

## **SURROGATE ANALYSIS AND INDEX DEVELOPER (SAID) TOOL AND REAL-TIME DATA DISSEMINATION UTILITIES**

**Marian Domanski, Hydrologist, USGS, [mdomanski@usgs.gov](mailto:mdomanski@usgs.gov), 217-328-9758**  
**Timothy Straub, Hydrologist, USGS, [tdstraub@usgs.gov](mailto:tdstraub@usgs.gov), 217-621-9587**  
**Molly Wood, Hydrologist, USGS, [mwood@usgs.gov](mailto:mwood@usgs.gov), 208-387-1320**  
**Mark Landers, Hydrologist, USGS, [landers@usgs.gov](mailto:landers@usgs.gov), 678-924-6616**  
**Gary Wall, Hydrologist, USGS, [grwall@usgs.gov](mailto:grwall@usgs.gov), 518-285-5621**  
**Steven Brady, Computer Scientist, USGS, [sbrady@usgs.gov](mailto:sbrady@usgs.gov), 785-832-3518**

**Abstract:** The use of acoustic and other parameters as surrogates for suspended-sediment concentrations (SSC) in rivers has been successful in multiple applications across the Nation. Critical to advancing the operational use of surrogates are tools to process and evaluate the data along with the subsequent development of regression models from which real-time sediment concentrations can be made available to the public. Recent developments in both areas are having an immediate impact on surrogate research, and on surrogate monitoring sites currently in operation.

The Surrogate Analysis and Index Developer (SAID) standalone tool, under development by the U.S. Geological Survey (USGS), assists in the creation of regression models that relate response and explanatory variables by providing visual and quantitative diagnostics to the user. SAID also processes acoustic parameters to be used as explanatory variables for suspended-sediment concentrations. The sediment acoustic method utilizes acoustic parameters from fixed-mount stationary equipment. The background theory and method used by the tool have been described in recent publications, and the tool also serves to support sediment-acoustic-index methods being drafted by the multi-agency Sediment Acoustic Leadership Team (SALT), and other surrogate guidelines like USGS Techniques and Methods 3-C4 for turbidity and SSC.

The regression models in SAID can be used in utilities that have been developed to work with the USGS National Water Information System (NWIS) and for the USGS National Real-Time Water Quality (NRTWQ) Web site. The real-time dissemination of predicted SSC and prediction intervals for each time step has substantial potential to improve understanding of sediment-related water-quality and associated engineering and ecological management decisions.

### **INTRODUCTION**

Streamflow, sediment, and water-quality data are needed to establish baseline information for water-resource managers to evaluate historical and current conditions and plan management alternatives. Real-time, continuous SSC data can be useful for monitoring river response downstream of areas affected by recent wildfires, construction or remediation activities, levee failures, or changing land uses. Additionally, real-time data can provide an early warning for operators of municipal water supply and hydroelectric facilities concerned with avoiding damage to infrastructure from sediment. Surrogates are becoming widely used to better understand physical and chemical processes in natural systems (Rasmussen and others, 2009). Acoustic technology is becoming increasingly used for velocity measurements and is also being used as a surrogate for sediment concentrations.

The Surrogate Analysis and Index Developer (SAID) tool is a standalone tool to assist in the development of ordinary least squares (OLS) regression models that relate response and predictor variables (Helsel and Hirsch, 2002) by providing visual and quantitative diagnostics to the user (figure 1). The tool is written in the Matlab® programming language. There is no limit on the number of explanatory variables to be used in the linear model and no requirement of which explanatory variables to use. SAID is under beta development and is not yet formally released as a USGS software product.

SAID has applications for relating surrogate-technology parameters such as turbidity, acoustics, and others. SAID can be used for processing acoustic parameters to be used as predictor variables for suspended-sediment concentrations (SSC). The sediment-acoustic method, which assumes a constant spatial suspended-sediment concentration and grain size distribution with respect to range along the acoustic axis of the beam, utilizes acoustic data from fixed-mount stationary acoustic Doppler velocity meters (ADVM). Some of the earliest USGS applications and research were done by Topping and others (2004, 2006, 2007), Wright and others (2010), Landers

(2012), and Wood and Teasdale (2013). The sediment-acoustic method, as described in these references, is used in SAID to compute the sediment attenuation coefficient and sediment corrected backscatter from ADVN acoustic parameters. SAID allows for quick adjustment of complex ADVN data-processing options, changes in the variables used in the regression, and evaluation of the created model. The tool also enables the user to transform loaded variables, build linear regression models, view linear model diagnostic statistics and plots, export the model information, and generate a predicted time series.

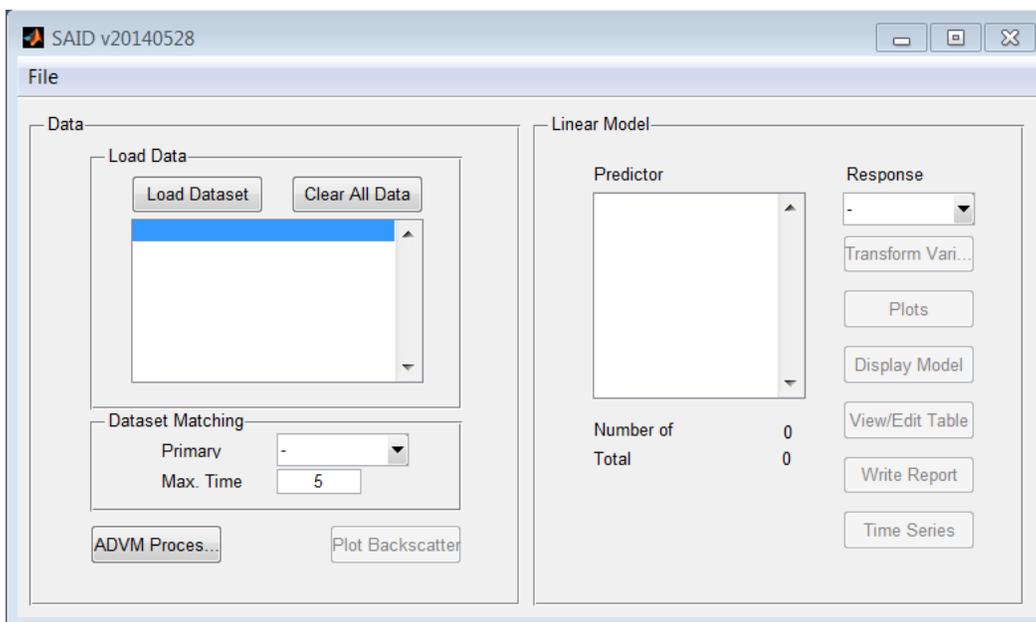


Figure 1 Main SAID window for beta version 20140528

This paper provides an overview on processing and loading data into SAID for developing regression models among surrogate data and measured constituents. In addition, this paper discusses the ADVN configuration parameters that are used in the calculation of acoustic surrogate parameters. Lastly, the paper gives an overview of how the regression models developed in SAID can be used in utilities that have been developed to disseminate predicted SSC in real-time.

## SURROGATE ANALYSIS AND INDEX DEVELOPMENT

In the development of linear regression models, explanatory and response variables must be selected. These variables are contained in time series dataset files stored on disk. Because surrogate observations are continuous, and constituent observations occur at irregular time intervals, it is typical to store surrogate and constituent time series in separate dataset files. In order to choose observation sets of variables to develop a linear regression model, observations from the surrogate and constituent time series must be matched. Once a linear regression model is created from a set of matched observations, it must be evaluated for validity and appropriateness. SAID provides the ability to load and match datasets, select the response and predictor variables, and evaluate the created linear regression model. An overview of the dataset workflow is briefly described below and the following sections describe the process to develop regression models in more detail.

- **Loading datasets**
  - Data that are stored on disk in ASCII files are loaded into memory by SAID.
- **Choose primary datasets**
  - A dataset is selected that serves as the primary time series to synchronize observations. The selected dataset is known as the primary dataset and other loaded datasets become secondary datasets.
  - Adjusting the maximum time difference value (Max. Time) changes the upper limit of the time difference to which observations are synchronized.

- **Choose linear model variables**
  - Available variables will be displayed in the Predictor Variables list box and the Response Variable drop-down list. SAID creates a linear model after a valid set of predictor and response variables are selected.
- **Evaluate linear model**
  - SAID provides several diagnostic plots to determine if the created linear model created fits the assumptions of the OLS method.

**Datasets:** SAID is capable of loading two types of data. The term “loaded datasets” refers to datasets that have been loaded from disk. The data can be stored as tab delimited ASCII files or a collection of Argonaut ASCII files. Loaded datasets are not necessarily stored in separate files because of a constituent/surrogate relationship. Having dissimilar time steps is a typical reason for storing and loading datasets separately.

Variables with names that match the patterns CellXXAmpY and CellXXSNRY (where XX is the cell number, from 00 to 99, and Y the beam number, either 1 or 2) are dedicated variables for backscatter counts (Amp) and signal-to-noise ratio (SNR) and are used in the computation of the sediment attenuation coefficient and mean sediment corrected backscatter. These variables are not available for use in the creation of a linear model but are necessary in the computation of the ADVN acoustic surrogate metrics.

Variables named ADVNTemp and Vbeam also are dedicated variables used for the temperature and water depth. The temperature must be in units of degrees Celsius and is directly used in computing the ADVN parameters and is therefore necessary. The water depth is used to determine if the cell is out of water when the vertical orientation is selected in the ADVN Processing dialog box. A minimum Vbeam value also is set by the user in order to exclude samples taken when the water is below a certain depth.

During the time a dataset is being loaded, the program checks for variable names that are already loaded. If a variable that is in the dataset that is to be loaded exists in an already loaded dataset, then the selected dataset will not be loaded. Once the datasets are loaded, the data are then available for matching.

**Matching Time-Series Observations:** In order to build a linear model, it is necessary that a dataset with observations of predictor (surrogate) and response (water-quality) variables exist. Matching occurs in order to synchronize observations from the loaded datasets. The result of matching is the creation of a single dataset containing the matched data, which is then used to develop the linear model.

The primary dataset is the loaded dataset that contains the observations whose date and time of observation form the basis for matching in the secondary datasets. In a typical application for SAID, the primary dataset is the dataset that contains the constituent observations. The primary dataset is chosen by selecting it from the Primary Dataset drop-down list (figure 1). A linear model will not be created until a primary dataset is selected.

Secondary datasets are loaded datasets that contain observations that are matched to primary dataset observations. The term secondary dataset refers to all of the datasets that are not the primary dataset. Observations from the secondary datasets are only copied to the synchronized dataset if they have a date-time that matches a primary dataset observation within the user specified time interval allowance (Max. Time).

Selecting a primary dataset initiates the matching algorithm. For each observation in the primary dataset, SAID calculates the minimum absolute time difference between the observation date and time variables and the date and time variables of the secondary dataset being compared. If the minimum absolute time difference is less than or equal to the user specified value for the maximum time difference, the observations from the secondary dataset being compared are matched with the observations of the primary dataset and the values are copied to the matched dataset. If the minimum absolute time difference is greater than the user specified maximum time difference (Max. Time), then the corresponding variables in the observation in the matched dataset are set to an invalid value. In other words, the observation in the primary dataset will not be matched to an observation in the dataset being compared.

After a primary dataset is selected, the program will indicate that it is matching datasets and will remain unresponsive until the matching is complete. The time it takes for the program to create a matched dataset depends on the number of loaded datasets and the number of observations in each dataset. When the program has completed the matching algorithm, the variables available for use in the linear model are shown in the Predictor Variables and Response Variable lists.

**Processing and Viewing Acoustic Backscatter Data (optional in SAID):** The following ADVM-related parameters are required by SAID before the acoustic backscatter data are processed and acoustic surrogate parameters are computed:

- ADVM Configuration - Frequency, Effective Transducer Diameter, Slant Angle, Blanking Distance, Cell Size, Number of Cells
- ADVM Processing - Intensity Scale Factor (if Amp is selected for Backscatter Values), Minimum Mid-Point Cell Distance, Maximum Mid-Point Cell Distance, Minimum Vbeam

The configuration parameters are taken from a configuration record file that is saved by the ADVM with each ADVM data file. Once the required parameters in the ADVM Processing window have valid values, the ADVM parameters with at least one valid observation will be available in the Predictor Variables list. By clicking on the ADVM Processing button (figure 1), the ADVM configuration and processing options used in the calculation of the ADVM parameters can be changed (figure 2). ADVM configurations needed for input to SAID can be found in the setup parameters section of the ADVM software.

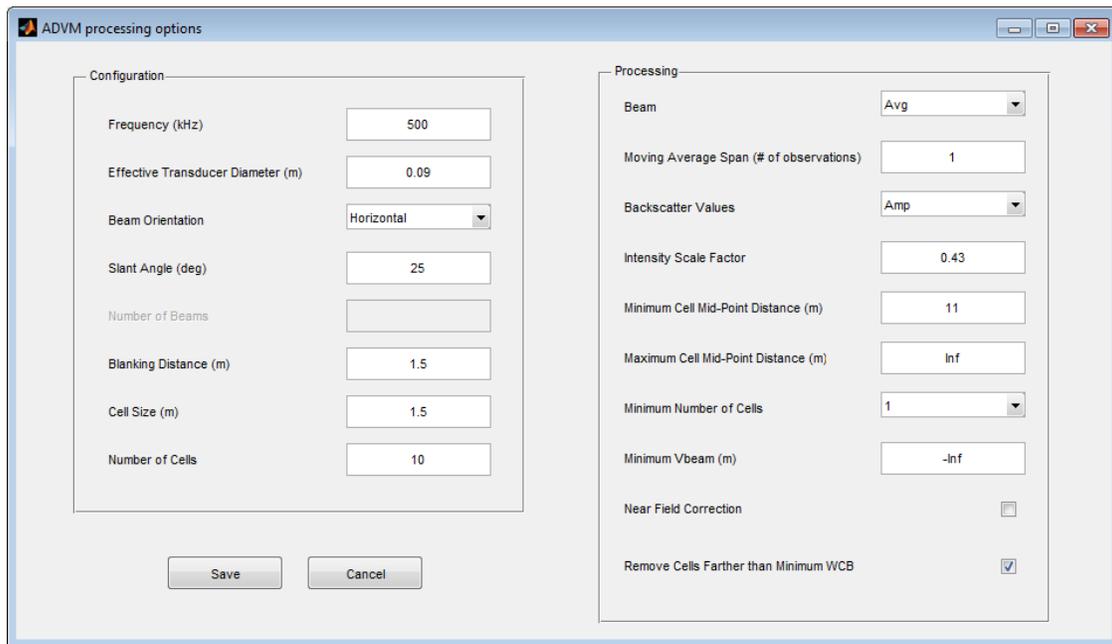


Figure 2 ADVM deployment configuration and acoustic parameter options window

**Configuration Parameters:** The following parameters indicate the ADVM type and setup and are necessary to compute the acoustic surrogate parameters (figure 2).

- **Frequency** – The frequency of the ADVM acoustic signal.
- **Effective Transducer Diameter** – The effective diameter in meters of the ADVM transducer. The effective transducer diameter is only used when the Near Field Correction option is selected in the Processing section.
- **Beam Orientation** – The orientation of the acoustic beams of the ADVM. If ‘Vertical’ is selected for this field, then the Vbeam for each observation is compared to the cell edges, and each cell that is out of water is marked as invalid.
- **Slant Angle** – The angle of the acoustic beam with respect to the vector that represents the cell distance from the instrument. This angle, along with the blanking distance, cell size, and number of cells, is used to find the mid-point distance of each cell along the acoustic beam.

- **Number of Beams** – The number of acoustic beams on the instrument. This value is not used. SAID assumes that the instrument has two beams.
- **Blanking Distance** – The distance in meters from the instrument to the beginning of the first cell. This value is used in the computation of the mid-point distance of each cell along the acoustic beam.
- **Cell Size** – The length of each cell in meters. This value is used in the computation of the mid-point distance along the acoustic beam of each cell.
- **Number of Cells** – The number of cells in the configuration of the ADVN under analysis. The number of cells directly affects the values displayed in the Minimum Number of Cells drop down list.

**Processing Parameters:** The following parameters control how ADVN backscatter data are screened and processed (figure 2).

- **Beam** – The beam number from which the backscatter values are taken. When ‘Avg’ is selected for this field, the average cell backscatter values are used.
- **Moving Average Span** – The span, in number of observations, used in a centered moving averaging of the backscatter time series. The span must be an odd positive integer.
- **Backscatter Values** – The backscatter values used in the computation of the ADVN parameters. When ‘Amp’ is selected, the backscatter values are multiplied by the value in the Intensity Scale Factor field. The Intensity Scale Factor field is made available only when ‘Amp’ is selected. (Caution: the model developed will be specifically for SNR or Amp units and cannot be switched without building a new model. All empirical testing for best model using SNR or Amp should be evaluated.)
- **Intensity Scale Factor** – The scaling factor to convert backscatter counts to decibels. This field is only available when ‘Amp’ is selected in the Backscatter Values drop-down list. The factor defaults to 0.43 (typical for SonTek® instruments); but should be taken from manufacturer literature for specific ADVNs.
- **Minimum Cell Mid-Point Distance** – The minimum distance in meters from the transducer that the mid-point of a cell has to be in order for it to be used in the computation of the ADVN parameters.
- **Maximum Cell Mid-Point Distance** – The maximum distance in meters from the transducer that the mid-point of a cell can be in order for it to be used in the computation of the ADVN parameters.
- **Minimum Number of Cells** – The required minimum number of valid cells that an ADVN sample has to have in order for its computed parameter to be included as an observation in the linear model.
- **Minimum Vbeam** – The minimum value for Vbeam that a sample must have in order for it to be used as an observation. Vbeam is the water height in meters that the ADVN reports.
- **Near Field Correction** – When the box is checked, a near field correction to the backscatter values is made (Downing and others, 1995). When the box is not checked, no near field correction is applied. In general, data from the near field should be avoided by setting the blanking distance and/or Minimum Cell Point distance greater than the near field for a given instrument.
- **Water Corrected Backscatter (WCB) Profile Adjustment** – When this box is checked, the range of cells that include and are beyond the cell with the minimum water corrected backscatter (minWCB) are not included in the calculation, unless the cell with the minWCB is the last or first cell in the range considered.
  - If the cell with the minWCB is the last cell, the value is retained and all cells are used to calculate the sediment corrected backscatter and attenuation coefficient.
  - If the cell with the minWCB is the first cell, all other cells are not considered, and the water corrected backscatter value in the first cell is used as the sediment corrected backscatter value for the observation, and no attenuation coefficient is calculated.

**Viewing acoustic backscatter profiles:** When a valid response variable is matched with valid predictor variables, the Plot Backscatter button will be made available. When this button is clicked, a window with three sets of axes is displayed. From the top, the axes show Sediment Corrected Backscatter (SCB), Water Corrected Backscatter (WCB), and Measured Backscatter (MB), all in decibels, versus the cell mid-point distance along the acoustic beam (figure 3). Also shown in the window is a list of observation numbers and times from the model. The observation times are taken from the primary dataset. Only the backscatter samples that correspond to observations in the linear model are shown. Selecting sample times in the list displays the plots of the backscatter values on the axes. Multiple observations can be selected and plotted.

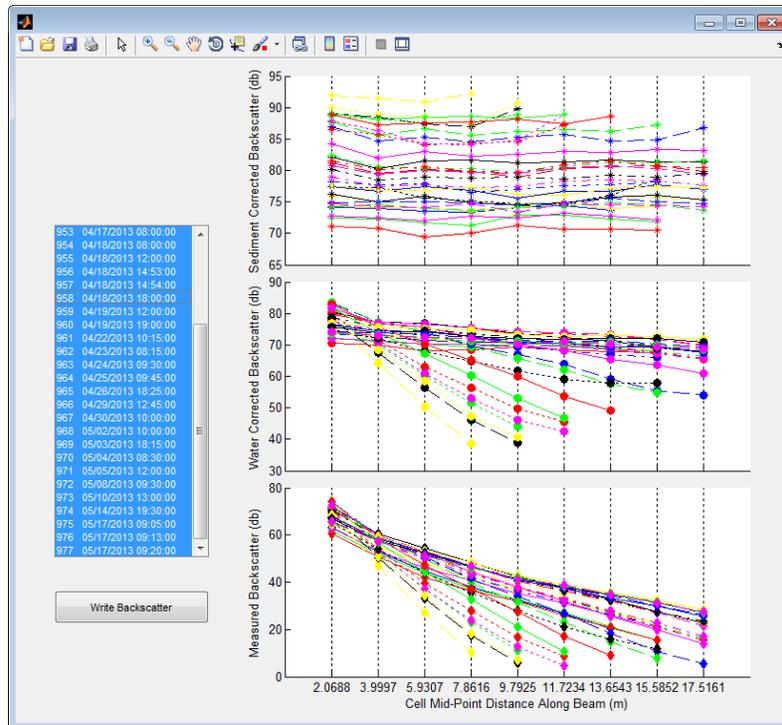


Figure 3 Backscatter profile plotting window

**Development of Linear Regression Models:** The available variables for use in the development of linear regression models in SAID appear in the Predictor Variable list and Response Variable in the Linear Model screen (Figure 4). There is no limit on the number of variables used in the creation of an Ordinary Least Squares (OLS) linear regression model, and there are no restrictions regarding which variables must be used. The Transform Variable button provides the option to transform a loaded variable using a transform function. When transformed, the variable will be available as a selection in the Predictor Variable list and the Response Variable drop down list.

As datasets are loaded, and if the Match Variable is a valid selection, the variables that are available for use in developing the linear model are shown in the Predictor Variables list and the Response Variable drop-down list. Selecting a variable in the Predictor Variables list, then one from the Response Variable drop-down list, will result in the generation of a model. Selecting the variable that is used for the Response Variable in the Predictor Variables list deselects the predictor variables and resets the response variable selection to the first in the list.

After a model is successfully created by selecting variables, a user can begin to evaluate the model results. This program includes tools to assist in model evaluation, available using the Plot Backscatter, View/Edit Table, Display Model, Write Report, Plots, and Time Series buttons. The number of observations used in the model is shown next to the Number of Observations label.

If a valid linear model exists within the program, the Number of Observations field will show the number of samples used in the development of the linear model. This corresponds to the number of valid observation values for the selected variables within the primary dataset. The Total Samples field shows the total number of samples in the loaded dataset. This number corresponds to the number of samples in the dataset that is selected in the Match Variable drop-down list.

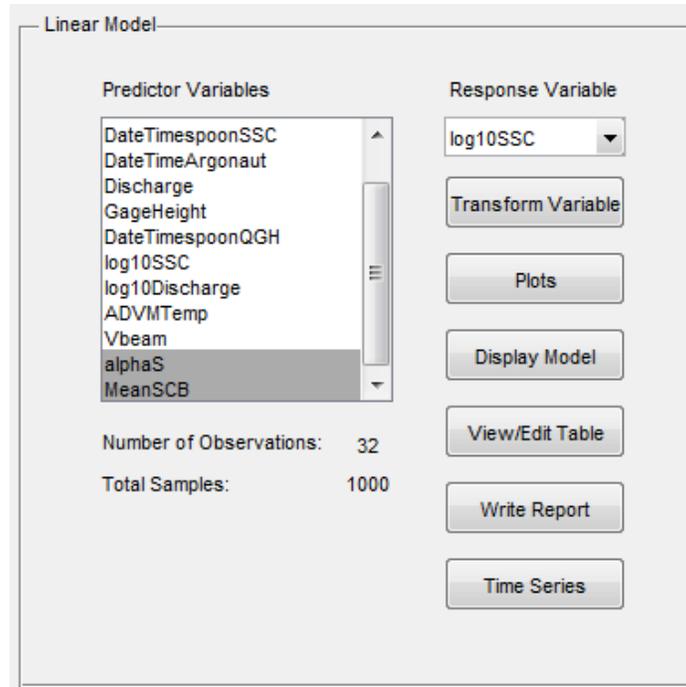


Figure 4 Linear Model options on the main SAID window

**Evaluation of Regression Models:** SAID provides several ways to graphically evaluate the linear model. Clicking on the Plots button within the main SAID window will display another window that provides several plotting options. In any plot figure, if Data Cursor Mode is enabled, any observation data point can be selected and the corresponding observation number will be shown along with the values plotted. The Model button will show different figures depending on if the linear model is a simple linear regression (SLR) or a multiple linear regression (MLR) or if the response variable is transformed. If the existing linear model is an SLR model, then a figure with the response observations plotted against the explanatory observed values will be shown (figure 5). When the existing model is an MLR, a partial residual plot for each variable in the model will be shown. If the response variable is transformed, then a linear-space plot will be shown with a smeared estimate fit line and confidence bounds.

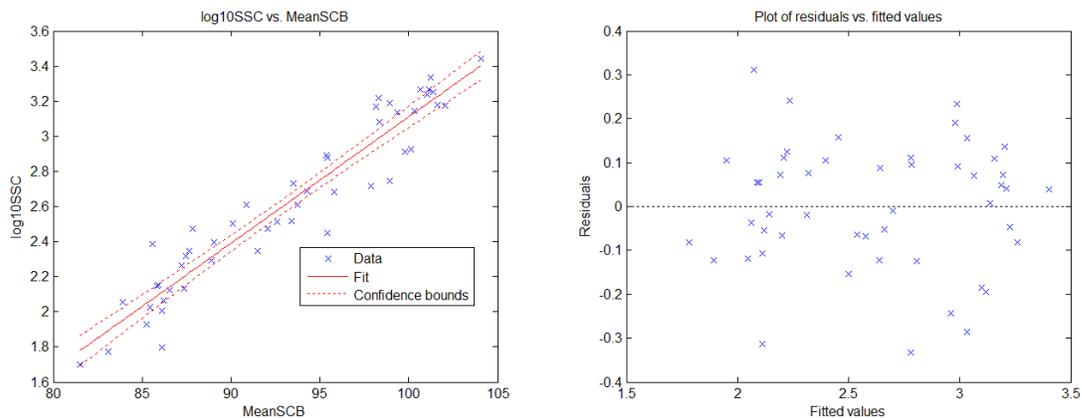


Figure 5 Linear model scatter plot and residual plot for a SLR model

Predicted versus observed plots can be selected to display the predicted response variable with the observed response variable. Also plotted is a one-to-one data line for comparison. If the response variable is transformed, then an additional figure will show the predicted versus observed values in linear space. Additionally the following residual plots can be selected:

- **Raw Vs. Fitted**—Illustrates a plot of the raw residuals against the fitted response values.
- **Probability**—Normal probability plot of raw residuals.
- **Stan. Ser. Corr.**—Standard serial correlation plot of the residuals shown with a LOWESS fit line to detect autocorrelation. If the LOWESS fit line shows a trend that deviates far from 0, serial correlation may be present.
- **Vs. Time**—Raw residuals plotted against time to see if a time dependent trend exists with the residuals.

The Display Model button will provide a window that displays the model results and statistics (figure 6). The information includes the linear equation, coefficient estimates, estimated confidence intervals,  $R^2$  values for the model, and root mean squared error. This information also is written to a report with the Write Report button on the main SAID window.

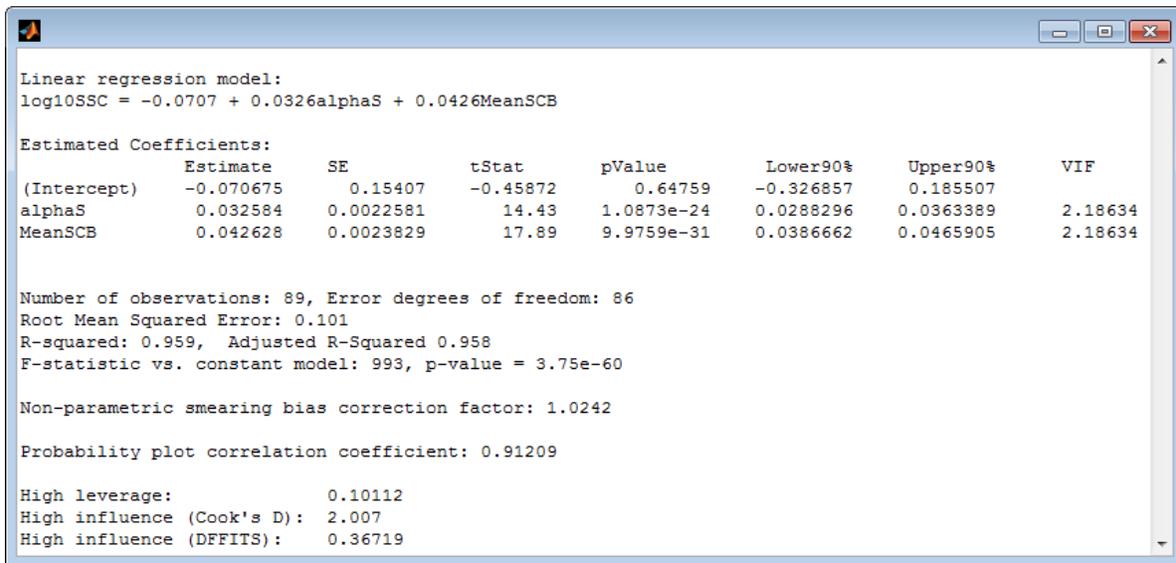


Figure 6 Linear model regression model statistics window

Clicking on the View/Edit Table button will display a window that contains the observation information used in the model. The information shown is the observation number, the corresponding primary date and time variable, the response variable, and the predictor variables. Also shown are diagnostic statistics for each observation for outlier detection (Helsel and Hirsch, 2002). Calculated indicator values that exceed the corresponding critical values for the model are highlighted in red.

Observations can be removed by checking the boxes in the far left column and clicking the Remove Observation button. This action flags the date and time within the program and sets the variables that correspond to the date and time to an invalid value. Once a date and time is flagged as removed, any future variables that are used in the model will have the corresponding values set as invalid. This will continue until the Restore All Observations button is clicked, which clears the date and times flagged.

Observation	DateTimespoonSSC	log10SSC	alphaS	MeanSCB	Leverage	Cook's Di...	Dffits
944	03/20/2013 14:30:00	2.2648	0.1778	73.9821	0.0788	0.0097	0.1690
945	03/23/2013 12:00:00	2.3856	0.1337	72.2537	0.1240	0.3071	1.0709
946	03/26/2013 11:30:00	2.0569	0.0953	70.4880	0.1908	0.0355	0.3233
947	04/02/2013 13:30:00	2.0253	0.1679	72.7195	0.1123	0.0290	-0.2934
948	04/06/2013 11:00:00	2.0645	0.1714	74.0404	0.0772	0.0343	-0.3222
949	04/10/2013 15:20:00	2.5159	0.4021	81.5799	0.0967	0.0601	-0.4299
950	04/11/2013 09:30:00	3.0828	0.8733	84.4967	0.1052	0.0596	0.4269
951	04/12/2013 10:30:00	3.1335	0.9743	85.5511	0.1262	0.0465	0.3734
952	04/15/2013 11:30:00	2.5105	0.3056	80.4132	0.0820	0.0108	-0.1783
953	04/17/2013 08:00:00	2.4757	0.2952	80.2825	0.0805	0.0194	-0.2397
954	04/18/2013 08:00:00	3.4425	2.9241	87.7971	0.28477	0.2523	-0.8828
955	04/18/2013 12:00:00	3.3365	2.2283	84.8483	0.1579	0.0266	0.2795
956	04/18/2013 14:53:00	3.3075	2.0726	86.1517	0.1123	1.8478e-04	0.0231
957	04/18/2013 14:54:00	3.2227	2.0726	86.1517	0.1123	0.0182	-0.2315
958	04/18/2013 18:00:00	3.2201	1.5909	83.4550	0.0640	0.0505	0.3982

Figure 7 Observation table window used to view and remove observations from the model dataset

**Generation of Report Output:** To write a full summary report for the linear model, click on the Write Report button within the main SAID window. The user will be prompted for a location and name of a comma separated value file to write the report to. Selecting and entering a valid location and file name will write the report. The contents of the report include:

- ADVM configuration and processing options
- Dataset file names and locations
- Linear model summary and statistics
- Critical outlier indicator values
- The dataset observations that were used in the creation of the model along with Observation number, fitted response variable values, raw residuals, an estimate of the non-transformed variable with bias correction applied (if the response variable is transformed), and calculated outlier indicator values
- The observations that were removed from the model dataset

### REAL-TIME DATA DISSEMINATION UTILITIES

After a surrogate regression model is developed and approved, the model can be used to generate continuous, real-time SSC estimates. The USGS has two utilities that make use of the computational algorithms in SAID to continuously estimate and display real-time sediment data:

- Real-time Acoustic Sediment Surrogate DATA Transfer (RASSDAT) program
- National Real-Time Water Quality (NRTWQ) program

RASSDAT is a Visual Basic Graphical User Interface (GUI) wrapped around a Python™ script that runs on a Windows® computer (figure 8), interfaces with the USGS National Water Information System (NWIS), and displays computed SSC on the NWIS Web Interface (<http://waterdata.usgs.gov/nwis>). NRTWQ is run from a centralized server and displays computed SSC on the NRTWQ Web site (<http://nrtwq.usgs.gov/>; figure 9).

RASSDAT is under beta development and is not yet formally released as a USGS software product. Questions about RASSDAT development can be directed to the authors.

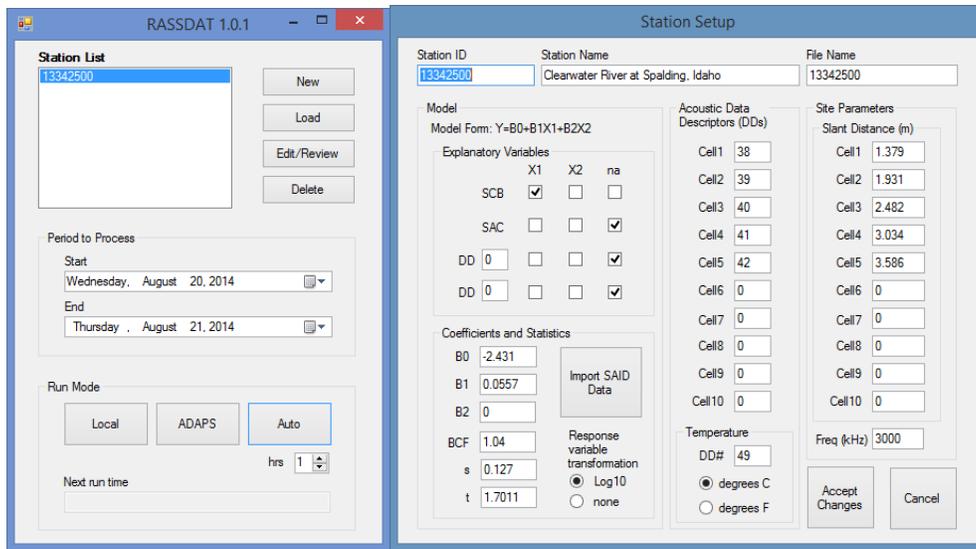


Figure 8 Screen captures of main processing (left) and station setup (right) windows from the USGS RASSDAT program, beta test version 1.0.1.

The data used to produce this plot are [provisional](#) and have not been reviewed or edited. They may be subject to change.

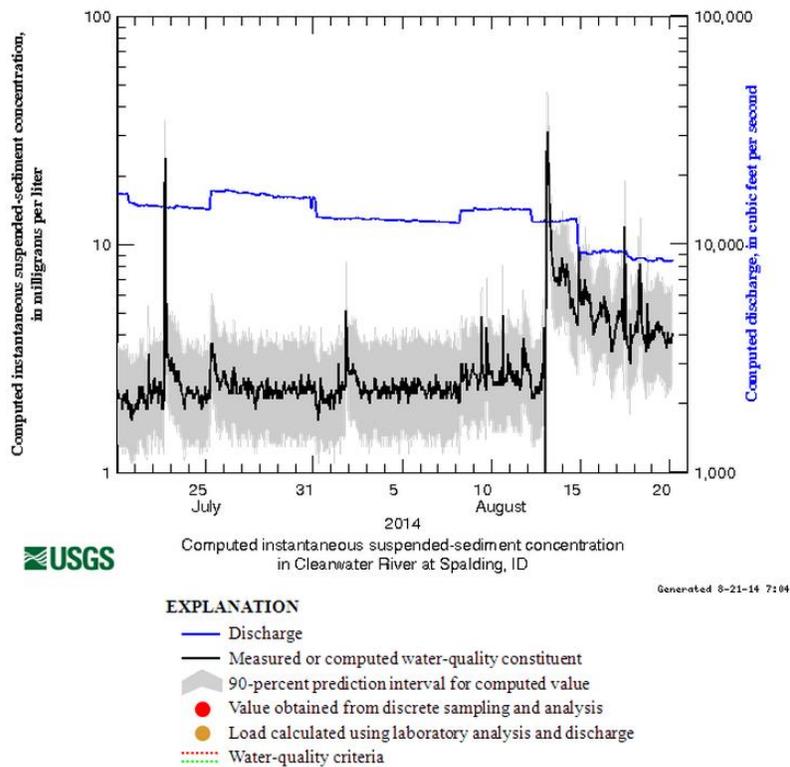


Figure 9 Screen capture from NRTWQ Web site showing example of SSC and SSC prediction intervals computed by using a sediment acoustic surrogate model developed for the Clearwater River at Spalding, Idaho (USGS Identification number 13342500).

## SUMMARY

The use of continuous parameters as surrogates for water quality constituents has been successful in multiple applications across the Nation. Critical to advancing the operational use of surrogates are tools to process and evaluate the data along with the subsequent development of regression models from which real-time sediment concentrations can be made available to the public. Recent developments of these tools are having an immediate impact on surrogate research, and on surrogate technologies for monitoring, assessment, rapid decision making, and adaptive management. The Surrogate Analysis and Index Developer (SAID) standalone tool processes complex datasets and creates regression models that related surrogate to constituent data by providing visual and quantitative diagnostics to the user. SAID is currently under development and beta testing at the U.S. Geological Survey.

SAID can be used to create regression models between surrogate data and constituent measurements. Additionally, SAID is a standalone tool to assist in the development of ordinary least squares (OLS) regression models with any response and predictor variables by providing visual and quantitative diagnostics to the user. There is no limit on the number of variables that can be used in the linear model, and there are no restrictions regarding which variables must be used. The sediment acoustic method utilizes acoustic parameters from fixed-mount stationary equipment with the assumption that the sediment concentration along the acoustic beam path is constant for a given time period. Within SAID, the user can set ADVM configuration and processing options, transform a loaded variable, build linear regression models, view linear model diagnostic statistics and plots, export the model information, and generate a predicted time series.

After a surrogate regression model has been developed and approved, the model can be used to generate continuous, real-time SSC estimates. Results from SAID provide direct inputs to two USGS utilities: the Real-time Acoustic Sediment Surrogate DATA Transfer (RASSDAT) program and the National Real-Time Water Quality (NRTWQ) program. The output from these utilities are displayed on USGS Web sites as real-time continuously computed sediment data. RASSDAT, currently under development and in beta testing at USGS, is a Visual Basic Graphical User Interface (GUI) wrapped around a Python™ script that runs on a Windows® computer, interfaces with the USGS National Water Information System (NWIS), and displays computed SSC on the NWIS Web Interface (<http://waterdata.usgs.gov/nwis>). NRTWQ is run from a centralized server and displays computed SSC on the NRTWQ Web site. The real-time dissemination of predicted SSC and prediction intervals for each time step has substantial potential to improve understanding of sediment-related water-quality and associated engineering and ecological management decisions.

## ACKNOWLEDGEMENTS

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