

CORRECT: A correction program for neutron diffraction data

Version 2.26

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1. Introduction

The CORRECT program has been developed from programs that were originally written at Oxford although some subroutines from other sources have been used. The program has been designed so that the input of data is done via a series of DCL-like commands. Once all the data has been entered the corrections procedure is performed. The advantage of this approach over the more conventional use of Fortran read statements is that changes can be made to the program without having to rewrite all the input data files. Also many values which have sensible default values need not be specified unless necessary.

This document first describes the use of the program as it stands for data from both reactors and pulsed neutron sources with some examples. After a description of all the commands available there are some notes on setting up the program and making alterations.

Version 2.26 includes the following modifications:

- Smoothing of background and container spectrum in cases of noisy data is now possible.
- The Placzek correction may now be applied to the vanadium spectrum only. This is useful for correcting samples containing light atoms, for which the inelasticity corrections fails (whereas the inelasticity correction for vanadium of course still is well defined). The 'true' correction may e.g. instead be approximated using a non-linear background during MCGR/RMCA modelling.
- There are now /MULTIPLIER and /TEMPERATURE options also for the vanadium spectrum.
- The 2θ offset parameter has been moved to the WAVELENGTH command.

2. Use of the program

The program is invoked by typing CORRECT at the prompt or from the Correct menu in the WinNFLP program. If used interactively it will respond with the prompt CORRECT>. A number of commands may be issued, for the most part in any order, giving details of the data to be used. EXECUTE starts the correction procedure. The final command is QUIT which leaves the program. An example set of commands is:

```

CORRECT> INST SLAD
CORRECT> VANADIUM T13232.RAW 0.3
CORRECT> BACK/VAN T13285.RAW
CORRECT> CONTAINER T13730.RAW 0.26 /DENS=0.0662/ABS=0.0571/SCAT=3.547
CORRECT> SAMPLE T13677.RAW 0.15 /TEMP=1170/DEN=0.0312
CORRECT> OUTPUT LACL3.CSX
CORRECT> BEAM 4. 2.
CORRECT> WAVELENGTH 0.94
CORRECT> COMPONENT 0.25 139 10.2 8.97
CORRECT> COMPONENT 0.75 Cl
CORRECT> TITLE "Molten LaCl3 at 1170K"
CORRECT> SPECTRUM 1
CORRECT> LIST
CORRECT> EXECUTE/NOLIST

```

The INSTRUMENT command (all commands may be abbreviated in the same way as DCL commands) tells the program which instrument, and thus which correction procedure, to use. The following six commands define data files containing raw data and, in the case of the OUTPUT command, to receive the corrected data. In the current version of the program two different formats are used: for time-of-flight and all input and output files are in the binary format used by the GENIE program whilst a text file format is used for reactor data except for SLAD where GENIE format is used. The other parameters to these commands specify a vanadium radius of 0.3 cm, furnace internal and external radii of 2.75 and 2.754 cm, a sample radius of 0.15 cm and a container (external) radius of 0.26 cm. The qualifier /VANADIUM to the BACKGROUND command means that this file contains a background to be used for the vanadium only. Qualifiers to the CONTAINER command give details of its density and scattering properties, which default to those of vanadium. Finally the SAMPLE command also defines the sample density and temperature.

The next two commands define the beam dimensions and the incident wavelength. The COMPONENT command defines the scattering properties of the components of the sample. It can be issued many times, each time it adds another item to the list of components. In this case there are two components so it is issued twice. TITLE defines a title to be written to the output file. Files in GENIE or text format can contain any number of spectra which, in the case of raw data, will be from different detectors and the SPECTRUM command determines which spectra from the input files are to be corrected. Like the COMPONENT command it can be issued many times, once for each spectrum to be corrected.

LIST will list all the program parameters to the terminal. Finally EXECUTE cause the correction routine to be run. Usually it will start by calling LIST but in this case, as LIST as already been called, the /NOLIST qualifier is used.

It is also possible to put commands in a command file which can be executed using @filename. The file type defaults to .COM. For example a file EXAMPLE.COM containing

```

INST SLAD
VANADIUM T13232.RAW 0.3
BACK/VAN T13285.RAW

```

```
CONTAINER T13730.RAW 0.26/DENS=0.0662/ABS=0.0571/SCAT=3.547
SAMPLE T13677.RAW 0.15/TEMP=1170/DEN=0.0312
OUTPUT LACL3.CSX
BEAM 4. 2.
WAVELENGTH 0.94
COMPONENT 0.25 139 10.2 8.97
COMPONENT 0.75 Cl
TITLE "Molten LaCl3 at 1170K"
SPECTRUM 1
LIST
EXECUTE/NOLIST
```

can be executed with

```
CORRECT> @EXAMPLE
```

Note that unlike DCL command files the lines do not start with a dollar symbol. For the VMS version of the program it is also possible to invoke CORRECT by typing CORRECT followed by a command which will be executed before the prompt is issued. This is most useful for executing a command file. For example

```
$ CORRECT @EXAMPLE
```

will enter the CORRECT program, obey all the commands in EXAMPLE.COM, and then, because the file contains an EXECUTE command, will return to DCL after completing the data correction. This is a convenient way of running CORRECT in batch jobs.

2.1 Reactor based diffractometry

Use of the program to correct data from reactor based diffractometers is straightforward. The program requires input data in the form of monitor normalised counts and standard deviations as a function of scattering angle. An example set of commands for correction of this sort of data was given in the previous section.

2.2 Time of flight diffractometry

Again the data must be put in the right format for input to the CORRECT program. For data from ISIS this can be done using their NORM program which combines data from different detectors after monitor normalisation and a correction for detector dead-time. The .NRM files that are produced are suitable for input to CORRECT, the running of which is again straightforward. An example command file is

```
INST LAD
XIN Q
```

```

VANADIUM VAN.RAW 0.5
BACKGROUND BACK.RAW
BACK/VAN VANBACK.RAW
CONTAINER CAN.RAW 0.4
SAMPLE CSCL.RAW 0.38/TEMP=900/DEN=0.03
OUTPUT CSCL.COR
COMPONENT 0.5 136 3.96 29.
COMPONENT 0.5 Cl
TITLE "Molten CsCl"
SPECTRUM 1 150. 10. 1.043
SPECTRUM 2 90. 10. 1.043
SPECTRUM 3 58. 10. 1.043
SPECTRUM 4 35. 10. 1.043
SPECTRUM 5 20. 10. 1.043
SPECTRUM 6 10. 10. 1.043
SPECTRUM 7 5. 10. 1.043
EXECUTE

```

This is similar to the reactor-based case. Note that the order of the two BACKGROUND commands is important: the first defines a background for everything, including vanadium, and then the second defines a different file as the vanadium background. Had they been in the opposite order the second would have counteracted the first. The command XIN Q specifies that the input data is expressed as a function of Q and in this case the SPECTRUM commands also give the scattering angles and incident and scattered flight path lengths of the relevant spectra.

3. Details of commands

BACKGROUND - Defines a file containing background data.

Parameter	The file.
/CONTAINER	Defines the background to be for the container only. The default is that it is the background for everything.
/SAMPLE	Defines the background to be for the sample only. The default is that it is the background for everything.
/SMOOTHING=value	Smooth the background spectrum, see VANADIUM/SMOOTHING for details (no Bragg peak removal in the background though). Only to be used with extremely noisy data.

/VANADIUM	Defines the background to be for the vanadium only. The default is that it is the background for everything.
BEAM	- Defines the beam dimensions.
Parameter 1	The beam height in centimeters. The default is 3 cm.
Parameter 2	The beam width in centimeters. The default is 1.5 cm.
CADMIUM	- Defines a file containing data for a cadmium rod or other absorber.
Parameter	The file.
CALIBRATION	- Specifies resolution parameters used by the vanadium smoothing.
Parameter 1	u, default = 2.6
Parameter 2	v, default = -2.1
Parameter 3	w, default = 0.7
COLLIMATOR	- Specifies that the absorption due to an oscillating radial collimator will be included in the corrections. (Only valid for reactor instruments. Default values are for SLAD.)
Parameter 1	The distance offset of the sample centre from the beam centre. The default is 0.0 cm.
Parameter 2	The angle offset of the sample centre from the beam centre. The default is 0.
Parameter 3	The collimator blade spacing at the inner radius. The default is 0.5 cm.
Parameter 4	The collimator blade thickness. The default is 0.05 cm.
Parameter 5	The inner radius of the collimator. The default is 15 cm.
Parameter 6	The outer radius of the collimator. The default is 25 cm.
Parameter 7	The distance to the detector. The default is 100 cm.
COMPONENT	- Defines the properties of one of the components of the sample. This command is used once for each component.

Parameter 1	The relative proportion of the component. This does not have to be absolute so long as the value given for each component is in the correct ratio. For example for CsCl any value can be used so long as it is the same for each component.
Alt. 1.	
Parameter 2	The atomic weight.
Parameter 3	The atomic scattering cross-section.
Parameter 4	The absorption cross-section at 2200ms^{-1} .
Alt. 2.	
Parameter 2	The atom symbol (eg. S=sulfur, O=oxygen, Fe=iron etc.). The atomic weight, scattering- and absorption cross-sections for the atom will be read from a file.
../RESET	Resets the list of components
CONTAINER	- Defines the file containing the container data and some of the properties of the container.
Parameter 1	The file containing the container data.
Parameter 2	The can external radius for CYLINDRICAL geometry, or the can thickness for PLATE geometry.
/ABSORPTION=value	The absorption cross-section of the can at 2200 ms^{-1} . The default is to use the value for vanadium.
/DENSITY=value	The number density of the can (\AA^{-3}). The default is to use the number density of vanadium.
/MULTIPLIER=value	A 'correction' factor by which the can scattering (after subtraction of any background) is multiplied. The default is 1.
/SCATTERING=value	The scattering cross-section of the can. The default is to use the value for vanadium.
/SMOOTHING=value	Smooth the container spectrum, see VANADIUM/SMOOTHING for details (no Bragg peak removal in the background though). Only to be used with extremely noisy data.

/TYPE=value	Instead of defining the density, absorption and scattering of the container you can define the type of material. Types recognized are VANADIUM and SILICA. The default is vanadium.
EXECUTE	- Performs the correction.
/NOLIST	Prevents a listing of the program parameters.
/OUTPUT=file	A file to receive the output from the program that would otherwise be sent to the terminal.
GEOMETRY	- The sample geometry. (Multiple scattering corrections not yet done correctly for plate geometry.)
Parameter 1	The geometry. Must be one of CYLINDRICAL or PLATE. The default is CYLINDRICAL.
Parameter 2	For PLATE geometry, the angle, in degrees, of the normal to the sample from the direction of the beam. The plate angle and the scattering angles must be defined in a consistent manner with respect to the beam direction. The default is 0°.
Parameter 3	For PLATE geometry, the angle, in degrees, of the normal to the vanadium from the direction of the beam. The plate angle and the scattering angles must be defined in a consistent manner with respect to the beam direction. The default is that the sample and vanadium are at the same angle.
INSTRUMENT	- The instrument that was used.
Parameter 1	The instrument. Must be one of D4, D20, LAD, SANDALS, SEPD, or SLAD. The default is D4. For reactor diffractometers the default file type is TEXT (except for SLAD where it is GENIE) and for time of flight diffractometers the default is GENIE.
LIST	- Lists the program parameters to the terminal.
LOW_ANGLE	- Causes a low angle correction to be done for reactor data between

angle 1 and angle 2. If a cadmium file has been defined this will be done using the cadmium data after subtraction of a background calculated between angles 3 and 4. If no cadmium file has been defined the correction will be done by extrapolating the data for vanadium or any other incoherent scatterers between angle 3 and angle 4.

Parameter 1	Angle 1
Parameter 2	Angle 2
Parameter 3	Angle 3
Parameter 4	Angle 4
/BACKGROUND	Will extrapolate the background data
/CONTAINER	Will extrapolate the container data
/VANADIUM	Will extrapolate the vanadium data
MONITOR	-Defines which spectrum in the data file is the monitor spectrum. This command only has effect for time of flight diffractometers.
Parameter	The number of the spectrum.
OUTPUT	- Defines the file to receive the corrected data produced by the program.
Parameter	The file
PLACZEK	- Specifies which type of Placzek correction will be used.
Parameter	The type of correction. Acceptable values are SERIES_EXPANSION (Yarnell et al for reactor; Howe et al for time of flight), DIATOMIC (Powles, time of flight only), and NONE. The default is NONE.
/VANADIUM_ONLY	Do the Placzek correction only for the normalising Vanadium data.
QUIT	- Leaves the program.
RANGE	- Defines the range of wavelengths used in time of flight data.
Parameter 1	The minimum wavelength to be used. The default is 0.1 Å.
Parameter 2	The maximum wavelength to be used. The default is 3.0 Å.
SAMPLE	- Defines the file containing the sample data and some of the properties of the sample.

Parameter 1	The file containing the sample data.
Parameter 2	The sample radius, for CYLINDRICAL geometry, or the sample thickness for PLATE geometry.
/DENSITY=value	The number density of the sample (\AA^{-3}). The default is 0.
/FULLNESS=value	The fullness of the container (default 1.)
/TEMPERATURE=value	The temperature of the sample in Kelvin. The default is 300K.
/CS_FILE	A file containing the total (scattering + absorption) cross-section of the sample as a function of wavelength, typically at 0.5 \AA intervals up to 10 \AA . This is used to calculate the attenuation coefficients. The default is to calculate the cross-section from the values given by the COMPONENT commands.
SPECTRUM	- Defines a spectrum to be corrected.
Parameter 1	The spectrum number.
Parameter 2	The scattering angle. Only for time of flight diffractometers. For PLATE geometry the plate angle and scattering angles must be defined in a consistent manner with respect to the beam direction.
Parameter 3	The incident path length in meters. Only for time of flight diffractometers. The default is 10 m.
Parameter 4	The scattered path length in meters. Only for time of flight diffractometers. The default is 1.043 m.
/DETECTOR	For time of flight diffractometers, the type of detector. Either HE_GAS or SCINTILLATION. The default is HE_GAS.
/DEFAULT	Runs through a default number of spectra. The default depends on the instrument used. (Only available for SLAD so far, spectra 1-48).
/TO=max_sp	Runs through spectra 1 to "max_sp".

TITLE	- Defines a title for the corrected data.
Parameter	The title.
VANADIUM	-Defines the file containing the vanadium data and some of the properties of vanadium (or any other material used as calibrant). If no vanadium is defined and a container has been defined calibration will be attempted using the can assuming it is a totally incoherent scatterer.
Parameter 1	The file containing the vanadium data.
Parameter 2	The vanadium radius, for CYLINDRICAL geometry or the vanadium thickness for PLATE geometry.
/ABSORPTION=value	The absorption cross-section of vanadium at 2200 ms ⁻¹ . The default is 5.08 b.
/DENSITY=value	The number density of vanadium (Å ⁻³). The default value is 0.0722 Å ⁻³ .
/MULTIPLIER=value	A 'correction' factor by which the vanadium scattering (after subtraction of any background) is multiplied. The default is 1.
/SCATTERING=value	The scattering cross-section of vanadium. The default is 4.95 b.
/SMOOTHING=value	<p>For two axis diffractometers the corrected vanadium spectrum may be smoothed with a polynomial of order SMOOTHING for positive values of SMOOTHING, i.e. 2 produces a straight line fit. The default is 0 (no smoothing) and the maximum is 10. If smoothing is used the routine will attempt to use statistical tests to remove small vanadium Bragg peaks. Recommended values are 2 for D4 and D20 and 4 for SLAD. For time-of-flight diffractometers the vanadium spectrum will be smoothed using cubic splines if SMOOTHING=1; the default is no smoothing.</p> <p>If SMOOTHING is negative the vanadium will be smoothed with a Savitzky-Golay filter, after subtraction of the V Bragg peaks. The smoothing window has a width of (-2*SMOOTHING+1) points. Recommended value -9.</p>

/TEMPERATURE=value	The temperature of the vanadium in Kelvin. The default is 300K. Has an influence on the Vanadium Placzek correction and Bragg peak subtraction (through the lattice parameter estimated from this temperature).
/CONTAINER	The vanadium scattering will be corrected for the container scattering. This may be used if the vanadium is flakes or foil in a container. In this case the vanadium number density should be the density of vanadium in the container. If this qualifier is not used then the number density should be the average density of vanadium in the beam, including both the flakes/foil and container.
WAVELENGTH	- The incident wavelength in Angstroms. Only appropriate for reactor based diffractometers.
Parameter 1	The wavelength. The default is 0.7 Å.
Parameter 2	2θ offset to be subtracted from the input angles.
WRITE	- Specifies what should be written to the output file in addition to the corrected cross-section.
Parameters	Things to be written. Acceptable values are ABSORPTION, CALIBRATION, LOW_ANGLE (reactor only), MULTIPLE_SCATTERING (reactor only), and PLACZEK. The default is to write only the corrected data.
XIN	- For time-of-flight diffractometers the input data can be expressed as a function of wavelength (in Å), time of flight (in ms), or momentum transfer (in Å ⁻¹) and this is specified with the XIN command.
Parameter	Can be WAVELENGTH, TOF, or Q. The default value is WAVELENGTH.
XOUT	- For reactor diffractometers the output data can be expressed as a function of angle (in degrees) or momentum transfer (in Å ⁻¹) and this is specified with the XOUT command.
Parameter	Can be ANGLE or Q. The default value is Q.

Appendix 1. Setting up the program

To set up CORRECT version 2.26 you must start with the following files:

NDPLIB.FOR	Subroutines including calculations of attenuation coefficients and multiple scattering
FILEIO_*.FOR	File reading and writing routines, *=WIN, LINUX or VMS
CORRECT.FOR	The main program unit
CORRECT.OPT	VMS Options file for use in linking CORRECT
CORRECT225.PDF	This document
CORRECT_2AXIS.FOR	Correction subroutine for reactor data
CORRECT_TOFDIF.FOR	Correction subroutine for time of flight data
DOUBLESCATTERING.DAT	Data file for the multiple scattering routine
HARWELL.FOR	Harwell subroutines used by the program
PARSE_LINE.FOR	Routine for parsing command lines
CORRECT_ROUTINES.FOR	Various subroutines used by both correction subroutines
NXSECTION.DAT	Data file containing x-sections and mass for different atoms.

To set up the program compile all the Fortran files and then link all the object files with the library of file reading and writing routines. For VMS this can be done using the options file by `$ LINK CORRECT,CORRECT/OPT`.

If CORRECT is to be used on an alpha-station change FILEIO.OLB to FILEIO_A.OLB and CORRECT.OPT to CORRECT_A.OPT. A symbol must be defined for the logical name for the data file used by the multiple scattering routine. To do this include in your LOGIN.COM file the lines

```
$ CORR*ECT:==SY$DIR:[CORRECT]CORRECT_223
$ DEFINE DOUBLESCATTERING SY$DIR:[CORRECT]DOUBLESCATTERING.DAT
$ DEFINE XSECTION SY$DIR:[CORRECT]XSECT.DAT
```

or something similar with the appropriate disk and directory names substituted.

Appendix 2. Some details about the program

The main program unit and its associated subroutines, contained in the file CORRECT.FOR, deal solely with the input of data into the program. The actual corrections are done by two completely separate subroutines, one for reactor based instruments (CORRECT_2AXIS.FOR) and one for time of flight instruments (CORRECT_TOFDIF.FOR). All the data is passed to these subroutines via the parameters in the module correctpar. Thus either of these routines could be used as they are,

independent of the remainder of the CORRECT package provided the relevant data is passed in the common blocks. There are some general purpose routines used by both correction subroutines and these, apart from the Harwell routines, are contained in CORRECT_ROUTINES.FOR.

The routines for reading and writing the data files used by the program are contained in the library FILEIO_*. To use different format files all that is necessary is to change a parameter to the routines for a format that is supported, or else to substitute appropriate file reading and writing routines.

At the moment only the instruments D4, D20, SLAD, SEPD, LAD, and SANDALS are understood. If you have data from another instrument but don't need to change the correction part of the program you can either fool it by pretending you have one of the existing instruments or add the new instrument to the list of instruments recognized. To do this all you have to do is alter CORRECT.FOR wherever it makes any reference to the instrument.

Versions of CORRECT for WIN95 or UNIX are now available but only the TEXT format can be used for these at this time.

Appendix 3. The format of data files

The file reading and writing routines used by CORRECT are contained in the library FILEIO_* and may be used in other programs by linking with this library. They read and write files in GENIE binary format, in an equivalent TEXT format, or in a simpler text DATA format. Data files in GENIE or TEXT contains an indefinite number of data sets one after the other. A file is read with `read_file`. A data file containing only one data set can be written with `write_file`. If it is to contain several data sets it must be opened with `open_file`, each data set written with `append_file`, and then closed with `close_file`. It is permissible to omit `close_file` after writing to a file in TEXT format but if writing to GENIE file the data will be lost if `close_file` is not called. Only one data file may be open for writing at one time. The specifications of the routines are:

```
Subroutine read_file(x,y,e,npts,histogram_mode,instrument,
user,run_number,spectrum_number,title,run_date,x_caption,
y_caption,file,data_set,format,ierror)
```

x	Real array of size at least npts+1 containing the x values.
y	Real array of size at least npts+1 containing the y values.
z	Real array of size at least npts+1 containing the standard deviations.
npts	Integer. The number of data points.
histogram_mode	Logical. If. <code>.true.</code> the data is in histogram mode which means that there are npts+1 x values representing boundaries of histogram bins. Otherwise there are npts x values.
instrument	Character*(*).The instrument name.

<code>user</code>	Character*(*). The name of the user.
<code>run_number</code>	Integer. A number identifying the run.
<code>spectrum_number</code>	Integer. A number identifying the spectrum.
<code>title</code>	Character*(*). A title for the data set.
<code>run_date</code>	Character*(*). A date associated with the data set.
<code>x_caption</code>	Character*(*). A label for the x data.
<code>y_caption</code>	Character*(*). A label for the y data.
<code>file</code>	Character*(*). The name of the file that is to be read.
<code>data_set</code>	Integer. The data set to be read from the file. These are numbered 1, 2, etc.
<code>format</code>	Character*12. One of GENIE, TEXT, or DATA.
<code>ierror</code>	Integer. If <code>ierror=1</code> on entry a failure in the routine will cause the program to terminate with an error message. If <code>ierror=0</code> on entry the routine will return a value of 1 on successful completion or a larger value on failure.

```
Subroutine write_file(x,y,e,npts,histogram_mode,instrument,
user,run_number,spectrum_number,title,run_date,x_caption,
y_caption,file,format,ierror)
```

```
subroutine open_file(file,format,max_size,ierror)
```

<code>max_size</code>	Integer. For a GENIE file every data set takes up the same amount of room so it is necessary to define this amount when the file is opened. <code>max_size</code> should be greater than or equal to the largest number of data points that will be written. For other formats this parameter is irrelevant.
-----------------------	--

```
subroutine append_file(x,y,e,npts,histogram_mode,instrument,
user,run_number,spectrum_number,title,run_date,x_caption,
y_caption,ierror)
```

```
subroutine close_file
```