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Calculation of calibration Coefficients from Internal and External Calibrations	Issue No	1.00
	Issued By	
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1 Introduction and scope:

This document provides instructions for obtaining calibration coefficients (bias corrections) for temperature dataloggers. These calibration coefficients relate the 'recorded' temperature to the 'true' temperature for each datalogger and provide an estimate of uncertainty in the resulting data. This document refers to Gemini TinyTag dataloggers and the TinyTag Explorer software but alternative loggers could be used assuming that the required input data structures can be generated.

Users should also refer to MSS-FFL Standard Operating Procedures for external and internal calibration processes (SOPFL 1010 and SOPFL 1020).

2 Principle of the method

Field Logger calibration follows a two stage procedure that involves external and internal calibrations. Firstly MSS Reference Dataloggers are calibrated externally in a UKAS accredited laboratory against appropriate reference materials. Secondly MSS Field Dataloggers are calibrated against the MSS Reference Dataloggers in a water bath using an internal calibration procedure (SOPFL 1020). All data from the internal calibration procedures is saved into .csv files. The 'loggercal' R package can then be used to generate calibration coefficients that characterise bias and uncertainty derived from both calibration procedures. At the end of the process each Field Datalogger will have 1) calibration coefficients that can be used to correct 'recorded' temperature to the 'true' temperature using a second order polynomial equation (quadratic function) and 2) standard error coefficients which can be used to return uncertainty in the corrected estimates of temperature (true temperatures) using a fourth order polynomial equation.

3 Reference materials

Calibration data files (.csv) for a "MSS reference datalogger" calibrated externally to UKAS standards

4 Reagents

N/A

5 Equipment

Gemini TinyTag Datalogger software version 4.8 or above
R (version >=3.0.0); RStudio; Window Operating System; R package mgcv

6 Environmental control

N/A

7 Interferences

N/A

8 Sampling and sample preparation

N/A

9 Analytical Procedure

9.1 Package installation

Joint bias and uncertainty between external reference materials / MSS Reference datalogger (step 1) and MSS Reference Datalogger / Field Dataloggers (step 2) is calculated using a package called 'loggercal' located on GitHub: https://github.com/Faskally/loggercal

The 'loggercal' package can be downloaded from the Faskally GitHub page (https://github.com/Faskally/loggercal) or installed directly using the following command in R:

```
devtools::install_github("faskally/loggercal")
```

Note that when working within a proxy server environment the following can be used:

```
if (TRUE) {
httr::set_config(
httr::use_proxy(url=INSERT PROXY ADDRESS, port=INSERT PROXYPORT)
)
devtools::install_github("faskally/loggercal")
}
```

Prerequisites: R (version >=3.0.0); RStudio; Window Operating System; R package mgcv

9.2 Required data inputs and structure:

Prior to running the calibration code, it is necessary get the input data into the required structure. This is split into two parts:
External laboratory (e.g. UKAS) calibration file (.csv) for MSS Reference Logger(s) (section 9.2.1)

Data file (.csv) from the internal calibration procedures using MSS Reference and MSS Field dataloggers (section 9.2.2)

9.2.1 External (UKAS) calibration of MSS Reference Dataloggers

9.2.1.1 MSS reference dataloggers are calibrated externally against a UKAS accredited standard at 5° C intervals ranging between 0 and 30° C (See SOPFL 1010 for further details). This defines bias and uncertainty in the relationship between UKAS reference materials and the MSS Reference Datalogger. Results of this calibration are provided as a calibration certificate from the UKAS accredited laboratory and should be saved in a comma separated (csv) file in the following format:

S/N	Mean Established Temperature	319151 "Mean Logged Temperature"	"Error"	"Time"	"Uncertainty"
	19.996	19.944	-0.052	00:30:00	0.025
	5.003	4.902	-0.101	00:30:00	0.025
	9.996	9.918	-0.078	00:30:00	0.025
	15.009	14.946	-0.063	00:30:00	0.025
	25.028	24.981	-0.047	00:30:00	0.025
	29.993	29.963	-0.03	00:30:00	0.025
	0.002	-0.118	-0.12	00:30:00	0.025
	19.99	19.939	-0.051	00:30:00	0.025

9.2.1.2 The file **must** be named following the convention UKASCalibration_loggerserialnumber e.g. UKASCalibration_733784

9.2.1.3 The file **must** then be stored in its own folder that contains no other files.

9.2.2 MSS Reference Dataloggers / Field Logger Calibration

9.2.2.1 MSS Field Dataloggers are calibrated against the 'MSS Reference Datalogger(s)' in a recirculating water bath over a temperature range of 0 - 30° C (See SOPFL1020 for further details). Once the calibration experiment is completed, these data are then downloaded using the TinyTag software.

9.2.2.2 The files **must** be named 'serial number_ddmmyy' (e.g. '123456_010119'). The reference logger file must be named 'serial number_ddmmyy_cal2'

9.2.2.3 The files **must** then be stored in a folder named according to the start date of the calibration experiment e.g. 010119

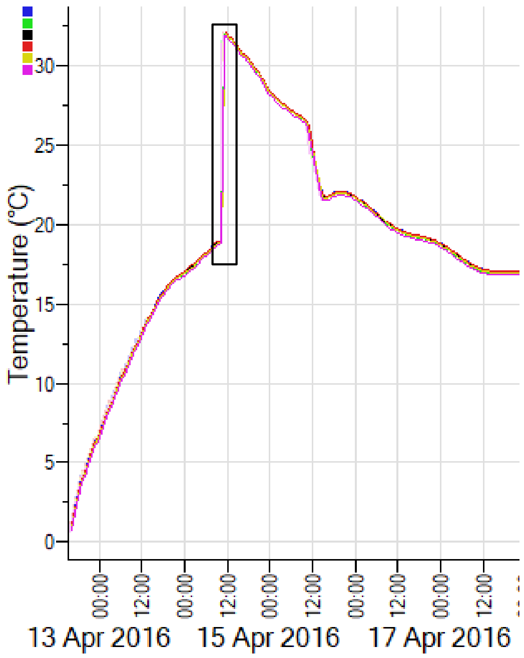
9.2.2.4 Once all the MSS Field Dataloggers are downloaded highlight **all** the datalogger files from the experiment (**including MSS Reference Datalogger**) and open them together in TinyTag Explorer (Highlight/Right Click/Open).

9.2.2.5 Next, click on 'view' and then 'create new overlay', 'select all files' and 'move'.

9.2.2.6 Inspect the data:

9.2.2.7 If there are obvious marked differences associated with a particular logger (i.e. the logger appears as an extreme outlier), put the logger aside for further investigation.

9.2.2.8 Note any periods of unusually rapid heating and cooling within the time series as these will need to be removed later. These can be at the start or end of the experiment but also in the middle of the experiment when a heater is turned on e.g. the data within the black box below:



9.2.2.9 Following the creation of an 'overlay', click on 'view' from the options at the top of the screen and then select 'Table of readings'.

9.2.2.10 Next select 'File' and 'Export all cells'. Create a csv file (option 'Comma Separated Text File (No units) (*.csv) of the calibration data and save it. The file **must** be named 'FullCalibration_[ddmmyy].csv' (e.g. FullCalibration_010119.csv). The file name nomenclature is necessary as it is called within the loggercal function.

9.2.2.11 The file **must** then be stored in the dated folder where the individual logger files from the calibration experiment files are saved.

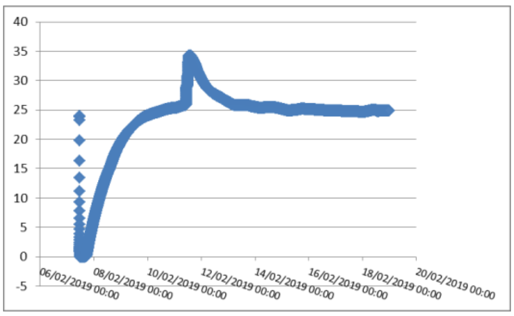
An example file following the required format is:

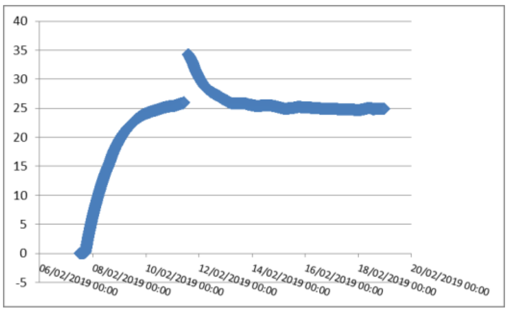
	Time	1	2	3	4
S/N		642283	642282	642277	642271
Type		TG-4100	TG-4100	TG-4100	TG-4100
Description		Gemini Data Loggers	Gemini Data Loggers	Gemini Data Loggers	Gemini Data Loggers
Property		Temperature	Temperature	Temperature	Temperature
1	12/10/2017 11:14:00	0.151	0.197	0.185	0.097
2	12/10/2017 11:15:00	0.13	0.173	0.17	0.074
3	12/10/2017 11:16:00	0.114	0.156	0.156	0.058
4	12/10/2017 11:17:00	0.104	0.147	0.142	0.048
5	12/10/2017 11:18:00	0.09	0.131	0.135	0.031
6	12/10/2017 11:19:00	0.076	0.126	0.121	0.025
7	12/10/2017 11:20:00	0.072	0.116	0.119	0.01
8	12/10/2017 11:21:00	0.065	0.105	0.105	0.006
9	12/10/2017 11:22:00	0.065	0.104	0.104	0.001
10	12/10/2017 11:23:00	0.046	0.098	0.1	-0.011
11	12/10/2017 11:24:00	0.05	0.095	0.093	-0.02
12	12/10/2017 11:25:00	0.045	0.088	0.086	-0.025
13	12/10/2017 11:26:00	0.038	0.086	0.086	-0.028
14	12/10/2017 11:27:00	0.034	0.079	0.086	-0.023

9.2.2.12 The first 5 rows of the file should contain information on the logger. Column A should contain sequential numbers for the observations, column B should contain data / time stamps in the format dd/mm/yyyy hh:mm:ss (**Note: seconds ARE required**). Column C onwards should contain temperature observations from individual loggers in ° C.

9.2.2.13 Next open the 'FullCalibration_ddmmyy.csv' file

9.2.2.14 The data that cannot be included in the calibration now needs to be removed. Any periods of rapid heating / cooling should be removed (Below left: before removal of rapid heating / cooling; below right: after removal of rapid heating / cooling) especially where these occur in the middle of the record. Problem data at the start or end of the experiment can be removed later (see below). The data are now ready to be used with the calibration coefficient R script.





9.2.3 Generate calibration coefficients

9.2.3.1 Open the R Script 'Calibration_Code_PointnClick'. Highlight the whole script and click 'Run' (or Ctrl+Enter) to run the entire script.

9.2.3.2 A pop-up screen will ask you to 'CHOOSE INTERNAL CALIBRATION DIRECTORY' – click to the folder where the 'FullCalibration_[ddmmyy].csv' file has been saved.

9.2.3.3 You will see a message printed to your R Console which shows the directory you have chosen. A pop-up screen will then ask you to 'CHOOSE EXTERNAL CALIBRATION DIRECTORY' – click to the folder that contains the correct external calibration file for the MSS Reference Logger that you want coefficients for. The external calibration serial number needs to match the reference logger serial number used in the experiment. The date when it was calibrated externally also needs to precede the date of the experiment (i.e. for experiment batch file dated 080317, the external calibration date would be earlier than 080317).

9.2.3.4 A message will be printed to the R Console which shows the directory chosen

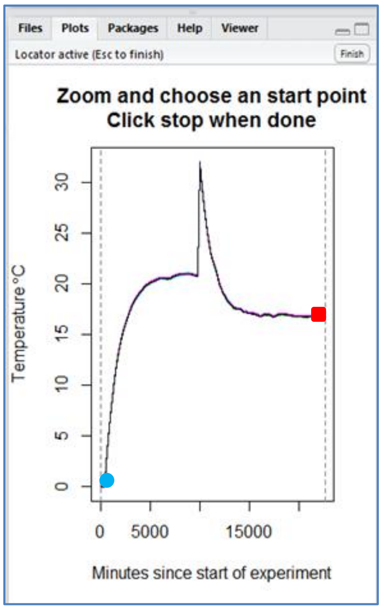
9.2.3.5 Next a message will be printed to the R Console which shows the files that are being read in for the external and internal calibration.

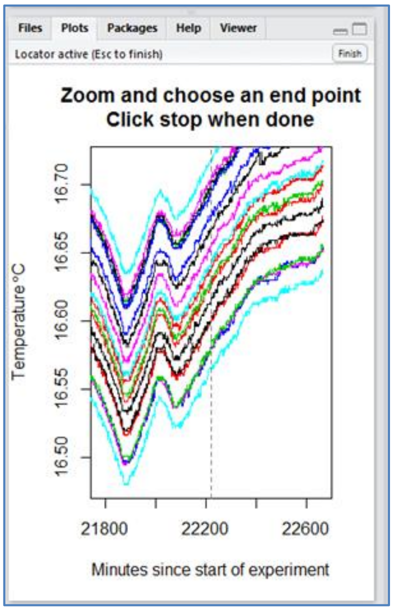
9.2.3.6 Once this has been done the word 'DONE!' will be printed to the console and the plotting window will be active. The next step is to set the start and stop times of the experiment (i.e. remove any unreliable data that has been identified at the start and end of the series). This is a carried out using the graphical interface within the plotting area of RStudio.

9.2.3.7 First click once at the start of the experiment (e.g. to the right of the first dotted line shown with a blue circle in the image below), the plot will then zoom into the area clicked, next click 'Finish' .

9.2.3.8 Next click once at the end of the experiment (e.g. to the left of the second dotted line shown with a red square in the image below), the plot will then zoom into the area clicked, and then click 'Finish'.

9.2.3.9 This will end the graphical interface selection.
Note: the data is plotted as a continuous line (joining all points) and therefore appears to show the rapid heating period, which was previously removed in Excel.





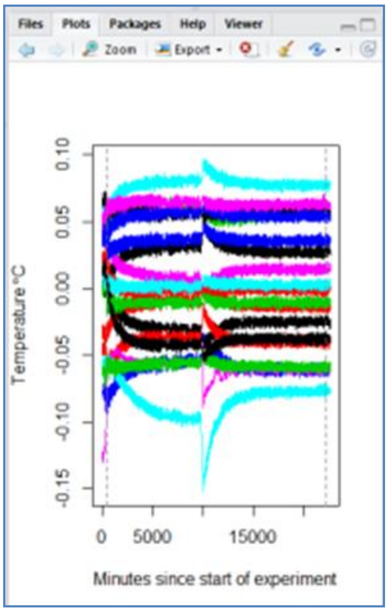
'Setting up calibration regressions' will then be printed to the R Console.

9.2.3.10 Next a progress counter will be displayed in the R console as it loops through each of the MSS Field dataloggers within the 'FullCalibration' file (e.g. if there are 5 MSS field dataloggers it will display: fitting 353130: 1 of 5 fitting 353119: 2 of 5 etc.).

9.2.3.11 'Calibration complete!' will be printed to the R Console when the process is finished. The location of the resulting files (calibration plot and coefficients), determined by the 'CHOOSE INTERNAL CALIBRATION DIRECTORY' that was provided earlier is also printed to the R Console

9.2.3.12 At the end of the calibration process a plot of logger biases is saved as a pdf into the same dated folder that contains the files from the internal calibration experiment. This plot identifies temperature differences between the MSS Reference Logger and each MSS Field Deployed Datalogger during the calibration experiment. This can be a useful plot to assess where loggers exhibit extreme biases or where there are unusual features in the calibration experiment requiring further consideration. In the case below inter-logger differences in temperature measurement are relatively small and there are no major causes for concern.

Note: these plots do not indicate how logger biases vary with temperature and do not incorporate any bias associated with the MSS Reference Logger.



9.2.3.13 The calibration coefficients are written out and saved in the same dated folder that contains all of the files from the internal calibration experiment. These coefficients can then be used to correct the 'recorded' temperature to the 'true' temperature (i.e. bias adjust) and to indicate the uncertainty in the corrected temperature observations (that reflects uncertainty in the internal and external calibrations).

9.2.3.14 These coefficients should be reproduced every time an MSS Field Datalogger is re-calibrated.

10 Calculation of results

10.1 Individual logger calibration coefficients are stored in the FLEObs database and used to calibrate data on export. The calibration equation is a second order polynomial (quadratic) function (a + bx + cx^2). The Uncertainty (standard errors) is represented by a fourth order polynomial function (a + bx + cx^2 + dx^3 + ex^4). An example of the exported MSS Field Datalogger coefficients table is shown below. Note in this example the standard errors on the double calibration procedure are <0.01°C and the corrected (true) temperatures are within ca. 0.2°C of the raw observations.

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W
Make	Model	SN	Unit	Start_date	Cal_	Cal_coef1	Cal_coef2	Cal_coef3	Cal_	Cal_	Cal_	Cal_	Cal_	Cal_	Cal_	SE_E	SE_coef1	SE_coef2	SE_coef3	SE_coef4	SE_coef5	SE_
Gemini Data Loggers	TG-4100	801340	°C	28/07/2017	2	0.147475	1.001454	-8.75E-05								4	0.004408	-0.00012	1.41E-05	-6.90E-07	1.16E-08	
Gemini Data Loggers	TG-4100	801759	°C	28/07/2017	2	0.119384	1.000022	-8.30E-05								4	0.004686	-0.00011	1.33E-05	-6.46E-07	1.08E-08	
Gemini Data Loggers	TG-4100	801362	°C	28/07/2017	2	0.158679	0.998369	-6.06E-05								4	0.004475	-0.00011	1.38E-05	-6.75E-07	1.13E-08	

10.2 A worked example is shown below on how to correct the 'recorded' temperature to the 'true' temperature and indicate the uncertainty using the derived calibration coefficients.

To determine 'true' temperature, for each 'recorded' temperature use the equation:

Cal_coef1 + (Cal_coef2*'recorded temperature') + (Cal_coef3*'recorded temperature'^2)

To determine the standard error for corrected estimates of temperature (true temperatures) use the following equation:

SE_coef1 + (SE_coef2*'recorded temperature') + (SE_coef3*'recorded temperature'^2) + (SE_coef4*'recorded temperature'^3) + (SE_coef5*'recorded temperature'^4).

Approximate 95% Confidence intervals can be obtained by adding and subtracting 1.96 * SE from the corrected temperatures.

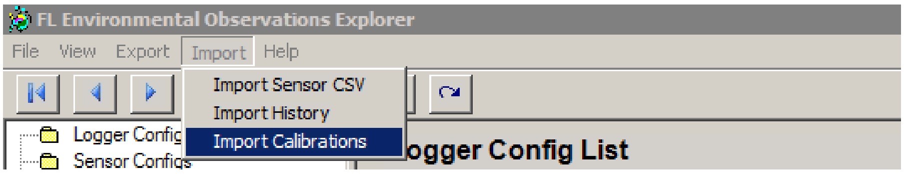
10.3 Uploading the calibration coefficients file into FLEObs

10.3.1 Copy the coefficients .csv file over to the SCOTS coefficients folder on the G drive:

[redacted]

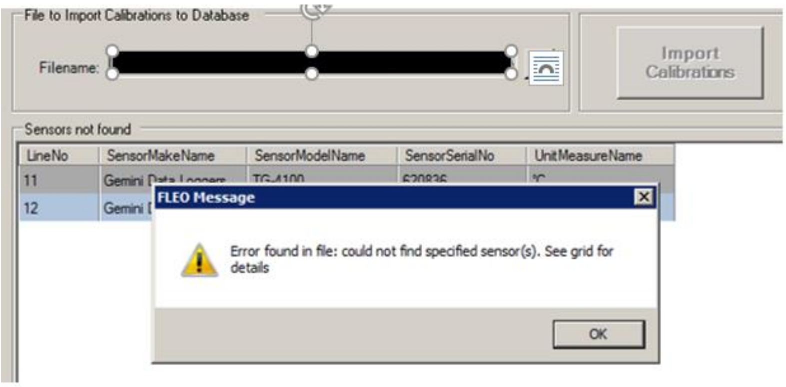
10.3.2 Open up the .csv you are wanting to upload and then save without making any changes (for some reason if you don't do this you get an error when you try and open file within FLEObs).

10.3.3 In FLEObs: Click on Import, then Import Calibrations.

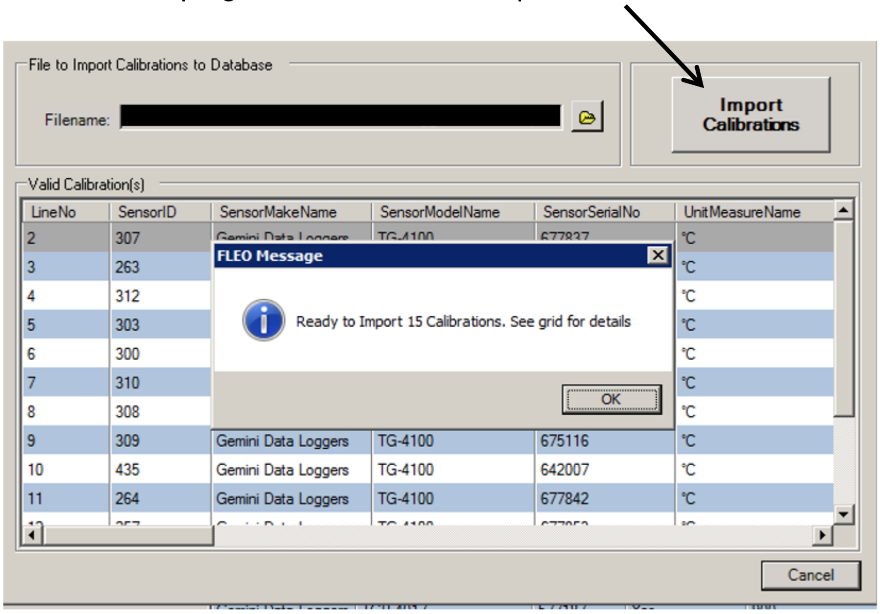


10.3.4 Select to the filename to be imported

10.3.5 Only loggers that have been set up on FLEObs can receive a calibration, therefore coefficients for logger serial numbers that are not set up on FLEObs cannot be included in the file. These are shown in the Import Calibrations box that appears (see below). Press Cancel. These columns should be manually removed from the .csv and then re-try. OR, these logger serial numbers could be set up on the system and set valid from date to just before the logger was calibrated in water bath.



10.3.6 Once all the logger serial numbers in the .csv are matched to those on the FLEObs system, these are now ready to be uploaded. Click on the Import Calibration box now available in top right hand side of the Import Calibrations window.



10.3.7 If import was successful, a box will appear saying that calibrations import completed successfully. Calibration coefficients for those logger serial numbers have now been uploaded into FLEObs.

10.4 Visualising calibration results

If you want to visualise the outcomes of the double calibration procedure, logger corrections and associated uncertainty, then a worked excel example is provided in the Calibration Coefficient Visulistaion Template (B 939) with the following column definitions. Cells highlighted in green should be updated with relevant coefficients.

Column A, Obs – raw temperature data recorded by the logger
Column B, Corrected – corrected temperature data
Column C, Upper CI –upper 95% confidence interval
Column D, Lower CI –lower 95% confidence interval
Column G, Cal1 – logger calibration coefficient 1 (column G, Cal_coef1 in the above example and ‘full_calibration_coefs’ file produced in Step 9)
Column H, Cal2 – logger calibration coefficient 2 (column H, Cal_coef2 in the above example and ‘full_calibration_coefs’ file produced in Step 9)

Column I, Cal3 – logger calibration coefficient 3 (column I, Cal_coef3 in the above example and 'full_calibration_coefs' file produced in Step 9)
Column K, SE1– logger standard error coefficient 1 (column R, SE_coef1 in the above example and 'full_calibration_coefs' file produced in Step 9)
Column L, SE2 – logger standard error coefficient 2 (column S, SE_coef2 in the above example and 'full_calibration_coefs' file produced in Step 9)
Column M, SE3 – logger standard error coefficient 3 (column T, SE_coef3 in the above example and 'full_calibration_coefs' file produced in Step 9)
Column N, SE4 – logger standard error coefficient 4 (column U, SE_coef4 in the above example and 'full_calibration_coefs' file produced in Step 9)
Column O, SE5 – logger standard error coefficient 5 (column V, SE_coef5 in the above example and 'full_calibration_coefs' file produced in Step 9)

11 Precision and bias
From results of calibration

12 Reports
N/A

13 Safety
N/A

14 Literature references
N/A