

# STSM ES1207-17346 Report

## Purpose of the STSM

The objective of the STSM is to implement a theoretical model for the Brewer spectrophotometer, relying on existing radiative transfer software, in order to make it possible to study the sensitivity of different parameters on the Brewer algorithm (temperature and altitude of the ozone layer, aerosol optical depth, etc.), to assess the measurement error budget and to validate several calibration methods.

## Description of the work carried out during the STSM

We developed a MATLAB script and several functions that are intended to be multiplatform in order to be used by the different users in the Brewer community.

The first step for the model is the calculation of the operative slits wavelengths and the full width at half maximum (FWHM) of the Brewer which nominal values are 303.2, 306.3, 310.1, 313.5, 316.8, and 320.1 nm. The operative wavelengths for a real Brewer (and its conversion to micrometer steps) are determined from the dispersion test and then calculated using the Dispro software. A model improvement would be the data reduction from the individual dispersion test files, which will be developed in the next months. From the Dispro file we also extract the coefficients to transform steps to wavelength which is what we really need as input for the radiative transfer model.

With the operative wavelengths and the FWHM we build the slit function. (Kerr et al., 1985)

We use Cdisort as the radiative solver, which is part of Libradtran 1.7 (Bernhard et al., 2012). We use 16 streams to solve the radiative transfer equation.

For the extraterrestrial spectrum we use SAO2010 a solar irradiance reference spectrum with resolution 0.01 nm which was developed combining high spectral resolution ground-based and balloon-based solar measurements with lower spectral resolution but higher accuracy irradiance information (K. Chance et al.), can be downloaded from <http://www.cfa.harvard.edu/atmosphere/links/>. We finally adapted it to the part of interest of our spectrum.

In the case of the ozone cross-sections we use a Bass and Paur modified file with a resolution adapted to the model resolution of 0,001 nm and for 228.15 K (Malicet et al.), but we also made

several simulations with different cross-sections, Molina & Molina (Molina et al., 1986), Daumont (Daumont et al., 1992) that will be showed in the results section.

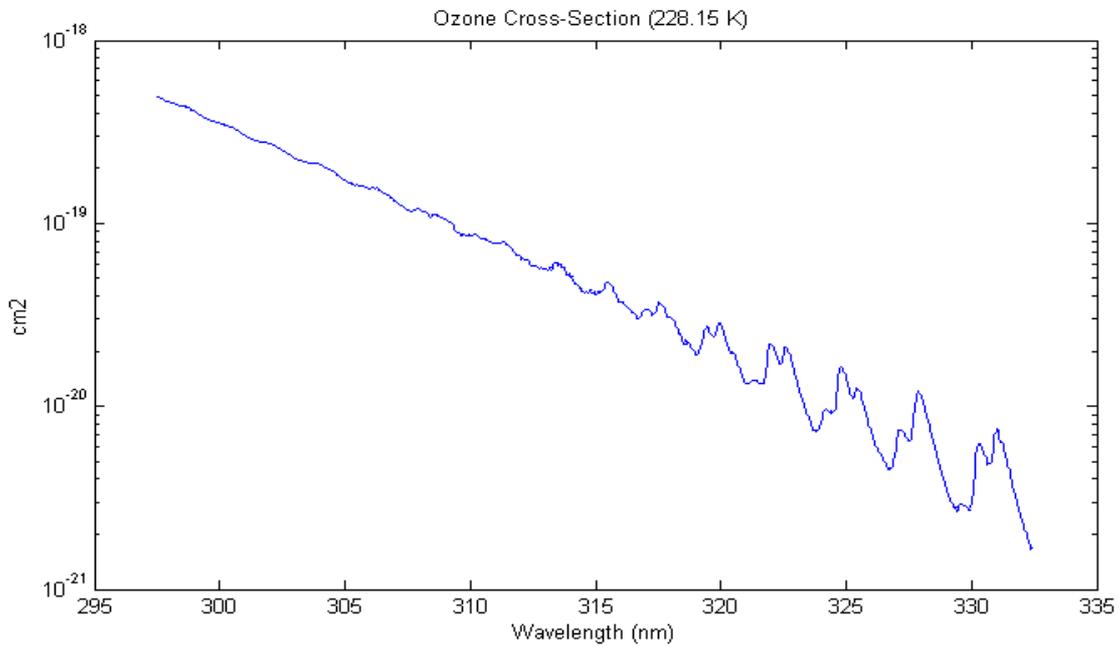


Figure 1: Ozone cross-sections at -45° used in the model.

We use the operative Rayleigh coefficients of the brewer 0, 0, 4870, 4620, 4410, 4220 and 4040, which doesn't provide the best results for our model using Langley calibration as we will see in the results.

We have slit weighted irradiances at the wavelength and FWHM defined by the dispersion test. The model output are intensities  $I_i$  in slit  $i$  and the brewer measures counts/seconds  $F_i$ . They are related by:

$$I_i = F_i \cdot R_i \quad (\text{or } I_i = F_i / R_i \text{ if } R_i \text{ is counts/wm}^2 \text{ nm})$$

$I_i$ ,  $R_i$  and  $F_i$  are the intensity, response and counts/second of the instrument for the slit  $i$ .

Now we have the count rates for each slit, we proceed with the standar Brewer data reduction scheme, where  $F_i$  are the count rates for each slit:

$$MS_5 = F_5 - F_3;$$

$$MS_6 = F_5 - F_4;$$

$$MS_7 = F_6 - F_5;$$

A higher order ratio is formed:

$$MS_9 = MS_5 - 0.5 \cdot MS_6 - 1.7 \cdot MS_7$$

This function has weightings which remove the effects of absorption which are linear with wavelength. In addition, it's stabilized with respect to small wavelength calibration errors, it's also weighted to remove SO2 absorption effects.

The O3 amount, MS11, is determined from the logarithms of the count rates for the four longer wavelengths, which we obtained from the Libradtran output.

$$MS_{11} = \frac{MS_9 - B1}{A1 \cdot M2}$$

Where:

B1 is the extra-terrestrial coefficient for the O3 wavelength combination (instrument-dependent)

A1 is the differential O3 absorption coefficient for the O3 wavelength combination (instrument-dependent)

M2 is the path-lengthening factor for an ozone layer of height 22 km.

MS<sub>9</sub> and B1 are the linear combination of the logarithm of the intensity of the slits (scaled on the brewer  $E = 10^4 \cdot \log(I)$ ).

$$E = \sum w_i E_i$$

with weights  $w_i$ , so the intensities are related to the counts  $F_i$

$$E_i = F_i \cdot R_i$$

$$E = \sum w_i \log(F_i \cdot R_i) = \sum (w_i \cdot F_i) + \sum (w_i \cdot R_i)$$

The calibration constant  $C = \sum (w_i \cdot R_i)$  cancels for the ozone calculation, is the same for E and E<sub>o</sub>.

## **Description of the main results obtained**

When we have our model working one of the first issues we have to solve is its calibration, as it is an instrument model we have to calibrate it in the same way we calibrate the instrument, modifying the input parameters until the output from the model matches an observed set of data.

Two ways of calibrating the model have been implemented, the two points calibration and Langley. We have different results depending on how we calculate the O<sub>3</sub> absorption coefficient. If we use the two points calibration method (The extraterrestrial constant and O<sub>3</sub> absorption coefficient are determined by comparison with a reference) we obtain very good results, and slight differences in ozone if we use Langley for calibration mainly due to the use of incorrect Rayleigh coefficients and the use of the standard weightings of the Brewer.

With the operative model we have made several simulations to study the sensitivity and strength of the model.

### ***Model Calibration***

When simulating the Brewer 185 measurements at Izaña using 340 DU as ozone input, we obtain for the two points calibration:

ETC: 7.9478370e+002

O<sub>3</sub> abs coeff: 3.3807766e-001

And with the Langley calibration:

ETC: 7.9483362e+002

O<sub>3</sub> abs coeff: 3.4106892e-001

Results in the ozone retrieval are shown in Figure 2, the differences of approximately 3 DU is mainly due to:

- Bad Rayleigh coefficients, the main error source.
- Use of standard weightings.
- The calculation of the differential ozone absorption coefficient.

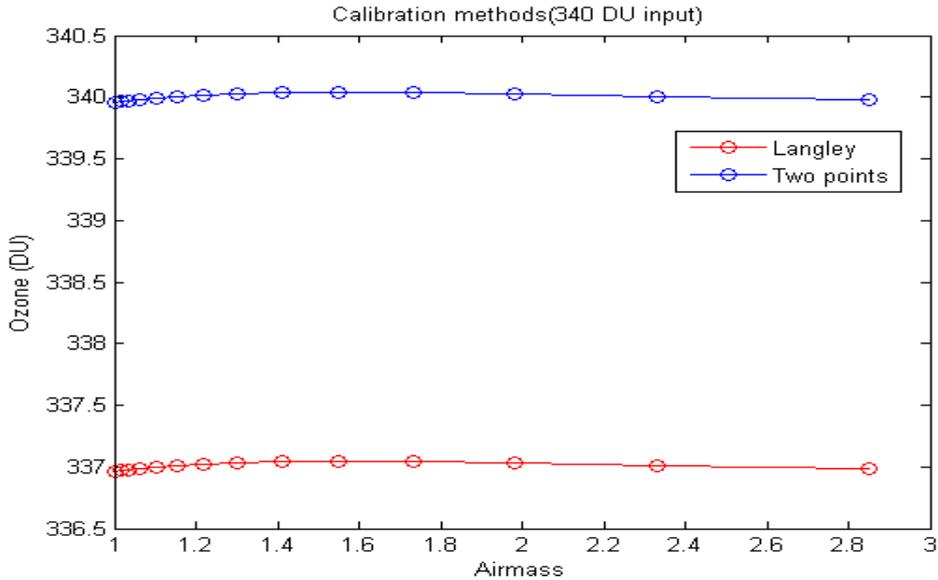


Figure 2: differences in ozone retrieval using different model calibration methods.

The next sections offer some examples, among many other, of the usefulness of our model, like the effect of the effective ozone height, the sun scan simulation, the use of Rayleigh coefficients and the use of different ozone cross-sections. The airmass is defined as in the MKIII Brewer operator manual appendixes.

### ***Effect of the effective ozone height***

Varying the effective ozone layer height has a significant effect in the ozone retrieval for a fixed ozone input, which is greater for the highest airmasses, having differences of approximately 20 DU for airmass near 5,5 between the height of 14 km and 30 km. Results are shown in figure 3.

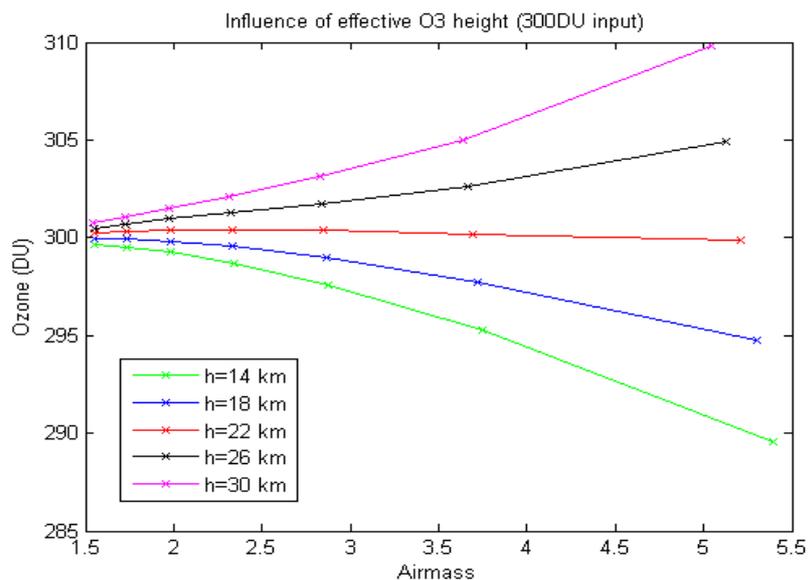


Figure 3: Differences in ozone retrieval for different ozone effective height varying the airmass.

### Use of 0 Du input

We have checked whether the model shows an offset by using 0 DU as input. We have a non zero output which is higher for the highest airmasses. We have also calculated for both calibration methods and we have a small difference of 0,03 DU which is constant for airmasses between 1 and 3 (Fig. 4).

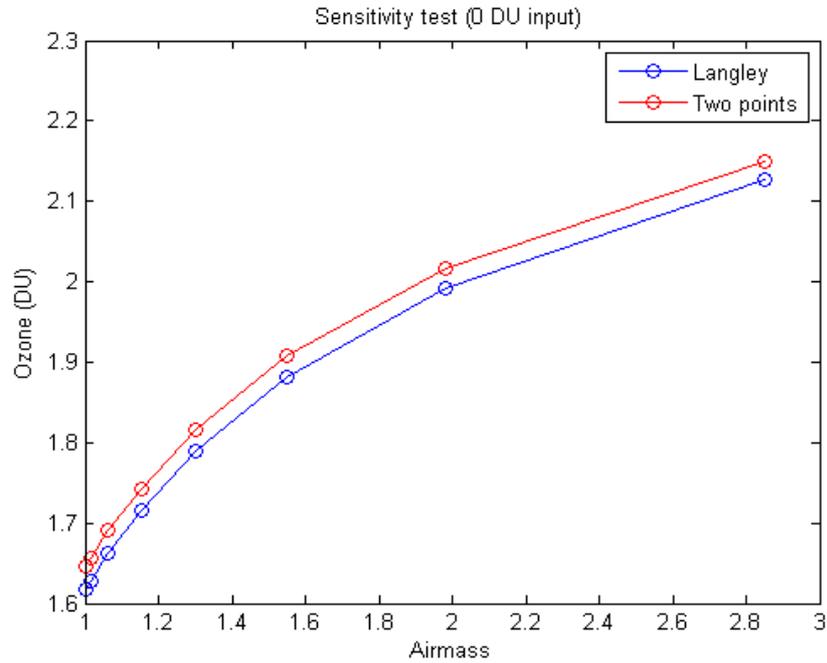


Figure 4: input 0 DU using both calibration method and varying the airmass.

### Sun scan simulation

We have simulated several Sun scans for different solar zenith angles (SZA) for brewer 185 whose operative step is 1020 and the Zero is 1733, and using 300 DU as ozone input. To perform this simulation we moved 12 steps backward and forward from each slit center every 2 steps (MKIII Brewer operator manual appendixes). In the Figure 5 we show the results, in red the Sun scan for 60° SZA (approx. airmass 2), which is the nearest to the operative calc step.

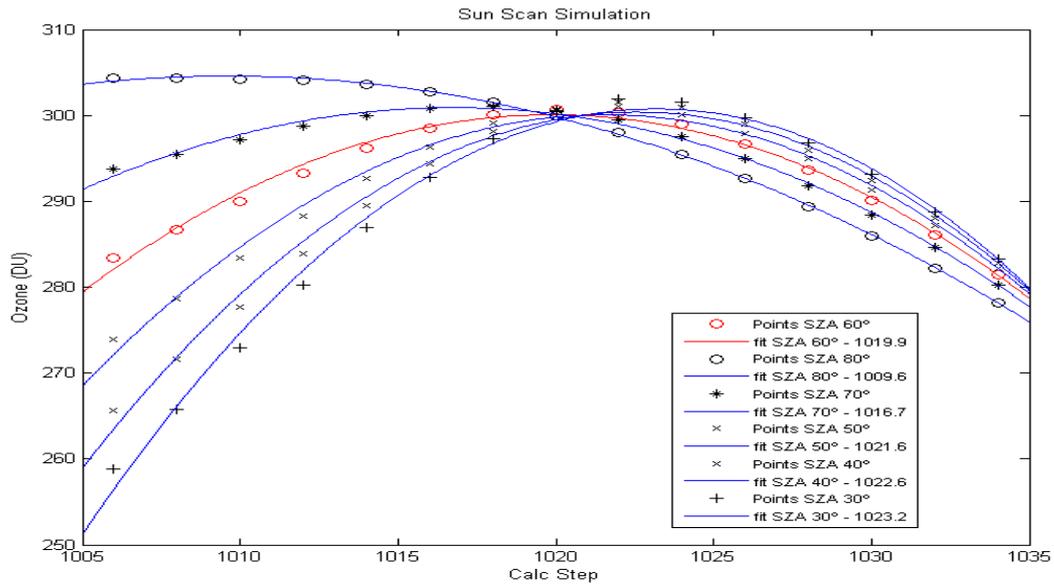


Figure 5: Sun scan simulation for the recommended airmass of 2 (approx. 60° SZA) and different SZA.

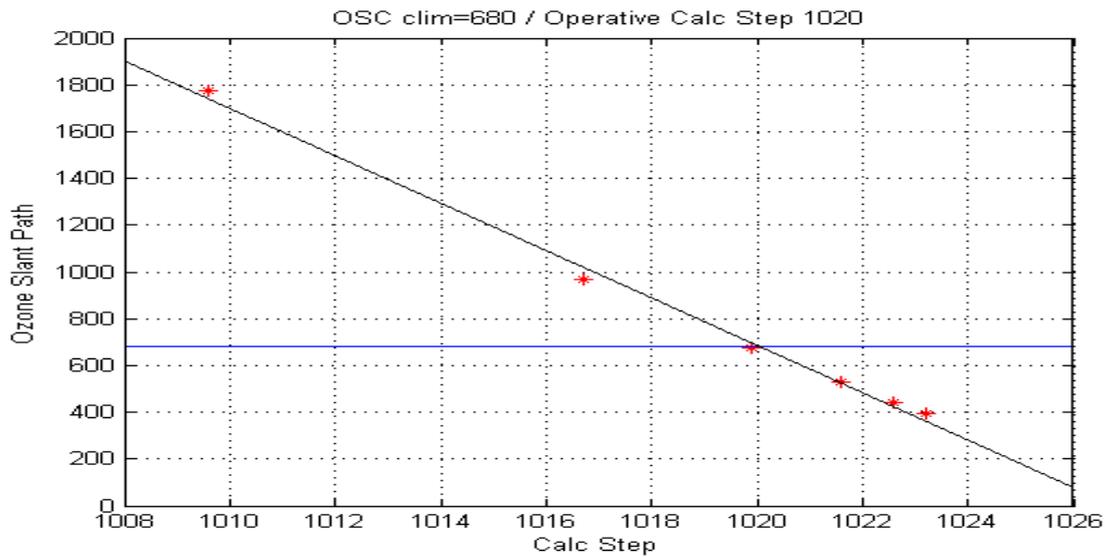


Figure 6: Sun scan simulation

From the results in figure 5 we recommend to use more points in the Sun Scan for solar zenith angles of 80° and greater.

In Figure 7 we moved 22 steps backwards to try to see the whole parabola for 80° SZA, we can't find a clear maximum, the highest part of the data plot is near flat.

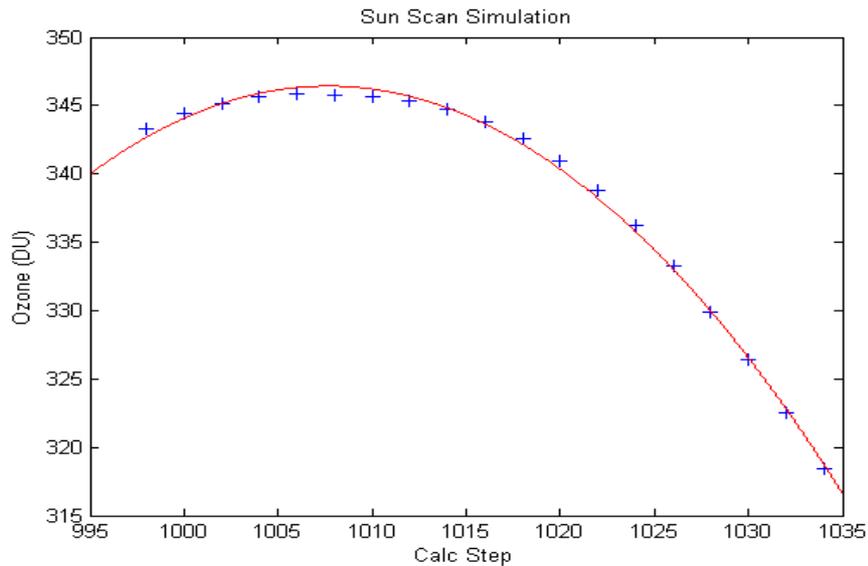


Figure 7: Expanded sun scan for 80° SZA, moving 22 steps left and 14 right.

### Rayleigh coefficients

As the main source of error in the results comes from the incorrect Rayleigh coefficients that are the ones used by the Brewer, we made a simulation using the Rayleigh corrections and without using it.

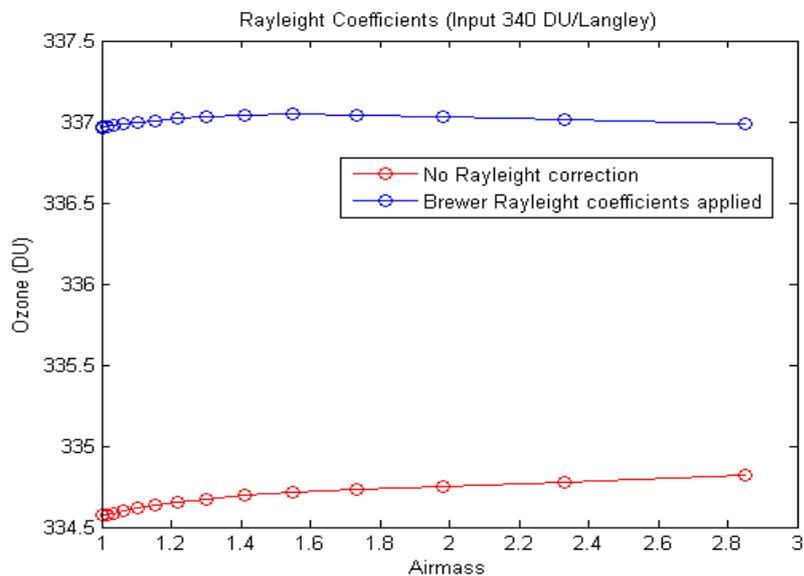


Figure 8: Simulation using Rayleigh coefficients and without correction for 340 DU ozone input.

### Cross-sections

We tested different cross-sections used for ozone, for Daumont we have a 3% overestimation, with Bass&Paur we have an underestimation of 1.2% and with Molina&molina we have an underestimation of 2,3%, in agreement with Redondas et al. 2014

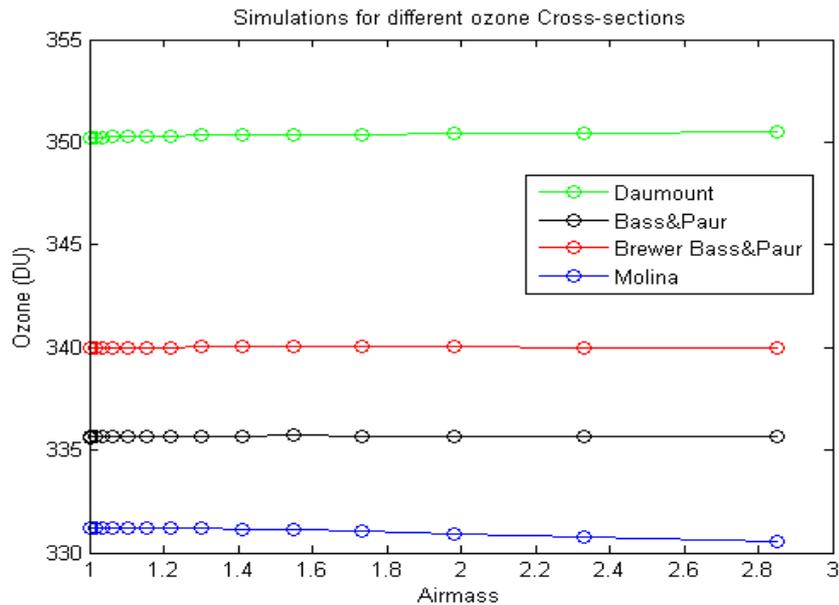


Figure 9: Different cross-sections included in Libradtran and the one used operatively in our model.

## Future collaboration with host institution

An expansion of the model will be completed in a short time before the next COST1207 meeting including an analysis of the effect of the extra light entering the field of view, sensitivity to the dead time, temperature dependence and some other details not included in the actual model that could be of interest.

We also want to study the effect of external factor during calibrations, AOD calculation and include interfering gases.

## Foreseen publications/articles resulting or to result from the STSM

A more detailed presentation including improvements will be presented in the next COST meeting that will be held at Azores in November 2014.

## References

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