

EQSANS Data Reduction – Quick Reference for MantidPlot (updated 20170118)

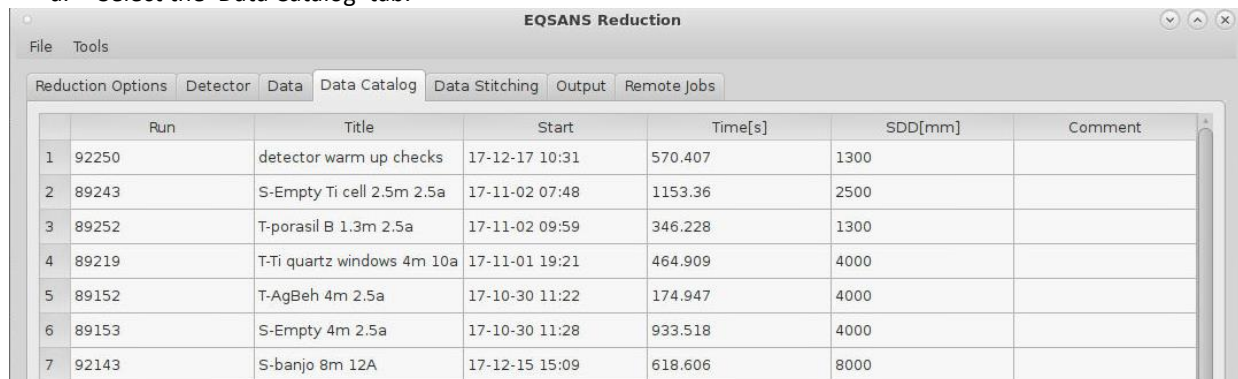
EQ-SANS data reduction can be accomplished through two equivalent means: via the EQ-SANS interface in MantidPlot or by using scripts that are run in the MantidPlot python window. Your local contact will work with you to configure the reduction for the various instrument configurations that you use during your experiment.

1. Open the EQSANS Reduction GUI within MantidPlot

- From the MantidPlot menu, go to Interfaces → SANS → ORNL SANS.
- Ensure the selected instrument is EQSANS and the top of the new window reads “EQSANS Reduction”. If needed, change to EQSANS from the new window by going to Tools → Change instrument and select ‘SNS’ and ‘EQSANS’.

2. See the available data sets using the Data Catalog

- Select the ‘Data Catalog’ tab.

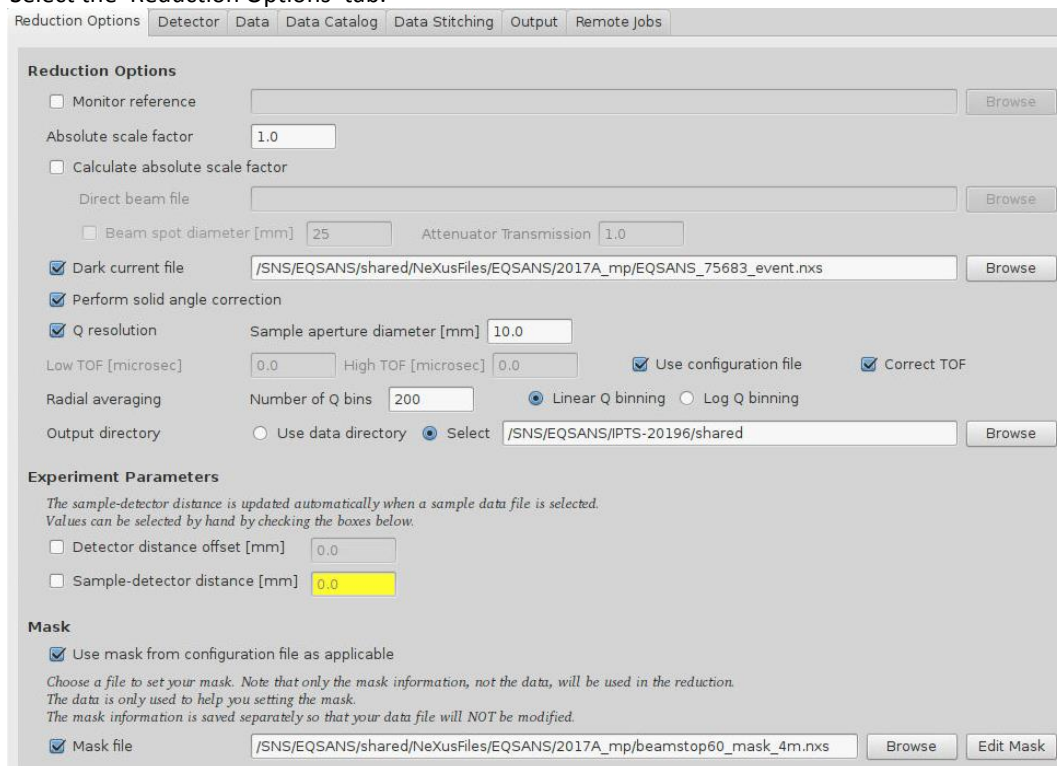


	Run	Title	Start	Time[s]	SDD[mm]	Comment
1	92250	detector warm up checks	17-12-17 10:31	570.407	1300	
2	89243	S-Empty Ti cell 2.5m 2.5a	17-11-02 07:48	1153.36	2500	
3	89252	T-porasil B 1.3m 2.5a	17-11-02 09:59	346.228	1300	
4	89219	T-Ti quartz windows 4m 10a	17-11-01 19:21	464.909	4000	
5	89152	T-AgBeh 4m 2.5a	17-10-30 11:22	174.947	4000	
6	89153	S-Empty 4m 2.5a	17-10-30 11:28	933.518	4000	
7	92143	S-banjo 8m 12A	17-12-15 15:09	618.606	8000	

- The data folder can be found in a consistent location for any experiment, which can either be typed directly in the field or browsed for:
 - Use the absolute path, which has the format: /SNS/EQSANS/IPTS-12345/data
 - The table can be sorted by any column by clicking the title of the column. The sorting can either be in ascending or descending order.
- To see any newly collected runs in the Data Catalog, click the Refresh button.

3. Setting the parameters for the data reduction

- Select the ‘Reduction Options’ tab.



Reduction Options

☐ Monitor reference

Absolute scale factor

☐ Calculate absolute scale factor

Direct beam file

☐ Beam spot diameter [mm] Attenuator Transmission

☒ Dark current file

☒ Perform solid angle correction

☒ Q resolution Sample aperture diameter [mm]

Low TOF [microsec] High TOF [microsec] ☒ Use configuration file ☒ Correct TOF

Radial averaging Number of Q bins ☒ Linear Q binning ☐ Log Q binning

Output directory ☐ Use data directory ☒ Select

Experiment Parameters

The sample-detector distance is updated automatically when a sample data file is selected. Values can be selected by hand by checking the boxes below.

☐ Detector distance offset [mm]

☐ Sample-detector distance [mm]

Mask

☒ Use mask from configuration file as applicable

Choose a file to set your mask. Note that only the mask information, not the data, will be used in the reduction. The data is only used to help you setting the mask. The mask information is saved separately so that your data file will NOT be modified.

☒ Mask file

- b. Under **Reduction Options**, if absolute scale factor has been calculated then enter its value for 'Absolute scale factor'. Otherwise, leave at 1 to not apply any scale factor.
- c. Check 'Dark current file' and enter the appropriate "dark current" run collected by the instrument team (found in /SNS/EQSANS/shared/NeXus/Files/EQSANS/[cycle]_mp/, where [cycle] is the current run cycle (2017A in the above example)).
- d. Check 'Perform solid angle correction'.
- e. Check 'Q resolution' and enter the 'Sample aperture diameter [mm]' (typically 10.0, but check with local contact), select 'Use configuration file' and 'Correct TOF'.
- f. For 'Radial averaging' → 'Number of Q bins', typical values are 200 and 'Linear Q binning'.
- g. For 'Output directory', check 'Select' and type (or browse to) your preferred output folder. A common folder to use is the IPTS shared folder (as in the example above). If you use the shared directory under the IPTS directory, your local contact can see the reduced data if they log into the analysis servers. If multiple people will be reducing data during an experiment, it is often helpful to create a subdirectory for each person in the shared directory to avoid file conflicts.
- h. Under **Mask**, check 'Use mask from configuration file as applicable'. Also check 'Mask file' and enter the appropriate beamstop mask file. See the current cycle machine physics folder for available beamstop masks. Your local contact also can show you how to make a custom mask, if needed.

4. Enter the parameters for the detector corrections to be applied

- a. Select the 'Detector' tab.

- b. Under **Beam Center**, check 'Use beam finder' and 'Fit direct beam'.
- c. For Data file, enter your empty beam transmission run corresponding to the configuration (SDD, wavelength band) you are reducing. You can find the run number on the Data Catalog tab.
- d. Under **Sensitivity**, check 'Perform sensitivity correction'.
- e. For Sensitivity data file, enter the appropriate "thin PMMA" run collected by the instrument team (found in /SNS/EQSANS/shared/NeXus/Files/EQSANS/[cycle]_mp/, where [cycle] is the current run cycle (2017A in the above example)).
- f. For Allowed sensitivity range, enter 0.4 and 2.0 for Min and Max, respectively.
- g. Under **Flood Data Beam Center**, ensure 'Use sample beam center' is checked.

5. Enter parameters into Data

- a. Select the 'Data' tab. Here, you can just enter run numbers (instead of full path), provided the files are in one of your IPTS folders.

The screenshot shows the 'Data Catalog' tab in MantidPlot. It contains two identical-looking panels for data reduction setup. The top panel is for sample data, and the bottom panel is for background data. Both panels have the following fields and options:

- Scattering data file:** Text box with '92154' and a 'Browse' button.
- Sample thickness [cm]:** Text box with '0.1'.
- Treat comma-separated files as separate reduction jobs:** Unchecked checkbox.
- Transmission:**
 - Calculate transmission:** Selected radio button.
 - Fix transmission:** Unselected radio button, with text boxes for '1.0000' and '+/- 0.0000'.
 - Sample direct beam data file:** Text box with '92152' and a 'Browse' button.
 - Empty direct beam data file:** Text box with '92150' and a 'Browse' button.
 - Beam radius (pixels):** Text box with '5.0'.
 - Fit frames together:** Unchecked checkbox.
 - Theta-dependent correction:** Checked checkbox.
- Background data file:** Checked checkbox, with text box '92153' and a 'Browse' button.
- Transmission (lower panel):**
 - Calculate transmission:** Selected radio button.
 - Fix transmission:** Unselected radio button, with text boxes for '1.0000' and '+/- 0.0000'.
 - Sample direct beam data file:** Text box with '92151' and a 'Browse' button.
 - Empty direct beam data file:** Text box with '92150' and a 'Browse' button.
 - Beam radius (pixels):** Text box with '5.0'.
 - Fit frames together:** Unchecked checkbox.
 - Theta-dependent correction:** Checked checkbox.

- Enter your sample scattering run # for 'Scattering data file'. Multiple runs can be added by entering as comma-separated (and leaving the 'Treat comma-separated files as separate reduction jobs' box unchecked).
- Enter your sample holder (cuvette) path length for 'Sample thickness [cm]'.
- Under **Transmission** (in upper panel), enter your sample transmission run for 'Sample direct beam data file' and your empty beam transmission run for 'Empty direct beam data file'.
- Enter 5 for 'Beam radius (pixels)' and check 'Theta-dependent correction'.
- Check 'Background data file' and enter your background (solvent) scattering run #. Multiple runs can be added by entering as comma-separated. If you are going to subtract the background using the reduced I(Q) data file, such as if you have very weak scattering or have a sample with a high volume fraction, you may leave this unchecked. Your local contact will discuss how best to reduce your data.
- Under **Transmission** (in lower panel), enter your background (solvent) transmission run for 'Sample direct beam data file' and your empty beam transmission run for 'Empty direct beam data file'.
- Enter 5 for 'Beam radius (pixels)' and check 'Theta-dependent correction'.

6. Reduce data

- Click the Reduce button at the bottom right of the GUI. Your reduced files will appear in the MantidPlot Workspaces panel normally found toward the right of the main MantidPlot window and in your designated Output directory.
- You can click the Save button to save this reduction setup for future use. Also, after performing a reduction, you can populate the GUI fields again by loading a reduction .xml file into the GUI by going to File → Open.

7. Export to script

- To create a Python script for performing batch reductions, click on the Export button at the bottom right. Save as a .py file.
- The saved script can be open in MantidPlot by clicking the 'Script Window' icon or going to View → Script Window. Within MantidPlot: Python Window, go to File → Open and choose your script.
- Advanced scripting that leverages the Python programming language is often used to automate reduction of a large number of files. Your local contact can help.

The example script below contains added comments to describe parameters that will need to be changed:

```

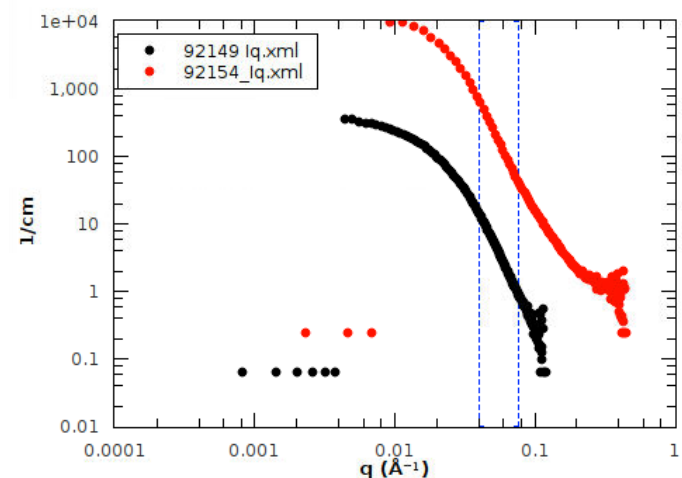
1 # EQSANS reduction script
2 # Script automatically generated on Thu Jan 11 10:47:16 2018
3
4 import mantid
5 from mantid.simpleapi import *
6 from reduction_workflow.instruments.sans.sns_command_interface import *
7 config = ConfigService.Instance()
8 config['instrumentName'] = 'EQSANS'
9
10 EQSANS()
11 SolidAngle(detector_tubes=True)
12 DarkCurrent("/SNS/EQSANS/shared/NeXusFiles/EQSANS/2017A_mp/EQSANS_75683_event.nxs")
13 TotalChargeNormalization()
14 SetAbsoluteScale(1) #porasil scale factor
15 AzimuthalAverage(n_bins=200, n_subpix=1, log_binning=False)
16 IQxQy(nbins=200)
17 OutputPath("/SNS/EQSANS/IPTS-20196/shared") #change directory to shared folder
18 UseConfigTOFTailsCutoff(True)
19 UseConfigMask(True)
20 Resolution(sample_aperture_diameter=10)
21 PerformFlightPathCorrection(True)
22 DirectBeamCenter("92150") #trans empty beam
23 SensitivityCorrection("/SNS/EQSANS/shared/NeXusFiles/EQSANS/2017A_mp/Sensitivity_patched_thinPMMA_4m_75789_event.nxs",
24 DivideByThickness(0.1)
25 DirectBeamTransmission("92152", "92150", beam_radius=5) #trans sample, trans empty beam
26 ThetaDependentTransmission(True)
27 AppendDataFile(["92154", "porasilB_2m_205A") #[scattering sample], "filename" e.g. ["1", "2", "3"] to add runs
28 CombineTransmissionFits(False)
29
30 Background("92153") #scattering background e.g. ("1", "2", "3") to add runs
31 BckDirectBeamTransmission("92151", "92150", beam_radius=5) #trans background, trans empty beam
32 BckThetaDependentTransmission(True)
33 BckCombineTransmissionFits(False)
34 SaveIq(process='None')
35 Reduce()

```

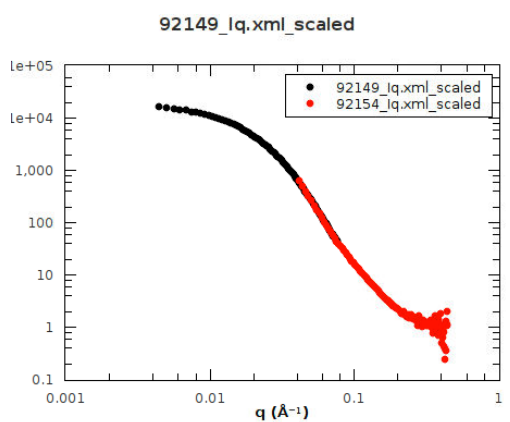
8. Data Stitching

If 2 or 3 configurations were measured on the same sample, the 'Data Stitching' tab allows you to merge the data.

- Under **Low Q** 'I(q) file:', enter run for the "lower" Q data (or frame 2, if data was collected in frame-skipping mode). The .xml file can be found by using the Browse button.
- Under **Medium Q** 'I(q) file:', enter run for the "higher" Q data (or frame 1, if data was collected in frame-skipping mode). The .xml file can be found by using the Browse button.
- Check the 'Normalize to this data set' for the data you will normalize to.
- Click the 'Pick Overlap Region' button between the **Low Q** and **Medium Q** fields. In the Range Selector window, slide the vertical range selectors to cover the desired overlap range.



- e. Go back to the 'Data Stitching' tab and click Auto Scale at the bottom right.



- f. If the merged data is accepted, go back to the 'Data Stitching' tab and click Save Result. If you wish to re-do the merge range then repeat steps e and f.
- g. There is an additional **High Q** field if 3 different configurations were measured. The lower 'Pick Overlap Region' button can be used for merging a 3rd configuration.
- h. Merging large numbers of files can also be scripted. Your local contact can help.