GOBIERNO DE ESPAÑA

MINISTERIO DE AGRICULTURA, ALIMENTACIÓN Y MEDIO AMBIENTE

AEMet Agencia Estatal de Meteorología

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PANDORA TOTAL OZONE ERROR

- Pandora ozone algorithm

ATMOZ-> Irradiance calibration

ATMOZ -> Stray Light

ATMOZ -> Ozone cross section

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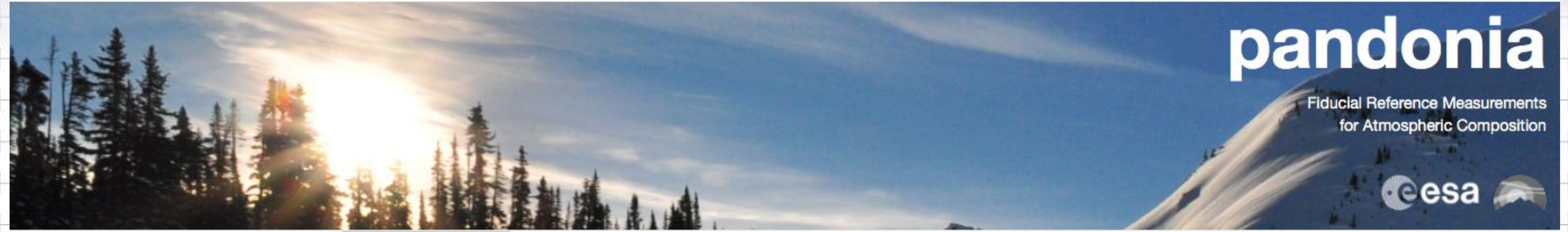

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PANDORA OZONE RETRIEVAL

- Lambert Beer law
- Direct fitting algorithm vs Pandora approximation (Blick software)
- Slant optical depth -> DOAS (only linear)
- Airmass factor (the same as Brewer)

Lambert-Beer's law

$$F(\lambda) = F_0(\lambda) \cdot exp\left(-\sum_{j=1}^{n_{EX}} \tau s_j(\lambda)\right)$$

$$\tau s_j(\lambda) = m_j(\lambda) \cdot q_j \cdot \tau_{STDj}(\lambda, T_j)$$

λ	Wavelength
$F_0(\lambda)$	Spectrum at wavelength λ reaching the top of the atmosphere; that is the "Extraterrestrial adjusted for the Sun-Earth distance
$F(\lambda)$	Spectrum at wavelength λ reaching the instrument's entrance window
n_{EX}	Number of extinction processes in the atmosphere
$\tau s_j(\lambda)$	Slant optical depth at wavelength λ for extinction process j
$qs_j^*(\lambda)$	(Absolute) slant column amount for extinction process j at wavelength λ (units e.g. mo per cm^2)
T_j	Effective temperature of extinction process j (see equation 3)
$\sigma_j(\lambda,T_j)$	Cross section for extinction process j at wavelength λ and effective temperature T_j (u cm^2 per molecule)
$\tau_{STDj}(\lambda,T_j)$	"Standard vertical optical depth" for extinction process j at wavelength λ
$qs_j(\lambda)$	(Relative) slant column amount for extinction process j at wavelength λ (no dimensior
$m_j(\lambda)$	Air mass factor (or optical mass) for extinction process j at wavelength λ
q_j	(Relative) vertical column amount extinction process j (no dimension)

Standard O_3 amount: 8.0603e18 [mol/cm^2] (=300 DU)

Pandora (Blick Software) approximation:

$$\mathrm{F_i} = \int \mathrm{F}(\lambda) \cdot \mathrm{S_i}(\lambda_\mathrm{i} - \lambda) \cdot \mathrm{d}\lambda$$

$$\mathrm{F_i} = \int_{\Delta\lambda_\mathrm{i}} \mathrm{F_0}(\lambda) \cdot exp\left(-\sum_{j=1}^{\mathrm{n_{EX}}} \tau \mathrm{s_j}(\lambda)\right) \cdot \mathrm{S_i}(\lambda_\mathrm{i} - \lambda) \cdot \mathrm{d}\lambda$$

"Direct fitting algorithm": all unknowns in equation (the mj(λ), qj, and Tj) are varied in an iterative process until the right and left side of the equation agree

$$\mathrm{F_i} = \mathrm{F_{0i}} \cdot exp\left(-\sum_{j=1}^{\mathrm{n_{EX}}} \tau \mathrm{s_{ji}}\right) \qquad \mathrm{F_{0i}} = \int_{\Delta\lambda_\mathrm{i}} \mathrm{F_0}(\lambda) \cdot \mathrm{S_i}(\lambda_\mathrm{i} - \lambda) \cdot \mathrm{d}\lambda$$

Pandora (Blick Software) approximation:

$$\tau s_j(\lambda_i, qs_j) = -ln\left[\frac{\int\limits_{\Delta\lambda} F_0(\lambda)\cdot exp\left(-qs_j\cdot\tau_{STDj}(\lambda, T_j)\right)\cdot S_i(\lambda_i-\lambda)\cdot d\lambda}{\int\limits_{\Delta\lambda} F_0(\lambda)\cdot S_i(\lambda_i-\lambda)\cdot d\lambda}\right]$$

This expression is calculated for qs_j values ranging from 1 to 8

$$\tau s_{ji} = A_{ji}\cdot qs_j^{1+B_{ji}+C_{ji}\cdot ln(qs_j)}$$

This expression is a more general approach than what is usually used in classical DOAS, where only linear absorbers are included

Table 16: Table "Trace Gases" in the fitting setups file

Short name	Symbol	Full name	Standard amount [molc/cm^2]	h_{EFF}[km]	T_{EFF}[K]
O3	O_3	Ozone	8.0603e18 (=300 DU)	20.4	225.0
NO2	NO_2	Nitrogen dioxide	1.3434e16 (=0.5 DU)	7.2	254.5
O2O2	O_2O_2	Oxygen dimer	1.2691e43 molc^2/cm^5 (=1 std atmosphere)	3.5	262.0
SO2	SO_2	Sulfur dioxide	1.3434e16 (=0.5 DU)	4.0	259.2
HCHO	HCHO	Formaldehyde	1.3434e16 (=0.5 DU)	4.3	256.9
H2O	H_2O	Water vapor	3.3428e22 (=1 cm precipitable water)	1.8	273.1
BrO	BrO	Bromine oxide	4e13	22.4	221.0
ClO	ClO	Chloride oxide	1e14	22.4	221.0
OClO	OClO	Chloride dioxide	1e13	22.4	221.0
GLY	CHOCHO	Glyoxal	6e14	4.3	256.9
IO	IO	Iodine monoxide	2e12	22.4	221.0
OH	OH	Hydroxyl radical	5e13	22.4	221.0
O2	O_2	Oxygen	4.5103e24 (=20.95 % of 1 std atmosphere)	6.2	250.6
CO2	CO_2	Carbon dioxide	8.1825e21 (=380 ppm of 1 std atmosphere)	6.2	250.6
NO3	NO_3	Nitrate	2e13	3.4	262.9

Convolution

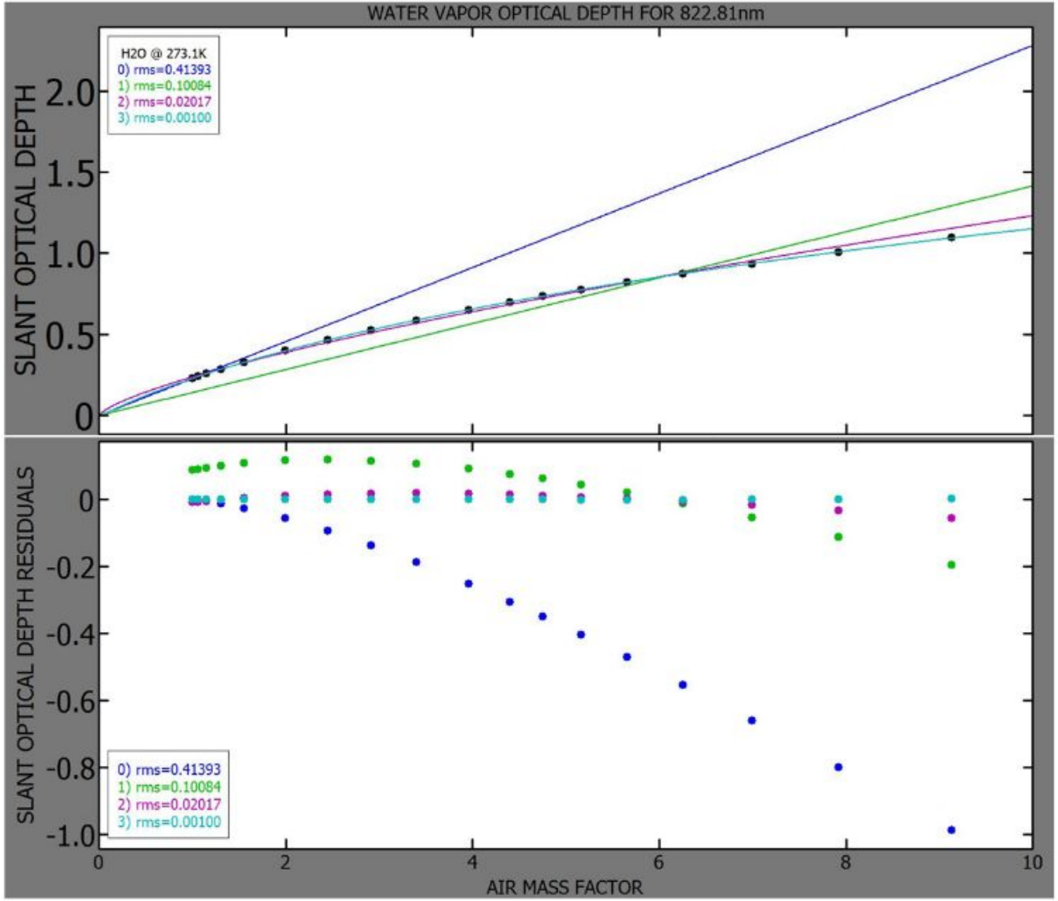
$$\tau s_{ji} = A_{ji} \cdot qs_j$$

With $A_{ji} = \tau s_{ji}(\lambda_i, qs_j=1)$

$$\tau s_{ji} = A_{ji} \cdot qs_j$$

$$\tau s_{ji} = A_{ji} \cdot qs_j^{1+B_{ji}}$$

$$\tau s_{ji} = A_{ji} \cdot qs_j^{1+B_{ji}+C_{ji} \cdot ln(qs_j)}$$



$$\tau s_{ji} = A_{ji} \cdot qs_j^{\,1+B_{ji}+C_{ji}\cdot ln(qs_j)}$$

$$A_{ji} = A_{jCi} + A_{jLi} \cdot \frac{T_j - T_{jREF}}{T_{SCALE}} + A_{jQi} \cdot \left(\frac{T_j - T_{jREF}}{T_{SCALE}}\right)^2$$

Parameters quadratic dependence

Fitting equation

$$lnF_{0i} - lnF_i = \sum_{j=1}^{n_{EX}} \tau s_{ji}$$

$$lnF_{0i} - ln\left(F_i - P_{OFFSi}\right) - \tau s_{FIXi} = \sum_{j=1}^{n_{GAS}} \tau s_{ji}(qs_j, T_j) + \tau_{RINGi} \cdot qs_{RING} + P_{SMOi} + P_{RESCi}$$

POFFSi : Offset polynomial (Stray Light)

PSMOi : Smooth polynomial (instrument spectral sensitivity)

PRESCi= Resolution Cange Polynomial

Ozone calculation:

- **External reference:** The current standard Pandora O3 retrieval uses an external absorption free reference spectrum (convoluted Kurutz spectrum radiometrically corrected towards SUSIM)
- No irradiance absolute calibration (PSMOI)
- Basic Stray light (POFF)
- DMB ozone cross section at -45

Least squares minimization

$$\xi_{\mathrm{i}} = ln\mathrm{F}_{0\mathrm{i}} - ln\left(\mathrm{F}_{\mathrm{i}} - \mathrm{P}_{\mathrm{OFFSi}}\right) - \tau s_{\mathrm{FIXi}} - \sum_{j=1}^{\mathrm{n}_{\mathrm{GAS}}} \tau s_{\mathrm{ji}} - \tau_{\mathrm{RINGi}} \cdot \mathrm{q}s_{\mathrm{RING}} - \mathrm{P}_{\mathrm{SMOi}} - \mathrm{P}_{\mathrm{RESCi}}$$

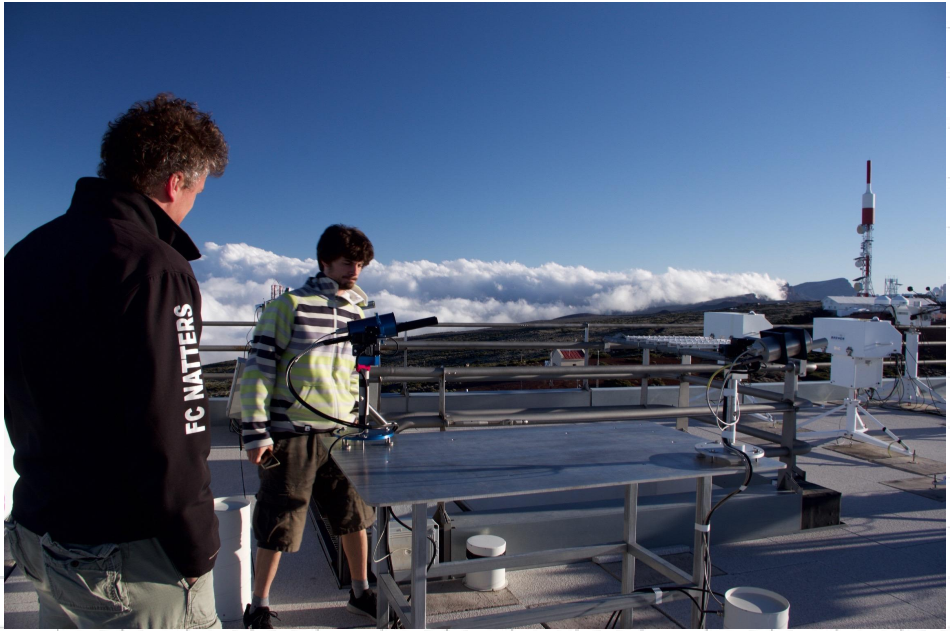
$$\sigma_{\mathrm{i}} = \sqrt{\sigma_{\mathrm{MEASi}}^2 + \sigma_{0\mathrm{i}}^2}$$

$$\sum_{i=1}^{\mathrm{n}} \left(\frac{\xi_{\mathrm{i}}}{\sigma_{\mathrm{i}}}\right)^2 \rightarrow Minimum$$

- Linear fitting

L0 to L1 corrections are associated with an error with a contribution to the measurement error

- Dark Correction
- No linearity correction
- Latency correction
- Flat field correction
- Count rates conversion
- Temperature
- Stray Light
- Filter Correction
- Conversion of Irradiances-fit
- Wavelength correction-fit



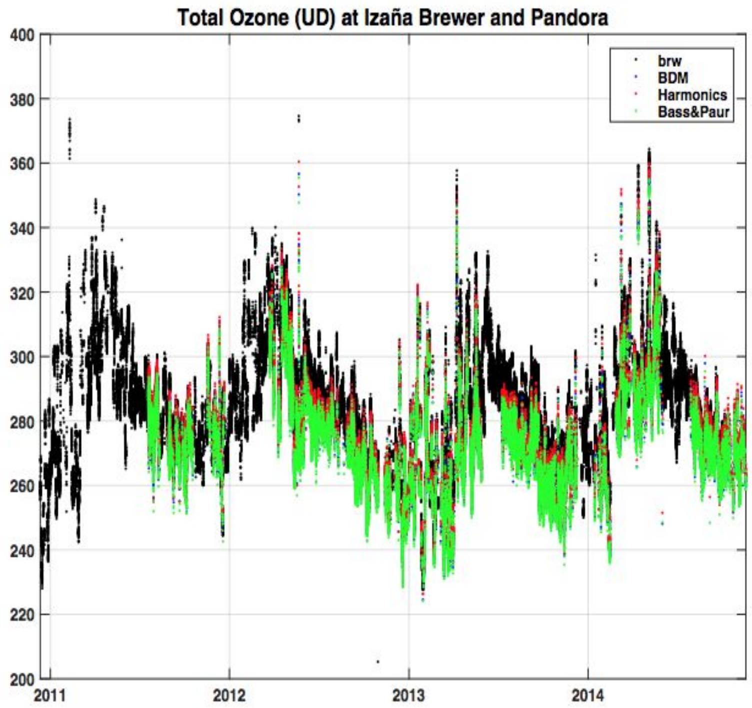
ATMOZ contribution:

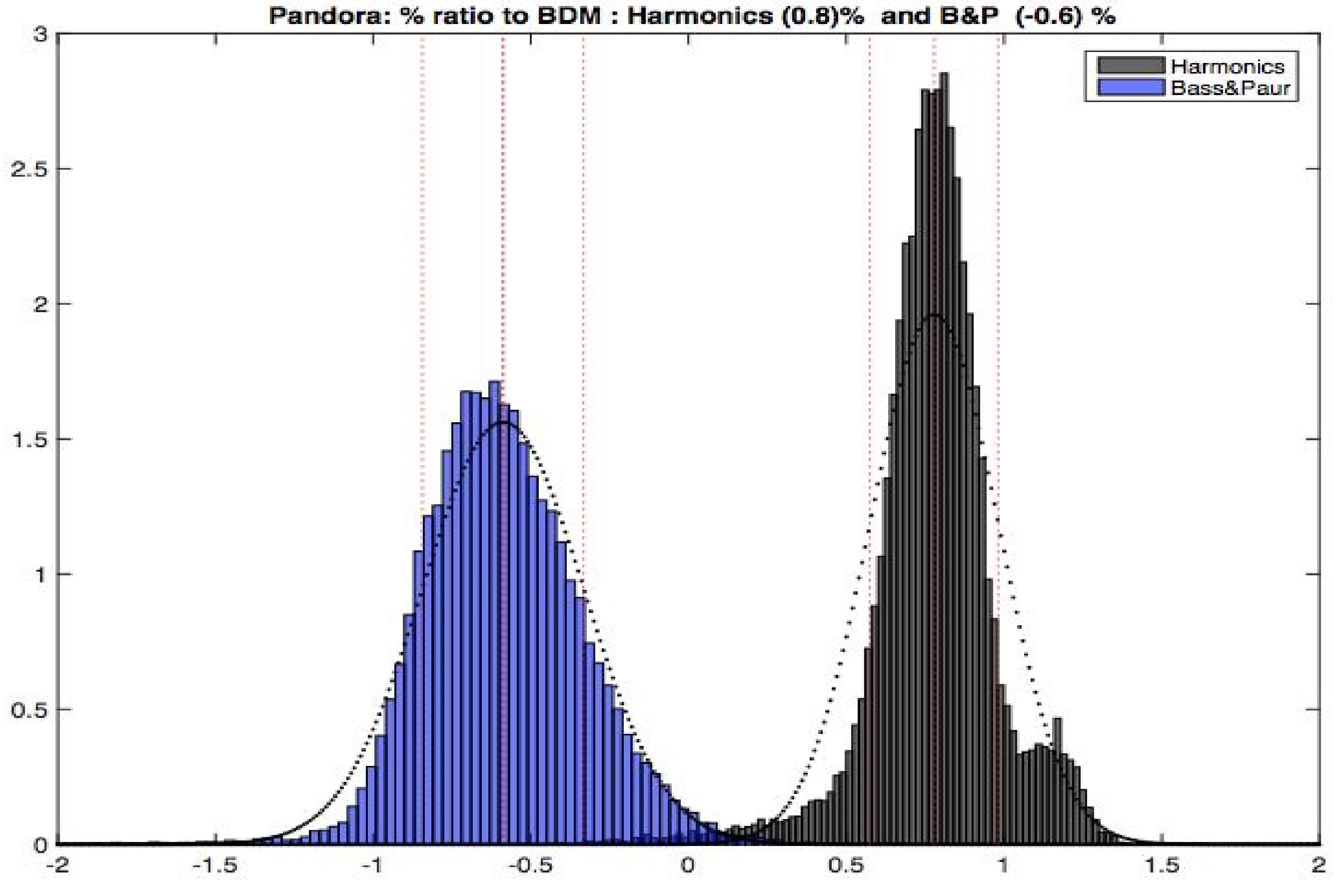
- Stray Light characterization
- Absolute calibration
- Cross-Section effect on pandora ozone retrieval

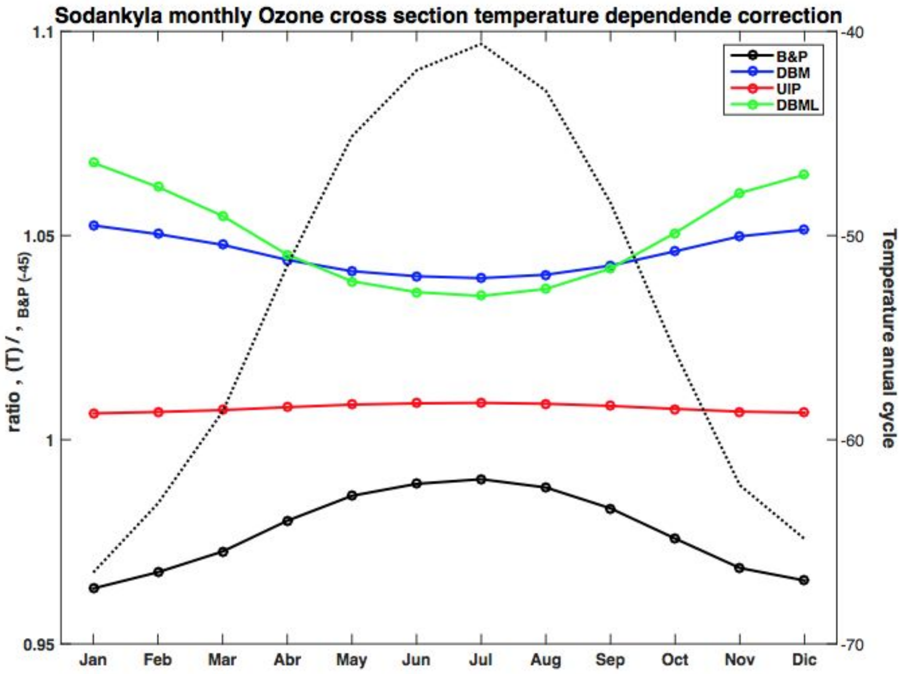
Cross-Section

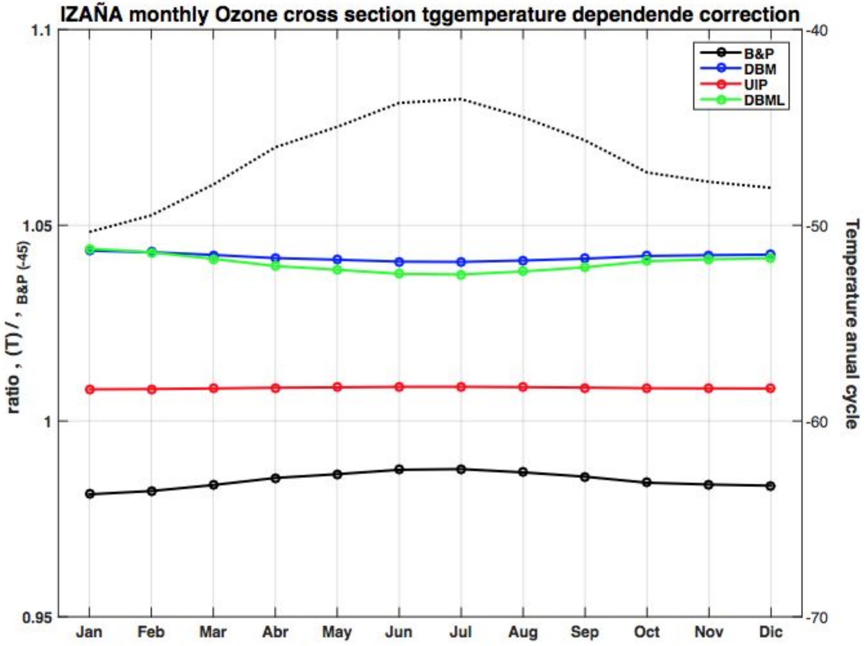
Brewer - Pandora

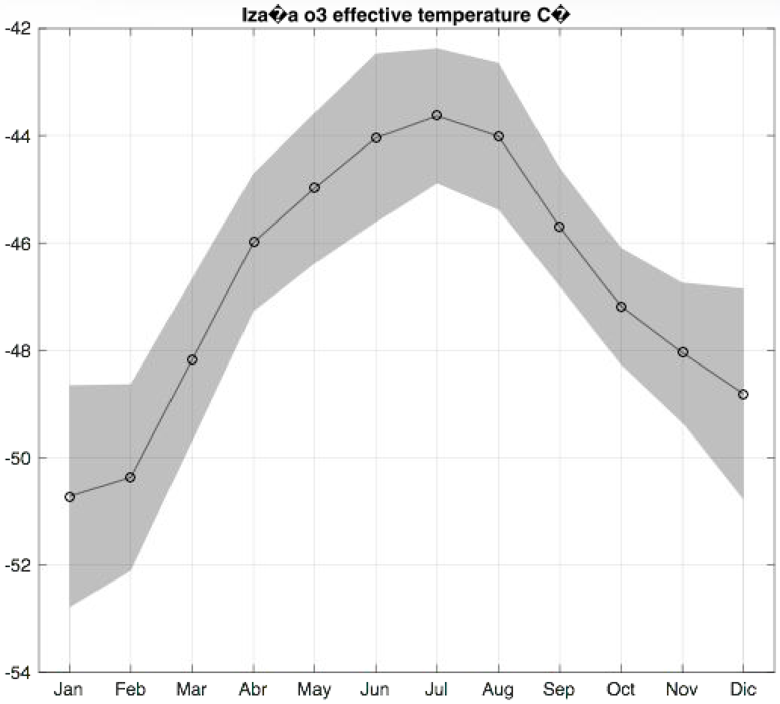
- Bass & Paur
- Brion Daumont & Malicet
- Serdyuchenko & Groshelev

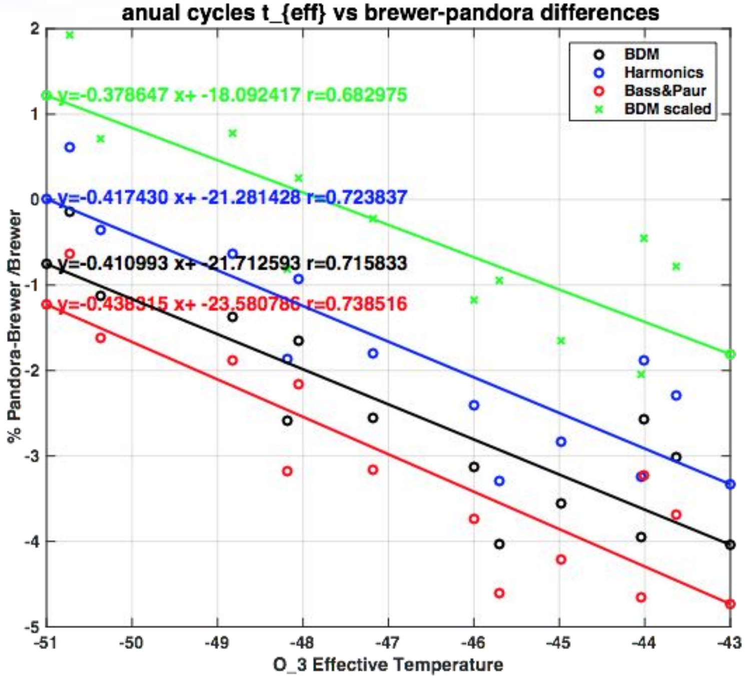


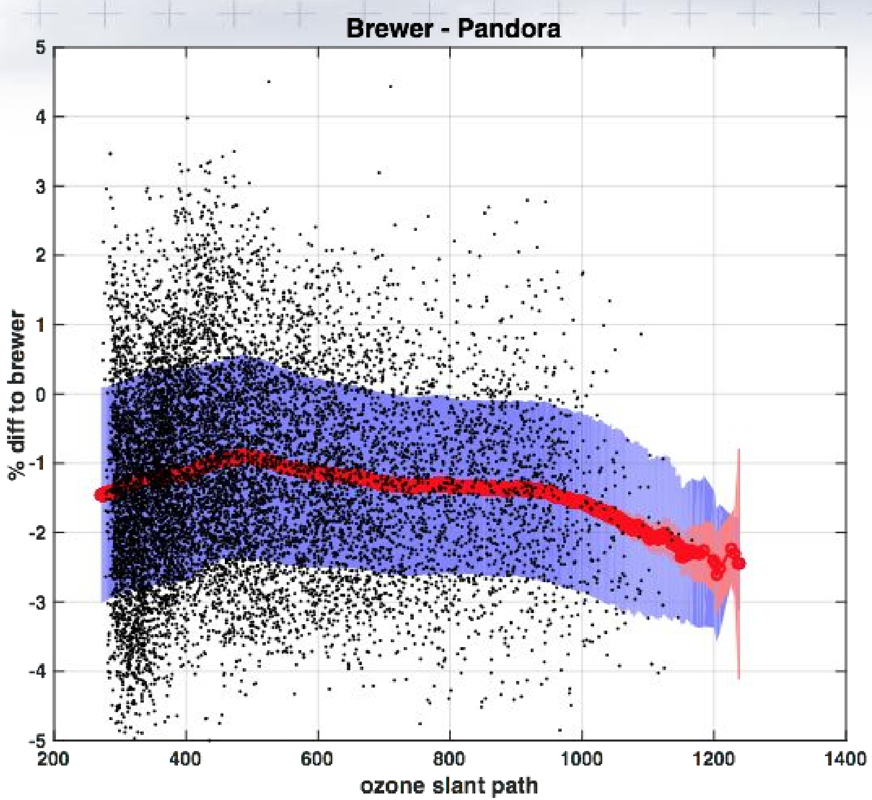

Pandora: % ratio to BDM : Harmonics (0.8)% and B&P (-0.6) %
Harmonics
Bass&Paur
3
2.5
2
1.5
1
0.5
0
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2


Sodankyla monthly Ozone cross section temperature dependende correction
B&P
DBM
UIP
DBML
ratio , (T) / , B&P (-45)
Temperature anual cycle
1.1
1.05
1
0.95
-40
-50
-60
-70
Jan
Feb
Mar
Abr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dic


IZAÑA monthly Ozone cross section tggemperature dependende correction
B&P
DBM
UIP
DBML
ratio , (T) / , B&P (-45)
Temperature anual cycle
1.1
1.05
1
0.95
-40
-50
-60
-70
Jan
Feb
Mar
Abr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dic


Iza�a o3 effective temperature C�
-42
-44
-46
-48
-50
-52
-54
Jan
Feb
Mar
Abr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dic


anual cycles t_{eff} vs brewer-pandora differences
BDM
Harmonics
Bass&Paur
BDM scaled
y=-0.378647 x+ -18.092417 r=0.682975
y=-0.417430 x+ -21.281428 r=0.723837
y=-0.410993 x+ -21.712593 r=0.715833
y=-0.438315 x+ -23.580786 r=0.738516
% Pandora-Brewer /Brewer
O_3 Effective Temperature
2
1
0
-1
-2
-3
-4
-5
-51
-50
-49
-48
-47
-46
-45
-44
-43



Pandora behaves like a ‘good’ sigle brewer.

Thanks

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Thanks !

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