Environnement et Changement climatique Canada
Environment and Climate Change Canada

Ozone Calibration SOP for the Brewer Spectrometer

The Canadian Brewer Spectrometer Network

Réseau Canadian de spectrophotometric – Brewer

Updated: May 13, 2020

Version 1.0

Canada

Ozone Calibration

An ozone calibration is mainly conducted to determine or confirm the O_3 and SO_2 extraterrestrial coefficient (ETC) values for a Brewer spectrophotometer. These ETC values are used by the Brewer software to calculate column O_3 and SO_2 amounts from the photon counts during a direct sun measurement. A calibrated and stable transfer standard is used to co-collect direct sun ozone data with the instrument being calibrated. Data collected from this intercomparison is processed using BFilePro software. BFilePro calculates the O_3 and SO_2 ETC's for the instrument being calibrated by producing a best-fit to the O_3 and SO_2 values measured by the transfer standard.

Note: Environment and Climate Change Canada (ECCC) uses BfilePro to process the collected instrument data. BFilePro is a software created by International Ozone Services (IOS) Inc. ECCC has access to BFilePro via a license from IOS Inc.

Brewer ozone calibrations should be done at a minimum every two years in order to confirm that the instrument is measuring ozone accurately. Ozone calibrations should also be performed if there are changes to signal conditioning (filters, gratings and mirrors), detection changes (PMT replacement or voltages affecting the PMT) or mechanical changes that affect the dispersion.

Pre-Calibration

It is important to confirm proper transfer standard (reference) operation prior to collecting data for an ozone intercomparison. A diagnostic test script, pdhphgslapdtrsapdipd for a double brewer (pdhgslapdtrsapdipd, single brewer), should be run and compared to previous data collected. A change in operation to the transfer standard should be investigated and corrected prior to starting the ozone calibration.

This sop assumes that the reference and brewer being calibrated are installed correctly and that the correct calibration step, absorption coefficients, uvres data, dead time and temperature coefficients are being used. Diagnostic tests indicate the reference and brewer being calibrated are in good working state.

1. Calculate Current O_3 and SO_2 ETC's for the Reference Brewer

Update the reference instruments ETC values if its standard lamp ratios have changed significantly since the last ozone calibration. Determine the current R5 and R6 ratio values using the results of the test string above if the instrument has traveled or average the last 20 entries from the standard lamp average file (Sloavg.###) if the instrument has not been moved and received any maintenance in the last 20 days. Calculate the updated O_3 and SO_2 ETCs as follows:

- Updated O_3 ETC = current R6 - R6 at time of last ozone calibration + O_3 ETC in icf file
- Updated SO_2 ETC = current R5 - R5 at time of its last ozone calibration + SO_2 ETC in icf file

The R5 and R6 values at the time of the last ozone calibration can be determined by averaging the 20 entries in the standard lamp average file (SLOAVG.###) after the date of the last ozone calibration. If the standard lamp was changed at the time of the last ozone calibration then delay the start date for selecting the range of entries to be averaged by a week or a few weeks until the standard lamp intensity and ratios become stable.
If the updated reference ETC's differ by more than 10 units, update the reference icf and OP_ST files to reflect this change. This will insure that the DOS window displays the correct DS value and that BFilePro will use the most recent ETC's when comparing to the Brewer being calibrated. If the ETC's differ by less than 10 units, make no changes to the reference files.

A change of ten units in the standard lamp ratios (or in the ETCs) is approximately equal to a change in ozone of one Dobson unit. For measured ozone values of about 350 DU (typical at mid-latitudes) 1 DU of ozone represents about one-third of 1% difference in ozone which is well within the uncertainty of the ozone calibration of about +/- 1 percent.

2. Calculate Updated O_3 and SO_2 ETCs for the Brewer being calibrated

Repeat the above process for updating the ETCs for the instrument to be calibrated. These calculated ETC's should be close to the values arrived at when using BFilePro.

Data Collection

A schedule containing ds measurements (i.e. calsc.skd) should be run simultaneously on both instruments to collect ozone intercomparison data. This schedule is designed to collect DS data starting when the sun rises to an 80 degree solar zenith angle (SZA) and until the sun falls to a SZA of 80 degrees in the evening. Sun sightings should also be performed on both Brewers every 1.5 to 2 hrs. during the data collection period.

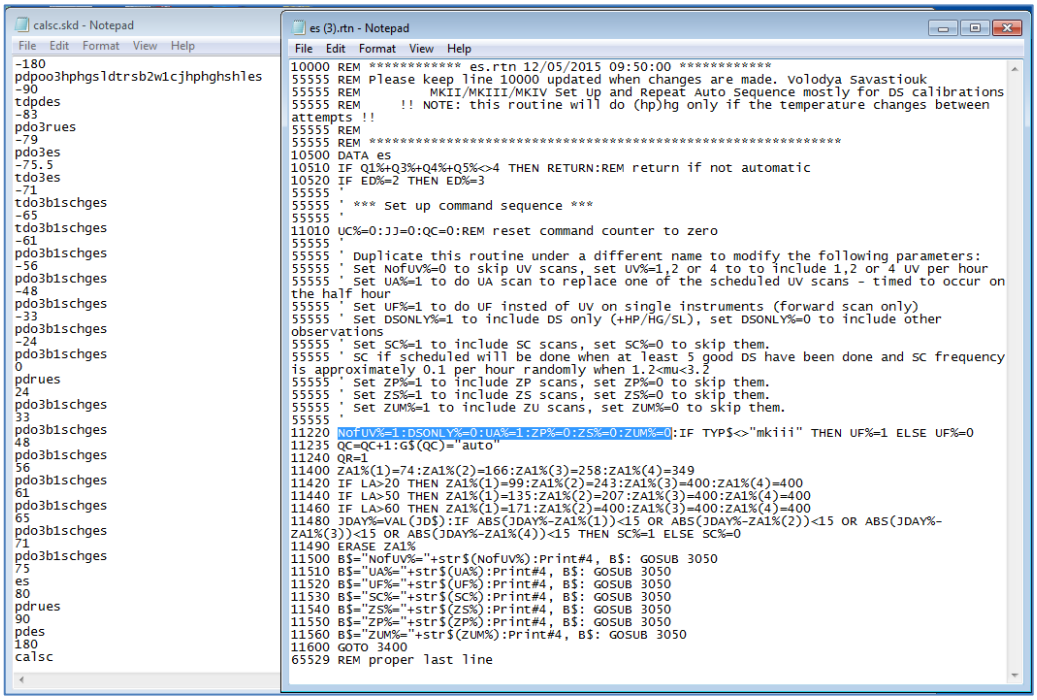
The schedule should include the following:

- An hg/hphg hourly to ensure that the micrometer(s) is/are positioned correctly for ozone measurement as instrument temperature changes through the day.
- At least one UV measurement should also be included every hour to ensure minimum disruption of the UV record for the station where the instrument is being calibrated.
- At least 5 standard lamp tests should be run before the beginning and after the end of data collection for each intercomparison day.
- A standard lamp test every two hours during the day would also be useful to monitor instrument stability throughout the day and highlight any changes with temperature.

At a minimum one half of one clear sky day (either morning or afternoon) is required to provide enough data for a good intercomparison. Ideally the intercomparison data should capture the full span of the suns movement though the sky. The ideal time to collect intercomparison data at

most locations in the Northern Hemisphere is June 20th ± 2 months since this is the time during which the maximum range of SZA at a given station occurs. For Arctic stations good intercomparison data can be collected June 20th ± 3 weeks. For mid-latitude stations good intercomparison data can be collected June 20th ± 2 months. In tropical regions the range of SZA are acceptable throughout the year therefore intercomparison data can be collected at any time.

1. Confirm the es.rtn and calsc.skd files used by the reference and Brewer being tested are configured as illustrated below. This will ensure that the schedule requirments mentioned above are executed.



calsc.skd - Notepad

```
-180
pdpoo3hphgsldtrsb2w1cjhphghshles
-90
tdpdes
-83
pdo3rues
-79
pdo3es
-75.5
tdo3es
-71
tdo3b1schges
-65
tdo3b1schges
-61
pdo3b1schges
-56
pdo3b1schges
-48
pdo3b1schges
-33
pdo3b1schges
-24
pdo3b1schges
0
pdrues
24
pdo3b1schges
33
pdo3b1schges
48
pdo3b1schges
56
pdo3b1schges
61
pdo3b1schges
65
pdo3b1schges
71
pdo3b1schges
75
es
80
pdrues
90
pdes
180
calsc
```

es (3).rtn - Notepad

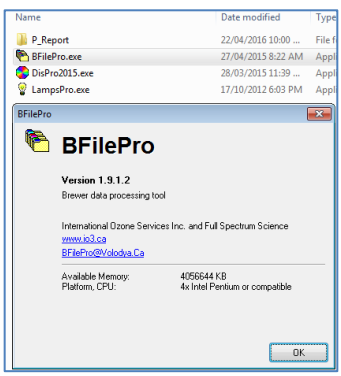
```
10000 REM ************ es.rtn 12/05/2015 09:50:00 ************
55555 REM Please keep line 10000 updated when changes are made. Volodya Savastiouk
55555 REM         MKII/MKIII/MKIV Set Up and Repeat Auto Sequence mostly for DS calibrations
55555 REM     !! NOTE: this routine will do (hp)hg only if the temperature changes between
attempts !!
55555 REM
55555 REM ************************************************************
10500 DATA es
10510 IF Q1%+Q3%+Q4%+Q5%<>4 THEN RETURN:REM return if not automatic
10520 IF ED%=2 THEN ED%=3
55555 '
55555 ' *** Set up command sequence ***
55555 '
11010 UC%=0:JJ=0:QC=0:REM reset command counter to zero
55555 '
55555 ' Duplicate this routine under a different name to modify the following parameters:
55555 ' Set NofUV%=0 to skip UV scans, set UV%=1,2 or 4 to to include 1,2 or 4 UV per hour
55555 ' Set UA%=1 to do UA scan to replace one of the scheduled UV scans - timed to occur on
the half hour
55555 ' Set UF%=1 to do UF insted of UV on single instruments (forward scan only)
55555 ' Set DSONLY%=1 to include DS only (+HP/HG/SL), set DSONLY%=0 to include other
observations
55555 ' Set SC%=1 to include SC scans, set SC%=0 to skip them.
55555 ' SC if scheduled will be done when at least 5 good DS have been done and SC frequency
is approximately 0.1 per hour randomly when 1.2<mu<3.2
55555 ' Set ZP%=1 to include ZP scans, set ZP%=0 to skip them.
55555 ' Set ZS%=1 to include ZS scans, set ZS%=0 to skip them.
55555 ' Set ZUM%=1 to include ZU scans, set ZUM%=0 to skip them.
55555 '
11220 NofUV%=1:DSONLY%=0:UA%=1:ZP%=0:ZS%=0:ZUM%=0:IF TYP$<>"mkiii" THEN UF%=1 ELSE UF%=0
11235 QC=QC+1:G$(QC)="auto"
11240 QR=1
11400 ZA1%(1)=74:ZA1%(2)=166:ZA1%(3)=258:ZA1%(4)=349
11420 IF LA>20 THEN ZA1%(1)=99:ZA1%(2)=243:ZA1%(3)=400:ZA1%(4)=400
11440 IF LA>50 THEN ZA1%(1)=135:ZA1%(2)=207:ZA1%(3)=400:ZA1%(4)=400
11460 IF LA>60 THEN ZA1%(1)=171:ZA1%(2)=400:ZA1%(3)=400:ZA1%(4)=400
11480 JDAY%=VAL(JD$):IF ABS(JDAY%-ZA1%(1))<15 OR ABS(JDAY%-ZA1%(2))<15 OR ABS(JDAY%-
ZA1%(3))<15 OR ABS(JDAY%-ZA1%(4))<15 THEN SC%=1 ELSE SC%=0
11490 ERASE ZA1%
11500 B$="NofUV%="+str$(NofUV%):Print#4, B$: GOSUB 3050
11510 B$="UA%="+str$(UA%):Print#4, B$: GOSUB 3050
11520 B$="UF%="+str$(UF%):Print#4, B$: GOSUB 3050
11530 B$="SC%="+str$(SC%):Print#4, B$: GOSUB 3050
11540 B$="ZS%="+str$(ZS%):Print#4, B$: GOSUB 3050
11550 B$="ZP%="+str$(ZP%):Print#4, B$: GOSUB 3050
11560 B$="ZUM%="+str$(ZUM%):Print#4, B$: GOSUB 3050
11600 GOTO 3400
65529 REM proper last line
```

2. Initate the calsc routine on both Brewer computers and allow this schedule to run until adequate ds data is co-collected. During data collection perform sun sighting every 1.5 to 2 hours. Note: a clear sky during collection is preferred.

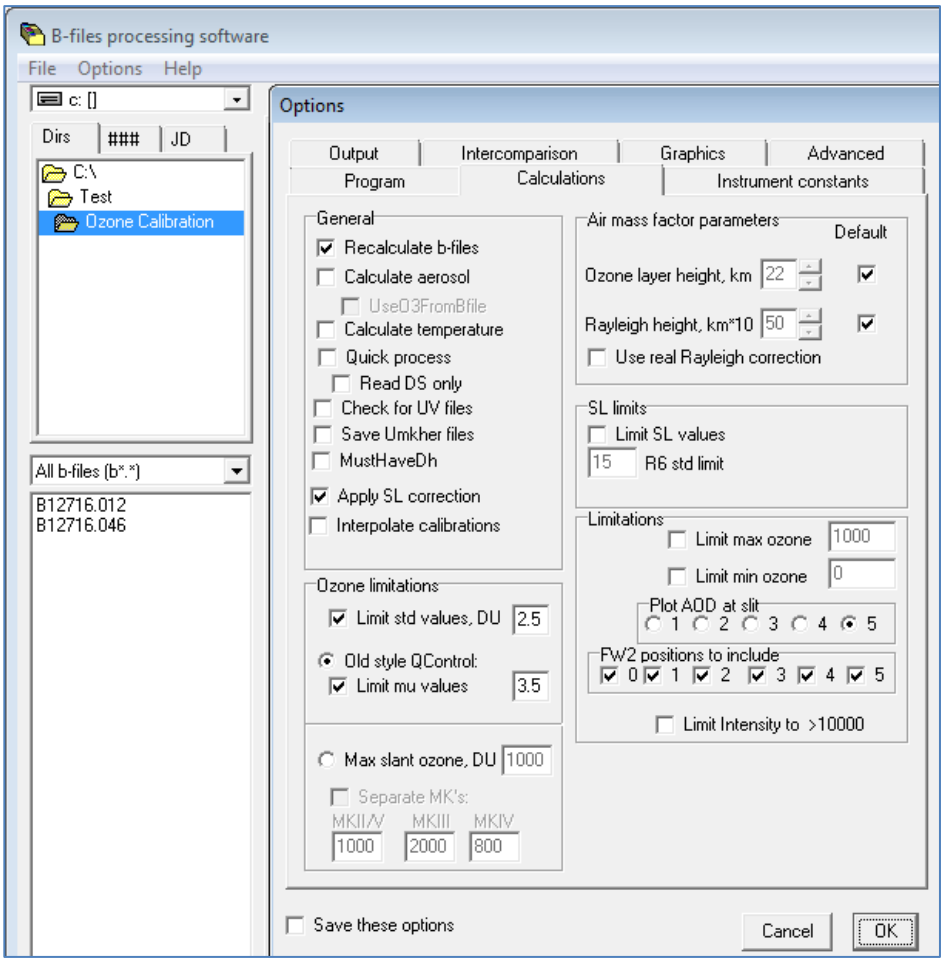
Data Processing using BFilePro

1. Create a test directory and copy all the working files (icf, dcf, uvres, relevant b-files and OP_ST) for the reference and the pre/post files for the brewer being calibrated into this test directory.

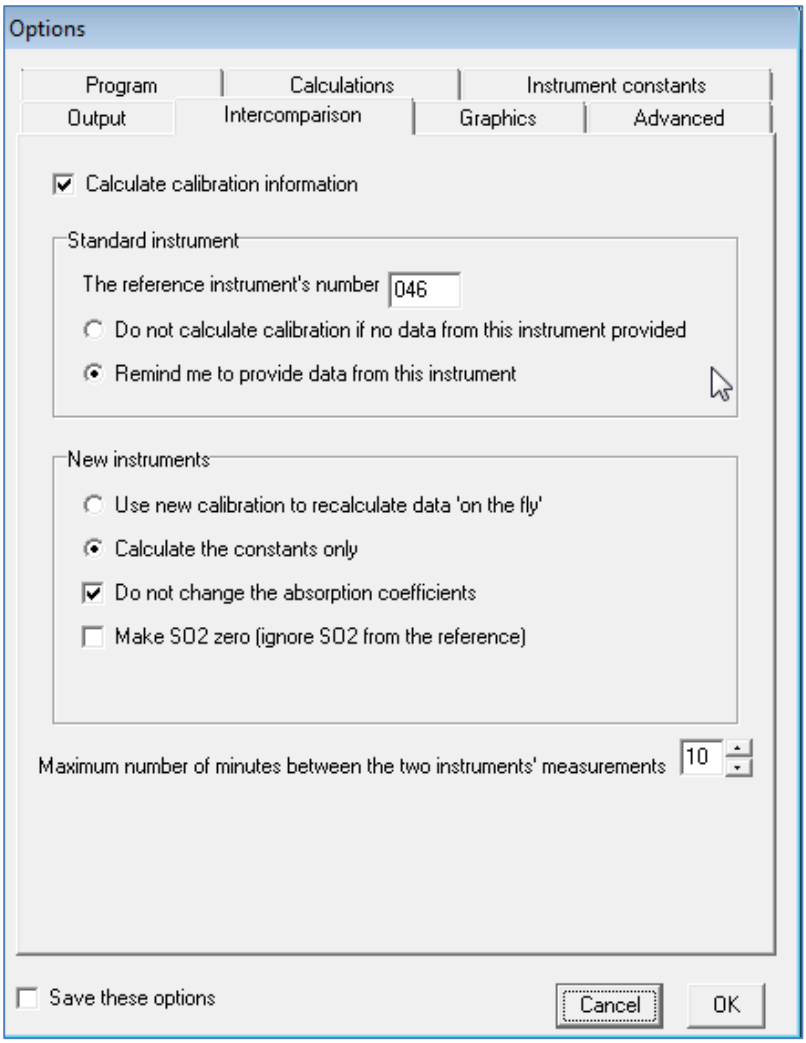
2. Double click on the BFilePro.exe icon to start the software and click OK to initiate the program.



3. Click on the *Options* menu and select the *Calculations* tab. Ensure the following boxes are checked and the values inputted as illustrated below.
    - Recalculate b-files checked,
    - Apply SL correction checked,
    - Limit std values DU, 2.5,
    - Limit mu values , 2.5 (Single Brewer) or 3.5 (Double Brewer),
    - Default for Ozone layer height and Rayleigh height checked,
    - FW2 positons 0,1,2,3,4,5 checked.



4. Next select the intercomparison tab and enter the three digit serial number of the reference instrument and insure that the following boxes are checked;
   - Calculate calibration information
   - Remind me to provide data from this instrument
   - Calculate the constants only
   - Do not change the absorption coefficients
   - Maximum number of minutes between the two instruments' measurements, 10.



Adding the Reference Brewer to the Instruments Constants Tab

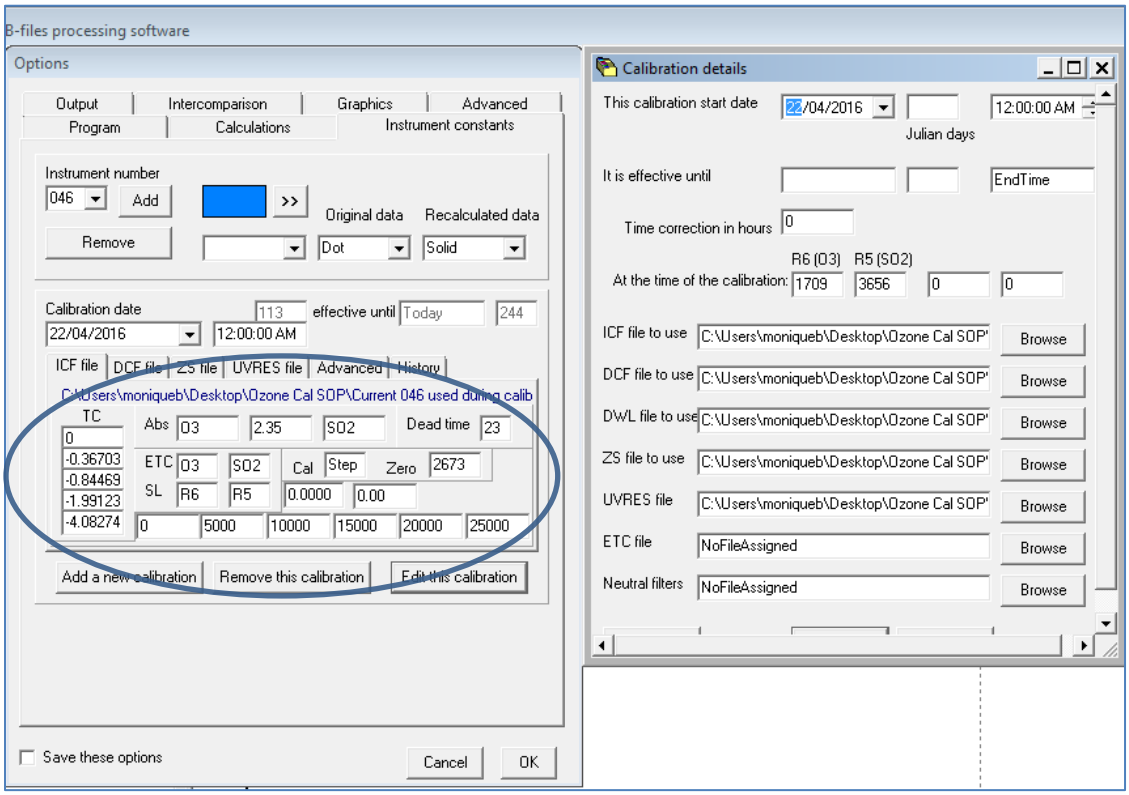
5. Next select the *Instruments constants* tab and click on the *Add* button beside the instrument number box and enter the three digit serial number of the reference instrument.

6. Then click on the *Add a new calibration* button which opens a Calibration details window.

7. Input the date of the last calibration in the *This calibration start date* field and the averaged SL ratio values for R6 and R5 calculated from the worksheet in the appendix (average of 20 SL ratio values following the last calibration).

8. Next use the *browse buttons* to navigate to the reference instruments current icf, dcf (cubic), dwl, zs and uvr files in use. These should be located in the test directory created earlier. Use the references in use OP_ST file to determine the correct files to be linked.

9. Click *OK* on the *Calibration details* window to save these constants for the reference brewer and any subsequent warning messages that appear.



10. The fields circled above will now be populated with values from the icf file linked to this instrument and date. Check mark *Save these options* and click *OK*.

Adding the Brewer being Calibrated to the Instruments Constants Tab

Pre-Calibration State

11. From the main BFilePro screen click on the *Options* menu and select the *Instruments constants* tab and click on the *Add* button beside the *instrument number box* and enter the three digit serial number of the Brewer being calibrated.

12. Then click on the *Add a new calibration* button which opens a *Calibration details window*.

13. Input the date of the last calibration in the *This calibration start date field* and the averaged SL ratio values for *R6* and *R5* calculated (average of 20 SL ratio values following the last calibration).

14. Next use the browse buttons to navigate to this Brewers current *icf, dcf (cubic), dwl, zs* and *uvr* files. These should be located in the test file created earlier. Use the Brewers in use OP_ST file to determine the correct files to be linked.

15. Click OK on the *Calibration details* window to save these constants for the reference brewer and any subsequent warning messages that appear.

16. The fields located in the *ICF file* tab will now be populated with values from the icf file linked to this instrument and date.

17. Check mark Save these options and click OK.

Post-Calibration State

18. From the main BFilePro screen click on the *Options* menu and select the Instruments constants tab and choose the number of the Brewer being calibrated.

19. Then click on the *Add a new calibration* button which opens a *Calibration details window*.

20. Input the start date of the intercomparison data just collected and the SL ratios R6 and R5 calculated at the time of this intercomparison.

21. Click the *Browse* buttons to open the pre-calibration icf file and the dcf, dwl, zs and uvr files that are to be used moving forward (post-calibration files).

22. Click *OK* and any error messages that may be displayed until you return to the Options window.

23. Edit any values located in the Instrument constants tab relating to the icf file. As an example, the abs constants (*use abs values from O3 line fit file*), cal step, dead time, TC's may have changed following instrument maintenance.

24. Click *OK* to save these changes and again when asked to confirm.

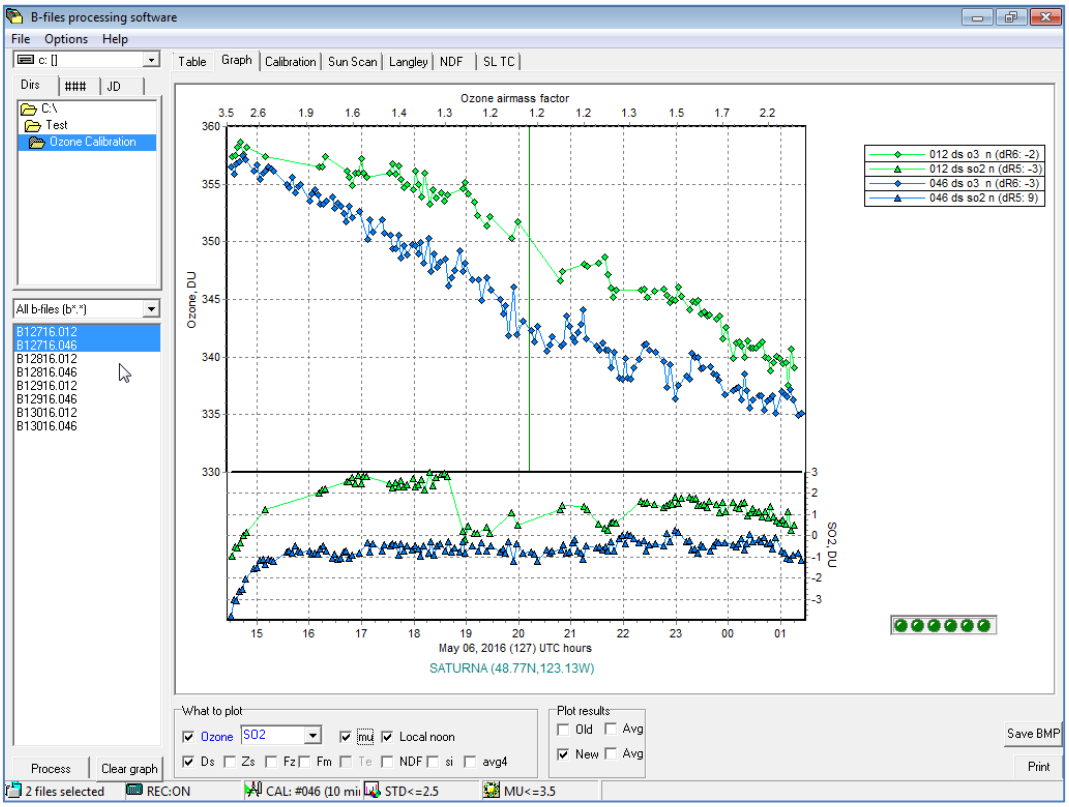
25. A prompt asking to save a new ICF file will activate, add the word test to the file name and save (i.e. icf12716_test.012, use the Julian date corresponding to the start of the intercomparison).

26. The fields located in the *ICF file* tab will now be populated with values from the icf file linked to this instrument and date.

27. Checkmark *Save* these options and click *OK*.

28. In the main BFilePro window use the directory dialog field to navigate to the directory containing the intercomparison B-files. Highlight the B-files for both the reference and the Brewer under test and click on the *Process* button.

29. Click on the *Graph* tab.



30. In the *What to plot* area checkmark the Ozone, Ds, mu, local noon boxes. Also using the drop down box beside Ozone, select SO_2.

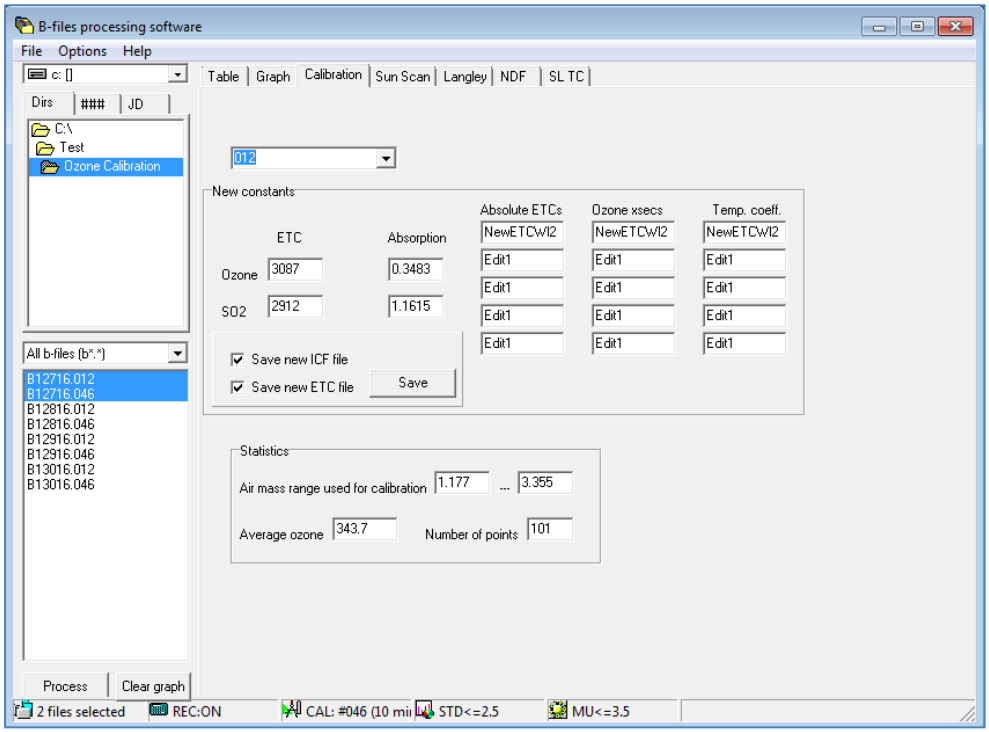
31. The O_3 and SO_2 data intercomparison data will now be displayed in the *Graph* tab.

32. In the Plot results area confirm that the *New* check box is checked. (toggle *New* and *Old* to view the changes in SL ratios where *Old* is without SL ratio correction and *New* is with the SL ratio correction applied).

33. Next click on the *Save BMP* button to save a screenshot of this graph. Name the file as follows;
    O3JJJYY A.&&&_ ###_ original.bmp
    - *JJJ* is the 3-digit Julian Day corresponding to the first day of the intercomparison data,
    - *YY* is the 2-digit year,
    - *A* is either initial or final, depending whether this calibration is before (initial) or after (final) instrument maintenance and calibrations,
    - *&&&* is the 3-digit serial number of the reference Brewer,
    - *###* is the 3-digit serial number of the Brewer under test,
    - *original* is in reference to using the original icf file (i.e. no changes to ETC's).

Correcting for ETC-related Curvature

34. Now navigate to the Calibration tab. Select the serial number of the Brewer being calibrated from the drop down window. The new calculated ETC's will be displayed for this Brewer relative to the reference Brewer.

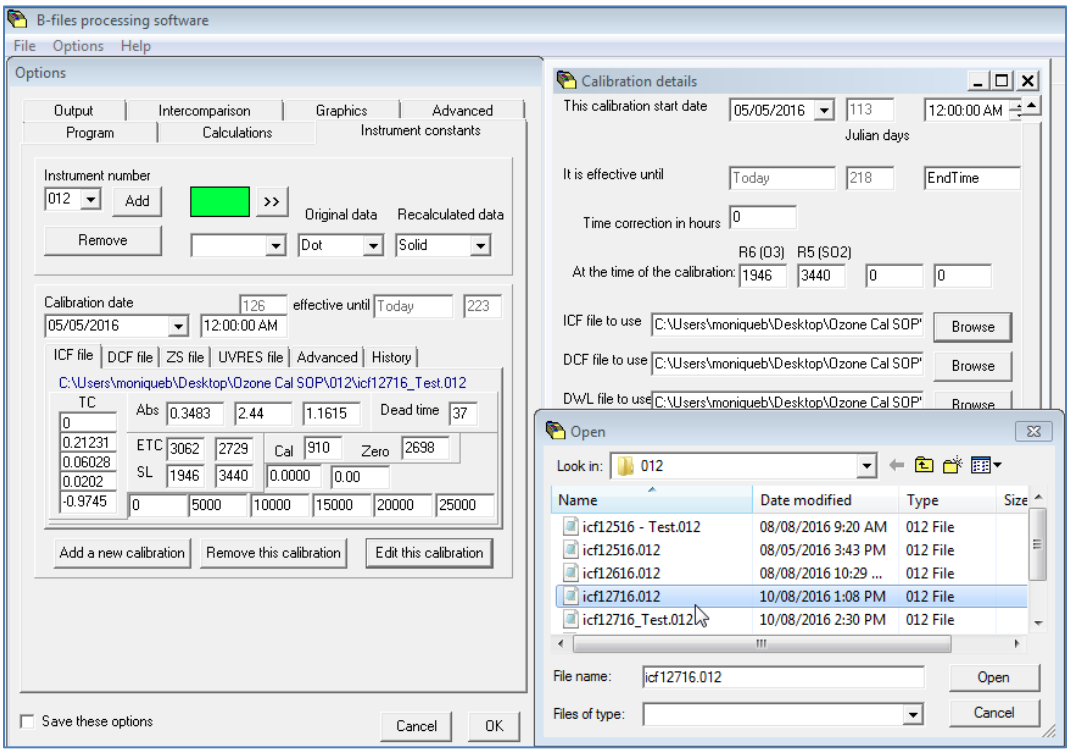


35. Place a checkmark in the Save new ICF file and Save new ETC file boxes and click on the Save button.

36. An ETC save window will open. Name the ETC file using the Julian date corresponding to the start of the intercomparison (i.e. etc12716.012) and save.

37. Following the ETC file creation another save window will open for the creation of a new ifc file. Name the new icf file using the Julian date corresponding to the start of the intercomparison (i.e. icf12716.012) and save.

38. These newly created files will now need to be associated with the Brewer being calibrated by updating the calibration files used in the Instruments constants tab.



39. From the main *B-files processing software* window click on *Options* and choose the *Instrument number* of the Brewer being calibrated and correct *calibration date*. Then click on *Edit this calibration*.

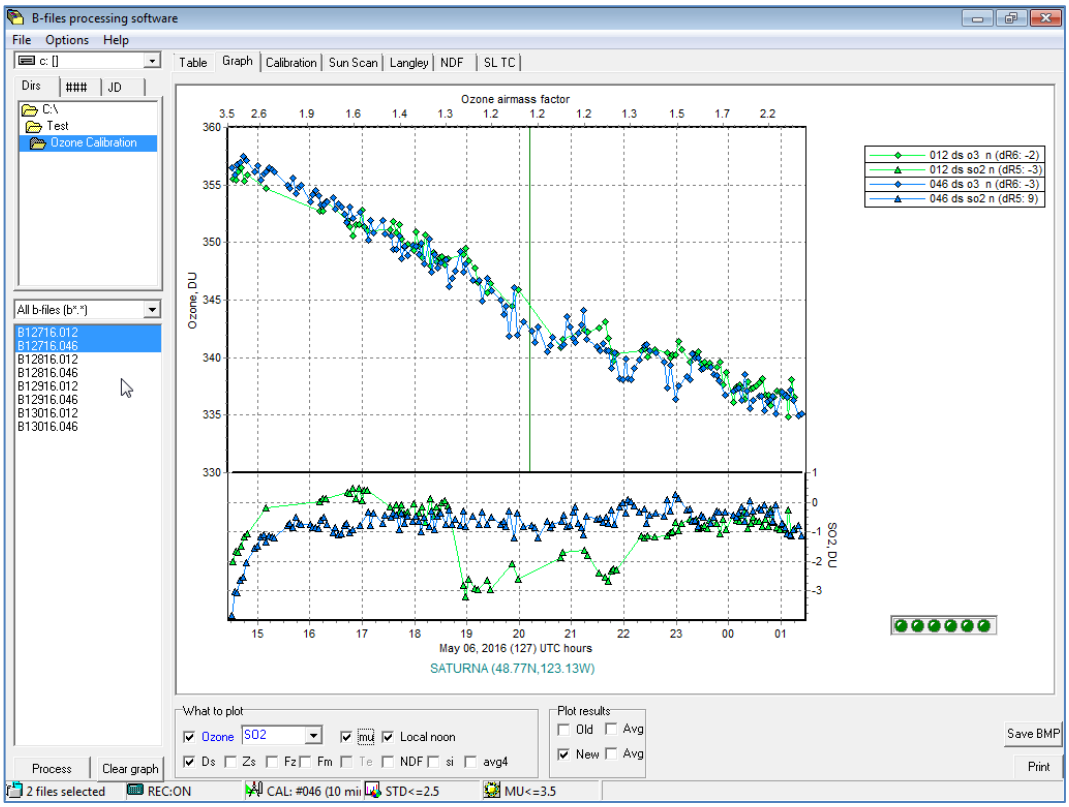
40. Click the *Browse* button for *the ICF file to use* and choose the icf file with the updated ETC values created in step 37 above. Then click open.

41. Next click the Browse button for the ETC file and choose the ETC file created in step 36 above and click *open*.

42. Click *OK* on the Calibration details window to associate these two files with the Brewer being calibrated.

43. Next click *OK* on the Options window and subsequent warning messages.

44. Click on the *clear graph* button and *process* the comparison b-files being used.



45. The resulting graph illustrates a good agreement between the Brewer being calibrated and the reference. The two plots should be within a few Dobson units throughout the entire intercomparison period.

46. Further ETC tweaking can be done to allow for tighter agreement between the reference and the Brewer being calibrated. ETC values should be rounded to the nearest 5 for O3 and 10 for SO2.

47. The ETC values obtained using BFilePro for the Brewer being calibrated can be graphically compared to the expected ETC's determined in the Pre-Calibration section. Simply input these expected ETC's in the Options window and save them to a new icf file when prompt (i.e. rename to icfexp.###). Then *Edit this calibration* and Browse to the new icf file just created.

48. Next click on the *Save BMP* button to save a screenshot of this graph. Name the file as follows;
    O3JJJYY A.&&&_ ###_ new.bmp
    - *JJJ* is the 3-digit Julian Day corresponding to the first day of the intercomparison data,
    - *YY* is the 2-digit year,
    - *A* is either initial or final, depending whether this calibration is before (initial) or after (final) instrument maintenance and calibrations,
    - *&&&* is the 3-digit serial number of the reference Brewer,
    - *###* is the 3-digit serial number of the Brewer under test,
    - *new* is in reference to using the new icf file (i.e. includes changes to ETC's).

Confirmation of Results

49. Next home out and close the DOS box for the Brewer being calibrated.

50. Copy the new icf file into the calibration instrument's constants directory and edit the Op_st.### file in the constants directory to the updated the icf filename.

51. Weather permitting, run several direct sun ozone measurements on the reference and the Brewer being calibrated to confirm that the direct sun ozone measurements agree to within 1-2% and that the intercomparison data was processed correctly.

Notes

BFilePro calculations are based one or a few days of data. The calibration technician must factor in expected results when determining the final ETC's to use.

Appendix

Real Example: Post maintenance results using a worksheet.

Saturna Calibration Trip, May 2-9, 2016.
Reference Brewer: 046
Brewer being calibrated: 012

Reference s/n 046

Current OP_ST

icf11316.046	SL Ratio following last Calibration			
dcf12715.046	Julian Date range used	08316-10316		
dwl12715.046				
zsf19514.046	R5 (SO_2)	3656	R6 (O_3)	1709
uvr18914.046				
etc none				
fi none				

Brewer being Calibrated s/n 012

Current OP_ST

icf21014.012	Current ETC values			
dcf09911.012	ETC_{SO2}	2729	ETC_{O3}	3062
dwl09911.012				
zsf12006.012	SL Ratio following last Calibration			
uvr15014.012	Julian Date range used	24815-26815		
etc None				
fi None	R5 (SO_2)	3436	R6 (O_3)	1944

SL ratios of period following new calibration, inter-comparison

Julian Date range used 12916-14816

R5 (SO_2) 3440 R6 (O_3) 1946

Expected ETC values based on ΔSL Ratios

ETC_{SO2} 2733 ETC_{O3} 3064

Calculated ETC values based on BFilePro

ETC_{SO2} 2912 ETC_{O3} 3087

Final "tweaked" ETC values based on graph agreement

ETC_{SO2} 2900 ETC_{O3} 3090

New OP_ST

icf12515.012
dcf12816.012
dwl12816.012
zsf21014.012
uvr12916.012
etc12515.012
fi None

Prepared by: Monique Berthiaume
Acknowledgements: Michael Brohart, Volodya Savastiouk, IOS, Tom Grajnar.