

Using COLETTE

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Using COLETTE

(A Simple Guide)

What is COLETTE?

COLETTE is the name of the data reduction program for the LOQ Small-Angle Neutron Scattering (SANS) instrument at the ISIS Spallation Neutron Source.

The acronym COLETTE is a contraction of "correct LETI", the Laboratoire d'Electronique et de Technologie de l'Informatique being the manufacturers of the original LOQ "area" detector.

Why COLETTE?

The ISIS data display and manipulation program, GENIE[®], was not designed to handle two-dimensional datasets, an essential operation in the processing of SANS data.

COLETTE runs on top of, and thereby incorporates, GENIE[®]. Data "workspaces" are shared between COLETTE and GENIE[®]. This means that a COLETTE user can "shell" into GENIE[®] and use all of its functionality and then return to their COLETTE session without any loss of data. However, for reasons of speed and ease of use COLETTE effectively functions independently of GENIE[®], it has its own command set and its own data input and output routines.

System Requirements

COLETTE is designed to run on the Digital Equipment Corporation (DEC) VAX family of computers under Digital's VMS (Version 5.x or higher) or OpenVMS (Version 6.1 or higher) operating systems. COLETTE also requires DEC GKS (Graphical Kernel System) Version 4.2 or higher. (Note: DEC GKS Version 5.0 is incompatible with GENIE[®]. The next compatible version is GKS 5.2). At the time of writing COLETTE does not run on DEC Alpha computers (even those running OpenVMS).

The disk space (VAX disk blocks = 0.5kB) and memory requirements (pages = 0.5kB) of COLETTE executable images at present are:

COLETTE / GENIE [®] Version 2.5(2) / DECGKS Version 4.2	1900 blocks	35000 pages
COLETTE / GENIE [®] Version 2.5(5) / DECGKS Version 5.2	17000 blocks	34000 pages

COLETTE will be distributed free to *bone fide* educational establishments.

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In the following document all of the commands to be typed are in **bold** type. Unless otherwise stated there is a <RETURN> at the end of each line. Most commands, their qualifiers and parameters can be abbreviated to just the first 3 letters. For additional information type HELP [command]. Should it become corrupted, the screen display may be "refreshed" by simply typing Control-W.

1) Run the program...

COL or **COL TEST** (ask your local contact or read the login notices)

COLETTE will respond with...

GKS\$CONID = "DECW\$DISPLAY"

CLASS = "WINDOWS"

OUTPUT = "POSTSCRIPT"

VERSION = "TOP"

...or something similar. GENIE will announce itself followed by various information notices about COLETTE and environmental setups. Finally the GENIE ">>" prompt will appear.

Please ignore any DECGKS error messages about incorrect Title & Border sizes.

NOTE:

Users who wish to import graphs produced by COLETTE into Microsoft WORD® or who wish to run COLETTE using PC KERMIT as a terminal emulator should not invoke COLETTE in this way. Please see Appendix 5 instead.

2) Call COLETTE from GENIE...

>> **COL** or >> **LOQ** but not COL TEST

3) Assign the sample run...

ASSIGN/SAMPLE 1234

COLETTE will look for the file LOQ01234.RAW by default. Specify any other file descriptor; e.g. ASS/SA 1234.ADD

If you are using the Workstation in the LOQ cabin it is possible to look at the run currently in progress. To do this you must take a "snapshot" of the data in the DAE (Data Acquisition Electronics) and copy it to an area of the computers memory called the CRPT (Current Run Parameter Table). COLETTE must still be told where to look for the data however, and there are two ways of doing this, either by

ASS/SA CRPT

or

ASS/SA 0

The legend CRPT will be displayed instead of a filename. To actually read the data from the DAE into the CRPT type

JUMP "UPDATE

The screen will go blank for a few seconds and then ask you to press <RETURN>.

4) {Optional}

Assign the sample can run. This will be a run containing scattering to be subtracted from the sample, such as a solvent filled sample cell for example...

ASS/CA 1235

COLETTE will look for the file LOQ01235.RAW

5) Invoke the mask...

ASS/SA

@MASK

This executes MASK.COM. The instrument scientists frequently check the behaviour of the detector and have written this command file to read in the detector-to-spectrum mapping tables and to apply the necessary detector and time masks. It should normally only need to be called each time you enter COLETTE.

A number of information messages will appear in the bottom four lines of the screen.

If you are a regular LOQ user with your own account on the HUB computer, please ensure that you copy a recent MASK.COM to your directory before you analyse any new data! Alternatively, the command @USER:MASK will execute the current mask file on the LOQ FEM. Now that the new ORDELA detector has been installed you must ensure that you use the correct detector mask file for the data you are analysing. The last LETI detector compatible mask was MASK912.COM (i.e., @MASKS:MASK912). Finally, if you are running LOQ at 50Hz you will need to use a special mask file, please ask your local contact.

6) {Optional}

View the raw data as an intensity contour plot of the main detector. This display is most useful when studying anisotropic systems...

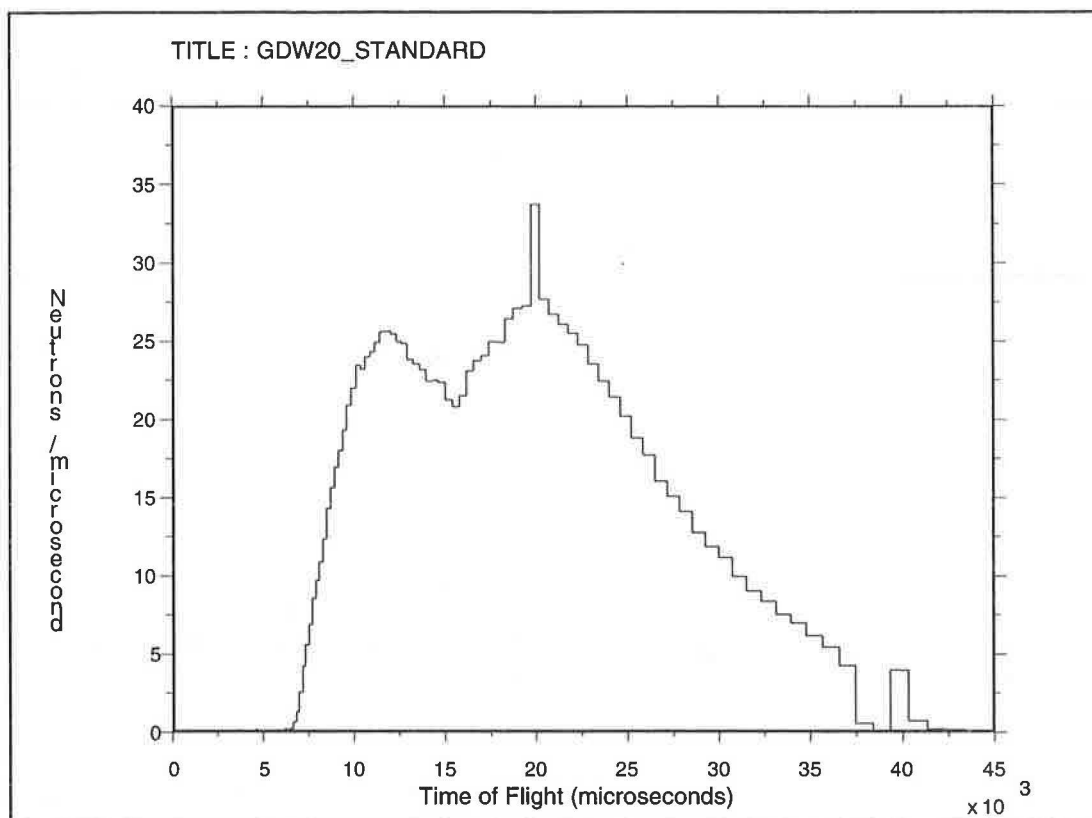
DISPLAY CONTOUR

- A sub-menu will appear:
- (a) To return to the main screen, type **0**.
 - (b) To normalise the contour levels, type **1** followed by the counts per unit area for contour level 1.
 - (c) To force the drawing of contour lines, type **2**
 - (d) To zoom on the centre, type **25**.

7) {Optional}

View the neutron time-of-flight spectrum as recorded by the main detector...

DISPLAY TIME

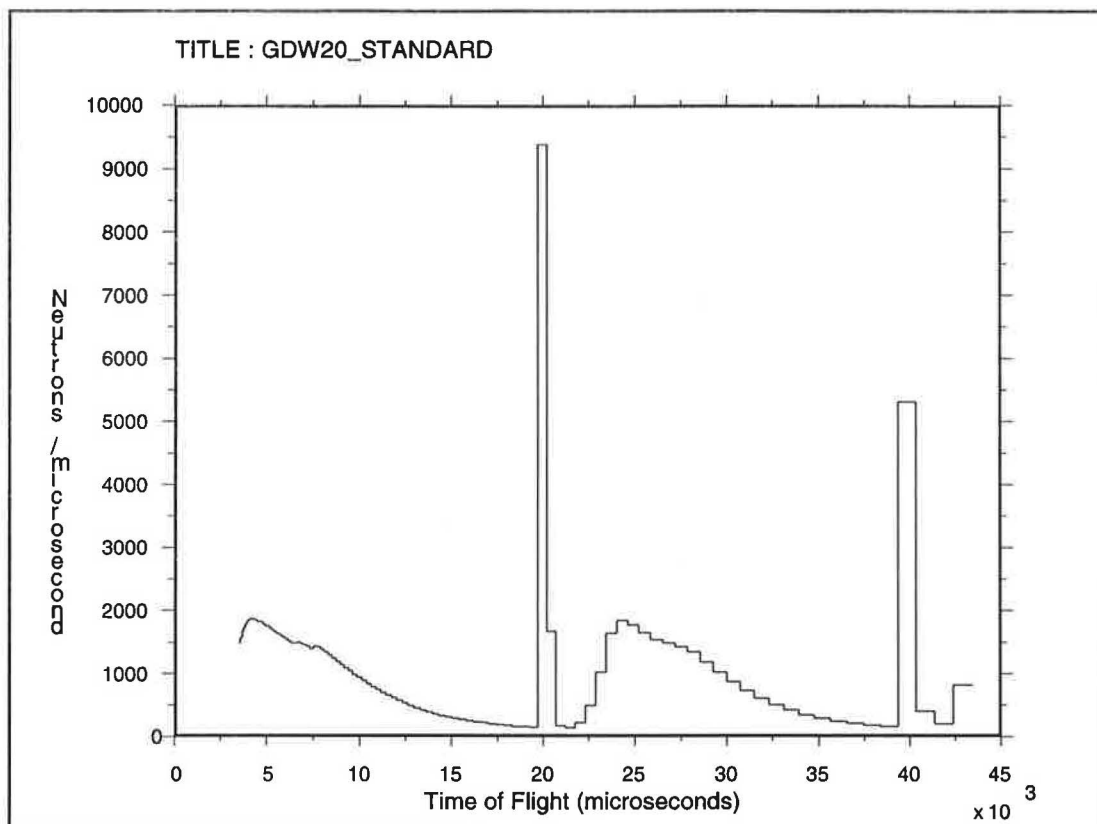


This may identify certain time channels which need to be masked out. The "prompt" pulse at 20ms must always be excluded. Again, this need only be done at the beginning of the experiment and will be done for you by the instrument scientists in MASK.COM.

LOQ also has two low-efficiency incident beam monitors. The neutron time-of-flight spectra that these record are stored in spectrum #1 and spectrum #2 and may be viewed by typing...

D/H S1

(where the /H qualifier signifies that the data is to be plotted in histogram format)

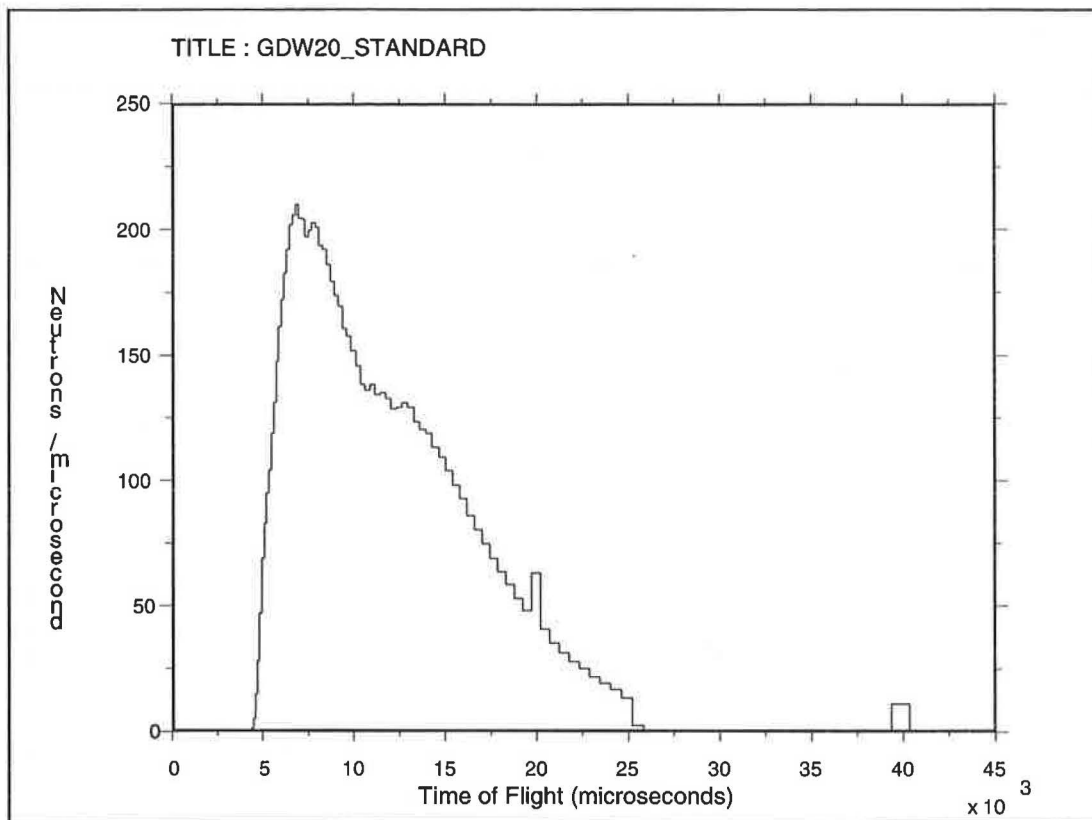


S1 contains the "raw" TOF spectrum, and is unaffected by your choice of wavelength or collimation. Because LOQ is normally a 25Hz instrument you should see two ISIS pulses. If not, ask an instrument scientist to check that the chopper is running and that LOQ is synchronised to the SMP (Secondary Master Pulse).

or...

D/H S2

S2 contains the TOF spectrum at the sample position and is used to normalise the small angle scattering from the sample as a function of wavelength. It should bear some resemblance to the spectrum obtained by DISPLAY TIME although the absolute scales will be different.



8) Calculate the transmission of the sample (also see the note under Step 10)...

TRANSMISSION/SAMPLE/MEASURE

COLETTE will respond with

"Enter transmission run number for sample run >> " **1236**

"Reading LOQ_DISK:[LOQMGR.DATA]LOQ01236.RAW"

"Enter direct beam run number >> " **1237.ADD**

"Reading LOQ_DISK:[LOQMGR.DATA]LOQ01237.ADD"

"Transmission contained in Workspace 21"

Write the transmission for the sample out as an ASCII datafile...

WRITE W21 TEMP:1236.TRAN or **WRITE W21 USER\$DISK:[ABC01]1236.TRAN**

NOTE 1:

If you have also assigned a can and it is anything other than an empty beam run (ie, a scattering run through an empty sample position) then you must also calculate the transmission of the can...

TRANSMISSION/CAN/MEASURE

COLETTE will respond with

"Enter transmission run number for can run >> " **1238.RAW**

"Reading LOQ_DISK:[LOQMGR.DATA]LOQ01238.RAW"

"Enter direct beam run number >> " **1237.ADD**

"Reading LOQ_DISK:[LOQMGR.DATA]LOQ01237.ADD"

"Transmission contained in Workspace 22"

Write the transmission for the can out as an ASCII datafile...

WRITE W22 TEMP:1238.TRAN or **WRITE W22 USER\$DISK:[ABC01]1238.TRAN**

NOTE 2:

If you forget to calculate the transmission then COLETTE will use whatever was calculated the last time you issued the above commands. If you forget what is in any workspace you can type SHOW W21, etc. See Appendix 3.

To clear a transmission use...

TRANSMISSION/CLEAR

This will set the transmission of the assigned run at all wavelengths currently in use to 1.0.

NOTE 3:

The TRANSMISSION/MEASURE command can be used in the format...

TRANSMISSION/MEASURE {sample transmission run #} {direct beam run #}

The {} brackets are not typed however!

NOTE 4:

A linearly-fitted transmission of the LOQ polymer standard "GDW20" is stored within COLETTE and may be used in place of an experimentally-measured transmission for this sample. To use this stored transmission, type...

TRANSMISSION/STANDARD

9) Display the transmission of the sample...

DISPLAY/MARKER W21 or better **D/M W21 2 10 0 1**

The /MARKER qualifier tells COLETTE to display the individual datapoints. For a moderately weak scatterer the transmission should be a straight line. In reality it probably also decreases at higher wavelengths. You can check how statistically significant any deviations are by overplotting the error bars.

<RETURN> (if using a TeKtronix-type terminal)

PLOT/ERROR

COLETTE will automatically assume that you want it to use Workspace 21 again in this instance.

10) {Optional}

Fit the transmission to a straight line. In some instances this will improve the quality of subsequent subtractions.

FIT W21 2.2 6.5

This command has an implicit /LINEAR qualifier. It is recommended that you only fit transmissions over the range 2.2 - 6.5Å. A quadratic fit is also possible using the command FIT/QUADRATIC.

Note that in this example the data in Workspace 21 is overwritten with data interpolated from the fit. To store the fit separately, say in Workspace 1, use...

FIT W21 2.2 6.5 W1NOTE:

Some MASK.COM files include the command FIT/TRANSMISSION. If you are using such a file, all transmissions that you calculate will automatically be fitted. In such cases the "actual" transmission is placed in W25 (regardless of whether you have calculated the transmission of a sample run or of a sample can run) and W21, W22, etc., only contain the fitted transmission. A message to this effect is always displayed at the bottom of the screen. To turn this feature off use FIT/TRANSMISSION/CLEAR.

Check the fit by overplotting on the original data...

PLOT/LINE W21 or **PLOT/LINE W1** or **PLOT/LINE W25** (respectively)

<RETURN> (if using a Tektronix-type terminal)

11) {Optional}

If you have assigned a can run then repeat steps 9) & 10) with Workspace W22.

- 12) Check that the beam size is correct. This is the first value after the run designation at the top right of the screen. Normally LOQ is run with an 8mm diameter beam at the sample. However, if you are not using standard 1mmx10mmx30mm quartz cells then your local contact may have altered the beam size. Unless the correct beam width was set in the instruments CHANGE utility it will be necessary to alter it in COLETTE using, for example, ...

SIZE/WIDTH=11 or **SIZE/SAMPLE/WIDTH=11**

... to set it to 11 mm. If it is necessary to change the beam size for the sample can as well then you can use...

SIZE/CAN/WIDTH=11

Any such change of collimation is normally recorded in the instruments log book alongside the remark SNOUT or A_{snout} .

IMPORTANT !

When running your samples try to ensure that the incident collimation is the same for both the sample run and the sample can run. As you can see, COLETTE will still be able to handle the data if they are not, but the resulting differences in beam divergence, views of the incident beam and scattering around the beamstop will give rise to unquantifiable effects at low-Q. You have been warned!

- 13) Check that the sample thickness is correct. This is the second value after the run designation at the top right of the screen. If it is not...

SIZE/THICK=2.0 or **SIZE/SAMPLE/THICK=2.0**

... will change it to 2.0 mm, for example. If it is necessary to change the thickness of

the sample can aswell then you can use...

SIZE/CAN/THICK=2.0

The sample thickness should be set every time you assign a new run, unless you entered the correct thickness into the .RAW file by specifying the thickness in PILOT.COM or by using the CHANGE utility (see the "PUNCH User Guide"). The default value for the thickness of a run is 1.0mm.

- 14) Check that the flight paths are correct. These are the values alongside the legend "Lm-s / Ls-d" and are the moderator-to-sample and sample-to-detector distances respectively. If these values are wrong then your Q-scale will be wrong!

These lengths are normally defined for you by the instrument scientists using the CHANGE or MENU utilities or by using the MODIFY command (see the "PUNCH User Guide") but you can easily check whether the values displayed are correct:

Lm-s

The back face (nearest your samples) of the Aperture #2 housing (the big rusty upright block in the sample pit) is 10.744 m from the moderator.

Ls-d

This is 15.473 - Lm-s.

If it is necessary to change these values then type...

SET LENGTHS

COLETTE will respond with

"NOTE: M-S = 11.0540 m S-D = 4.4190 m M-M = 10.4310 m"

"Mod-Sam length ==> " **10.96**

"Sam-Det ==> " **4.513**

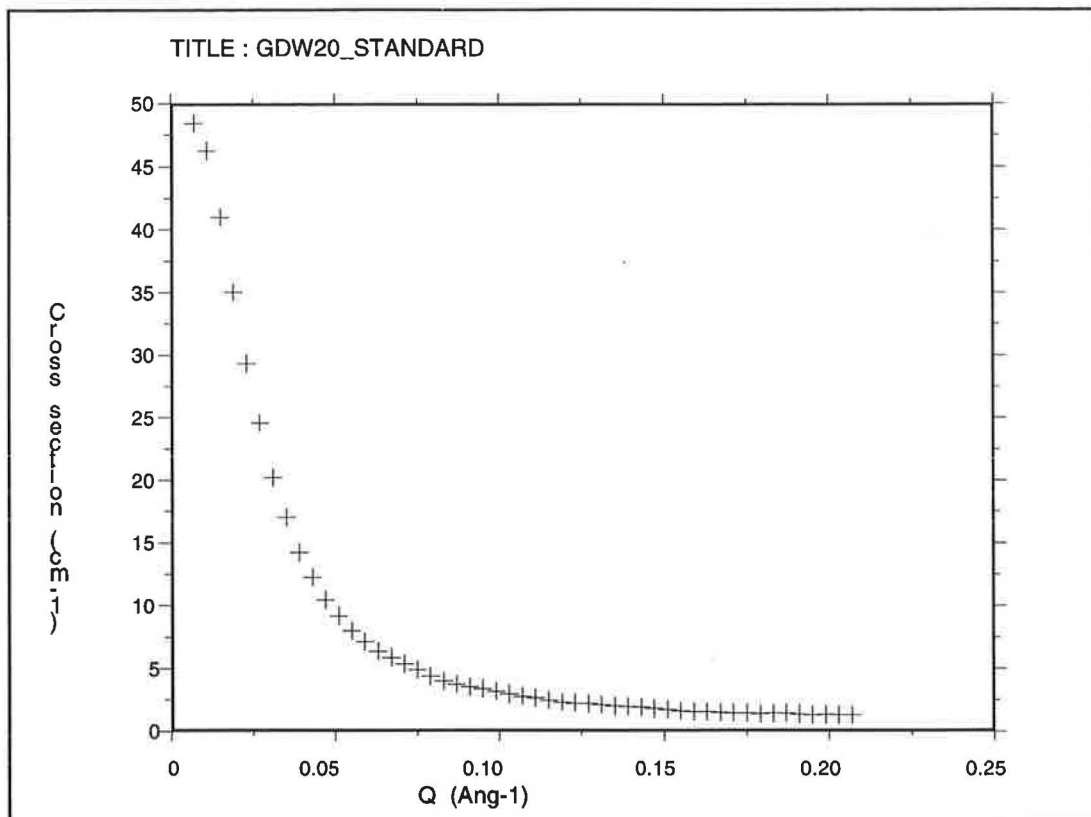
"NOTE: M-S = 10.9600 m S-D = 4.5130 m M-M = 10.4310 m"

If you are using the LOQ sample changer with LOQ's own sample racks then Lm-s = 11.046 and Ls-d = 4.427 m.

- 15) Reduce the data (but please read Appendix 6, Appendix 7 and Appendix 8 first)...

CORRECT/SA W1

This would process the sample data (by rebinning into lambda, dividing by the monitor count, scaling by the direct beam for detector efficiency, scaling by the transmission and sample volume, weighting the masked data by zero and finally rebinning the data into Q weighting by solid angle) and put the data as a function of Q into Workspace 1.



A more preferable (where possible) reduction would be to subtract the sample can data from the sample data. To do this use...

CORRECT/SC W1

Write the corrected data out as an ASCII datafile of cross-section versus scattering vector...

WRITE W1 TEMP:1234.IQ or WRITE W1 USER\$DISK:[ABC01]1234.IQ

or

WRITE/TITLE="My Plot" W1 TEMP:1234.IQ

NOTE 1:

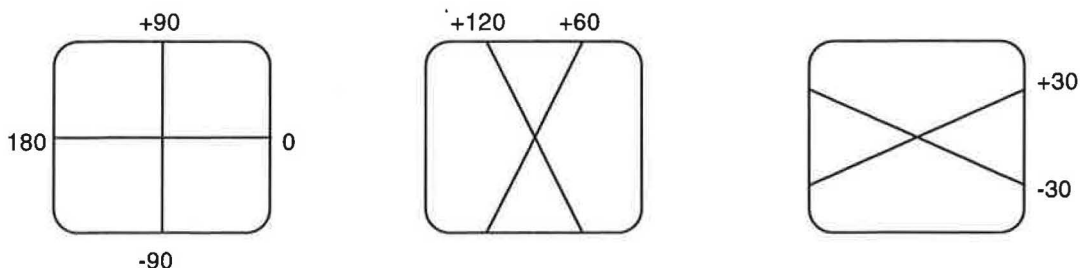
Data reduction by the above method involves a radial average and so the result is just one-dimensional (cross-section versus Q). COLETTE is however capable of making a two dimensional reduction; i.e., cross-section as a function of both Q parallel and Q perpendicular to the direction of an applied tensor (e.g., shear flow, magnetic field, etc.). For details of how to perform such a reduction, see section 19.

NOTE 2:

It is possible to only reduce data in selected sectors of the detector. This is done by altering the range of azimuthal angles used by typing...

LIMIT/PHI {minimum angle} {maximum angle}

For a full radial average (the default) the minimum angle should be set to -90 and the maximum angle to +90. Other sectors may be chosen with reference to the diagram below:



The LIMIT/PHI command only takes effect when another CORRECT is issued.

NOTE 3:

It is possible to calculate a "fully normalised" scattering cross-section, see Section 20.

16) Display the corrected cross-section...

DISPLAY/MARKER W1

<RETURN> (if using a TeKtronix-type terminal)

...and overplot the error bars...

PLOT/ERROR W1

<RETURN> (if using a TeKtronix-type terminal)

Other qualifiers available include...

/YLIN - for a linear Y axis
/XLIN - for a linear X axis
/XYLIN - for linear X and Y axes
/YLOG - for a logarithmic Y axis
/XLOG - for a logarithmic X axis
/XYLOG - for logarithmic X and Y axes
/SPECIAL - for other specialised representations (e.g., Guiner, Porod, Kratky). You will be prompted to select the representation you require and prompted to enter a background to be subtracted from the data. This can either be a single value (if in doubt enter 0) or a workspace as Wn. If you give a workspace it must have identical Q bins to the data workspace.

NOTE:

Different types of marker can be selected with the command...

ALTER MARKER n

<RETURN>

where $-13 \leq n \leq -1$ ($-1 = \bullet$) and $1 \leq n \leq 5$ ($1 = \circ$, $2 = +$, $3 = \star$, $4 = o$ and $5 = \times$).

17) {Optional}

To generate a hard copy of the display on a Laser Printer, type...

PRINT

This tells COLETTE to write the graphics screen to a file called DEC_POSTSCRIPT.DAT in the directory from which you are running COLETTE. You will then be asked to select a printer. Choose...

- 0 - if you are in R3 (the ISIS administration building)
- 2 - if you are in the DAC (the Data Assessment Centre in the experimental hall)
- 4 - if you are in the LOQ cabin (the printer is in the CRISP cabin)
- 9 - if you are in the LOQ cabin (the printer is in the HET cabin)

NOTE 1:

The PRINT command can be used in the form...

PRINT/ON=n/COPIES=m

...where n is the laser printer number (shown above) and m is the number of copies - between 1 and 9 - required. The default value of m is 1.

18) {Optional}

To read COLETTE format ASCII datafiles of, say, corrected data or transmissions back into COLETTE workspaces, type...

OLD W1 TEMP:1234.IQ or OLD W21 USER\$DISK:[ABC01]1236.TRAN

NOTE:

If a transmission file is read back into W21, W22, W23 or W24 then COLETTE will not use that data in a CORRECT unless you first issue...

TRANSMISSION/WORKSPACE

...in place of the TRANSMISSION/MEASURE command.

19) {Optional}

Perform a two-dimensional reduction of the data. It is first necessary to establish Q limits in the directions parallel and perpendicular to the applied tensor, what COLETTE refers to as the Q_x and Q_y directions using the commands...

LIMIT/QX 0 {maximum value of Q_x }

LIMIT/QY 0 {maximum value of Q_y }

...and then to determine the number of Q bins (points) in either direction with...

STEP/QX/LIN {interval}

STEP/QY/LIN {interval}

Due to the way in which data is stored inside COLETTE there is a limit to the number of Q bins which can be handled. As a rough guide

$(\text{maximum value of } Q) / (\text{interval}) \leq 100$

NOTE:

The use of logarithmic (/LOG) Q bins in 2D reductions is not recommended. Only use them in normal 1D reductions (i.e., STEP/Q/LOG). See Section 15.

If necessary, reset the azimuthal limits...

LIMIT/PHI -90 90

The data may then be corrected as before using...

CORRECT/SA W61 or CORRECT/SC W61

...but, the result must be written to a 2D workspace (see Appendix 3), such as W61.

NOTE:

CORRECT/SA W61 and CORRECT/SC W61 are identical with CORRECT/AREA/SA W61 and CORRECT/AREA/SC W61 respectively. Providing that a 2D workspace is given as an argument the /AREA qualifier can be omitted.

To display the result of a 2D reduction, use...

DISPLAY W61

...as the data can only be displayed as line contours. The /E, /H or /M qualifiers will have no effect on the display of 2D workspaces.

To write the data out as an ASCII datafile of cross-section versus Q_x and Q_y , use...

WRITE W61 TEMP:1234.LQA or WRITE W61 USER\$DISK:[ABC01]1234.QXY

...or, to write the data out in a shorter binary format, use...

WRITE/BIN W61 TEMP:1234.LQB

NOTE:

WRITE W61 is identical with WRITE/AREA W61. Providing that a 2D workspace is given as an argument the /AREA qualifier can be omitted.

20) (Where appropriate)

It is possible to calculate a "fully normalised" scattering cross-section (as is often done on reactor-based SANS instruments) where the scattering from the sample is divided by that from a normalisation sample. However, this procedure should be used with caution on LOQ because it is very difficult to find a normalisation sample with a well-defined cross-section over all of the LOQ wavelength range. This limitation applies to the two most common normalisation samples, vanadium and water.

The only purpose of the normalisation is to eliminate the detector efficiency from the scattering law. On a time-of-flight SANS instrument, like LOQ, it is preferable to determine the detector efficiency directly. When you use the CORRECT command in COLETTE the program automatically reads in a file containing the efficiency of the LOQ main detector unless you issue CORRECT/SCNB or CORRECT/FULL (the two qualifiers are equivalent (see below)).

To make a full normalisation, first assign a normalisation run (eg, a vanadium run)..

ASSIGN/NORMALISATION 1239

...followed by a background run (ie, whatever must be subtracted from the normalisation run. The background run may be considered to be a can run for the normalisation)..

ASSIGN/BACKGROUND 1240

...then calculate their respective transmissions...

TRANSMISSION/NORMALISATION/MEASURE 1241.RAW 1237.ADD

FIT W23 2.2 6.5

TRANSMISSION/BACKGROUND/MEASURE 1242.RAW 1237.ADD

FIT W24 2.2 6.5

Assuming that the width and thickness of both the normalisation and background runs are correctly set (see Sections 12 & 13 if they are not), a fully normalised reduction may then be made using...

CORRECT/SCNB W2 or **CORRECT/FULL W2**

Should a full two-dimensional normalisation be required then the above CORRECT commands should be replaced by (but also see Section 19), say, ...

CORRECT/SC W62

CORRECT/NB W63

AREA/ARITHMETIC

...followed by, for example, ...

64 0.0 1.0 62 63

...to do $W64 = 0.0 \times W64 + 1.0 \times W62/W63$

APPENDIX 1

Analysing Old Data

(a) **DATA COLLECTED WITH THE LETI DETECTOR AND OLD BEAMSTOP (ONE WITH HOLES!)**

This is data collected prior to ISIS Cycle 1 1990 - Run Numbers < 4493

- (1) Assign an empty beam run (**ASS/MT {empty beam run number}**)
- (2) Use an appropriate mask file (**@MASKS:MASK89**)
- (3) Use **TRANSMISSION/CALCULATE** (instead of TRANSMISSION/MEASURE)

(b) **DATA COLLECTED WITH THE LETI DETECTOR AND NEW BEAMSTOP**

This is data collected prior to ISIS Cycle 3 1991 - 4493 < Run Number < 9607

- (1) Use an appropriate mask file (**@MASKS:MASK912**)
- (2) Use the correct detector efficiency file:-
MONITOR/DIRECT=LOQ\$DISK[LOQMGR]BEAM_FUDGED.RKH

NOTE 1:

If you are changing detector types during the same COLETTE session you must clear all detector and time masks before reading a new mask file using...

MASK/CLEAR

MASK/TIME/CLEAR

NOTE 2:

Old masks and masks generated for special purposes are stored in the directory LOQ\$DUA0:[LOQMGR.MASKS] which has been equivalenced to the logical name MASKS: To find a mask file for a particular period type...

DIR/DATE MASKS:

... at a DCL prompt (\$ or LOQ>). Do not under any circumstances delete, rename or edit any of the files in this directory. If you need help please contact an instrument scientist.

APPENDIX 2

Logging On At ISIS

An increasing number of terminals at ISIS now connect to the PUNCH computer system via an EtherNet protocol called LAT (Local Area Transport). This includes terminals in the DAC and LOQ. These so-called "LAT terminals" will be routed through one of two types of terminal server; a Lantronix Server (which displays a Vista> prompt) or a DECserver (which displays a Local> prompt).

*** If logged out of a Lantronix**

[press return]
Vista VCP-1000
Enter Username> mickey_mouse
Vista>

If logged out of a DECserver

[press return twice]
DECserver 90TL ...etc
Enter Username> fred_flintstone
Local>

*** To log onto the HUB (central computer)**

C ISISE <RETURN>

*** To log onto the LOQ FEM**

C LOQ <RETURN>

*** To view the Protons Per Pulse display**

C PPP <RETURN>

(There are only a limited number of PPP connections so please do not "hog" them and always disconnect when you have finished. Thank you.)

*** To make an additional alternate connection (3 alternate connections are allowed)**

<BREAK>
C [new nodename]

*** To clear a connection**

<BREAK>
DISCO

*** To resume alternate connection number 1**

<BREAK>
RES 1

A plea! When you have finished your experiment and are analysing data in the DAC or back in your home institution, please DO NOT logon to the LOQ FEM either as LOQ or under your own username. Use the much more powerful ISIS HUB computer called ISISE instead. Otherwise you only slow LOQ down for the current users (and for yourselves)! Thank you.

APPENDIX 3

COLETTE Workspaces

COLETTE has 67 workspaces for data. Most can be used without any restriction, although some are reserved for specific purposes.

W1	Normal (1D) workspace	
.	.	
.	.	
.	.	
W14	Normal (1D) workspace	
W15	Graphics buffer	RESERVED
W16	Monitor spectrum versus wavelength for sample run	RESERVED
W17	Monitor spectrum versus wavelength for can run	RESERVED
W18	Monitor spectrum versus wavelength for normalisation run	RESERVED
W19	Monitor spectrum versus wavelength for background run	RESERVED
W20	Main detector efficiency versus wavelength	RESERVED
W21	Transmission versus wavelength for sample run	RESERVED
W22	Transmission versus wavelength for can run	RESERVED
W23	Transmission versus wavelength for normalisation run	RESERVED
W24	Transmission versus wavelength for background run	RESERVED
W25	Fitted transmission versus wavelength for assigned run	RESERVED
W26	Normal (1D) workspace	
.	.	
.	.	
.	.	
W60	Normal (1D) workspace	
W61	2D workspace for use with CORRECT/AREA only	
W62	2D workspace for use with CORRECT/AREA only	
W63	2D workspace for use with CORRECT/AREA only	
W64	2D workspace for use with CORRECT/AREA only	
W65	Used by CORRECT/AREA (counts buffer)	RESERVED
W66	Used by CORRECT/AREA (solid angle buffer)	RESERVED
W67	2D graphics buffer	RESERVED

APPENDIX 4

Absolute Intensities

COLETTE reduces data in such a way that the scattered intensity (or, more formally, the scattering cross-section) you see displayed on the Y-axis has units of cm^{-1} ; ie, absolute dimensions. The data should also be on an absolute scale. However, to correct for small instrumental non-linearities, geometrical factors, repeatability of sample positioning, etc, it is in your own interests to run the *LOQ Standard Sample*.

The LOQ Standard Sample is a solid blend of 19.8% w/w deuterated polystyrene dispersed in protonated polystyrene matrix. It was calibrated by Dr George D. Wignall at the Oak Ridge National Laboratory in the USA in July 1990 and is a true secondary standard.

The correction procedure requires that you make 2 runs (for say 1M Counts each) at each instrument geometry that you use:

1. a scattering run on the Standard Sample
2. a scattering run on an empty sample position (ie, an EMPTY BEAM run) or on an empty cell (if the Standard Sample is placed in a cell; ie, between windows).

Then reduce the data as follows...

ASS/SA {standard sample scattering run}
SIZE/THICK=1.27 (the thickness of the LOQ Standard Sample in mm)
SIZE/WIDTH=x (where x is beam diameter in mm at the sample)
TRANS/STANDARD
ASS/CA {empty beam or cell run}
SIZE/THICK=1.27
SIZE/WIDTH=x

then

TR/CLEAR

(for an empty beam run - resets the can transmission in W22 to unity all wavelengths)

or

TR/CAN/MEASURE {sample can transmission run} {direct beam run}

(for an empty cell run)

LIMIT/PHI -90 90

LIMIT/Q 0.0065 0.25

STEP/Q/LIN 0.002

CO/SC Wn (where n is a workspace number)

WRITE Wn TEMP:STANDARD.Q

Now fit the I(Q) data to a Debye Gaussian coil model and determine I(Q=0) and the (z-average) radius of gyration, Rg. Both RKH's "FISH" program and SMK's "SANDRA" program will do this. To use SANDRA type...

SANDRA

... at a DCL prompt (\$ or LOQ>) and then enter...

1

TEMP:STANDARD.Q

1

24

1

REM 0.1 0.3

SET

1 Intensity @ Q=0 : **350**

2 Z-average Rg : **50**

3 Background : **1**

GO

Now check the quality of the fit...

P D

P O F

... and if you are satisfied with it then record the values of I(Q=0) and Rg.

KEEP

P R

KEEP

EX

<RETURN>

-1

To plot the fit and the residuals on laser printer n...

```
PLASERn SYS$SCRATCH:FRILLS.PS;-1
PLASERn SYS$SCRATCH:FRILLS.PS
```

The expected values of $I(Q=0)$ and R_g for the LOQ Standard are $I(Q=0) \sim 42.0 \text{ cm}^{-1}$ and $R_g \sim 70.5 \text{ \AA}$. So, now scale the observed scattering from your samples (in say W_m) by the ratio that the observed standard scattering must be scaled by in order to bring the $I(Q=0)$ values into agreement...

QUIT

```
>> Wm =Wm × 42.0 / {measured I(Q=0)}
>> COL
```

APPENDIX 5

Special Versions of COLETTE or COLETTE Startups

(a) TO GENERATE MICROSOFT WORD® COMPATIBLE GRAPHICS FILES

Normally when you issue a PRINT command COLETTE creates a graphics file called DEC_POSTSCRIPT.DAT in your current directory and then queues it to the printer that you select. This is because the default hardcopy output language is PostScript. Although Microsoft Word can import PostScript files they tend to require a great deal of memory (for example, it would be stupid to try and import a COLETTE contour plot in PostScript - we've tried!).

If you want to import COLETTE graphs into Microsoft Word run...

COL WORD

... instead of COL or COL TEST. This will cause COLETTE to load the Hewlett Packard graphics driver for hardcopy operations and to create files called DEC_HP7475.DAT. COLETTE will still queue the file to print but the operation will fail. These files can be transferred to a PC and imported into Word using *INSERT PICTURE*.

(b) TO RUN COLETTE THROUGH A PC USING KERMIT AS A TERMINAL EMULATOR

Instead of running COLETTE using COL or COL TEST try **COL KERMIT** or type the following at a DCL prompt (\$ or LOQ>)...

```
SET COMMAND LOQ$DISK:[LOQMGR.COLETTE.XCOLETTE]XCOLETTE
```

... and then invoke COLETTE using...

```
NEWCOLETTE/DEV=KERMIT/SCALE=1.0
```

(equivalent to COL)

... or...

```
TESTCOLETTE/DEV=KERMIT/SCALE=1.0
```

(equivalent to COL TEST)

(c) TO RUN COLETTE ON A VAX 4000 WORKSTATION (EG, SURF)

SURF has a more recent version of the DECGKS graphics library and so some display aspects of COL and COL TEST may not work properly (eg, cursor commands, etc). Instead, run...

COL SURF

(d) RUNNING COLETTE OVER DECNET OR TELNET IN A DECWINDOWS ENVIRONMENT

In order to redirect the graphical output to your workstation screen you will need to type...

SET DISPLAY/CREATE/NODE={your node name; eg, SURF}

... or...

SET DISPLAY/CREATE/NODE=aaa.bbb.cc.d/TRANSPORT=TCPIP

... where aaa.bbb.cc.d is your InterNet IP address (eg, ISISE is 130.246.84.3)

(e) TO RUN COLETTE WITH A REGIS GRAPHICS EMULATOR

Some commercial PC terminal emulation software uses REGIS escape codes when generating graphical displays. If you are using such software then invoke COLETTE using...

COL VT

APPENDIX 6

Detector Coordinate Corrections

When a neutron arrives at the main detector its time of arrival and position on the detector are noted by the electronics. But, because of the way in which all neutron detectors work, the position that is recorded is not the actual physical position at which the neutron arrived. In general the recorded position is out by a few mm. This discrepancy increases as you move out from the centre of the detector. This behaviour is known as "detector non-linearity".

From October 1994, COLETTE now corrects for detector non-linearity by default, using a procedure devised by RKH. A more detailed description of both the problem and the correction procedure may be found in a handout available from RKH. Also see Appendix 8.

To see if the detector coordinate correction is active, type...

SHOW TRANS or **SHOW MONITOR**

...and look at the second page of output (press <RETURN>) for..

"X coordinate correction is in use"

"Y coordinate correction is in use"

To deactivate the detector coordinate correction, type...

SET/XCOR/OFF or **SET/XCOR/CLEAR**

and

SET/YCOR/OFF or **SET/YCOR/CLEAR**

APPENDIX 7

Pixel by Pixel Detector Efficiency Corrections

Because of the way in which all neutron area detectors are built and operated, the efficiency with which a neutron is detected varies from position to position (pixel to pixel).

From October 1994, COLETTE now corrects for the detector efficiency on a pixel by pixel basis by default, using a procedure devised by RKH. A more detailed description of both the problem and the correction procedure may be found in a handout available from RKH.

To see if the detector coordinate correction is active, type...

SHOW TRANS or **SHOW MONITOR**

...and look at the second page of output (press <RETURN>) for..

"Cell by cell normalisation is ON"

To deactivate the pixel by pixel detector efficiency correction, type...

MON/FLAT/OFF or **MON/FLAT/CLEAR**

NOTE:

This efficiency correction is completely separate from the "normal" wavelength-dependent detector efficiency correction which is always used, irrespective of whether this pixel by pixel efficiency correction is activated or not.

APPENDIX 8

Semi-automatic Determination of the Beam Centre Coordinates

The apparent coordinates of the transmitted (or "through") beam on the main detector are periodically checked by the instrument scientists and entered in the mask file. If necessary, these coordinates may be changed with the command...

SET CENTRE [X value in mm] [Y value in mm] 0 0

Determining the beam centre coordinates is relatively straightforward but somewhat involved. To make things easier the procedure has now been semi-automated. The following description assumes that you have assigned a sample run and a can run, read in an appropriate mask file and calculated the relevant transmissions. Then type...

FIT/MID

WARNING! *This command runs very slowly on LOQ.
It will also overwrite W31, W32, W33 and W34.*

...and watch what happens! If you are using a Tektronix-type terminal it will be necessary for you to press return after each new plot is displayed. A more detailed description of this command can be found in a handout available from RKH.

