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SAC Activation Analysis and Validation

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Instrument and Source Division

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1. INTRODUCTION

The Spallation Neutron Source (SNS) [1] and the High Flux Isotope Reactor (HFIR) [2] at Oak Ridge National Laboratory (ORNL) uses the Sample Activation Calculator (SAC) [3] to calculate the activation of a sample before the sample has been exposed to the neutron beam in one of the SNS or HFIR beamlines. The SAC webpage takes user inputs (choice of beamline, the mass, composition and area of the sample, irradiation time, decay time, etc.) and calculates the activation for the sample. In recent years, the SAC has been incorporated into the user proposal and sample handling process, and beamline scientists and users have noticed conservativeness in the predicted activation of their samples. The Neutronics Team at SNS was tasked with validating the SAC tool and diagnosing the origin of the discrepancies seen by the beamline scientists and the users. Measurements were performed on the EQ-SANS (Extended Q-Range Small-Angle Neutron Scattering Diffractometer) [4] and VULCAN (Engineering Materials Diffractometer) [5] instruments at SNS to help validate the SAC, and diagnose the discrepancies in the calculated and measured activations. Through the analysis of these measurements, we found serious differences in the calculated and measured activities, even for our well-defined test irradiation. We also found that the errors in the SAC beamline flux spectra are a significant contributor to the activation discrepancies observed by many of the beamline scientists and users. The results of the analysis of the validation measurements on the select beamlines will be discussed in detail.

2. SAC DESCRIPTION

The SAC is used to calculate the activation of user samples after irradiation on any SNS beamline, and the SAC has been incorporated into the user proposal and sample handling process. The SAC is a webpage that takes user inputs, such as the choice of beamline, the mass, composition and area of the sample, irradiation time, decay time, etc., and invokes the Sample Activation Program for Easy Use (SAPEU) to calculate the activation of the sample. SAPEU uses the user input file (supplied by SAC) along with a file containing the SNS beamline neutron flux spectra, either the CINDER 90 [6] or 08_flat-weighted cross section library, and other reference files containing information on radiotoxicity, gamma spectroscopy detector efficiency, atomic mass, and natural isotopic abundances to perform activation analysis of a given sample.

3. DESCRIPTION OF MEASUREMENTS AND ANALYSIS

In order to diagnose the discrepancies in the calculated and measured sample activities and to validate the SAC tool, measurements have been performed on both the EQ-SANS and VULCAN instruments to acquire the data needed for analysis. In these measurements, gold foils were irradiated using single neutron energy band passes, the activity of the gold foils was assessed using a gamma-ray spectrometer, and image plate autoradiography was performed on the foils [7]. The irradiation time of the foils was set such that sufficient counting statistics could be acquired from the gamma-ray spectrometer. Image plate autoradiography was used to verify the distribution of neutron flux across the beam spot. The gold foil measurement configurations, as well as the details of the gold foil sample, are outlined in Table 1 for the EQ-SANS instrument and in Table 2 for the VULCAN instrument.

Table 1 EQ-SANS Irradiation Conditions

Thickness (cm)	Area (cm^2)	Density (g/cm^3)	Norm. Factor	
8.18E-04	0.79	19.3	1.00	
Configuration #	**Beam Power (MW)**	**Wavelength Window (Å)**	**Irradiation Time (min)**	**Decay Time (min)**
1	0.85	2.50 - 6.10	10	6
2	0.85	6.00 - 9.60	60	9
3	0.85	10.0 - 13.4	60	9

Table 2 VULCAN Irradiation Conditions

Thickness (cm)	Area (cm^2)	Density (g/cm^3)	Norm. Factor	
8.18E-04	0.32	19.3	1.00	
Configuration #	**Beam Power (MW)**	**Wavelength Window (Å)**	**Irradiation Time (h)**	**Decay Time (min)**
1	0.85	0.48 - 1.92	1	9
2	0.85	1.68 - 3.12	1	9
3	0.85	2.88 - 4.32	2	9
4	0.85	4.08 - 5.52	10	9
5	0.85	5.28 - 6.72	15	9

We make two types of comparisons among the SAC results and measured sample activities for the EQ-SANS and VULCAN instruments. First, we compare the flux spectra in the SAC database to the most recent McStas simulations [8-10]. The flux spectra in the SAC database are a combination of simulation results for the most part and other methods. Second, we compare the activities predicted by SAC irradiated by single well-defined energy bands to those by sequential irradiations of a single foil in multiple (still well-defined) energy bands.

4. ANALYSIS

4.1 NEUTRON FLUX SPECTRUM ANALYSIS

The neutron flux spectrum used in the SAC code is compared with the McStas simulated neutron flux spectra [10] and a measured neutron flux spectrum [11] for the EQ-SANS instrument in Fig. 1. Iverson's measured neutron flux spectrum shown in Fig. 1 is a combination of measurements taken over several wavelength bands and the corresponding chopper cutoffs have been removed. These measurements were done using a calibrated beam monitor located just upstream of the nominal sample position while SNS was operating at 1 MW. The sample pinhole was set to 10 mm in diameter and the source pinhole was set to 25 mm in radius. It should be noted that Iverson's measured neutron flux was normalized by the area of the sample pinhole rather than the area of the beam spot at the sample position [11].

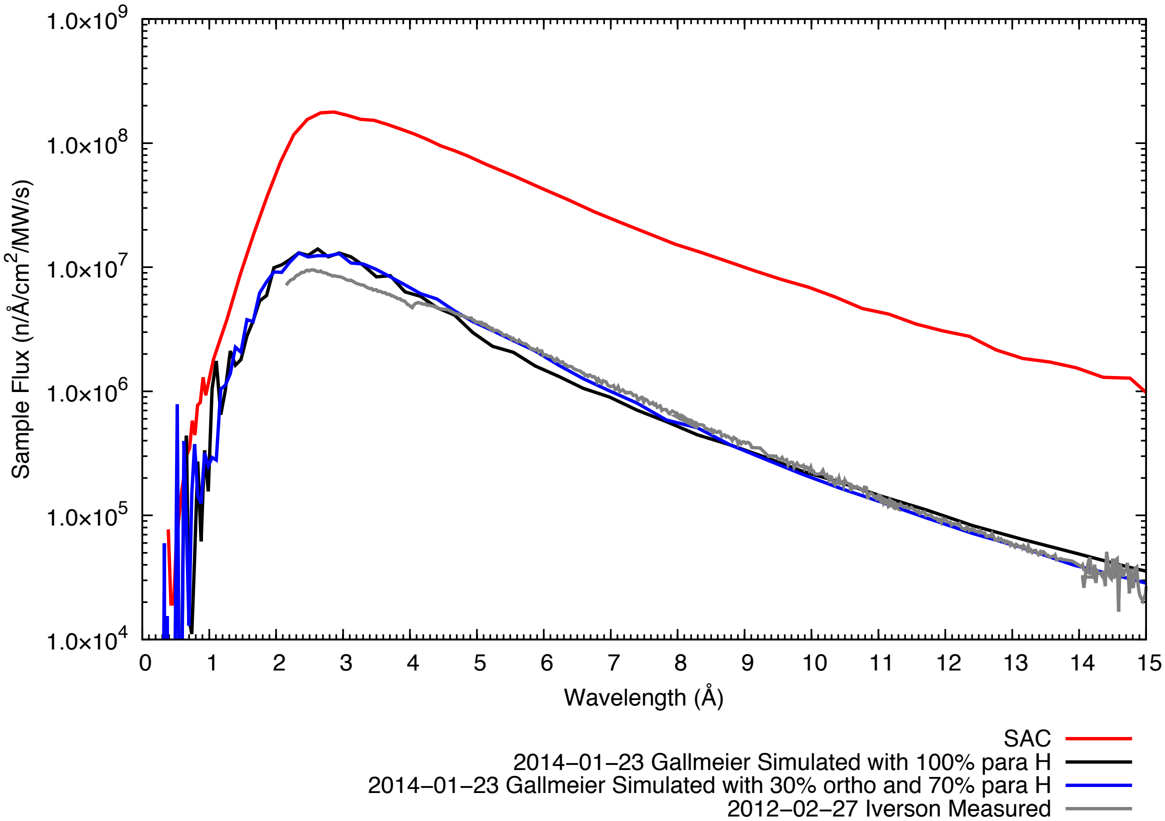


Fig. 1. **EQ-SANS Wavelength Flux Comparison (The chopper cutoffs have been removed from the measured neutron flux spectrum)**

The neutron flux spectrum used in SAC is compared with a McStas simulated (Gallmeier Simulated) [9] neutron flux spectrum and a measured neutron flux spectrum (Iverson Measured) [12] for the VULCAN instrument in Fig. 2. The simulated and measured spectra in Fig. 2 nominally differ with the SAC spectrum by approximately a factor of two but all three spectra have approximately the same shape. Iverson's measured neutron flux spectrum used a calibrated beam monitor located at the nominal sample position viewing a pinhole of 2.32 mm in diameter with the default chopper settings and the upstream guide configuration in the high-intensity mode [12].

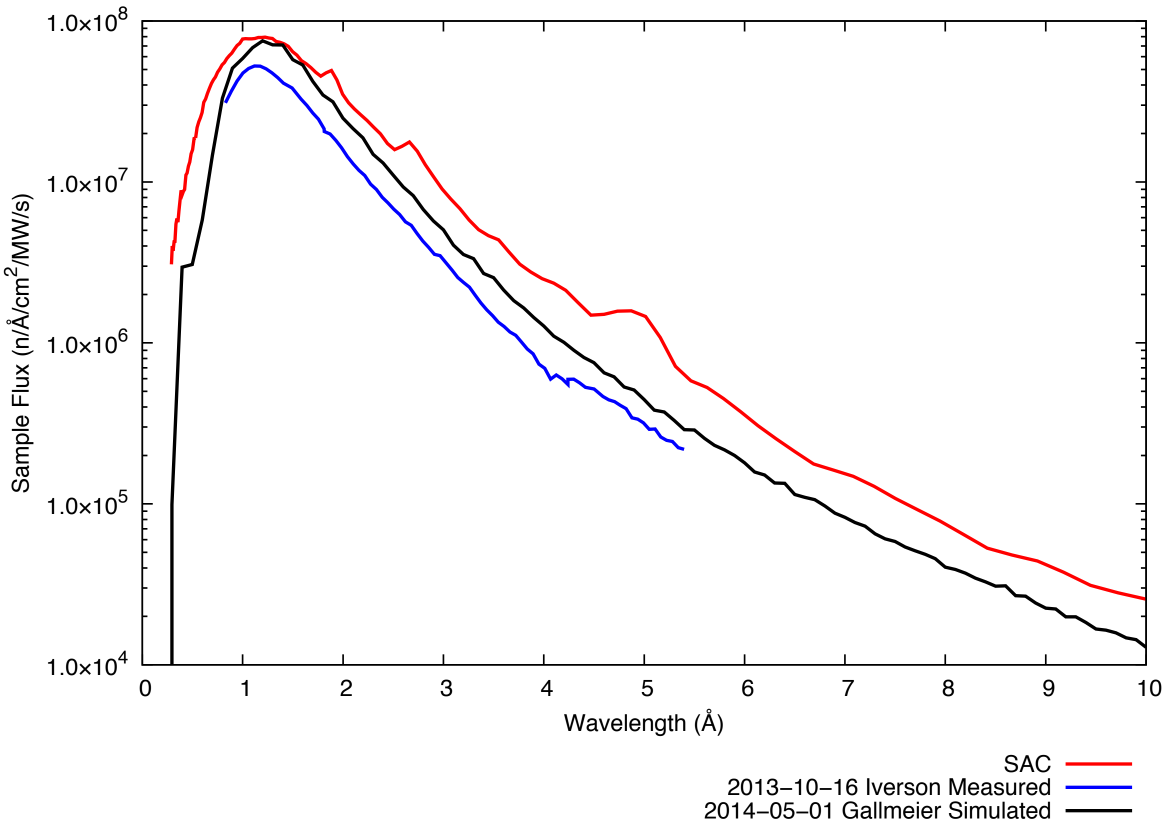


Fig. 2. VULCAN Wavelength Flux Comparison (The chopper cutoffs have been removed from the measured neutron flux spectrum)

The discrepancies observed in the measured and calculated sample activation for samples irradiated on the VULCAN instrument can only attribute a small portion of the discrepancies to the input neutron flux spectrum used in SAC.

4.2 GOLD FOIL ACTIVATION ANALYSIS

Table 3 shows the calculated activities using the SAC inherent neutron flux spectrum compared to those using both the Gallmeier simulated neutron flux spectrum with 100 percent para hydrogen and the Iverson measured neutron flux spectrum (both shown in Fig. 1) for all three configurations of the EQ-SANS instrument [10, 11]. Both cross section libraries, CINDER 90 and CINDER 08_flat-weighted, were used in the calculation. When an appropriate spectrum, such as one of the Gallmeier simulated neutron flux spectra, was used to calculate the sample activities, the results were within approximately 30% error of the measured activities for EQ-SANS. The test case activation was calculated within an average of 9% error of the measured activities for EQ-SANS when Iverson's measured flux was used to calculate the sample activation.

Table 3 EQ-SANS Au Foil Activation

	Configuration 1 2.50 – 6.10 Å		Configuration 2 6.00 – 9.60 Å		Configuration 3 10.0 – 13.4 Å	
	Total Activity (nCi)	% Difference with Measured	Total Activity (nCi)	% Difference with Measured	Total Activity (nCi)	% Difference with Measured
Measured by Gamma Spec	6.10	-	9.60	-	1.80	-
Calculated by SAC with CINDER 90 Cross Sections	132	2060	190	1880	33.6	1770
Calculated by SAC with CINDER 08 Cross Sections	138	2160	290	2920	54.3	2920
Calculated by SAPEU using Gallmeier [10] simulated flux spectrum for 100 percent para H with CINDER 90 Cross Sections	7.94	30.2	7.50	-21.9	1.40	-22.2
Calculated by SAPEU using Gallmeier [10] simulated flux spectrum for 100 percent para H with CINDER 08 Cross Sections	8.14	33.4	12.1	26.0	2.25	25.0
Calculated by SAPEU using Iverson [11] measured flux spectrum with CINDER 90 Cross Sections	6.24	2.3	6.84	-28.8	1.06	-41.2
Calculated by SAPEU using Iverson [11] measured flux spectrum with CINDER 08 Cross Sections	6.51	6.7	11.0	15.1	1.71	-5.0

Note: $\text{Percent Difference} = \frac{Calculated - Measured}{Measured} \times 100$

The comparison between the sample activation calculated with the SAC neutron flux spectrum and the Gallmeier simulated [9] and Iverson measured [12] neutron flux spectra (both shown in Fig. 2) for the VULCAN instrument separated by the use of the CINDER 90 or 08_flat-weighted cross section libraries is shown in Table 4. The calculated sample activities using Iverson's measured neutron flux spectrum for Configuration 4 and 5 are absent from Table 4 due to lack of data in Iverson's measurement. If there are wavelengths in the irradiation band pass that are not in the input flux spectrum to SAC, SAC assumes a zero flux for those wavelengths. The zero flux assumption leads to an underestimation of the sample activity.

Table 4 VULCAN Au Foil Activation

	Configuration 1 0.48 - 1.92 Å		Configuration 2 1.68 - 3.12 Å		Configuration 3 2.88 - 4.32 Å		Configuration 4 4.08 - 5.52 Å		Configuration 5 5.28 - 6.72 Å	
	Total Activity (nCi)	% Difference with Measured	Total Activity (nCi)	% Difference with Measured	Total Activity (nCi)	% Difference with Measured	Total Activity (nCi)	% Difference with Measured	Total Activity (nCi)	% Difference with Measured
Measured by Gamma Spec	37.0	-	29.2	-	19.0	-	72.7	-	34.5	-
Calculated by SAC with CINDER 90 Cross Sections	68.1	84.1	49.4	69.2	29.7	56.3	67.9	-6.6	27	-21.7
Calculated by SAC with CINDER 08 Cross Sections	67.8	83.2	49	67.8	29.5	55.3	60.9	-16.2	43.6	26.4
Calculated by SAPEU using Gallmeier [9] simulated flux spectrum with CINDER 90 Cross Sections	55.9	51.1	33.1	13.4	16.0	-15.8	28.4	-60.9	13.4	-61.2
Calculated by SAPEU using Gallmeier [9] simulated flux spectrum with CINDER 08 Cross Sections	55.7	50.5	32.9	12.7	15.9	-16.3	25.7	-64.6	21.7	-37.1
Calculated by SAPEU using Iverson [12] measured flux spectrum with CINDER 90 Cross Sections	36.1	-2.5	19.8	-32.2	9.84	-48.2	-	-	-	-
Calculated by SAPEU using Iverson [12] measured flux spectrum with CINDER 08 Cross Sections	35.9	-2.9	19.7	-32.7	9.76	-48.6	-	-	-	-

Note: $\text{Percent Difference} = \frac{Calculated - Measured}{Measured} \times 100$

For configurations one through three in Table 4, the use of the Gallmeier simulated flux spectrum with either the CINDER 90 or 08_flat-weighted cross section libraries yields considerable improvements in the prediction of the sample activities. However, the sample activities calculated for configurations four and five in Table 4 using the Gallmeier simulated neutron flux with either the CINDER 90 or 08_flat-weighted cross section libraries were not as accurate as those for configurations one through three.

The gold foil measurements made on both the EQ-SANS and VULCAN instruments yielded significant differences in the calculated and measured activities for well-defined test irradiation conditions. The SAC tool using a normalized neutron flux spectrum occurring at the exit of the neutron guide, which is some distance away from the irradiated sample position, caused the discrepancies observed in relation to the EQ-SANS instrument. While the beam divergence at this location is quite small (a few degrees), such divergence over the four-meter distance to the sample position resulted in an (order of magnitude) over-estimate of the spectral intensity at the sample location.

4.3 HYPOTHESIS OF SYSTEMATIC ERROR IN SAC

The EQ-SANS and VULCAN instruments provide a well-isolated system with low background radiation for these activation measurements. Fig. 4 & 4 show that the difference between the measured and calculated sample activities is linear with the center wavelength of the irradiation wavelength band. The sample activities used for the comparison to the measured sample activities in Fig. 4 and 4 are calculated with the Gallmeier simulated neutron flux spectra for EQ-SANS and VULCAN using either the CINDER 90 or 08_flat-weighted cross section libraries. Based on the linear relationship observed in both libraries and neutron flux spectra, it may be assumed that there is a wavelength-dependent systematic error in how SAC uses the cross section data in calculating of the sample activities. The details of the linear fit parameters are shown in Table 6 & 6. The X-Intercepts in Table 6 & 6 are the nominal wavelengths where SAC most accurately calculates the sample activation when compared to the measured values.

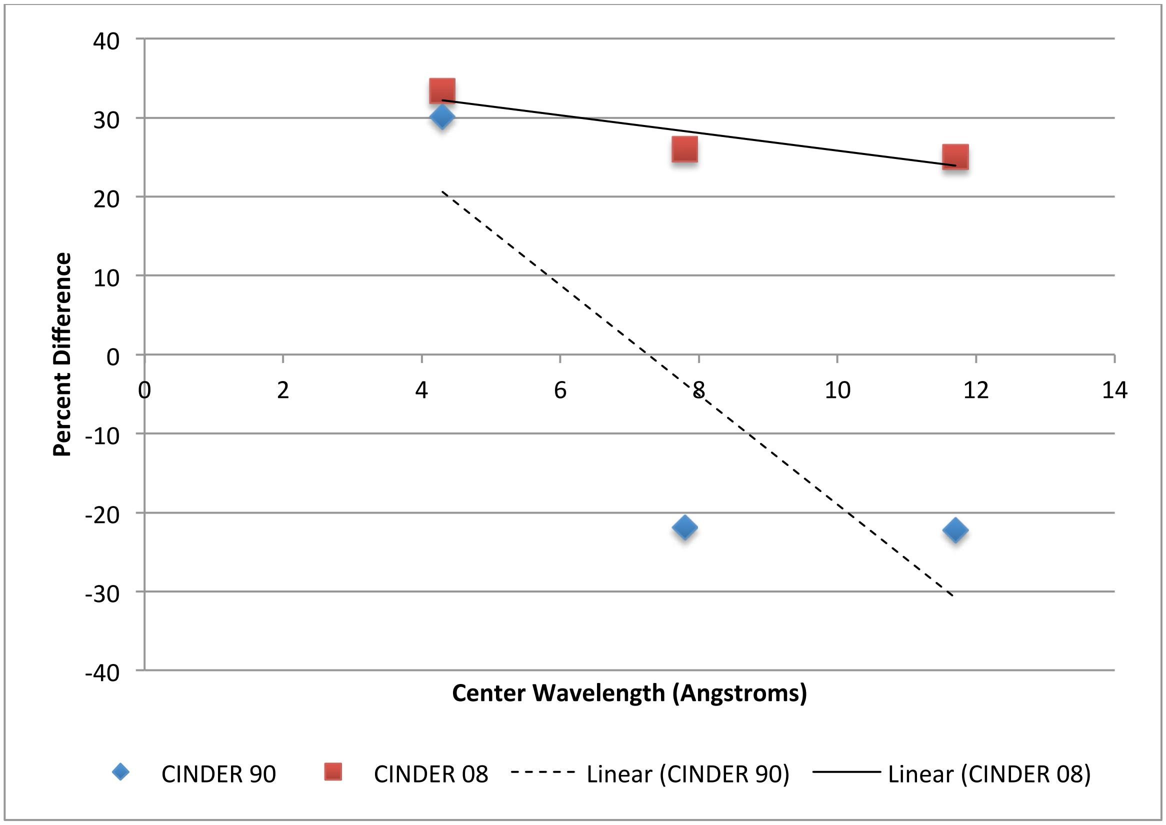


Fig. 3. **EQSANS sample activation (calculated with Gallmeier [10] simulated neutron flux spectrum for 100 percent para H) percent differences relative to the measured values.**

Table 5 Fig. 3 (EQ-SANS) Linear Fit Parameters

	R^2 -	Slope (% $Å^{-1}$)	Slope Abs. Error (% $Å^{-1}$)	X-Intercept (Å)	X-Int. Abs. Error (Å)
CINDER 90	0.73	-7	4	7	7
CINDER 08	0.81	-1.1	0.5	33	16

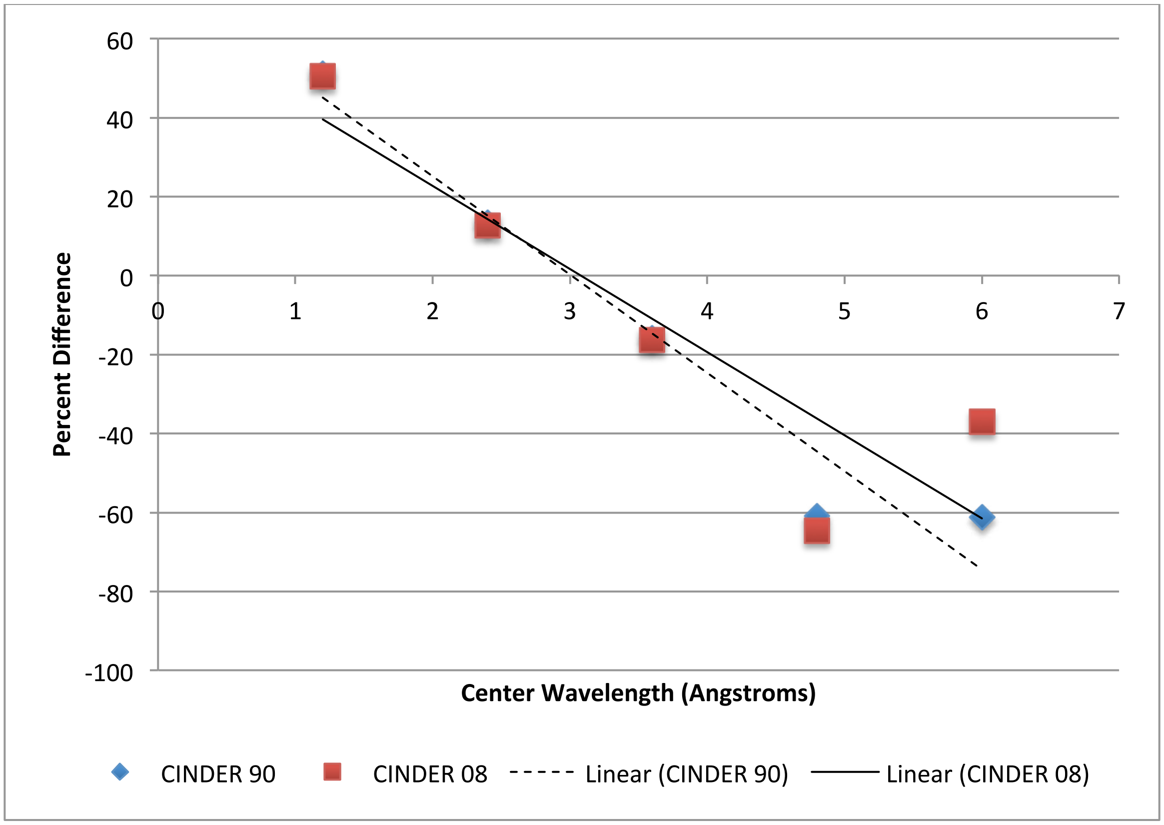


Fig. 4. **Difference of the calculated VULCAN sample activities (using the Gallmeier-simulated neutron flux spectrum [9]) to the measured values.**

Table 6 Fig. 4 (VULCAN) Linear Fit Parameters

	R^2 -	Slope (% Å^{-1})	Slope Abs. Error (% Å^{-1})	X-Intercept (Å)	X-Int. Abs. Error (Å)
CINDER 90	0.95	-25	3	3	1
CINDER 08	0.80	-21	6	3	1

For comparison, the same method of studying the systematic error that was employed using the Gallmeier simulated neutron flux spectra (Tables 5 & 6, Figs. 3 & 4) are now performed with the Iverson measured flux spectra (Tables 7 & 8, Figs. 5 & 6).

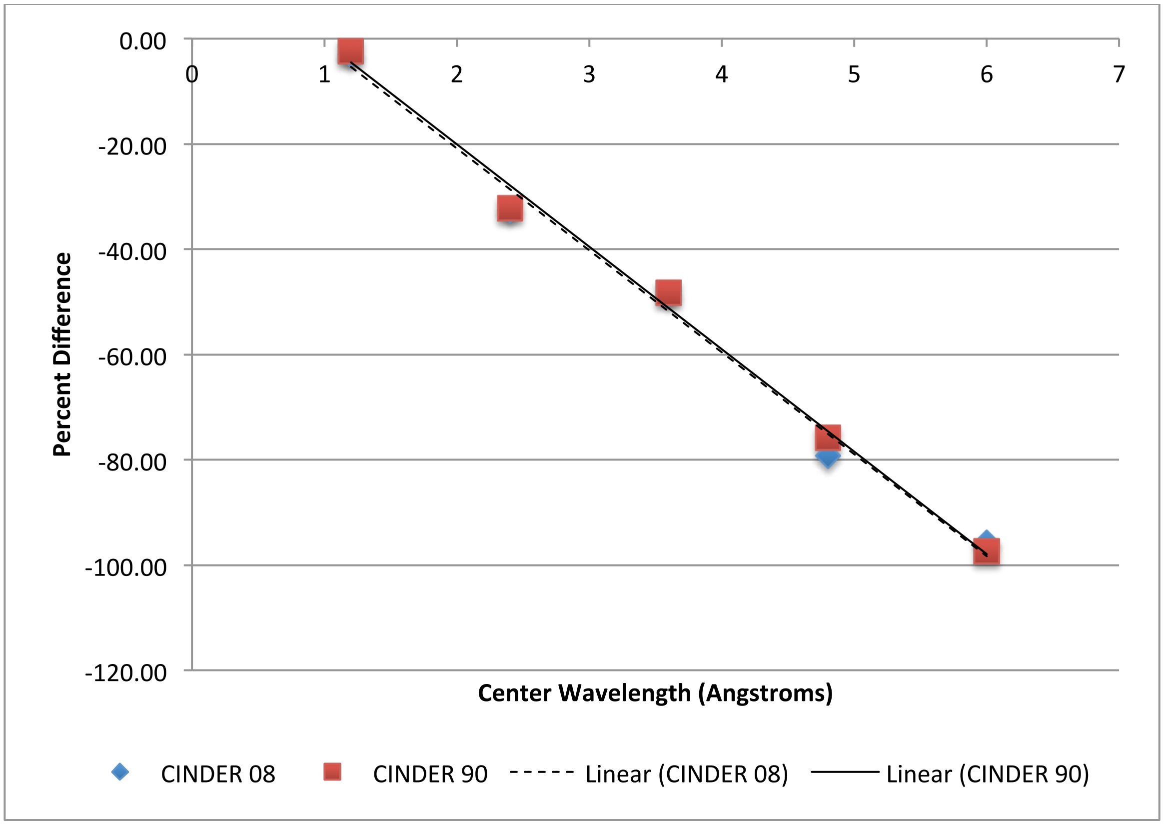


Fig. 5. **VULCAN sample activation (calculated with the Iverson [12] measured neutron flux spectrum) percent differences relative to the measured values.**

Table 7 Fig. 5 (VULCAN) Linear Fit Parameters

	R^2 -	Slope (% Å^{-1})	Slope Abs. Error (% Å^{-1})	X-Intercept (Å)	X-Int. Abs. Error (Å)
CINDER 90	0.99	-19	1	1.0	0.2
CINDER 08	0.99	-19	1	0.9	0.2

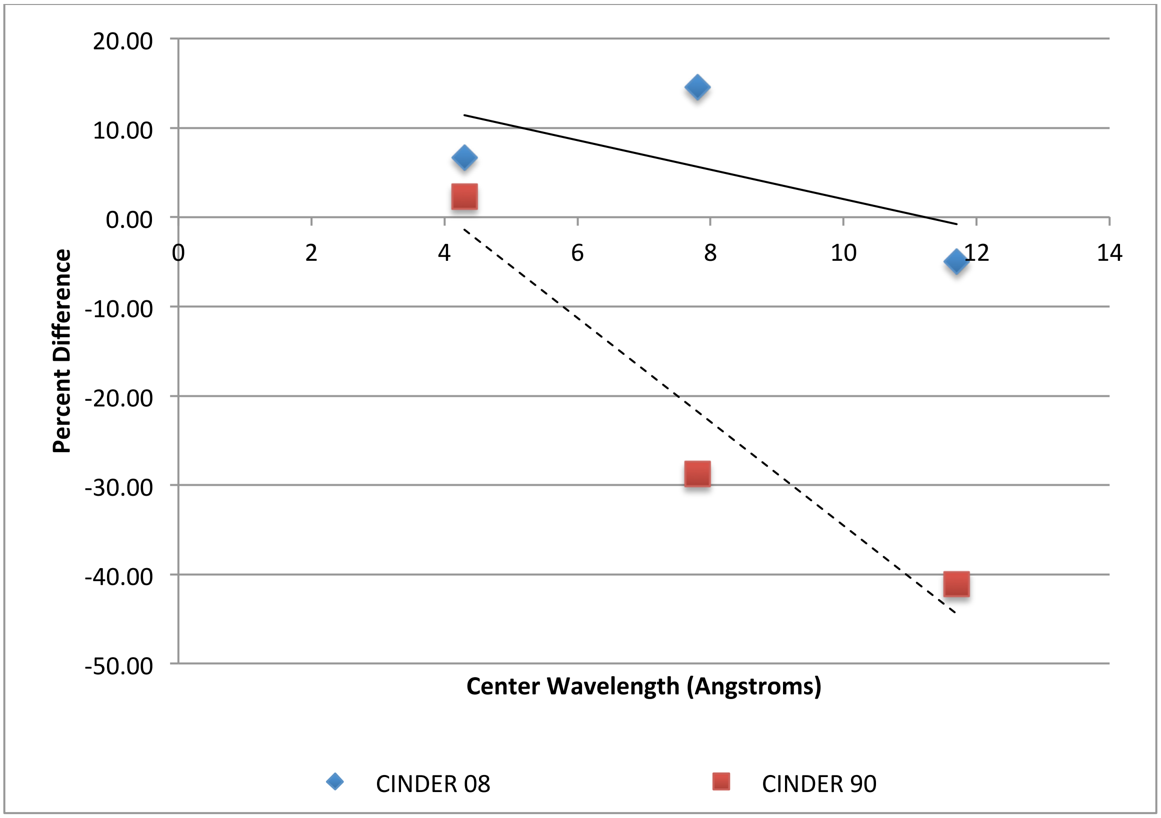


Fig. 6. EQSANS sample activation (calculated with the Iverson [11] neutron flux spectrum) percent differences relative to the measured values.

Table 8 Fig. 6 EQ-SANS Linear Fit Parameters

	R^2 -	Slope (% $Å^{-1}$)	Slope Abs. Error (% $Å^{-1}$)	X-Intercept (Å)	X-Int. Abs. Error (Å)
CINDER 90	0.93	-6	2	4	3
CINDER 08	0.38	-2	2	11	18

We hypothesize that the systematic error is caused by SAC's use of a cross section library with a limited number of energy groups below 1 eV. To explore this systematic effect, one could modify SAC to use a cross section library with a much finer energy group structure below 1 eV, and analyze how SAC predicts the sample activity with a variety of weighted cross section libraries. We hypothesize that the systematic effect at low energies (long wavelengths) is stemming from the discrete nature of the cross section representation and causes the discrepancies to quickly worsen as the irradiation energy bandwidth approaches the energy bin width of the cross section library.

4.4 GOLD FOIL IMAGE PLATE AUTORADIOGRAPHY ANALYSIS

Image plate autoradiography measurements were taken for each of the irradiated gold foils in both EQ-SANS and VULCAN instruments. The measurements of the irradiated gold foils for the EQ-SANS instrument show a slight gradient of ~ 25% in the neutron flux distribution for each of the neutron wavelength bands measured as seen in Fig. 7-9. The images in Fig. 7-9 were rotated to keep the foil orientation consistent, because the initial orientation of the foils was not tracked. The plot on the right in Fig. 7-9 shows the beam profile across the centerline of the beam spot.

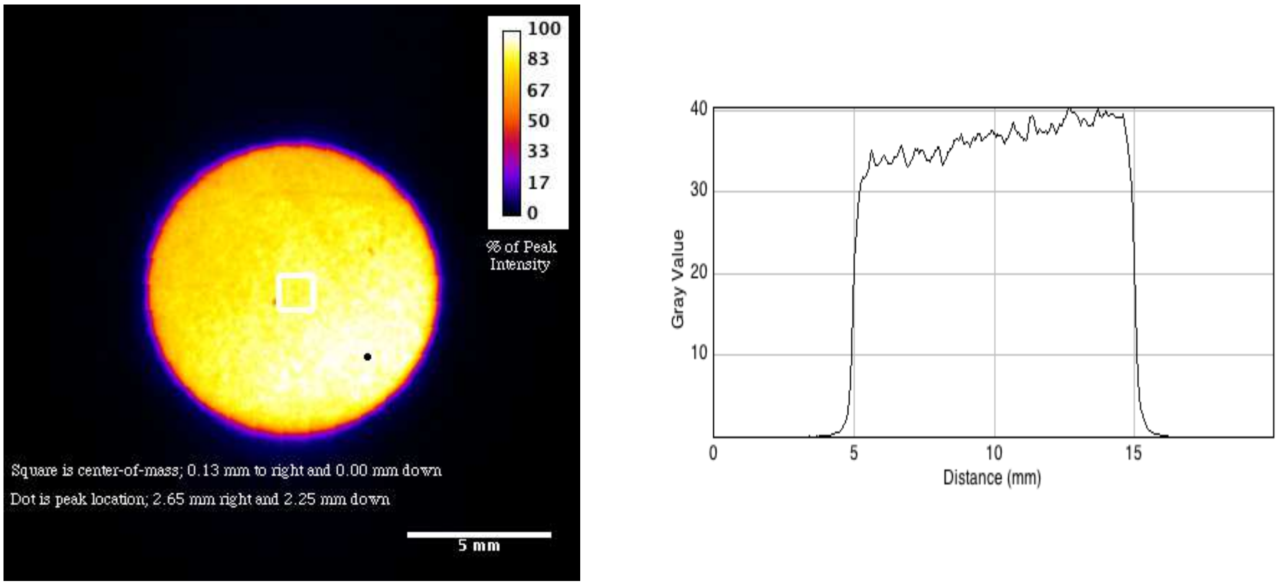


Fig. 7. EQ-SANS Beam spot for Configuration 1

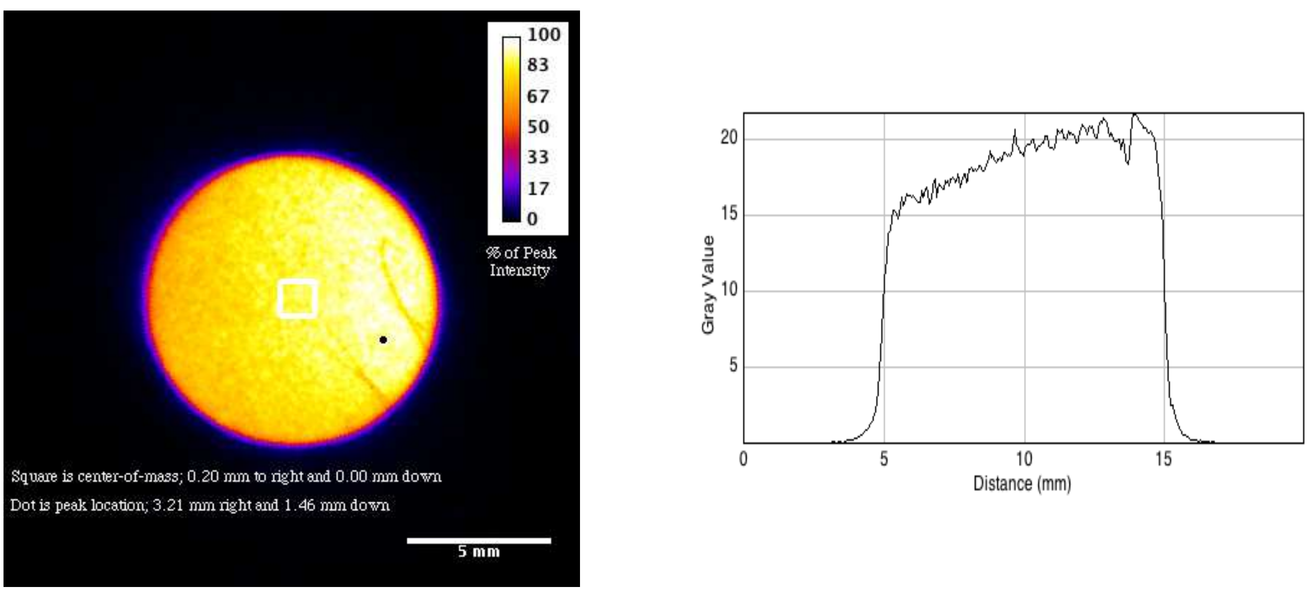


Fig. 8. EQ-SANS Beamspot for Configuration 2

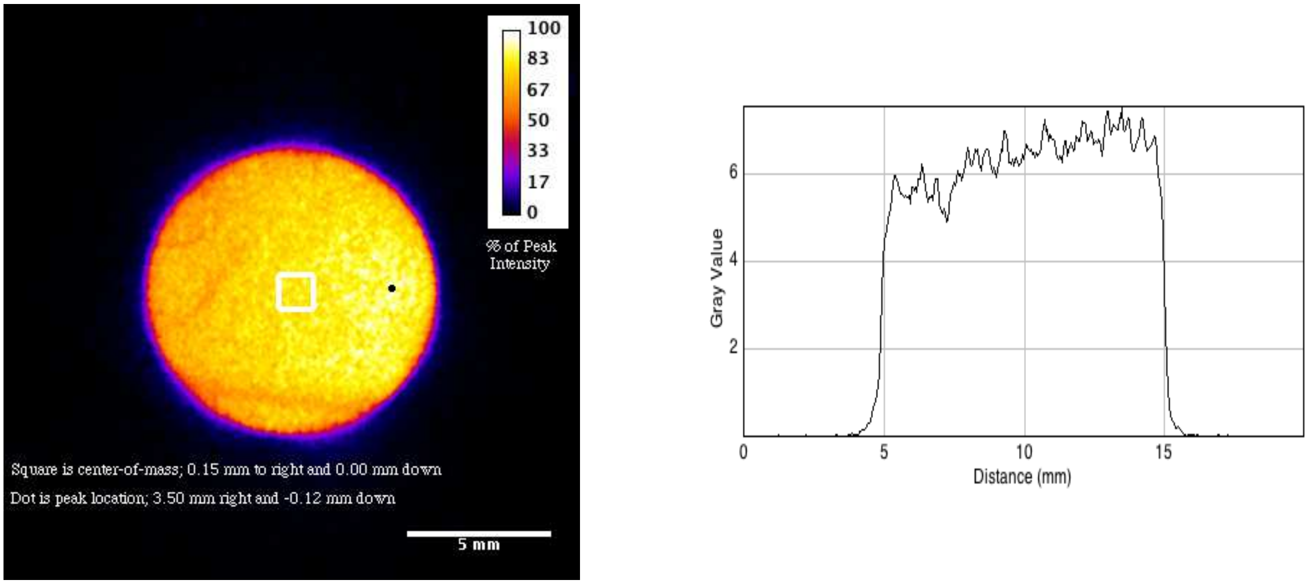


Fig. 9. EQ-SANS Beamspot for Configuration 3

In Fig. 7-9, the black dot on the beam spot represents the relative peak neutron flux. The position of the peak in each figure suggests that the EQ-SANS sample aperture may be off beam center, but there has not been enough analysis to strongly confirm this notion. Further analysis and testing will be done later.

The next instrument inspected was VULCAN. After performing image plate autoradiography on the irradiated gold foils, we found that two of the five image plate measurements showed the peak of the neutron flux distribution to be slightly (a few millimeters) off center, which can be seen in Fig. 10 & 11. Fig. 10 & 11 show the measured beam spot for the lowest wavelength bands used in the irradiation of the gold foils. The non-symmetrical distribution of neutron flux across the beamspot, shown in Fig. 10 &11, only occurred in the shortest wavelength bands. We suspect that the 42-meter-long neutron beam transported through curved, straight, and tapered guide section along with neutron mirrors of varying quality cause a biasing of the neutrons in these extreme wavelength bands and an off-center peak of the neutron flux distribution. Fig. 12-14 show an approximately normal distribution of the neutron flux across the beamspot for the higher irradiation wavelength bands with the peak of the neutron flux in approximately the center of the beamspot. The plot on the right in Fig. 10-14 shows the beam profile across the centerline of the beamspot.

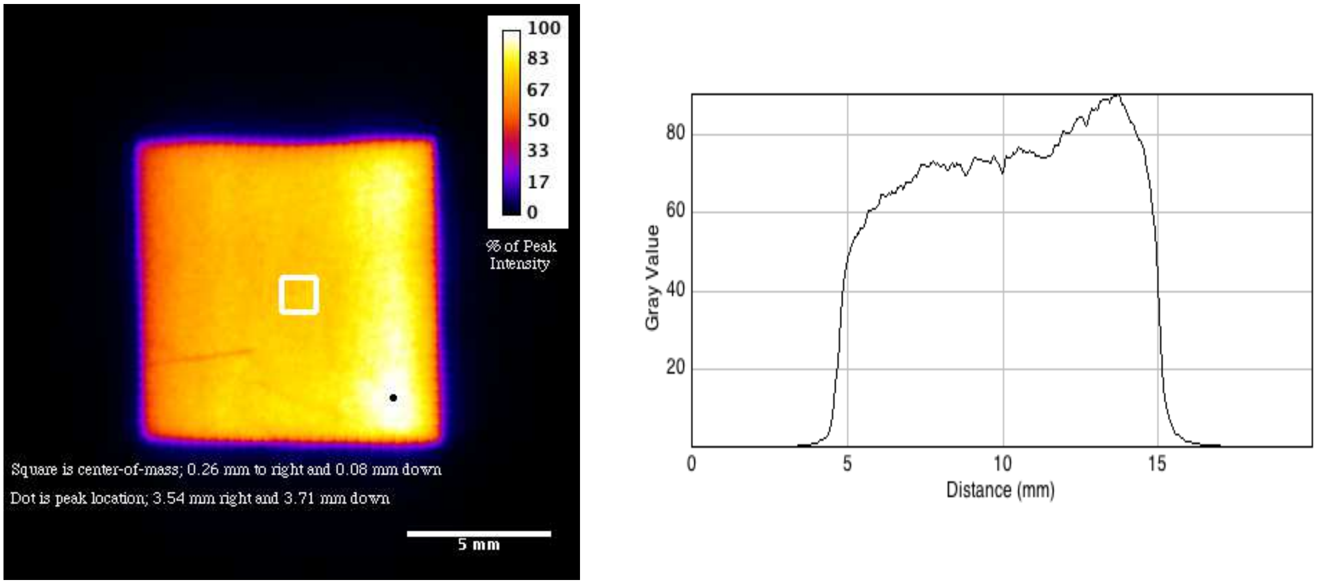


Fig. 10. VULCAN Beamspot for Configuration 1

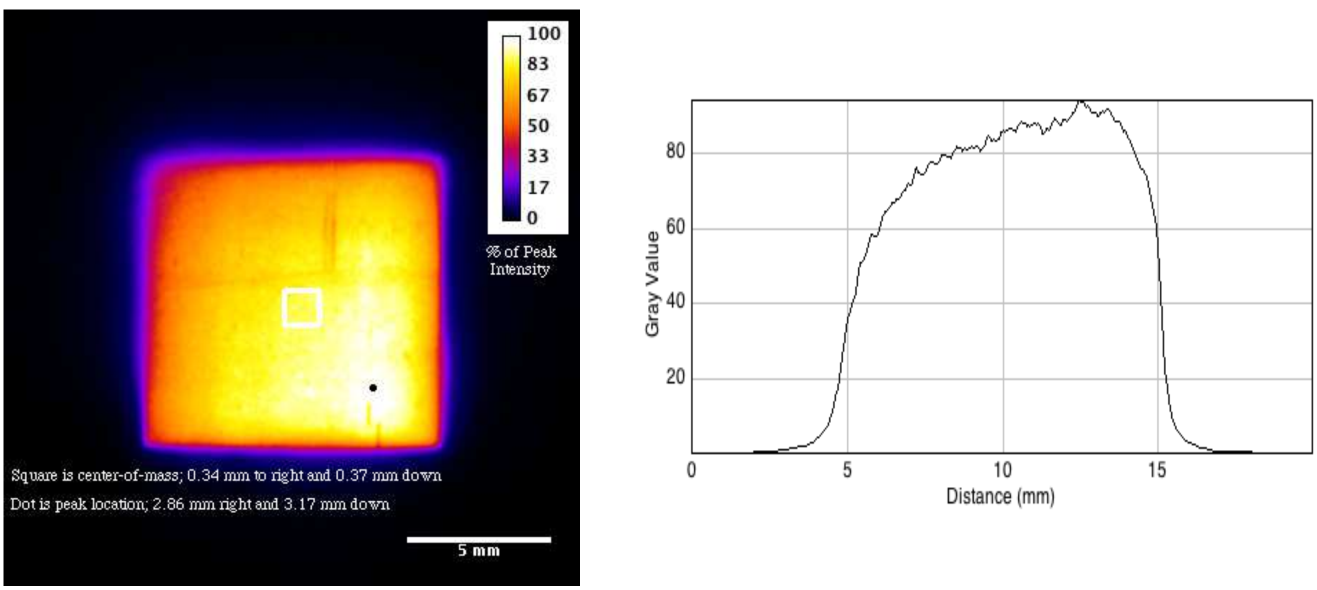


Fig. 11. VULCAN Beamspot for Configuration 2

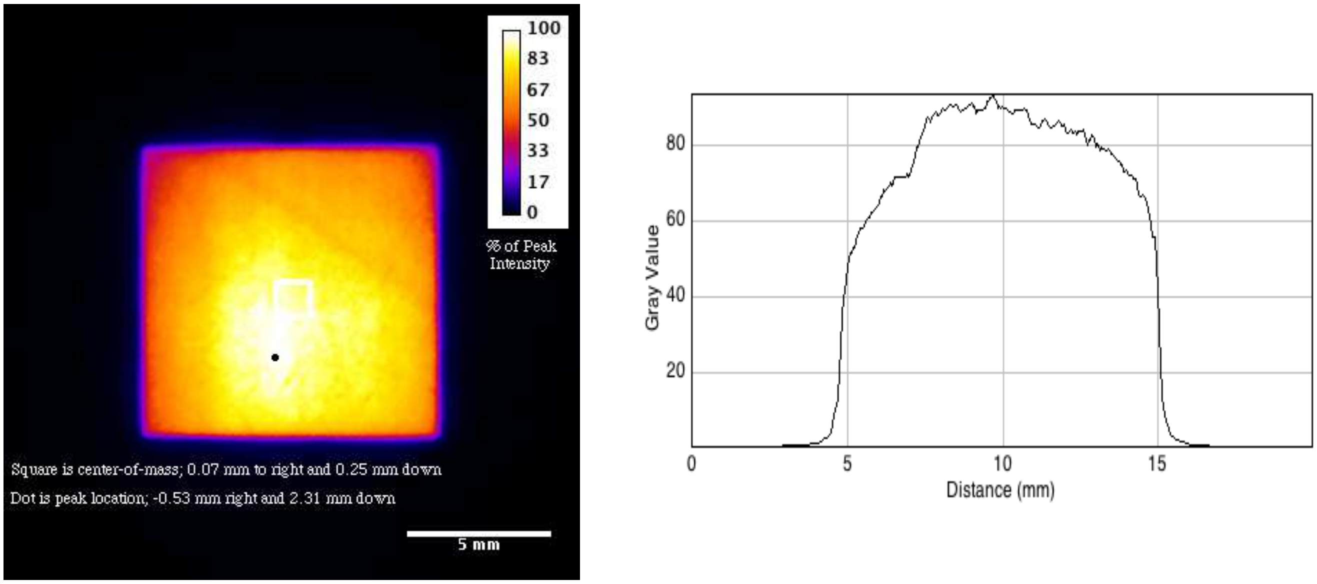


Fig. 12. VULCAN Beamspot for Configuration 3

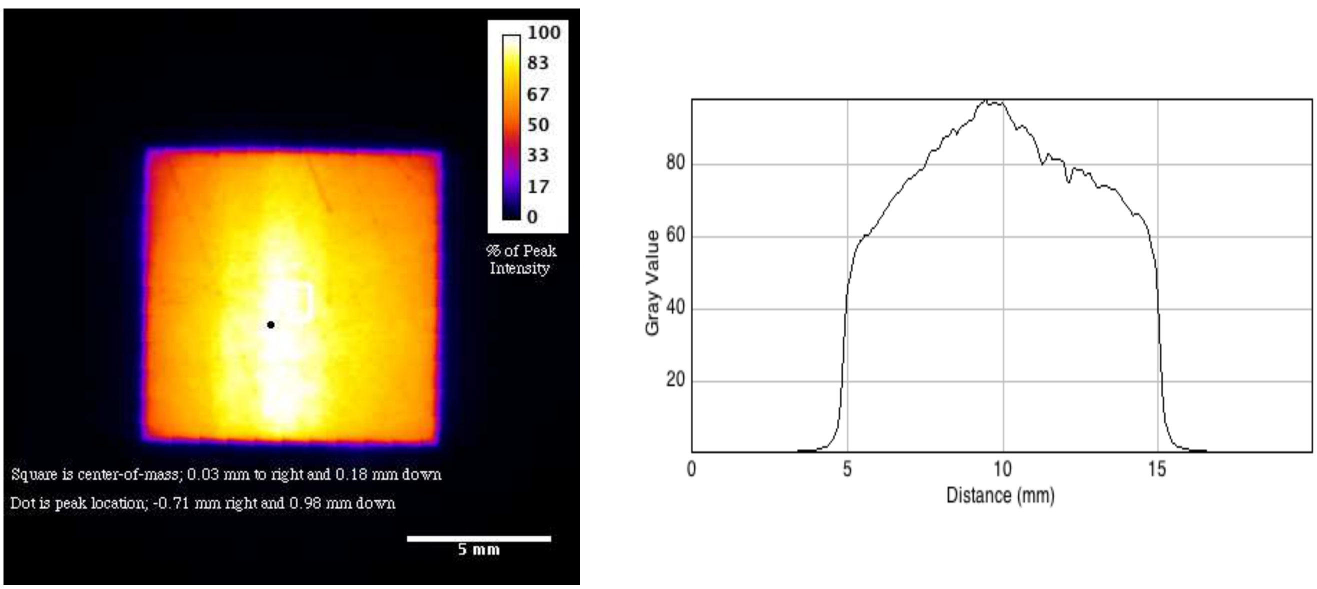
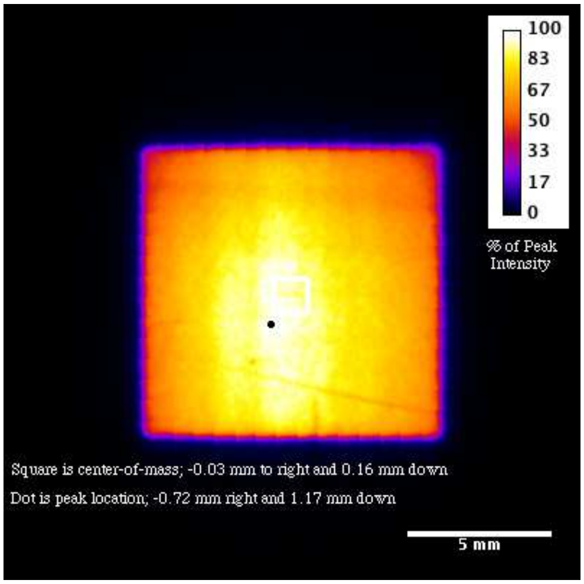


Fig. 13. VULCAN Beamspot for Configuration 4



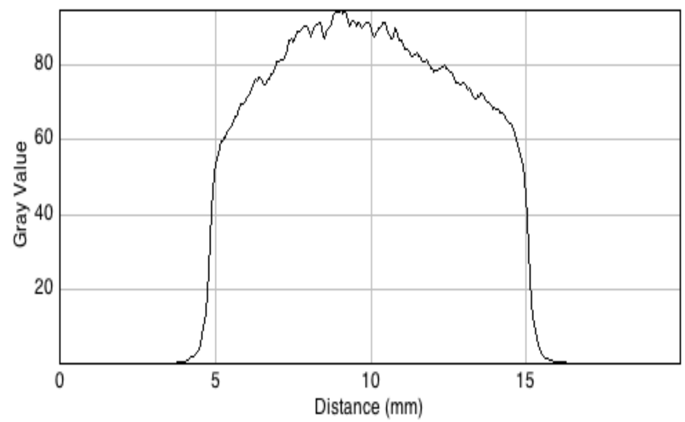


Fig. 14. VULCAN Beamspot for Configuration 5

4.5 MULTIPLE IRRADIATION BANDS ANALYSIS ON THE EQ-SANS INSTRUMENT

Typical operation of the EQ-SANS instrument, like most SNS instruments, will involve sequentially irradiating the same sample with neutrons from different wavelength bands. SAC does not support such an irradiation sequence. In SAC, the only way to mimic sequential irradiation with different wavelength bands is to assign each irradiation the same wavelength band. Furthermore, the separate sequential irradiations may in fact be at different power levels (because of SNS operations). SAC has no way to provide different power levels (or normalization factors) for the different sequential irradiations in a single SAC calculation. While for gold, with a half-life relatively long compared to typical EQ-SANS irradiation periods, this could be simulated by proportionally changing the irradiation duration. In this case, we performed separate SAC calculations and added the results to get the prediction shown as Total Activity 1 in Table 9. Total Activities 2-4 in Table 9 show the results approximated from arbitrarily choosing one of the wavelength bands to use for all three irradiation periods. The differences in the right-most column of Table 9 show that under its current configuration, SAC cannot calculate correctly for samples irradiated with multiple wavelength bands on the EQ-SANS instrument in one single run. There is an additional mode of operation for the EQ-SANS instrument called frame skipping that allows for operating two wavelength bands at the same time, and the current configuration of SAC does not either support this mode [4].

Table 9 EQ-SANS Multiple Irradiation Bands

Wavelength Bandwidth (Å)	Irradiation Time (m)	Calculated Activity (μCi)	% Difference with Total Activity 1
2.50-6.10	10	0.170	
6.00-9.60	60	0.240	
10.0-13.4	120	0.085	
	Total Activity 1	0.495	-
2.50-6.10	10	0.170	
2.50-6.10	60	1.00	
2.50-6.10	120	2.00	
	Total Activity 2	3.17	540
6.00-9.60	10	0.041	
6.00-9.60	60	0.240	
6.00-9.60	120	0.480	
	Total Activity 3	0.761	54
10.0-13.4	10	0.007	
10.0-13.4	60	0.043	
10.0-13.4	120	0.085	
	Total Activity 4	0.135	-73

5. SUMMARY

The measurements made on the EQ-SANS and VULCAN instruments yielded significant results to support some of the theories behind the discrepancies in the calculated and measured sample activities observed by the beamline scientists and users. Most of the discrepancies on the EQ-SANS instrument stemmed from the neutron flux spectrum used in the current configuration of SAC. It was observed that with a properly simulated neutron flux spectrum of the EQ-SANS instrument, SAC overestimates the sample activity within 30% of the measurement. The measurements on the VULCAN instrument yielded a similar conclusion as that for the EQ-SANS instrument. The implementation of a properly simulated neutron flux spectrum in the SAC yielded more accurate results for the shorter wavelength bands than those for the longer wavelength bands. This anomaly lead to the hypothesis that there could be systematic error in the generation and SAC’s use of the cross section library based on the linearity of the differences between the calculated and measured sample activities using both the simulated and measured neutron flux spectra. Further investigation of the systematic error in SAC will be performed later. Image plate autoradiographies of the EQ-SANS beam spot suggest that the sample apertures may need to be moved to coincide with the beam intensity center. The image plate autoradiography of the VULCAN beam spot found discrepancies on the order of 20% of the distribution of neutron flux across the beam spot. Finally, it was determined that the current configuration of the SAC tool does not properly calculate the activity of samples irradiated with multiple wavelength band passes.

6. REFERENCES

[1] T. E. Mason, D. Abernathy, I. Anderson, J. Ankner, T. Egami, G. Ehlers*, et al.*, "The Spallation Neutron Source in Oak Ridge: A powerful tool for materials research," *Physica B: Condensed Matter,* vol. 385–386, Part 2, pp. 955-960, 11/15/ 2006.

[2] R. D. Cheverton and T. M. Sims, "HFIR Core Nuclear Design," ORNL, HFIR, ReportJuly 1971.

[3] W. Lu, P. D. Ferguson, F. X. Gallmeier, E. B. Iverson, I. I. Popova, and Y. Wang, "A Sample Activation Program for Neutron-Scattering Experiments," *Nuclear Technology,* vol. 168, pp. 970-976, 2009.

[4] J. K. Zhao, C. Y. Gao, and D. Liu, "The extended Q-range small-angle neutron scattering diffractometer at the SNS," *Journal of Applied Crystallography,* vol. 43, pp. 1068-1077, Oct. 2010.

[5] X. L. Wang, "Conceptual Design of the VULCAN Diffractometer," Oak Ridge National Laboratory IS-1.7.9-6055-RE-A-00, 2000.

[6] P. D. Ferguson, "CINDER'90 for SNS activation studies," Oak Ridge National Laboratory SNS-106100200-TR0142-R00, March 2006 2006.

[7] E. B. Iverson and C. Geoghegan, "Diagnostic Use of Neutron-Sensitive Image Plates at ORNL Neutron Facilities," in *AccApp'11*, Knoxville, TN USA, 2011.

[8] K. Lefmann and K. Nielsen, "McStas, A General Software Package for Neutron Ray-tracing Simulations," *Neutron News,* vol. 10, p. 20, 1999.

[9] A. C. Hamilton and F. X. Gallmeier, "A Suite of SNS Neutron Instrument Models," in *Tenth International Topical Meeting on Nuclear Applications of Accelerators*, Knoxville, TN, 2011.

[10] F. X. Gallmeier, "McStas Fluxes for Selected Instruments," T. C. McClanahan, Ed., Email containing an Excel file that has a lot of the flux spectra for the SAC comparison ed. Oak Ridge National Laboratory, 2014.

[11] E. B. Iverson, "Flux Measurements on SNS BL06 EQ-SANS," Oak Ridge National Laboratory SNS-106100200-TR0205-R00, Jan. 2014.

[12] E. B. Iverson, A. D. Stoica, and W. Lu, "Intensity Gain from VULCAN Guide 9," Oak Ridge National Laboratory SNS-106100200-TR202-R00, Oct. 2013.