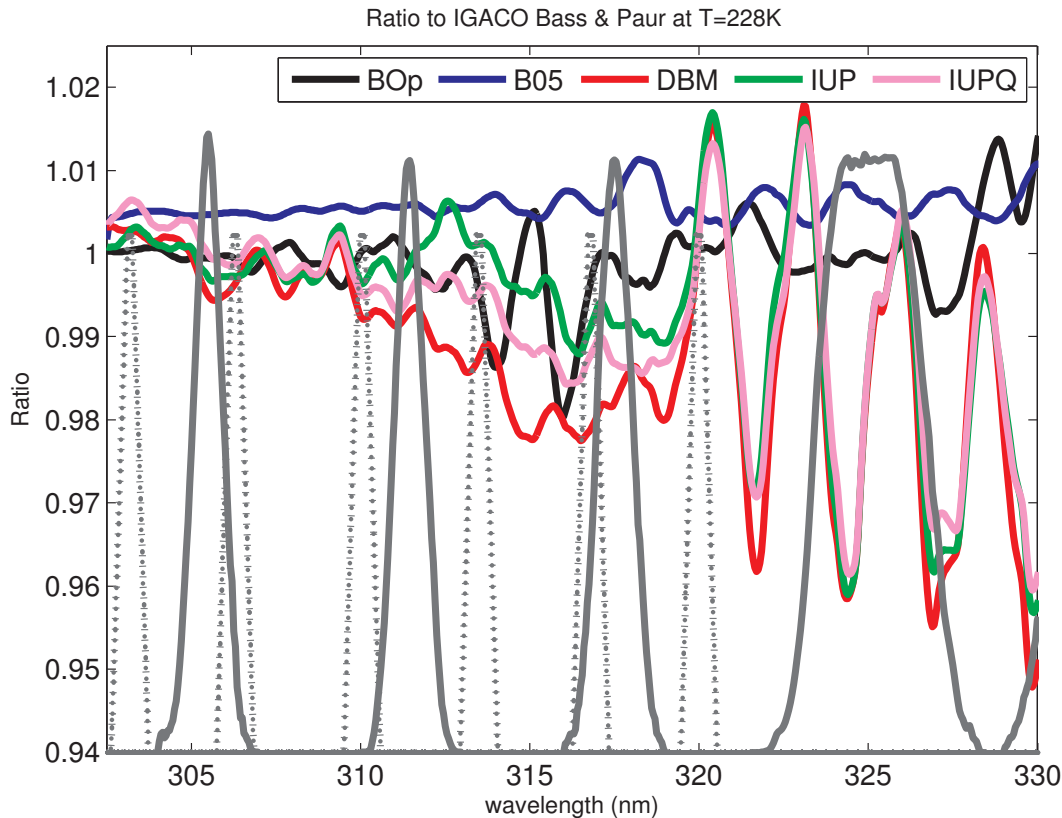
Figure 2 : Ratio of the cross-sections of this study to the IGACO Bass & Paur (IGQ4) , the cross section are interpolated to a common resolution (0.1 nm) and smoothed to the Brewer resolution

Dobson Operative Algorithm

Comparison with the operational values

- The AD pair change is $+1\%$ with a little variation with XS.
- The CD pair from $+1.7\%$ (IGQ4) to $+0.8\%$ (IUP).
- We check the methodology with Berhard05, our results agreed with his published results whithin 0.15%.

Table 1 :   Change in Dobson calculated Ozone for the Double wavelength pair combinations from the standard Absorption coefficients to one derived from the various cross section data sets

Wv	Measured slit			Prior Determinations			
set	IGQ4 B&P	DBM	IUP	Komhyr approx	Komhyr	Bernhard approx	Bernhard
AD	0.9%	0.7%	0.8%	-0.1%	-0.5%	0.3%	0.3%
CD	1.7%	1.5%	0.8%	-0.7%	-1.5%	0.9%	0.9%

Brewer operative Algorithm

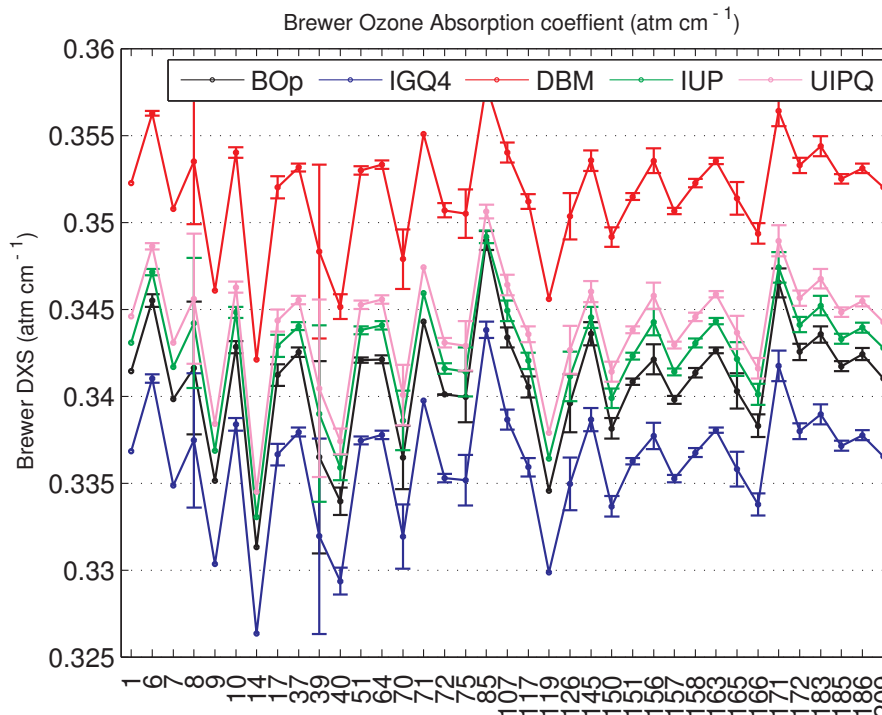- RBCC-E data set: 123 wavelengths calibration performed on 33 instruments.

Figure 3 : Brewer ozone absorption coefficient or diferencial cross section (DXS) for the Brewers of the RBCC-E set, the values is the mean and the bars indicate de standard desviation, for the analyzed cross sections. Brewer labeled as #1 is the

Brewer Operative Algorithm

- UIP Serdyuchenko data set changes the calculated TOC by -0.5%
- UIPQ quadratic fitted changes the caluclated TOC by -0.9%
- DBM data set changes the calculate TOC by -3.2%
- IGQ4 data set at -45C changes the calculated TOC by +1.3%

Table 2 : Statistics of the RBCC-E dataset

	IGAQ	DBM	IUP	IUPQ
Mean	0.987	1.032	1.005	1.009
Std	0.001	0.002	0.001	0.001

Table 3 : Ratio of the DXS to operative, comparative study

	R.06	R.09	Savastiouk10	Scarnato09			This Work
Brewer	#185	#157	set average	#040	#072	#156	set average
DBM	0.970	0.969	0.970	0.939	0.917	0.933	0.969
Burrows	0.978	-	-	1.087	0.947	1.009	-

The ozone absorption coefficient is calculated from the ozone absorption cross section and the ozone and the temperature vertical profile:

$$\alpha(\lambda) = \frac{\int \sigma(\lambda, T(z)) X(z)\, dz}{\int X(z)\, dz} \qquad (3)$$

We use a simplest approach of Komhyr93 based on

1. The temperature dependence of the cross section is approximated by a quadratic polynomial.

$$\sigma(T) = c_o + c_1 T + c_2 T^2 \qquad (4)$$

2. The effect of the temperature and ozone profile is simplified by the introduction of the effective temperature.

$$T_{eff} = \frac{\int_{z_o}^{\infty} T(z)\, X(z)\, dz}{\int_{z_o}^{\infty} X(z)\, dz} \qquad (5)$$

The effective absorption coefficient is therefore

$$\alpha_i(T_{eff}) = C_{io} + C_{i1} * T_{eff} + C_{i2} * T_{eff}^2 \tag{6}$$

Where the coefficients C are

$$C_{ij} = \frac{\int c_j(\lambda)\, S_i(\lambda, \lambda')\, d\lambda}{\int S_i(\lambda, \lambda') d\lambda} \tag{7}$$

and finally the absorption coefficient

$$\alpha(T) = \sum_{i=1}^{n} w_i \sum_{j=0}^{2} C_{ij} * T^j$$

$$= \sum_{i}^{n} w_i C_{io} + T \sum_{1}^{n} w_i C_{i1} + T^2 \sum_{i=1}^{n} w_i C_{i2} \tag{8}$$

The temperature dependence is expressed as the gradient of the XS.

$$\frac{\Delta A}{\Delta T} = \sum_{i=1}^{n} w_i \left[C_{i1} + 2 * C_{i2} * T \right] \tag{9}$$

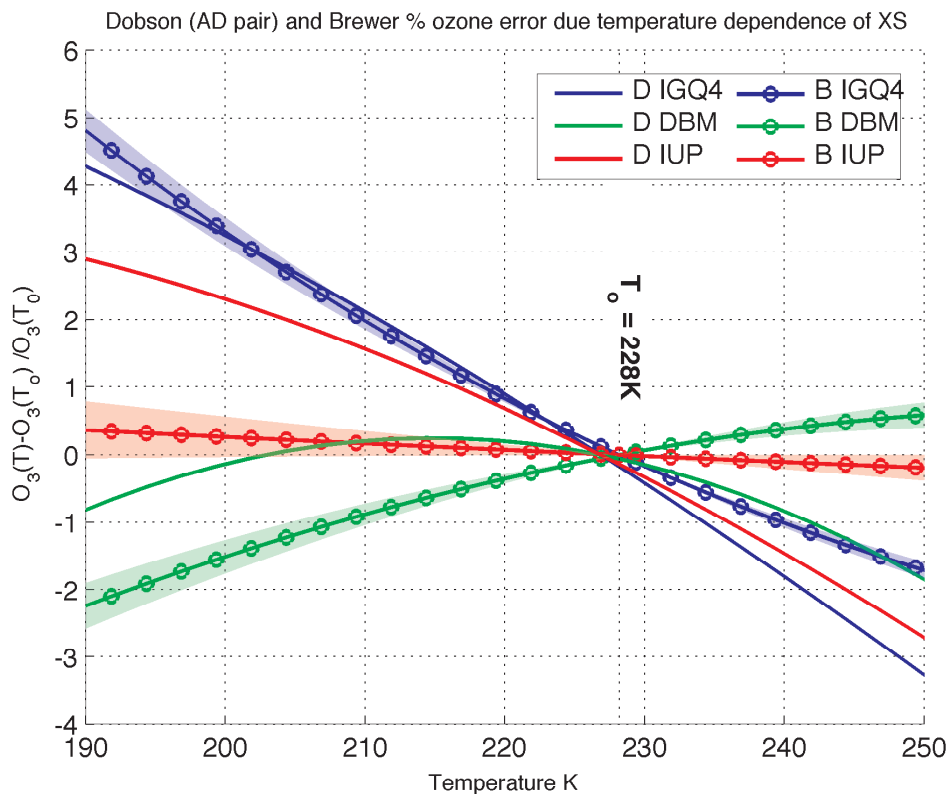Dobson (AD pair) and Brewer % ozone error due temperature dependence of XS

Figure 4 : Dobson AD pair and Brewer (average and shadowed the standard deviation of the RBCC-E set) total ozone error due temperature dependence of the XS. In a cooler

Brewer Dobson temprature dependence

- The calculated IUP temperature dependence for the Brewer is very low,less than 0.01%. For the Dobson, the value is smaller than that Komhyr 93.

- The calculated DBM temperature dependence is a small negative value for the Brewer,but is a small positive value for Dobson.

- The calculated B&P temperature dependence for Brewer is lower than Dobson.

Table 4 :   Temperature dependence Dobson and Brewer previous studies in %/K

%/K	Kerr 1998		Kerr 2002	Rozendael		Scarnato			
Inst.	Dob	#008	#014	Dob	Brw	Dob	#040	#072	#156
B&P	0.13	0.07	0.094	0.13	0.11		0.081	0.099	0.088
DBM						-0.11	-0.131	-0.12	-0.128

%/K	Scarnato			Redondas.	Fragkos	This work	
Inst	#040	#072	#156	#185	#005	Dob	Brw
B&P	0.081	0.099	0.088	0.09	0.097	0.133	0.094
DBM	-0.131	-0.12	-0.128	-0.04	-0.07	-0.042	-0.038
IUP					0.019	0.104	0.009

Applicantion to existing dataset

Arosa - Payerne (Switzerland)
Brewer Dobson Soundings Time Series

Izaña (Tenerife) Langley
Dobson-Brewer campaign
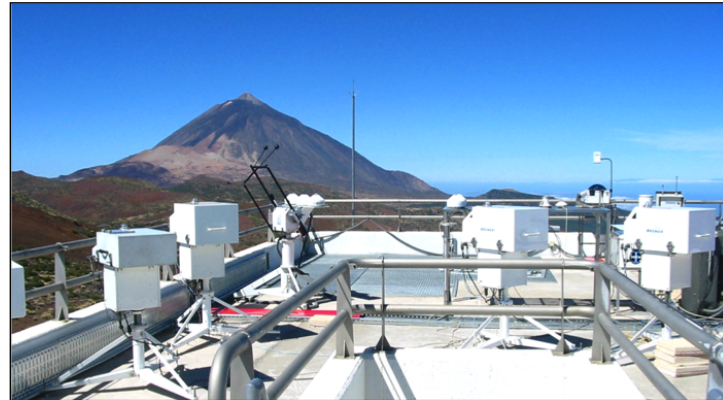
We can evaluate the effect on the Brewer Dobson comparison by applying the cross sections determined in this study to the synchronized measurements made during of the Izaña 2012 Langley Campaign.

- Both the Dobson and Brewer instrument use the Langley plot method to verify the extraterrestrial constant used in the algorithms to convert measurements to total ozone.

- The effect on the TOC calculated by Dobson and Brewer instrument of change from ozone cross-section α to α' is simply the ratio between the old and new absorption coefficients.

- At Izaña the effective temperature had a small variation as it was very close to the operative value so his effect is small on the measurements.

- The Brewer -Dobson comparsion shows an underestimation of 1.5% of the Dobson respect to the Brewer.
- The comparison of the instrument is flat vs ozone slant path which suggest that the difference between instruments are due cross section.
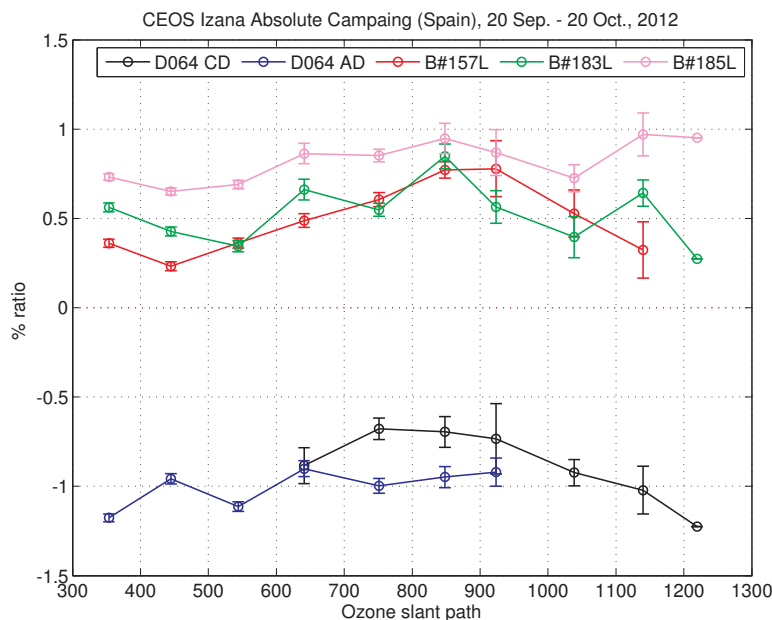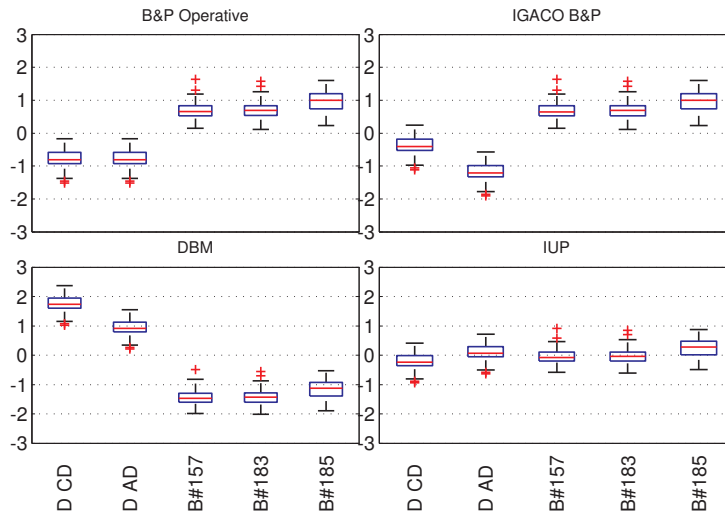

Figure 5 :

- IGAGCO XS slightly increases the Dobson CD/AD.
- The DBM increases the difference from 1.5 % of to 2% (CD) and 3% (AD)
- the IUP reduces significantly the differences

CEOS Izana Absolute campaign (Spain), 20 Sep. - 20 Oct., 2012
o3(α)-ref/ref ref is the mean of Brewer and Dobson operative values

Arosa Dobson-Brewer Time Series

Dobson and Brewer observational data from Arosa Switzerland.

- This consists of three years TOC observations with Dobson D101 and Brewer B040 (single monochromator) and Brewer B156 (double monochromator).
- Dobson and Brewer are corrected using the caculated Coeffients for the XS and using T_{eff} from the Payerne ozonesonde.
- Several methods were tested to assing the three on the week ozonesonde T_{eff} to Dobson/Brewrer observations (nearest,only ozone sonde coincident data, linear interpolation) ,without significant effect on the results. Interpolation is used.
- Two sets were investigated using an averge brewer DXO and using the DXO especific for the Arosa brewer. In this case the use of especific calculation do not have significant effect.
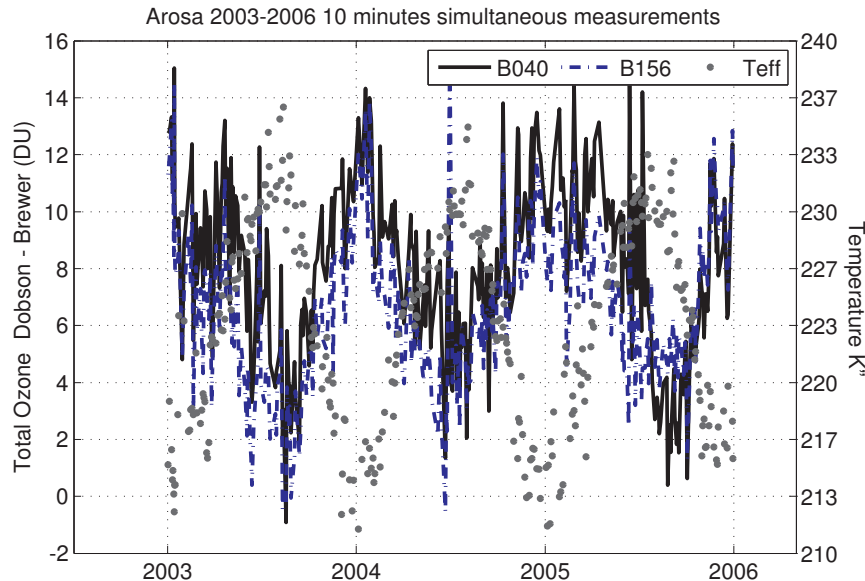
Figure 6 : Daily mean of the Dobson Brewer differences for the Arosa obseravtions and efective temperature for single (B040) and double (B156)
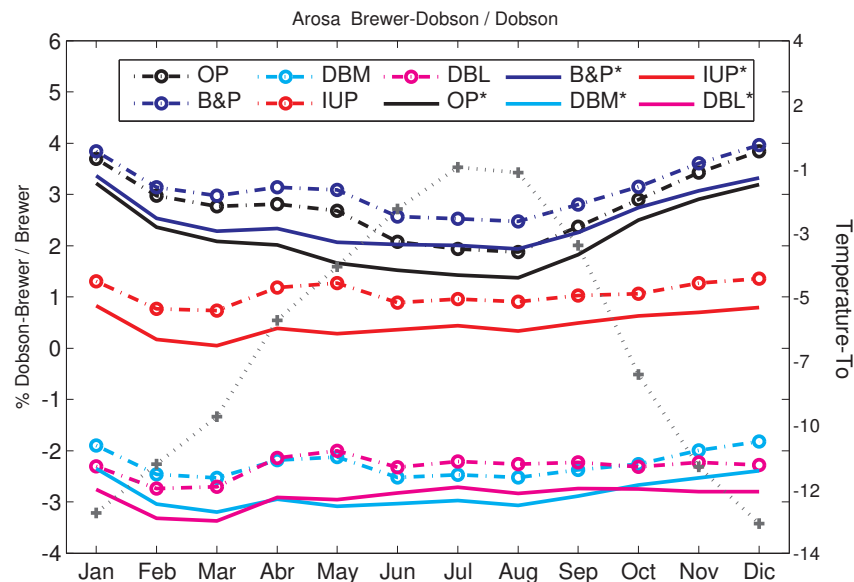
Figure 7 : Montly mean of the Brewer Dobson TOC differences of Arosa. The colored doted lines are for single brewer and solid lines for double Brewers , the different collors indicate the XS. In gray the monthly mean temperature departure from the operational temperature

- The Bass & Paur produce a difference of about + 2-3%, .
- The DBM difference of about - 2-3% .
- The IUP produce a difference of about 0-1%.

Conclusions

- The Brewer and Dobson instrument results agree best when the absorption coefficients used are based on the IUP XS.

- The application of the temperature dependent absorption coefficients substantially reduces the seasonality found in the Arosa Brewer-Dobson record. The DBM set also reduces the seasonality but the change in absolute scale in the Brewer instrument results away from the Dobson results makes its use unsuitable for the network.

- The temperature dependence values obtained confirm the hypothesis of Kerr 2002 the systematic annual differences between Brewer and Dobson are due the different temperature dependence in the instrument's ozone retrieval algorithm.

- The temperature dependence for the Brewer this is small; less than 0.01%/C, this difference is due the temperature dependence in the Dobson algorithm.

- Dobson record will change **less than 1%**. A change to the temperature dependent absorption coefficients provides the most benefit by removing an artificial seasonality in the ozone record.

- The application of the temperature dependent absorption coefficients will be station dependent, as knowledge of the stratospheric temperature record over the station is required. The determination of the best method to determine this record is a subject for another study.

- The calculation of the DXS for a particular Brewer instrument is very sensitive to both the XS and the handling of the XS (editing, smoothing, etc.); these differences can be as large as 1% in ozone.

- The Brewer record of TOC can be adjusted to the IUP scale though the record of the wavelength calibrations. Using the average Brewer value the maximum uncertainty based on 123 instruments was 0.4%; using the known operational absorption coefficient that uncertainty be reduced to 0.1%.