# ISAW GLAD Operators

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# GLADAnalyze

## Introduction

The GLADAnalyze operator is used to calculate experimental attenuation, multiple scattering, and inelasticity terms.

## Launching Operator

To launch GLADAnalyze from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD>GLADAnalyze**

## User Inputs

**dso** – See documentation for GLADConfigure.

**ds** – Select an input dataset.

**imask** – The imask field is used to enter a special integer flag indicating the type of scatterer; each bit corresponds to one experiment sample setup component:

0: Calibration/Vanadium

1: Sample

2: Can

4: Furnace

8: Flat Plate Setup

**Example:**

To indicate a sample with a can, you would enter 3 in the imask field.

Sample = 1, Can = 2

Sample + Can = 3

To indicate a sample with a can in a flat plate setup, you would enter 11 in the imask field.

Sample = 1, Can = 2, Flat Plate Setup = 8

Sample + Can + Flat Plate Setup = 11

**mulstep** – Use the mulstep field to specify a step size (cm in the cylindrical axial direction) for the multiple scattering calculation.

**absstep** – The absstep field is used to specify a step size (cm in the cylindrical axial direction) for the absorption calculation.

**usemutfile** – The usemutfile checkbox is used to choose whether or not to apply a user specified MUT file.

**mutfile** – Use the mutfile browser to choose a file to be used when the usemutfile option is enabled.

**minw** – The minw field is used to assign a minimal wavelength (in angstroms) when generating the MUT table.

**maxw** – The maxw field is used to assign a maximum wavelength (in angstroms) when generating the MUT table.

**dw** – The dw field is used to specify a wavelength step size (in angstroms).

## Additional Information

See sections 3.6 and 3.7 on pages 13-15. [1]

See equations 14 and 15. [1]

$$I_s^i(Q) = \frac{I_{sc}^i(Q) - \frac{I_c^i(Q)}{A_{c,c}}}{A_{s,sc}}, \tag{14}$$

$$I_{dcs}^i(Q) = \frac{I_s^i(Q)}{N_s}. \tag{15}$$

# GLADCalibration

## Introduction

The GLADCalibration...

## Launching Operator

To launch GLADCalibration from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADCalibration**

## User Inputs

**calibfile0**

**calibfile1**

**calibds**

## Additional Information

See section 3.9 on page 19. [1]

See equation 18. [1]

# GLADCombine

## Introduction

The GLADCombine operator uses the weighting function generated by the GLADDistinct operator to produce a final differential cross section.

## Launching Operator

To launch GLADCombine from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADCombine**

## User Inputs

**int_smp** – The int_smp menu is used to choose the dataset containing the sample differential cross section.

**flx_van** – The flx_van menu is used to choose the dataset containing the weighting function.

**NUMQ** – The NUMQ field is used to specify the number of Q bins in one unit (in angstrom$^{-1}$).

**GLADQMAX** – The GLADQMAX field is used to specify a maximum Q value.

### Additional Information

See section 3.9 on page 19. [1]

See equation 18. [1]

$$F(Q) = \frac{\sum_i W^i(Q) I^i_{\text{int}}(Q)}{\sum_i W^i(Q)}. \qquad (18)$$

# GLADConfigure

### Introduction

The GLADConfigure operator is used to define the experimental standards to be used for subsequent analysis.

### Launching Operator

To launch GLADConfigure from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADConfigure**

## User Inputs

**calibopt** – Enter the calibration standard used.

**smpcomposition** – Enter the sample composition.

**smpdensity** –Enter the sample effective density.

**canopt** – Enter the sample container (can) used.

**scc** – Enter the sample calibration constant.

*Note: scc = (number density, 1/cm$^3$)*(beam ht, cm)*π*(radius of sample, cm)^2*

**configfile** – Use the configfile browser to choose a configration file.

**hasCan** – Check this box if the experiment uses a can ("false" for calibration run with fused silica rod).

**hasFur** – Check this box if the experiment uses a furnace.

**isFP** – Check this box if a flat plate setup was used.

**doDebug** – Check this box to print out inputs relating to absorption and multiple scattering correction routines.

## Outputs:

**dso**

At the beginning of data analysis, the GLADConfigure operator reads a user specified/edited configuration file to set up an array of objects containing the following elements:

0: A GLADRunProps object holding instrument information

1: Vanadium (a GLADScatter object)

2: Sample (rod or with can)

3: Can (empty)

4: Furnace

The dummy dataset contains only a single attribute -"GLAD_Running_Info" - with the object array as its value. This special dataset "dso" is used to transport instrument and experiment information around within ISAW to various GLAD related operators.

# GLADCrunch

## Introduction

The GLADCrunch operator is used to eliminate dead detector data.

## Launching Operator

To launch GLADCrunch from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADCrunch**

## User Inputs

**dso** – See documentation for GLADConfigure.

**runfile** – Use the runfile browser to choose the IPNS runfile to be "crunched."

**noDeadDetList** – Check this box if you are not using a vanadium run

**redpar** – Use the redpar browser to choose a DAS bad data list file.

**lcutoff** – A data group is flagged as bad if its total number of counts is smaller than the value entered in the lcutoff field.

**MonSmoothing** – Check the MonSmoothing box to smooth monitor data with Fourier filtering.

**DetSmoothing** – Check the DetSmoothing box to smooth detector data with Fourier filtering.

## Additional Information

See sections 3.1, 3.2, 3.4, and 3.5 on pages 7-12. [1]

# GLADDistinct

## Introduction

The GLADDistinct operator rebins the vanadium monitor spectrum for each data group from wavelength to Q at a given scattering angle, and then generates a weighting function. This weighting function is subsequently used by the GLADCombine operator.

## Launching Operator

To launch GLADDistinct from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADDistinct**

## User Inputs

**dso** – See documentation for GLADConfigure

**dcs_smp** – The dcs_smp menu is used to choose a sample dataset.

**smo_van** – The smp_van menu is used to choose a vanadium dataset.

**dm_van** – The dm_van menu is used to choose a vanadium monitor dataset.

**temperature** – Enter the temperature to be used in Placzek correction.

**wmin/wmax** – If the wavelength value is outside the boundaries of wmin/wmax, the weightings are set to zero, which in turn sets the contribution to merged differential cross section values to zero.

### Additional Information

See section 3.9 on page 19. [1]

See equation 17. [1]

$$W^i(Q) = Cal^i_v(Q) C^i_{m,v}(Q). \quad (17)$$

# GLADDQ2R

### Introduction

The GLADQ2R operator is used to Fourier transform the structure factor for the lattice into real space. The operation results in a number of distribution functions including the differential distribution function, the total distribution function, and the radial distribution function.

## Launching Operator

To launch GLADQ2R from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADQ2R**

## User Inputs

**dso** – See documentation for GLADConfigure.

**ioq_smp** – Use the ioq_smp menu to choose a sample dataset.

**NumberDensity** – This field is used to enter the number density.

**RCut** – Use this field to define the R cutoff in calculating real space functions.

**QCut** – Use this field to define the Q cutoff in Fourier transform.

**NUMQ** – Use the NUMQ field to define the number of Q bins in each unit (in angstroms$^{-1}$).

## Additional Information

See section 3.12 on page 22. [1]

# GLADSumRun

## Introduction

The GLADSumRun operator is used to combine any number of runs.

## Launching Operator

To launch GLADSumRun from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADSumRun**

## User Inputs

**mon_nrm_list** – The mon_nrm_list text field is used to define the .NRM and .MON files that will be combined by the operator. The filenames are entered as an array.

# GLADVanCal

## Introduction

The GLADVanCal operator is used to generate a vanadium calibration function for each data group.

## Launching Operator

To launch GLADVanCal from ISAW, follow the menus:

**Macros>Instrument Type>TOF_NGLAD> GLADVanCal**

## User Inputs

**dso** – See documentation for GLADConfigure.

**nrm_van** – Use the nrm_van menu to choose a vanadium dataset.

**DOsmooth** – Check the DOsmooth box to enable smoothing for the vanadium data.

**temperature** – Enter the temperature to be used in Placzek correction.

**mulstep** – Use the mulstep field to define a step size to be used in the vanadium multiple scattering calculation.

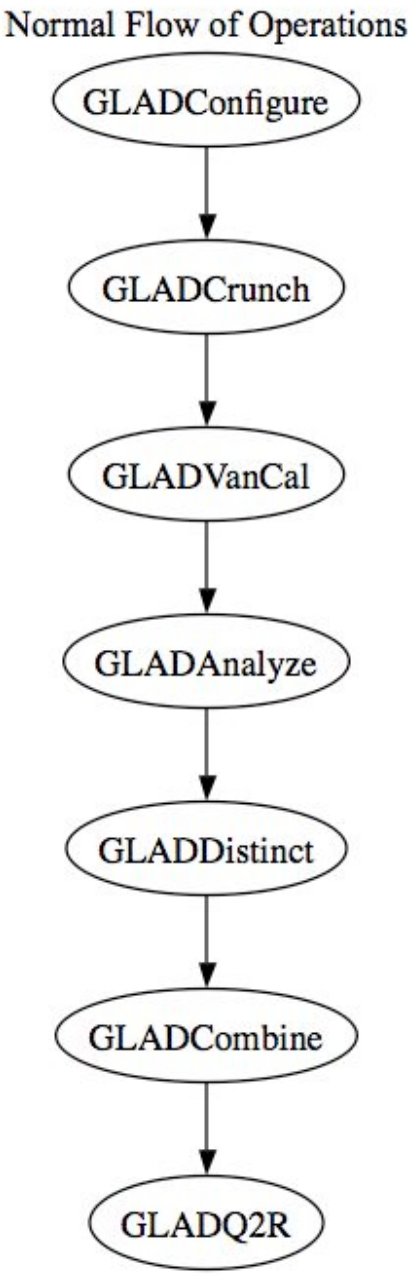
## Additional Information

See section 3.8 on page 15. [1]

See equation 9. [1]

$$Cal_{v}^{i}(Q) = \frac{I_{nrm,v}^{i}(Q)}{M_{v,0}^{i}(\lambda)\,p^{i}(\lambda) + M_{v,1}^{i}(\lambda)}\,, \tag{9}$$

# Flowchart


Normal Flow of Operations
GLADConfigure
GLADCrunch
GLADVanCal
GLADAnalyze
GLADDistinct
GLADCombine
GLADQ2R

# References

[1] J. Tao, C. J. Benmore, T. G. Worlton, J. M. Carpenter, D. Mikkelson, R. Mikkelson, J. Siewenie, J. Hammonds, A. Chatterjee, Time-of-Flight Neutron Total Scattering Data Analysis implemented in the software suite ISAW. 2005.