A VERSATILE SUITE OF LABORATORY-NONSPECIFIC SOFTWARE FOR PROCESSING SEDIMENT GRAIN-SIZE DATA

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Abstract We have designed and written four computer programs to facilitate analysis of sediment grain-size data. These programs: 1) describe distributions within the two classification schemes most commonly used by sedimentologists (SEDCLASS); 2) generate moment and inclusive graphics statistics and extrapolate particle distributions to the clay-colloidal boundary (GSSTAT); 3) plot the data on ternary diagrams (SEDPLOT); and 4) calculate settling velocities based on Stokes Law for gravitational procedures and derive angular velocities or total settling times for particles by centrifuge (CENTRISET). Ancillary files include spreadsheet templates that help users organize sample identifiers, incorporate corrections (e.g. for salt, organics, shell debris), and combine relative percents within the gravel, sand, and fine fractions into complete grain-size distributions. The programs run on Windows 98/2000/XP computers, provide interface windows to facilitate execution, and allow users to select options primarily with mouse-click events, or through interactive dialogue boxes. Detailed schematics of the functions and documentation are available within each program. Input files are expected in comma-delimited ASCII text; detailed error messaging warns the user of potential problems and provides diagnostics. All of the programs in this suite are laboratory nonspecific in that usage is not limited to particular analytical equipment or to any uncommon proprietary formats.

INTRODUCTION

Geologists, hydrogeologists, geochemists, and geotechnical engineers commonly use sediment grain-size data. Techniques that describe and summarize grain-size distributions are important to these scientists because the large amount of information contained in textural data sets can be difficult to understand and interpret. Thus, scientists commonly use nomenclature, statistical measures, and graphical representations to reduce complexities, reveal trends and patterns in the data, and develop hypotheses. Although statistical and plotting software packages are commercially available (e.g. SigmaStat, Grapher), these packages are not integrated, designed for sedimentologists, or inexpensive. Furthermore, privately developed “in-house” software is often proprietary, unintuitive, designed for and limited to specific analytical equipment, or runs under less common operating systems.

The purpose of this paper is to describe an integrated suite of recently completed, freely distributed, grain-size analysis software that is tailored to meet the needs of sedimentologists, but not limited to particular analytical equipment or to any uncommon operating environment.

SOFTWARE

Windows 98/2000/XP computers with minimal specifications and the necessary support and associated files can run compiled versions of the programs described below without difficulty. Users of these programs with early versions of Windows 98 may need to install updated versions of two support files into their C:\Windows\System directory. These files include the Common Dialog control file COMDLG32.OCX and the Visual Basic “Run-Time” driver MSVBVM60.DLL. Both support files are included with the affected software packages. SEDCLASS, GSSTAT, SEDPLOT, and CENTRISET provide interface windows to facilitate execution, allowing users to select options primarily with mouse-click events, or through interactive dialogue boxes. To further facilitate their use, windows opened by the programs in this suite are similar in appearance, with similar options and functions. For example, selecting command buttons labeled “Run” or “Calculate” executes the data processing; selecting command buttons labeled "Reset-Restart" or “Clear All” restarts the programs; selecting the "Information" button allows the user to view schematics, look-up tables, output files, and the documentation; and clicking “Close” or “Exit” ends the program and closes the window.

SEDCLASS Nomenclature describing size distributions is important to geologists because grain size is the most basic sediment attribute. Traditionally, geologists have divided sediments into four size fractions that include gravel, sand, silt, and clay and have classified these sediments based on ratios of the various proportions of the fractions. Definitions of these fractions have long been standardized to the grade scale described by Wentworth (1922), and two main classification schemes have been generally adopted to describe the approximate relationship between the size fractions.

The original scheme devised by Shepard (1954) utilized a single ternary diagram with sand, silt, and clay in the corners to graphically show the relative proportions among these three grades within a sample. This scheme, however, does not allow for sediments with significant amounts of gravel. Therefore, Shepard’s classification scheme (Fig. 1A) was subsequently modified by the addition of a second ternary diagram to account for the gravel fraction (Schlee, 1973). The system devised by Folk (1954, 1974) is also based on two triangular diagrams (Fig. 1B), but it has 15 major categories, and uses the term mud (defined as silt plus clay). The patterns within the triangles of both systems differ, as does the emphasis placed on gravel. For example, in the system described by Shepard, gravelly sediments have more than 10% gravel; in Folk’s system, slightly gravelly sediments have as little as 0.01% gravel. Folk’s classification scheme stresses gravel because its concentration is a function of the highest current velocity at the time of deposition and of the maximum grain size of the detritus that is available. Shepard’s classification scheme emphasizes the ratios of sand, silt, and clay because they reflect sorting and reworking (Poppe et al., 2005).

The program SEDCLASS (Poppe et al., 2003) is written in Microsoft Visual Basic 6.0 and characterizes sediment grain-size distributions using the terminologies defined by Shepard and Folk. Upon successful installation, the program may be executed by simply clicking on the executable program (sedclass.exe) or its icon. The program opens a window that presents the user with several options (Fig. 2). First, the user can select a sediment classification scheme for the output. Second, selecting the “Input File” button opens a text window allowing the user to identify the file to be processed and its location. The input file must be in comma-delimited ASCII text (.txt or .csv) and have seven fields that include: sample identifier, latitude, longitude,

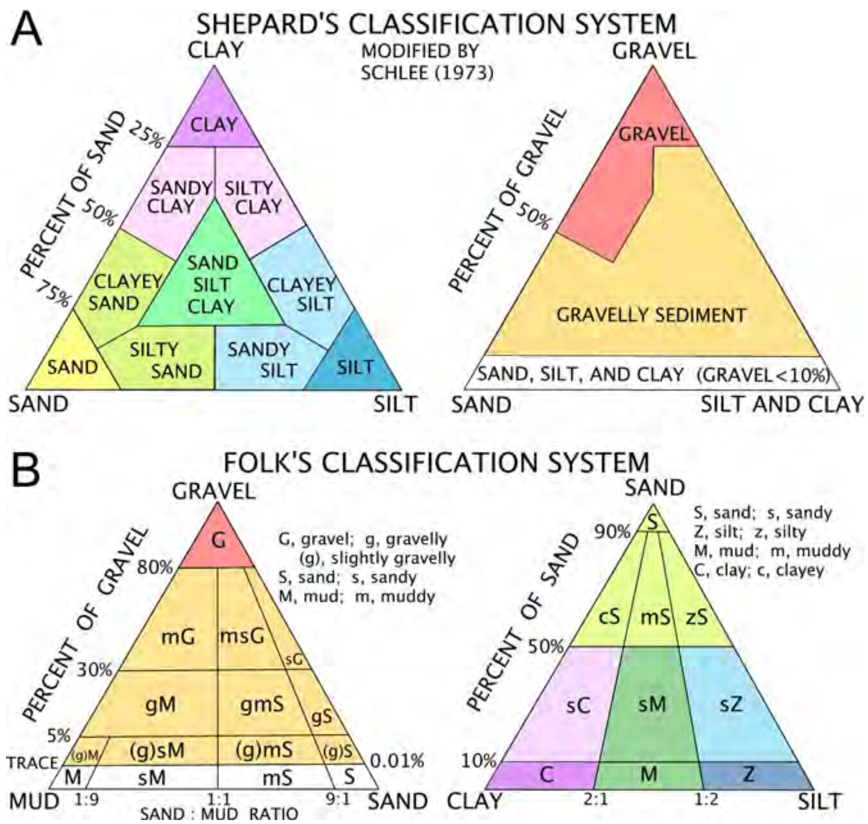

Figure 1 Sediment classification schemes used by the program SEDCLASS. A) Scheme from Shepard (1954) and modified by Schlee (1973). B) Scheme from Folk (1954, 1974).

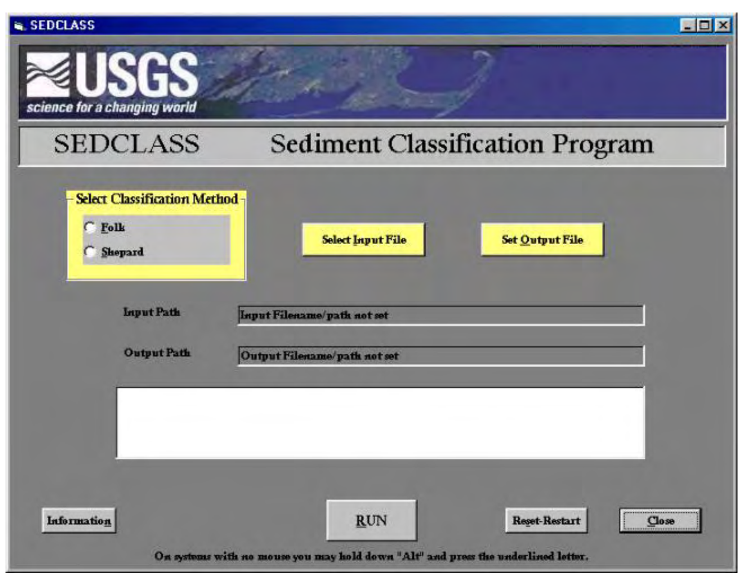

Figure 2 Window for the program SEDCLASS.

%gravel, %sand, %silt, and %clay (Appendix 1A). The latitude and longitude fields may be left blank (i.e., not omitted, but comma delimited), but the remaining fields must be populated, and the sum of the percentages of gravel, sand, silt, and clay must total 100% (+/- 0.1%). The program expects the first line of the input file to be a header showing the attribute names; no embedded commas are allowed in any of the data fields. Third, selecting the "Output File" button opens a text window that allows the user to name the file to be generated and to specify the destination directory. As the classification scheme, input file, and output file functions are successfully completed, the buttons change color from yellow to green. Selecting the "Run" command button executes the data processing. The program generates the output file in the requested destination directory and allows the user to view results in a display window or to view diagnostics if errors have occurred. The output file also has a header for its first line, but now contains eight fields; the original fields plus an additional field for sediment classification in the desired scheme (Appendix 1B).

GSSTAT Statistical methods are usually employed to simplify the necessary comparisons among samples and quantify the observed differences. The two statistical methods most commonly used by sedimentologists to describe grain-size distributions are mathematical moments (Krumbein and Pettijohn, 1938) and inclusive graphics (Folk, 1974). The choice of which of these statistical measures to use is typically governed by the amount of data available (Royse, 1970). If the entire distribution is known, the method of moments may be used; if the next to last accumulated percent is greater than 95 percent, inclusive graphics statistics can be generated. Unfortunately, most earlier programs designed to describe sediment grain-size distributions statistically will not run in a Windows environment, do not allow extrapolation of the distribution's tails, or do not generate both moment and graphic statistics (Kane and Hubert, 1963; Collias et al., 1963; Schlee and Webster, 1967; Poppe et al., 2005).

Owing to analytical limitations, electro-resistance multichannel particle-size analyzers (e.g. Coulter Counters) commonly truncate the tails of the fine-fraction part of grain-size distributions. These devices do not detect fine clay in the 0.6 to 0.1 micron range (part of the 11-phi and all of the 12-phi and 13-phi fractions). Although size analyses performed down to 0.6 microns are adequate for most freshwater and near shore marine sediments, samples from many deeper water marine environments (e.g. continental rise and abyssal plain) may contain significant material in the fine-clay fraction, and these analyses benefit from extrapolation.

The program GSSTAT (Poppe et al., 2004) generates statistics to characterize sediment grain-size distributions and can extrapolate the fine-grained end of the particle distribution. It is written in Microsoft Visual Basic 6.0 and provides a window to facilitate program execution (Fig. 3). The program presents the user with several options. The user must: 1) select either method of moments or inclusive graphics statistics; 2) select the method of extrapolation with radio buttons (either none, linear, exponential, or the average of these two); 3) if extrapolating, enter the smallest particle size actually measured (in microns); 4) select the format of the phi-class percentages in the input file (i.e. frequency or cumulative frequency percent); and 5) enter the format of the phi-class percentages in the output file.

Selecting the "Input File" button opens a text window that allows the user to identify the file to

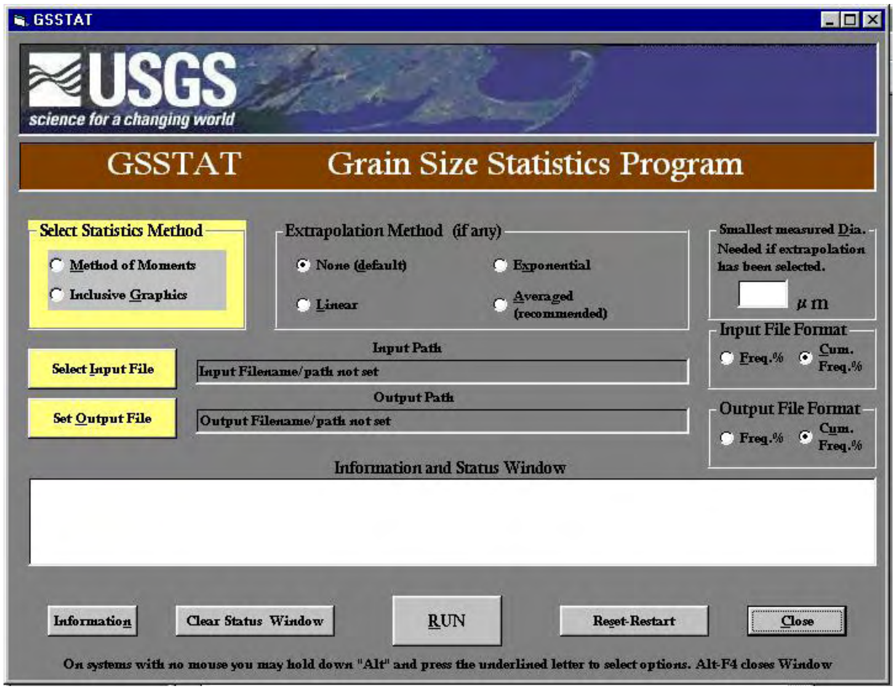

Figure 3 Window for program GSSTAT.

be processed and specify its location. The input file must be in comma delimited ASCII text (.txt or .csv) and have twenty fields that include: sample identifier, latitude, longitude, and the percentages (cumulative or frequency) of the 11 phi to -5 phi fractions (Appendix 1C). The latitude and longitude fields may be left blank (i.e., unpopulated, but not omitted), but the sum of the phi fraction percentages must total 100% (+/- 0.2%). The program expects the first line of the input file to be a header showing the attribute names; no embedded commas are allowed in any of the data fields. Selecting the “Output File” button opens a text window that allows the user to name the file to be generated and specify the destination directory.

The program generates an output file in the requested destination directory and allows the user to view results in a display window for verification purposes. The output file has a header for its first line, and contains thirty-three fields including: sample identifier, latitude, longitude, percentages of gravel, sand, silt, and clay, sediment classification, median, mean, standard deviation, skewness, kurtosis, verbal descriptions, and the frequency or cumulative frequency percentages of the fractions in whole-phi notation (Krumbein, 1934; Inman, 1952) from 13 phi through -5 phi (Appendix 1D). If the user has selected extrapolation, the two additional phi-fraction fields will be populated. If the user has selected inclusive graphics statistics, the verbal description field will be populated.

The program will generate error messages if problems associated with file format, required parameters, or data content occur. Most of the error messages appear in a pop-up window, but some warnings appear in the “Information and Status Window” of the main program display window and(or) in the thirty-fourth field of the output file. A complete listing of error messages with common causes and suggested solutions is provided in the documentation.

SEDPLOT Sedimentologists commonly use graphical representations to reduce complexities and recognize patterns or trends in numerical information. Of the graphical techniques, one of the most common methods used by sedimentologists is to plot the basic gravel, sand, silt, and clay percentages on equilateral triangular diagrams. This means of presenting data is simple and facilitates rapid comparison of samples. The program SEDPLOT (Poppe and Eliason, 2008), which is written in Microsoft Visual Basic 6.0, generates ternary diagrams to characterize sediment grain-size distributions. The inputs for the sediment fractions are percentages of gravel, sand, silt, and clay in the Wentworth (1922) grade scale, and the program permits the user to select output in either the Shepard (1954) classification scheme, modified as described above, or the Folk (1954, 1974) scheme.

The program opens a series of two windows that present the user with several options. In the first window the user can select an output scheme for plotting, identify the file to be processed and its location, and specify the file to be generated. Selecting the “Load Data” command button executes the data processing and notifies the user of any problems with the data. Selecting the “View-Plot” command button opens the second window showing the ternary diagram of the currently selected classification scheme and a set of control buttons and interfaces. The “Plot Data Array” button initiates plotting to the current window of the data loaded from the main window (Fig. 4). The “Clear Plot” clears the ternary diagram of all data, but does not erase the diagram. A button that alternates between “Show FINE Plot” and “Show COARSE Plot” toggles between ternary diagrams for the fine and coarse fractions for the selected classification scheme. The “Print Graphic” button prints the current plot window to whatever printer is active as the current system printer for this computer. The “Classification Method” interface has two radio buttons that allow the user to toggle between the ternary diagrams of Folk (1974) or Shepard (1954). The “Point Annotation” interface has three radio buttons that allow the user to choose annotation of the plotted points. The plotted points are plus signs (+) plotted with their centers at the points of closest available proximity to the actual point coordinates. Annotation options are: point only, point number (i.e. the number of the record in the data file), or the sample identifier from the first field of the data record. Changing this option does not change the plotted data.

Additional datasets may also be added to an existing plot, thereby allowing the user to compare and distinguish between their distributions. This is accomplished by rerunning the program without selecting the “Clear Plot” button or closing the plot window. When the “Plot Data Array” button is now pressed, the new dataset will be added to the existing plot. Selecting the "Reset-Restart" button restarts the program; selecting the "Information" button allows the user to view schematics of the classification systems, output files, and the documentation; and clicking "Close" exits the program and closes the window.

CENTRISET The program CENTRISET (Poppe and Eliason, 2009) is written in Just BASIC, calculates settling velocities based on Stokes Law for gravitational procedures, and derives angular velocities or total settling times for specific particles from any given medium by centrifuge. Detailed documentation, schematics, and tables for water density and viscosity at various temperatures, as well as tables for specific gravities of common materials, are available within the program through the “Information” button (Fig. 5). A file containing an explanation of

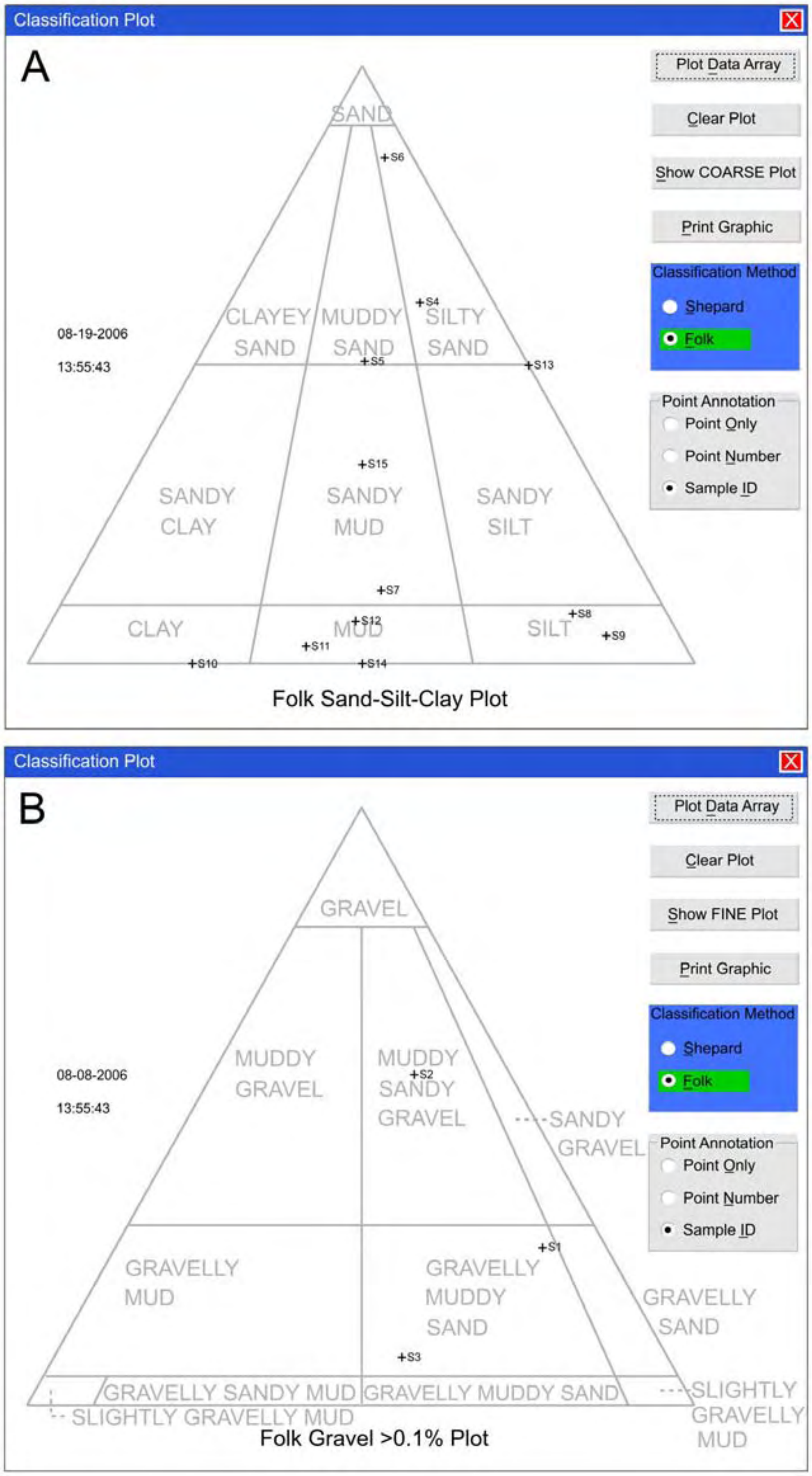

Figure 4 Ternary diagrams of the sediment classification scheme from Folk (1954, 1974), produced by the program SEDPLOT. In the example shown, selecting the "Plot Data Array" button has plotted data from 15 samples from a test input file. (A) Twelve samples with no gravel. (B) Three samples with greater than 0.1% gravel.

the theory behind the centrifugation function of this software and a derivation of its equation is also provided.

A

WATER		
TEMPERATURE T°C	VISCOSITY (poise) η	DENSITY (g/cm³) ρ_o
16	0.01110	0.999
17	0.01082	0.999
18	0.01056	0.999
19	0.01030	0.998
20	0.01005	0.998
21	0.00981	0.998
22	0.00958	0.998
23	0.00936	0.998
24	0.00914	0.997
25	0.00894	0.997
26	0.00874	0.997
27	0.00855	0.997
28	0.00836	0.996
29	0.00818	0.996
30	0.00801	0.996
31	0.00784	0.995
32	0.00768	0.995
33	0.00752	0.995
34	0.00737	0.994
35	0.00723	0.994
36	0.00709	0.994
37	0.00695	0.993
38	0.00681	0.993
39	0.00669	0.993
40	0.00656	0.992

B

SPECIFIC GRAVITIES OF COMMON SEDIMENTARY MATERIALS			
LIGHT MINERALS		HEAVY MINERALS	
MINERAL	SPECIFIC GRAVITY (g/cm³)	MINERAL	SPECIFIC GRAVITY (g/cm³)
ALBITE	2.62	ACTINOLITE	3.1
ANORTHITE	2.76	ANHYDRITE	2.94
CALCITE	2.72	APATITE	3.19
CHALCEDONY - CHERT	2.63	ARAGONITE	2.95
CHLORITE	2.6-2.9	AUGITE	3.3
CLAYS (MEAN)	2.46	BARITE	4.5
GYPSUM	2.32	BIOTITE	3.0
ILLITE	2.6-2.9	DOLOMITE	2.85
KAOLINITE	2.61	EPIDOTE	3.4
LABRADORITE	2.69	GARNET GROUP	3.1-4.3
MICROCLINE	2.55	GLAUCONITE	2.9
MONTMORILLONITE	2.5	HEMATITE	5.2
ORTHOCLASE	2.57	HORNBLENDE	3.2
PLAYGORSKITE	2.2	ILLMENITE	4.7
PLAGIOCLASE (MEAN)	2.69	KYANITE	3.61
QUARTZ	2.65	MAGNETITE	5.18
SEPIOLITE	2.0	MUSCOVITE	2.93
VERMICULITE	2.4	RUTILE	4.2
ZEOLITES (MEAN)	2.2	SIDERITE	3.96
HEAVY LIQUIDS (20°C)		STAUROLITE	3.7
		TOPAZ	3.5
BROMOFORM	2.89	TOURMALINE	3.12
TETRABROMOETHANE	2.96	ZIRCON	4.68

Figure 5 Examples of reference tables available within the CENTRISET program through the "Information" button. (A) Water density and viscosity at various temperatures (B) Specific gravities of common materials.

Gravitational settling methods, such as by pipette or hydrometer, are still commonly used to analyze fine-grained sediments because the required equipment is relatively inexpensive and because it is generally accepted that hydrodynamic characteristics of particles are often more useful than geometrically defined measures of size. Also, difficulties associated with decanting the finest sediment fractions and with separating minerals in heavy liquids make centrifugal settling methods attractive.

To calculate a settling velocity for gravitational analyses, the user must enter the following five variables: fluid viscosity, fluid density, particle density, particle radius, and gravitational acceleration. For settling by centrifuge, the user must enter: fluid viscosity, fluid density, particle density, particle radius, time of acceleration, time of deceleration, initial distance from axis of rotation, final distance from axis of rotation, and either angular velocity or total time. Running the program generates the calculated variable in standard units for the selected process and displays it in the results window.

Ancillary Files These files include spreadsheet templates that help users organize sample identifiers, incorporate corrections (e.g. for salt, organics, shell debris), and combine relative percents within the gravel, sand, and fine fractions into complete grain-size distributions. For example, the spreadsheet GRAINSIZE.XLS will perform the calculations necessary to obtain a normalized phi distribution from 11 phi through -5 phi using the weights of sand and gravel phi classes and volume percentages of silt and clay phi classes obtained during grain-size analysis. Input for this spreadsheet includes: gross wet and dry sample weights, beaker weight, salinity, shell/organic material weight (to be subtracted from sample weight, if desired), weight of sand and gravel phi classes (from 0 phi to 4 phi and -1 phi to -5 phi), and percentages (weight or volume cumulative frequency %) of fine phi classes (5 phi to 11 phi). Output from this spreadsheet is the normalized frequency percentages of 11 phi through -5 phi size classes that are formatted to be copied and pasted into GSSTAT_INPUT.CSV. GSSTAT_INPUT.CSV is a comma-delimited ASCII file that can be used as an input file for GSSTAT, the program described above that generates statistics for grain-size data.

Other spreadsheets provided in the GRAINSIZE.XLS file allow users to: 1) calculate percent calcium carbonate; 2) convert ¼ phi weights within the sand and gravel fractions into ¼ phi frequency percents, and whole-phi weights and frequency percents; 3) convert ¼ phi weights into whole-phi weights and calculate net coarse, sand, and gravel weights; and 4) normalize phi distributions where no salt correction is necessary (e.g., freshwater samples).

SUMMARY

The software suite described herein facilitates the organization and interpretation of sediment grain-size data. Individual programs run on 98/2000/XP Windows computers and are easy to install and intuitive to operate. Compiled and un-compiled versions of this software, helpful readme files, test input files, installation instructions, necessary support files, documentation, and derivations of primary equations are available free of charge from the U.S. Geological Survey at: http://woodshole.er.usgs.gov/software/sediment-software.html

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APPENDIX 1

Examples of the comma-delimited ASCII input and output files from the programs SEDCLASS and GSSTAT. (A) Typical SEDCLASS input file. Note that the latitude and longitude fields of the second record are blank. (B) SEDCLASS output file generated from the input file above with the Shepard (1954) option selected. (C) Typical GSTAT input file. (D) GSTAT output file with thirty-three fields generated from input file above with inclusive graphics (Folk, 1974), frequency percent, and no extrapolation options selected.

A SAMPLE_ID,LATITUDE,LONGITUDE,%GRAVEL,%SAND,%SILT,%CLAY AA435,40.437,-68.139,26.5,64.01,7.02,2.47 AA525,,,0,7.15,45.56,47.29
B SAMPLE_ID,LATITUDE,LONGITUDE,%GRAVEL,%SAND,%SILT,%CLAY,SHEPCLASS AA435,40.437,-68.139,26.5,64.01,7.02,2.47,GRAVELLY SEDIMENT AA525,,,0,7.15,45.56,47.29,SILTY CLAY
C SAMPLEID,LATITUDE,LONGITUDE,11_PHI,10_PHI,9_PHI,8_PHI,7_PHI,6_PHI,5_PHI,4_PH I,3_PHI,2_PHI,1_PHI,0_PHI,M1PHI,M2PHI,M3PHI,M4PHI,M5PHI AQ364,40.83333,-70.38333,2.76,4.67,7.04,10.8,9.12,2.66,0.7,18.63,41.72,0.51,0,1.38,0,0,0,0,0 AM306,41.16755,-72.2307,0.16,0.38,0.43,0.46,0.54,0.5,0.38,4.08,28.2,22.37,12.06,13.19,9.96,7.29,,,
D SAMPLEID,LATITUDE,LONGITUDE,GRAVEL_PCT,SAND_PCT,SILT_PCT,CLAY_PCT,SEDCLASS,MEDI AN,MEAN,STDDEV,SKEWNESS,KURTOSIS,VERBAL_DES,PHI_13,PHI_12,PHI_11,PHI_10,PHI_9,PHI_8,P HI_7,PHI_6,PHI_5,PHI_4,PHI_3,PHI_2,PHI_1,PHI_0,PHIM1,PHIM2,PHIM3,PHIM4,PHIM5,ERRORS AQ364,40.83333,-70.38333,0.00,62.24,23.28,14.47,SILTY SAND,3.21,4.50,2.46,0.71,0.68,VERY POORLY SORTED; STRONGLY FINE SKEWED; PLATYKURTIC,,,2.76,4.67,7.04,10.80,9.12,2.66,0.70,18.63,41.72,0.51,0.00,1.38,0.00,0.00,0.00,0.00,0.00, AM306,41.16755,-72.2307,17.25,79.90,1.88,0.97,GRAVELLY SEDIMENT,1.39,0.95,1.76,-0.34,0.84,POORLY SORTED; STRONGLY COARSE SKEWED; PLATYKURTIC,,,0.16,0.38,0.43,0.46,0.54,0.50,0.38,4.08,28.20,22.37,12.06,13.19,9.96,7.29,0.00,0.00,0.00,