KEIT | INDUSTRIAL ANALYTICS

IRmadillo™

DOC0926 Offline sampling for IRmadillo calibration

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1. INTRODUCTION

This instruction is intended to guide customers in how to take samples for the purpose of calibrating IRmadillo systems.

1.1. Required training

Use of the IRmadillo control software *KeitSpec*.

1.2. Tooling

Offline analyser (not in scope of supply by Keit Ltd).

Reference Data Template.

1.3. Consumables

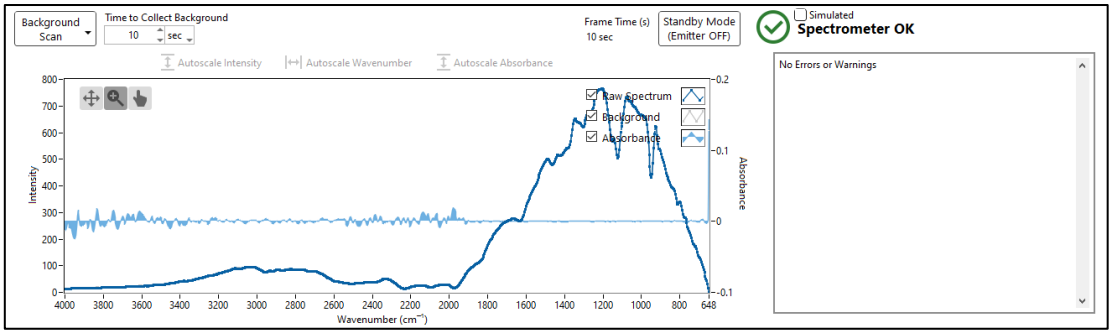
Manual sampling for offline analysis will require small levels of analyte consumption.

2. REFEENCE DATA COLLECTION

2.1. Preparation

If Keit has remote access, Keit can check the IRmadillo before you begin collecting samples for calibration; if not, please confirm that the IRmadillo is operating correctly by completing the checks below. Additionally, please send Keit a screenshot confirming the that the spectrometer is purged correctly.

1. Ensure a Keit Project File is running (saving spectra) where the scan averaging duration is set to 120 seconds in the Configure Acquisition Tab.
    a. More information on this can be found in Section 1.3 of the Software User Manual.
2. Ensure no errors or warning are displayed and there is a green tick in the top right corner of the spectrometer tab as in the image below.



3. The probe temperature is within the product specifications as shown in the health data for the spectrometer.
4. Ensure Keit has provided a template to store the data.
5. Ensure that the process liquid is flowing past the probe tip.
6. Set up a sample extraction location that is as near to the IRmadillo as possible.
7. Synchronise watches! It is essential that the times logged when samples are manually extracted from the process are synchronised with the time of the IRmadillo controller.

2.2. Sampling and Sample Analysis

In general, effective model building requires 25-30 samples, but more is better!

Sampling frequency will depend on the specific process being measured. It is important to incorporate as many variations in the process as possible, e.g.:

- Natural changes in the concentrations of chemicals of interest while your process is running.
- Physical process variations, e.g. temperature, pressure ...
- Other process variations, e.g. feedstock changes.

Collect samples following your internal processes and measure the samples using your analytical method of choosing.

If manually extracted samples are unstable over time, it is essential that analysis occurs promptly after extraction.

Record the exact time that each sample is extracted and analysed in the template provided with this document.

The extracted sample must be representative of the liquid flowing past the spectrometer and being measured at that instant. This allows us to match the offline analysis measurement to the spectrum measured by the IRmadillo.

Do not mix samples taken at different times prior to offline analysis. These composite samples cannot be matched to specific spectra and so cannot be used for calibration.

When reporting values from an analytical instrument, please use the maximum number of decimal places, avoiding rounding where possible. This is to prevent unnecessary binning of numerical data, which can be detrimental to model-building.

3. PROVIDING REFERENCE DATA TO KEIT

Record the data in the template provided (an example is provided below) ensuring the following:

- The timestamps are the following format YYYY-MM-DD HH:MM using 24-hour time.
- The units of each chemical concentration are included in the column headers **only**.
- Data values must be numeric only.
- The decimal separator is a period or full stop "." not a comma ",".
- The IRmadillo serial number is provided for each row.
- Data from each IRmadillo (if you have more than one) is saved in its own file.

IRmadillo serial number	Sample Extraction Time YYYY-MM-DD HH:MM	Sample Analysis Time YYYY-MM-DD HH:MM	DP4+ (g/l)	DP2 (%)	DP1 (ppm)
0167	2022-12-31 08:02	2022-12-31 14:35	21.432	2.194	5.998
0167	2022-12-31 13:58	2022-12-31 15:27	20.80	1.858	0.100
0167	2022-12-31 21:02	2022-12-31 23:26	9.904	2.88	2.276
0167	2022-12-31 23:18	2023-01-01 09:22	6.265	4.262	2.061
0167	2023-01-01 07:53	2023-01-01 11:19	5.795	3.63	1.78

3.1. Providing a process event log

Along with the filled in template, please provide an event log over the time of data collection to help us to identify differences we might see in the spectral data – for example if there is a cleaning cycle or a shutdown etc.

4. SENDING DATA TO KEIT

4.1. Reference data

Once you have gathered at least 25 sets of sample data, please transfer the data and event log to Keit so model-building can start. If Keit has remote access to your system, please send the reference data to Keit by email and let your contact know that the spectral data are available to be downloaded.

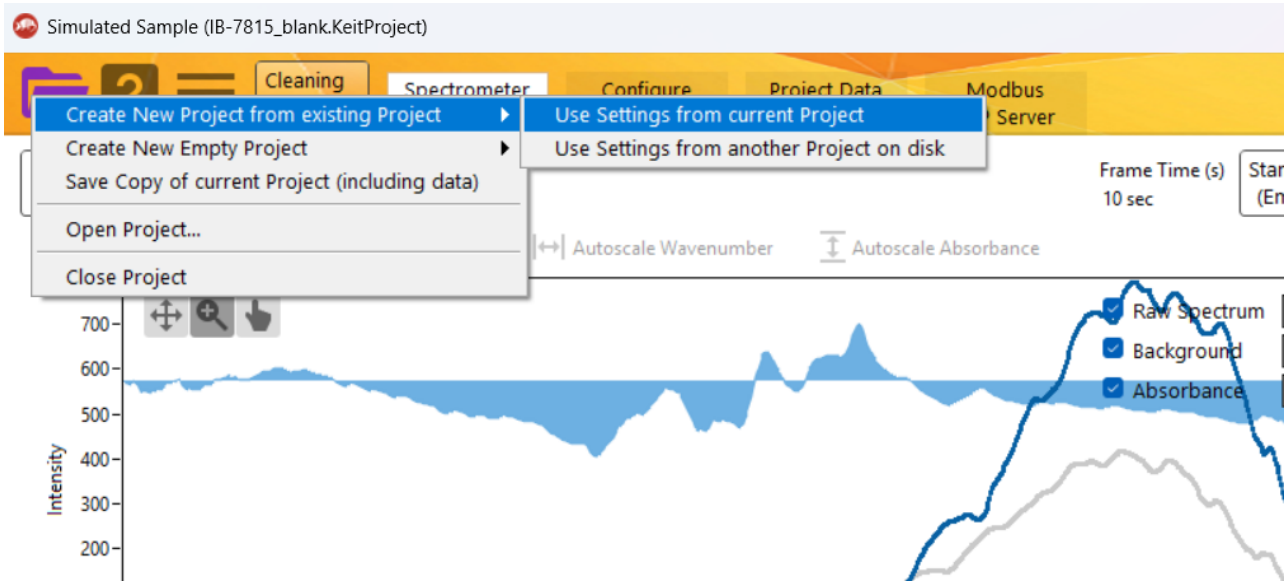
If Keit does not have remote access to your system, please follow the instructions below to send spectral data to Keit.

4.2. Spectral data (in cases where Keit does not have remote access)

KeitSpec stores spectral data in the proprietary KeitProject format. Please send the KeitProject file to Keit.

To avoid corruption, copy KeitProject files from within *KeitSpec*. To do this, click on the purple folder icon and then select 'Create New Project from existing Project' > 'Use Settings from current Project'. A Windows file save dialogue will open.

This will create a new KeitProject file into which live spectra are saved. It is the *previous* file that contains the data that Keit needs.



4.3. Sending the project file to Keit

It is likely that KeitProject files will be too large to send by email. If this is the case, please copy the project file in your external file share folder. If you do not know how to find your external file share folder, or if you find that you cannot copy files to it, please contact support@keit.co.uk. Once the file has been successfully received, please delete the file from your controller.