USER'S MANUAL FOR ESTIMATION OF DISSOLVED-SOLIDS CONCENTRATIONS AND LOADS IN SURFACE WATER

By Timothy D. Liebermann, Robert F. Middelburg, and Scott A. Irvine

A computerized method using data from WATSTORE--National Water Data Storage and Retrieval System of the U.S. Geological Survey

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CONVERSION FACTORS

Multiply	*By*	*To obtain*
acre-foot	1,233.5	cubic meter
cubic foot per second (cfs)	0.028317	cubic meter per second
ton	907.18	kilogram
ton per acre-foot	735.29	kilogram per cubic meter

The following terms and abbreviations are also used in the report:

degree Celsius	(°C)
milligram per liter	(mg/L)
milliequivalent per liter	(meq/L)
microsiemens per centimeter at 25 degrees Celsius[1]	(μS/cm)

[1]The U.S. Geological Survey recently has adopted the unit of microsiemen per centimeter at 25 degrees Celsius for specific conductance; however, the unit in WATSTORE is micromho per centimeter at 25 degrees Celsius. The two units are equivalent.

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ABSTRACT

Dissolved solids are the sum of the individual dissolved ionic constituents present in water and are a measure of the salinity of water. Salinity of surface water is an important indicator of overall water quality. Ordinarily, however, dissolved-solids concentrations and loads are estimated by indirect methods that are based on periodic chemical analyses. Three computer programs, FLAGIT, DVCOND, and SLOAD, were developed to provide a consistent and accurate method of estimating dissolved-solids concentrations and loads. The programs are written in a data analysis programming language and are used on the U.S. Geological Survey's mainframe computer. FLAGIT retrieves daily values of specific conductance and discharge and periodic water-quality analyses from the U.S. Geological Survey's National Water Data Storage and Retrieval System data base, deletes incomplete data, flags possible data errors, and creates data sets on which DVCOND and SLOAD operate. DVCOND fills in missing daily values of specific conductance, when appropriate, by linear interpolation. SLOAD uses water-quality data to compute 3-year moving regressions of dissolved-solids loads as a function of specific conductance and discharge; the program then applies the regression coefficients to the daily-values data to estimate daily dissolved-solids loads. Dissolved-solids loads are summed by month and by year. Separate regressions are used to estimate the mass fractions of six major ions. The theoretical basis and underlying assumptions of the procedures are presented, with documentation of the programs and their use.

INTRODUCTION

Dissolved solids are the sum of the individual dissolved ionic constituents present in water. The salinity of water, as represented by dissolved solids, may have adverse effects on irrigation, recreation, and municipal and industrial uses (U.S. Environmental Protection Agency, 1976). Water-quality standards for salinity exist at the State, Federal, and international levels (U.S. Bureau of Reclamation, 1985). Thus, determination of dissolved-solids concentrations and loads is a necessary step in assessing historical salinity data and predicting the effects of future water policies and land-use practices on salinity.

Dissolved materials generally accumulate in a river as it flows downstream. The dissolved-solids load increases as the river flows through areas underlain by rocks containing soluble minerals and as surface runoff and return flows from irrigation and other sources flow into the river. Even without the addition of salts, the concentration may increase because of evaporation and diversion of relatively pure water upstream (Duffy, 1984).

Dissolved-solids loads are difficult to measure directly; instead they are computed as the product of dissolved-solids concentration and discharge. Direct determination of dissolved-solids concentration requires an extensive program of sample collection and chemical analysis. Dissolved-solids data for a given streamflow-gaging station commonly have been collected at infrequent intervals or do not represent the entire flow regime; however, specific conductance and discharge may be measured by automatic monitoring equipment and their daily mean values routinely are reported for a large number of streamflow-gaging stations. If a significant relation is established between specific conductance, dissolved solids, and discharge, then daily dissolved-solids concentrations and loads may be predicted from daily specific-conductance and discharge values, resulting in reasonably accurate and complete estimates of salinity at a stream location. Using these estimates, which are based on the historical record, trends over time may be established (Kircher and others, 1984). Furthermore, it is possible to establish relations between salinity and land-use practices throughout time, and, also, if daily specific conductance and discharge are known or can be estimated, to extend salinity estimates beyond the period of historical salinity record.

This report presents three computer programs, FLAGIT, DVCOND, and SLOAD that estimate dissolved-solids concentrations and loads from an existing data base. The programs are written in Statistical Analyses System (SAS)[1] language (SAS Institute, Inc., 1982) and are run on the U.S. Geological Survey AMDAHL computer using IBM System 370 Job Control Language (Brown, 1977). The program FLAGIT retrieves data from the daily-values file and water-quality file of the U.S. Geological Survey's National Water Data Storage and Retrieval System (WATSTORE) (Hutchinson, 1975), examines the data, deletes incomplete observations, and flags possible errors in the remaining observations. FLAGIT also produces the data base used by the programs DVCOND and SLOAD. The program DVCOND fills in missing values in the daily specific-conductance record by linear interpolation. DVCOND needs to be used only when the flow at a streamflow-gaging station is extensively regulated. The program SLOAD derives regression relations from water-quality data, modeling dissolved solids and six major ions as functions of specific conductance and discharge. SLOAD then applies these relations to the daily specific conductance and discharge data and computes daily loads of dissolved solids and the other six major ions. The computed daily loads are summed by month and by year. Monthly and annual dissolved-solids and major ion concentrations are computed from the monthly and annual loads and streamflows. Monthly, annual, and seasonal concentrations and loads, in addition to regression statistics, are printed and saved on SAS data sets. Separate versions of SLOAD enable annual summation either by water year or calendar year.

The computerized method can be used for streamflow-gaging stations that have a complete record of daily-values discharge and periodic water-quality analyses. The reliability of the estimates is considerably increased if daily values of specific conductance also are available.

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[1]Use of trade names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

RELATIONS BETWEEN SPECIFIC CONDUCTANCE, DISSOLVED-SOLIDS CONCENTRATIONS, DISCHARGE, AND DISSOLVED-SOLIDS LOADS

Specific conductance and dissolved-solids concentration are measures of the ionic strength of a solution. For a single ionic constituent, the simple form of the Onsager equation (Davies, 1967) for equivalent specific conductance is:

$$\Lambda = \Lambda_0 - S\ C^{\frac{1}{2}} \qquad (1)$$

where Λ = equivalent specific conductance, in microsiemens per centimeter per equivalent at 25 degrees Celsius;

Λ_0 = equivalent specific conductance at infinite dilution, in microsiemens per centimeter per equivalent at 25 degrees Celsius;

S = a constant known as the Onsager slope; and

C = dissolved-solids concentration, in moles per liter.

Specific conductance, then, is:

$$K = 1{,}000\ \Lambda\ C\ z \qquad (2)$$

where K = specific conductance, in microsiemens per centimeter at 25 degrees Celsius; and

z = the charge on the ion (absolute value).

At relatively weak ionic strength, the specific conductance of a solution is a linear function of dissolved-solids concentration, and the specific conductance of a solution composed of n ionic species equals:

$$K = 1{,}000 \sum_{i=1}^{n} \Lambda_i\ C_i\ z_i \qquad (3)$$

where

i is the ith ionic species. At greater ionic strength, the equivalent specific conductance decreases because interactions and interferences between ions decrease the ionic mobility, and the relation becomes less linear (Hem, 1970).

Similarly, the dissolved-solids concentration may be expressed as:

$$DS = 1{,}000 \sum_{i=1}^{n} C_i\ F.W._i \qquad (4)$$

where

DS = dissolved-solids concentration, in milligrams per liter; and

F.W. = the formula weight, in grams per mole.

By comparing equations 3 and 4, we may expect that, for a fairly constant mix of ions, there is a direct relation between specific conductance and dissolved-solids concentration. At weak ionic strength, the relation may be expressed as:

$$DS = r\ K \tag{5}$$

where

$0.55 < r < 0.75$ for most streams (Hem, 1970). At greater ionic strength, a linear relation between the logarithms of dissolved-solids concentration and specific conductance is more valid. This logarithmic model is assumed to apply throughout the range of concentrations present in natural waters.

Because load is the product of concentration and discharge, and because concentration is a function of specific conductance (eq. 5), it is possible to predict load using the readily available parameters for specific conductance and discharge. Furthermore, due to the dilution effect of increasing discharge in unregulated streams, there is a relation between concentration and discharge (Lane, 1975), in the form:

$$DS = a_{*}\ Q^{-b_{*}} \tag{6}$$

where

Q = discharge, and

a_{*} and b_{*} = constants.

Using equations 5 and 6, we have two methods of applying readily available values to the prediction of load:

$$LOAD = \underline{a}\ Q^{1-b_{*}} \tag{7}$$

where

LOAD = dissolved-solids load, and

$\underline{a}$ = a constant,

and:

$$LOAD = r\ K\ Q \tag{8}$$

A logarithmic transformation of the variables results in relations that are more nearly linear and residuals that are approximately normal and homoscedastic. Thus, an appropriate method for estimating load is to use linear regression on the transformed data, resulting in the models:

$$\ln(LOAD) = a + b\ [\ln(Q)] \tag{9}$$

where

ln = the natural logarithm;

a and b = regression coefficients; and

b = generally between 0 and 1

and:

$$\ln(LOAD) = c + d\,[\ln(Q)] + e[\ln(K)] \quad (10)$$

where

c, d, and e = regression coefficients; and

d and e = generally close to 1.

Equations 9 and 10 are used to derive the linear-regression coefficients from which loads are estimated. Because concentration is more directly related to specific conductance than to discharge, equation 10 is used when specific conductance is available. Otherwise, equation 9 is used. In some instances, such as when a streamflow-gaging station is directly downstream from a large reservoir, concentration may be independent of discharge; therefore, equation 9 is not appropriate, and some effort needs to be made to fill in missing specific-conductance values. The program DVCOND is provided for this purpose.

ESTIMATION OF DISSOLVED-SOLIDS CONCENTRATIONS AND LOADS

Program FLAGIT

The program FLAGIT accesses the U.S. Geological Survey WATSTORE data base stored on the AMDAHL computer in Reston, Va. (Hutchinson, 1975). FLAGIT retrieves one station per run. The user needs to supply the 8-digit streamflow-gaging station identification number, the backfile volume number, and the beginning and ending years for the data. A listing of the variables retrieved by FLAGIT and their corresponding parameter codes is shown in table 1.

Flagging of Potential Errors in the Data Base

The program FLAGIT has four editing functions in addition to producing the data base used to estimate dissolved solids. It combines variables stored as different parameter codes into a single listing, deletes incomplete or redundant data, prints the data, and flags possible data errors. Incomplete data consist of daily-values observations with missing discharge or periodic water-quality observations with missing dissolved-solids concentration or missing discharge. Redundant data consist of two or more daily values having the same date or a single chemical analysis listed as two or more water-quality analyses. By deleting redundant analyses, each separate water-quality analysis is given equal weight in the subsequent regression computations.

FLAGIT merges daily-values and water-quality data into a temporary data set, which then is sorted by date and printed. Data are compared within and between dates, according to user-defined criteria. If a comparison indicates a potential problem, a 1-character flag is printed beside the date. For example, if the ratio of dissolved solids to specific conductance is less than 0.55 or greater than 0.75, an "R" flag is generated. These flags enable the user to locate potential errors that, if uncorrected, might degrade the accuracy of subsequent regression models and lead to erroneous results. The user easily can adjust the values of the flagging coefficients to print more

Table 1.--*Variables retrieved from WATSTORE by FLAGIT*

[WATSTORE, U.S. Geological Survey's National Water Data Storage and Retrieval System]

WATSTORE Code	Description
	DAILY-VALUES FILE
00060	Discharge[1], in cubic feet per second
00095	Specific conductance[1], in microsiemens per centimeter at 25 degrees Celsius
	WATER-QUALITY FILE
00060	Discharge, in cubic feet per second
00061	Discharge, instantaneous, in cubic feet per second
00095	Specific conductance, in microsiemens per centimeter at 25 degrees Celsius
00410	Alkalinity, titration to pH 4.5, in milligrams per liter as calcium carbonate ($CaCO_3$)
00440	Bicarbonate ion, in milligrams per liter
00445	Carbonate ion, in milligrams per liter
00915	Calcium, dissolved, in milligrams per liter
00925	Magnesium, dissolved, in milligrams per liter
00930	Sodium, dissolved, in milligrams per liter
00933	Sodium plus potassium, dissolved, in milligrams per liter
00935	Potassium, dissolved, in milligrams per liter
00940	Chloride, dissolved, in milligrams per liter
00945	Sulfate, dissolved, in milligrams per liter
00955	Silica, dissolved, in milligrams per liter
70300	Solids, residue on evaporation at 180 degrees Celsius, dissolved, in milligrams per liter
70301	Solids, sum of constituents, dissolved, in milligrams per liter
90410	Alkalinity, titration to pH 4.5, laboratory, in milligrams per liter as calcium carbonate ($CaCO_3$)
90440	Bicarbonate, incremental titration, laboratory, in milligrams per liter
95440	Bicarbonate, titration to pH 4.5, laboratory, in milligrams per liter

[1]If daily mean values (statcode 00003) are not available, then once-daily values (statcode 00011) are used.

or fewer flags, depending on the desired degree of scrutiny and the characteristics of the stream being studied. Flagging symbols and the default values of their coefficients are presented in table 2.

Table 2.--*Flagging symbols and the possible errors they represent*

[DV, daily-values; Q, discharge; QW, water-quality; K, specific conductance; DS, dissolved-solids concentration; CDS, calculated dissolved-solids concentration; ROE, residue on evaporation at 180 degrees Celsius; SOC, sum of constituents. Coefficients represent default values and may be redefined by the user.]

Flag	Possible error
D	Duplicate date
M	Missing date in DV file
Q	DV Q and previous DV Q differ by >100 percent
W	DV Q and QW Q differ by >50 percent
C	DV K and previous DV K differ by >50 percent
I	DV K and QW K differ by >50 percent
R	Ratio of DS to QW K is <0.55 or >0.75
T	CDS and ROE differ by >10 percent
Z	CDS and SOC differ by >10 percent
%	Charge balance differs by >5 percent
s	Charge balance differs by >2 standard deviations
+	Cations > anions
-	Anions > cations

Charge balance, or anion-cation balance, is one flagging procedure used to detect errors in the analyses of individual ionic constituents. Because water is electrically neutral, the sum of the anions must balance the sum of the cations. The charges are computed in milliequivalents per liter from the ionic concentrations in milligrams per liter as:

$$\text{Sum of cations} = 0.04990(\text{calcium}) + 0.08229(\text{magnesium}) + 0.04350(\text{sodium}) + 0.02558(\text{potassium}) \quad (11)$$

and:

$$\text{Sum of anions} = 0.02821(\text{chloride}) + 0.02082(\text{sulfate}) + 0.03333(\text{carbonate equivalent}). \quad (12)$$

FLAGIT uses two methods to check the charge balance: Percent error and error expressed in standard deviations (American Public Health Association and others, 1981):

$$\text{Error} = \frac{\text{Sum of anions} - \text{Sum of cations}}{0.1065 + 0.0155\ (\text{Sum of anions})} \quad (13)$$

where

Error = the number of standard deviations from the expected value.

Calculation of Dissolved-Solids Concentrations

Three separate estimates of dissolved-solids concentration may be used for a given water-quality analysis within the FLAGIT program. Two are retrieved from WATSTORE, and one is calculated using FLAGIT. Parameter code 70300, dissolved solids, residue on evaporation at 180 degrees Celsius (ROE), is considered the least reliable for the load calculations. Parameter code 70301, dissolved solids, sum of constituents (SUM), was calculated by the analyst prior to 1970 but since then has been calculated automatically by WATSTORE at the time of retrieval. Although SUM is considered more accurate than ROE, its method of calculation has varied. Furthermore, SUM is reported to only two significant figures. The FLAGIT program computes the third estimate, referred to as calculated dissolved solids (CDS). This third estimate is preferred because it is more precise than SUM, and because it is computed consistently as the sum of a fixed number of constituents. The default order of preference used in choosing the dissolved-solids parameter is CDS > SUM > ROE. The user may change this default order by altering the programming code.

CDS is computed as the sum of the eight major constituents normally present in natural streams: Calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^{+}), potassium (K^{+}), silica (Si), chloride (Cl^{-}), sulfate (SO_4^{2-}), and carbon, expressed as carbonate equivalent. Measures of dissolved carbon include carbonate (CO_3^{2-}), bicarbonate (HCO_3^{-}), and alkalinity [milligrams per liter as calcium carbonate ($CaCO_3$)]. These eight constituents are summed in the steps listed below. If any step cannot be computed because of missing data, then no value is computed for CDS. If potassium is missing, its value is set to zero. Because carbonate ion is not found in most natural streams, its value is set to zero when missing. The steps are:

1. Calcium plus magnesium plus chloride plus sulfate plus silica.

2. Sodium plus potassium.
   Two possible categories exist in WATSTORE for sodium and potassium. Either their sum is reported (parameter code 00933) or they are reported separately (parameter codes 00930 and 00935). Computation follows this preference: 00930 plus 00935 > 00933 > 00930.

3. Carbonate equivalent.
   This step is somewhat complicated, because of the various analytical procedures and parameter codes associated with inorganic carbon. The result is that the parameters are converted into their equivalent as carbonate, in milligrams per liter. Computation of carbonate follows this preference:
   a. Carbonate plus bicarbonate/2.03.
      Three parameter codes are retrieved for bicarbonate. The parameter codes, listed here in order of decreasing preference, are: 00440 > 90440 > 95440. If carbonate is missing, its value is set to zero.
   b. Alkalinity/1.67.
      The choice of parameter codes follows this preference: 00410 > 90410.

Program DVCOND--Estimation of Missing Specific-Conductance Values

The program DVCOND fills in missing values in the daily-values specific-conductance record by linear interpolation between known values. The program progresses in two steps. For small gaps in the data (less than 10 consecutive missing days), the daily values at either end of the gap are used as the endpoints for the interpolation. For larger gaps in the record, instantaneous specific-conductance values from the water-quality analyses are inserted into the missing daily record. These inserted values, in addition to the daily values at either end of the gap, then are used as endpoints for a second set of linear interpolations, which fills in all remaining missing values.

This program needs to be used where dissolved-solids concentration is independent of discharge, such as streamflow-gaging stations directly downstream from large reservoirs. At these locations, specific-conductance values are needed in order to predict dissolved solids. In such instances, it is assumed that specific-conductance values are not characterized by large day-to-day fluctuations and that the interpolation procedure adequately includes slow changes in daily specific conductance. If a station is not directly downstream from a large reservoir, the program DVCOND is not used.

The data base for some streamflow-gaging stations is characterized by a period of unregulated flow preceding the construction of reservoirs. Interpolation of missing specific-conductance values is needed only for the postconstruction period. To accommodate such streamflow-gaging stations, the user of DVCOND specifies a beginning date; all missing specific-conductance values following that date are filled in.

Program SLOAD

General Approach to Estimation of Dissolved-Solids Loads

Load equals concentration times discharge as shown in the following equation:

$$LOAD = 0.0027\ Q\ DS \tag{14}$$

where

LOAD = dissolved-solids load, in tons per day;

Q = discharge, in cubic feet per second; and

DS = dissolved-solids concentration, in milligrams per liter.

The fundamental problems in predicting loads (or concentrations) are that dissolved-solids data from the water-quality file are not complete throughout time and that it is unlikely that the daily-values file will contain dissolved-solids data. Because day-to-day changes in concentration and discharge occur in most streams, estimates of dissolved solids over time may be incorrect if based only on periodic water-quality analyses, which may be collected irregularly or infrequently. The approach presented in this report combines the best features of each type of data. Three-year moving-regression coefficients that model load as a function of specific conductance and instantaneous discharge are calculated from data in the water-quality file. Those regression coefficients then are applied to the data in the daily-values file to predict daily loads. Finally, the total load divided by the total discharge gives the flow-weighted concentration.

This approach is based on several assumptions:

1. After making obvious corrections, the WATSTORE data base is reasonably accurate.

2. For a given stream location, there is a significant relation between specific conductance and discharge, and dissolved-solids concentration (or load). This relation does not change significantly in a short time.

3. This relation, derived from random instantaneous measurements, also holds for daily mean values.

This approach is most useful for streamflow-gaging stations with a consistent record of daily values of specific conductance and discharge, and concurrent water-quality analyses. In such instances, the results compare favorably with results obtained by other methods (Kircher and others, 1984).

Estimation of Dissolved-Solids Loads by Linear Regression

Two approaches may be used when estimating dissolved-solids loads by regression. One approach is to regress using the logarithm of concentration, compute predicted concentrations, and then multiply by discharge to obtain predicted loads. The second approach is to regress using the logarithm of load directly, and then compute predicted loads directly. This second approach gives an artificially large coefficient of determination, R^2, value compared to the first approach because, in effect, discharge is present on both sides of the equation. However, both approaches give the same predicted loads and have the same standard error associated with the estimates. In the program SLOAD, both approaches are used, largely because the program was developed in two stages. Dissolved solids are estimated using the logarithm of load as the dependent variable in the regression. The individual constituents are estimated using the logarithm of concentration as the dependent variable.

The program SLOAD divides the water-quality data into groups, one group per water year. Each group consists of the 3 consecutive water years. Any group having less than three analyses during the 3-year period is deleted from further analysis. Then a separate regression is performed on each group, resulting in a series of 3-year moving regressions. For n water years of record, there are n separate regressions, each on a 3-year set of water-quality data. This method increases the degrees of freedom in the regression for each year but does not mask existing time trends (Kircher and others, 1984).

The least-squares regression coefficients then are applied to daily values of specific conductance and discharge to generate daily loads, which then are summed, printed, and stored in the data base as monthly, annual, and seasonal loads. Annual loads may be summed either by water year or calendar year, by using alternative versions of SLOAD. Flow-weighted concentrations are computed by dividing total load by total discharge.

Estimation of Mass Fractions of Ionic Constituents

In addition to dissolved solids, SLOAD calculates regression coefficients for six major ions: calcium, magnesium, sodium plus potassium, chloride, sulfate, and carbonate equivalent. Dissolved silica is not included in the regressions. Each ion is regressed separately, using the models:

$$\ln(ION_i) = a_i + b_i\,[\ln(Q)] \qquad (15)$$

and:

$$\ln(ION_i) = c_i + d_i\,[\ln(Q)] + e_i\,[\ln(K)] \qquad (16)$$

where

ION_i = the concentration of the ith ion, in milligrams per liter.

Daily loads are then estimated for each ion, summed by month, and saved and printed as the percent mass fraction of the dissolved solids. The user can convert these percentages into concentrations or loads for each ion by multiplying by the mean concentration or the load. The percentages of the six major ions, excluding silica, sum to 100. Therefore, when dissolved silica constitutes a substantial part of the dissolved solids, the use of these percentages will result in ion concentrations and loads that are too large.

USER NOTES

Data Requirements and the Sequence of Program Execution

To estimate dissolved solids for a streamflow-gaging station using the given programs, data need to be available from the WATSTORE system's water-quality file and daily-values file. Water-quality analyses need to include discharge and some measure of dissolved-solids concentration--ROE, SUM, or the major dissolved constituents. The daily-values file needs to include a complete record of discharge. If daily values of specific conductance are available, the accuracy of the estimates is improved.

The programs described in this report need to be executed in the following sequence:

1. Create a SAS data set and flag potential errors using the program FLAGIT.

2. Correct errors in the data set.

3. If necessary, fill in missing daily values of specific conductance using the program DVCOND.

4. Estimate dissolved solids by linear regression and save the results on a new data set using the program SLOAD.

Availability of Programs

The programs FLAGIT, DVCOND, and SLOAD were developed by the U.S. Geological Survey. They, and the accessory programs listed below, are stored on the U.S. Geological Survey's PRIME computer network, on node DCOLKA, in the directory FTS_DEPOT>SLOAD. These accessory programs may be useful for users with special needs.

SLOAD.CAL	Same as SLOAD, except that it provides annual summaries by calendar year instead of by water year.
LOADS.TO.PUNCH	Transfers output data from SLOAD to the user's punch queue.
MAG.TAPE.DUMP	Copies an entire data set to a reserved magnetic tape.

To copy a file to a local pathname on a PRIME node, use the command "FTR FTS_DEPOT>SLOAD>file pathname -SS DCOLKA."

PRIME users may send questions via electronic mail to RMIDDELBURG@DCOLKA. Other potential users may phone FTS-776-4886 or 303-236-4886 to arrange access to the programs.

Disk Storage and Space Requirements

The programs listed in the section "Availability of Programs" produce SAS data sets and store them using online disk space on the U.S. Geological Survey AMDAHL computer in Reston, Va. A retrieval of 40 years of record requires output storage of about 150 tracks on a 3350 disk device for FLAGIT and about 20 tracks for SLOAD. SLOAD also requires 2 blocks of 150 tracks each as temporary storage. Abnormal endings sometimes occur on online public disks if there is insufficient space to store the entire data set. If the user has access to private disk space, the chances of abnormal endings are decreased. The user who does not want to pay long-term storage charges for disk space may either delete a data set or copy it onto a less expensive magnetic tape using the SAS procedure PROC COPY.

Producing Submit Files

Once the original programs have been copied into the user's space, they need to be modified for the individual user. This requires changing the jobname, password, programmer's name, and class on the JOB statement, and inserting an appropriate user ID into the DD statements. These resulting template files then may be edited repeatedly to produce submit files. Editing is straightforward and consists of changing all occurrences of a unique string in the first 100 lines of the file. Required editing changes for FLAGIT, DVCOND, and SLOAD are listed in table 3. If a data set has been previously produced, the user needs to change the DISP parameter on the DD statement from (NEW,CATLG) to (OLD,KEEP). The user may alter the default flagging coefficients in FLAGIT by editing that part of the file directly below the line "*****MAKE CHANGES TO FLAGGING COEFFICIENTS HERE*****." The user may alter the default order of preference used in choosing the dissolved-solids parameter by altering the programming code in FLAGIT directly below the line "*****DEFINE TDS HERE*****."

Table 3.--*Editing requirements for submit files*

Unique String	Description	Example
	FLAGIT[1]	
FFFF	An appropriate file name, which conforms to standards for data-set names	EAGLGYP
SSSSSSSS	8-digit streamflow-gaging station identifier	09069000
XXXX	Beginning water year	1960
YYYY	Ending water year	1970
ZZZZ	Beginning calendar year	1959
VVVVVV	Volume number of daily-values backfile	115614
WWWWWW	Volume number of water-quality backfile	113924
	DVCOND[2]	
FFFF	An appropriate file name	LEES
YYYY	Year that regulation began	1963
ZZ	Month that regulation began	3
	SLOAD[3]	
FFFF	An appropriate file name	EAGLGYP

[1]The example program retrieves data for streamflow-gaging station 09069000, Eagle River near Gypsum, Colo., for water years 1960 through 1970. Volume numbers are listed in Hutchinson, 1975. The volume number refers to the State in which the streamflow-gaging station is located and does not necessarily coincide with the State that collects the data. By default, the data set is saved online on the data set USERID.SALT.EAGLGYP.

[2]The example program would fill in all missing daily values for specific conductance during the period of regulation for the Colorado River at Lees Ferry, Ariz., just downstream from Lake Powell. Regulation began in March 1963. By default, the example program modifies the data set USERID.SALT.LEES. Use of the program DVCOND is necessary only when there is not a strong relation between dissolved solids and discharge.

[3]By default, the example program executes on the data set USERID.SALT.EAGLGYP and saves the output on the online data set USERID.SALT.SLOAD.EAGLGYP.

Contents of Output Data Sets

The program FLAGIT creates four subfiles, or SAS data sets, within the DDNAME, or system data set, specified in the DD statement of the Job Control Language:

.QW	Water-quality data
.DV	Daily-values data
.QWBAD	Deleted water-quality data
.DVBAD	Deleted daily-values data

The program DVCOND does not create a new data set; instead it modifies the data set created by FLAGIT. The program SLOAD creates five subfiles within the DDNAME:

.MLOAD	Monthly values, including dissolved-solids load, flow-weighted dissolved-solids concentration, discharge, and mass fractions of ions.
.ALOAD	Annual values, summed by water year.
.BYMONTH	Mean values for each month of the year, averaged over the entire period of record.
.REGR	Regression coefficients and statistics, seven observations per group (load plus six ions).
.SUBST	Number of observations and substitutions (for example, ROE substituted for DS) per group.

Both FLAGIT and SLOAD execute the SAS procedure PROC CONTENTS, which displays the space occupied by these subfiles, and displays a listing of the variables they contain.

Editing Data Sets

Once potential errors have been identified by the program FLAGIT, there is no easy procedure to make necessary changes to the SAS data set. The user may write a batch job, edit the data set in Time-Sharing Option (TSO) using the SAS procedure PROC EDITOR, update the WATSTORE records, or devise other methods to make changes to the data set. Attachment A-1 in the section "Attachments" at the end of the report presents general procedures for editing files in TSO.

SUMMARY

Current emphasis on the causes and effects of dissolved-solids concentration in streams requires estimates of historical dissolved-solids concentrations and loads. Because of the nature of data-collection practices, it is difficult to derive reliable estimates of salinity. This manual presents a set of SAS-language computer programs that retrieve WATSTORE data from the U.S. Geological Survey's AMDAHL computer and estimate dissolved-solids concentrations and loads based on regression analysis.

When possible, dissolved-solids concentration is computed as the sum of eight major dissolved constituents; otherwise, the dissolved-solids concentration parameter retrieved from WATSTORE is used. Using regression coefficients derived from water-quality analyses, daily dissolved-solids loads are estimated by applying the coefficients to daily-values data. This method requires a consistent record of daily values of discharge and specific conductance and concurrent water-quality analyses.

The program FLAGIT indicates potential errors in the data for verification by the user. Tests for errors include day-to-day comparisons, comparison of the three values for dissolved-solids concentration, the ratio of concentration to specific conductance, and ionic-charge balance.

For streamflow-gaging stations having extensively regulated flow, concentration is independent of discharge, and daily values of specific-conductance data are needed. For these stations, the program DVCOND fills in missing specific-conductance data by linear interpolation.

The regression models in program SLOAD are based on the relation among specific conductance, dissolved-solids concentration, discharge, and dissolved-solids load. Load is simply the product of concentration and discharge. Concentration may be expressed either as a function of specific conductance or, less accurately, as a function of discharge. Thus load is modeled as a function of specific conductance and discharge or, when specific conductance is not available, as a function of discharge. Using 3-year moving groups, loads for each water year are estimated by separate regressions. Using ionic concentrations, either as a function of discharge or of specific conductance and discharge, the percent mass fractions of six major ionic constituents also are estimated. Regression coefficients and monthly and annual concentrations, loads, and mass fractions are printed and stored on SAS data sets.

The programs FLAGIT, DVCOND, and SLOAD, as well as several related programs, are stored on the U.S. Geological Survey's PRIME computer network. The programs execute and store output on the AMDAHL computer. Techniques for executing programs and editing SAS data sets are supplied.

These programs provide a reliable basis for computerized estimation of dissolved-solids concentrations and loads, using a minimum of user effort. The generation of numerous graphs enables rapid visual examination of the output data. The flagging procedure enables potential data errors to be located easily.

The monthly and annual output variables may be used to analyze trends or to provide correlation with changes in water- and land-use practices. Seasonal mean values also are output by month, giving a perspective on the yearly cycle. The regression coefficients could be used to extend the dissolved-solids estimates beyond the period for which water-quality analyses are available.

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ATTACHMENTS

ATTACHMENT A-1. -- TIME-SHARING OPTION PROCEDURES
1 -- MISCELLANEOUS TIME-SHARING OPTION COMMANDS

Time-Sharing Option (TSO) is one of AMDAHL's interactive modes and is one method of directly inspecting or changing a SAS data set. It is a relatively inflexible mode; once an error is made, TSO will insist on a correct response before it will proceed. Other methods for changing a SAS data set may be available, but are beyond the scope of this report.

Prompt	Command	Explanation
OK,	netlink -to amdahl	Connect to AMDAHL from PRIME network
AMDAHL connected	tlogon	Log on to TSO
Enter USERID	id/password	
PROCEDURE NAME	bigalc	Big allocation
READY	listc	List cataloged files
READY	listd filename	Specific file information
READY	delete filename	Delete a file
READY	rename oldname newname	Change file name
READY	profile char(!) line(~)	Specify keys for backspace and rubout (line delete). Because the normal keyboard keys for backspace and rub-out do not function in TSO, the PROFILE command is used. These characters will remain in effect during future TSO sessions, until a new PROFILE command is given.
READY	SAS	Enter SAS subsystem
?		Standard SAS prompt
?	ENDSAS; or /*	Exit SAS subsystem
READY	logoff	Log off TSO
ID LOGGED OFF	@	Netlink command level
@	quit	Exit from Netlink, back to PRIME

ATTACHMENT A-1. -- TIME-SHARING OPTION PROCEDURES--Continued
2 -- FILE ALLOCATION

To access a SAS data set in TSO, it first needs to be allocated. This is the equivalent of the batch command "DD DSN=file." The easiest method is to allocate before entering the SAS subsystem. The TSO command

```
AL F(D1) DA(SALT.SLOAD.CISCO) UNIT(ONLINE) VOL(PUB050)
```

is equivalent to

```
//D1 DD DSN=SALT.SLOAD.CISCO,UNIT=ONLINE,VOL=SER=PUB050...
```

Unit and volume only need to be specified if the file is not cataloged.

After entering SAS, the data set is accessed by commands such as:

```
DATA DDD; SET D1.MLOAD;
```

or

```
PROC EDITOR DATA=D1.ALOAD; RUN;
```

To sort, plot, or merge data sets while in interactive SAS, the user first needs to allocate sufficient temporary storage space to the file name USER (SAS Institute, Inc., 1982, p. 875). Give the TSO commands

```
ATTRIB SASDCB DSORG(DA) RECFM(U) DELETE TEMP.SAS
```

and

```
AL F(USER) DA(TEMP.SAS) SPACE(6 2) CYL USING(SASDCB)
```

before entering the SAS subsystem.

Files also may be allocated while in the SAS subsystem, using the command

```
TSO AL F(D1) DA(data.set.name) ;
```

The semicolon is required.

ATTACHMENT A-1. -- TIME-SHARING OPTION PROCEDURES--Continued
3 -- EDITING DATA SETS

Inspecting a File

Two procedures are available in interactive SAS for file inspection: PROC EDITOR and PROC BROWSE. EDITOR enables the user to make changes to the SAS data set, and any changes made are permanent on that data set. BROWSE is for inspection only and does not permit changes to be made.

Prompt	Command	Explanation
READY	SAS	Enter SAS subsystem
?		Standard SAS prompt
?	PROC BROWSE DATA=D1.QW;RUN;	Enter BROWSE mode on D1.QW
>		BROWSE and EDITOR prompt
>	L 1,3;	List observations 1 to 3
>	B;L;	List last observation
>	FIND 1,LAST TDS=.;	Find first occurence of missing value for TDS
>	FIND 100,200 P00095<250;	Search observations 100 to 200 for first occurence of a value of P00095 less than 250
>	FIND 1,LAST WY=1978;	Jump to water year 1978
>	END;	Exit from BROWSE mode
?	ENDSAS;	Exit SAS subsytem
READY		

Changing Existing Data

Prompt	Command	Explanation
?	PROC EDITOR DATA=D1.DV;RUN;	Enter EDITOR mode
>	L 1375;	Move to observation 1375
>	VERIFY ON;	Display all changes
>	R DCOND=1200;	Change value of DCOND in current line to 1200
>	R 1380,1385 DCOND=.;	Set DCOND to missing for observations 1380 to 1385
>	R DCOND=675 DISCHARG=12000;	Change several variables in current line
>	L;	Display this observation
>	END;	Exit EDITOR mode
?		

Deleting Observations

The delete command in PROC EDITOR does not actually delete an observation; it merely sets all values to missing (.). Thus a subsequent DATA step is necessary.

Prompt	Command	Explanation
?	PROC EDITOR DATA=D2.QW;RUN;	Enter EDITOR mode
>	F 1,LAST DIS=.;	Locate first occurence of missing discharge
>	D;	Delete current observation
>	D 135,137;	Delete several observations
>	END;	Exit EDITOR mode
?	DATA D2.QW; SET D2.QW;	Delete those observations permanently
?	IF DATE EQ. THEN DELETE;RUN;	
?	ENDSAS;	Exit SAS subsystem

Adding Observations

There is no simple way to add an observation to a SAS data set while in TSO. DATE cannot be entered directly. Any observations added while using PROC EDITOR will be concatenated to the end of the data set. PROC SORT then is necessary. The following procedure is cumbersome, but reliable. Its use is applicable only for temporary data sets; the changes can be transferred to the permanent data set when the procedure is complete. The data set F(USER) needs to be previously allocated in order for PROC SORT to execute properly. (See Attachment A-1.2.)

Prompt	Command	Explanation
?	DATA DDD; SET D2.DV;	Temporary data set
?	M=MONTH(DATE); D=DAY(DATE);	Convert DATE
?	Y=YEAR(DATE);	
?	DROP COUNT;	Will revise it later
?	RUN;	Execute DATA step
?	PROC EDITOR DATA=DDD;RUN;	Enter EDIT mode
>	VERIFY ON;	Verify changes
>	B;	Move to bottom
>	A M=10 D=1 Y=1951 DISCHARG=13000	
>	DCOND=560 STATCODE=3;	Add an observation
>	L;	Display observation;
>	END;	Exit EDITOR mode
?	DATA DDD; SET DDD;	
?	IF DATE EQ. THEN DATE=MDY(M,D,Y)	Reconstruct DATE
?	DROP M D Y;	Delete temporary variables
?	STATION='ssssssss';	
	SNAME='nnnnnnnn';	Add other variables
?	RUN;	Execute DATA step
?	PROC SORT DATA=DDD;BY DATE;RUN;	Sort by date
?	DATA DDD;SET DDD;	
?	RETAIN COUNT 9000; COUNT+1;	Use 9000 for .DV,
?	RUN;	0000 for .QW
?	DATA D2.DV; SET DDD;RUN;	Revise the permanent data set, when satisfied
?	ENDSAS;	Exit SAS subsystem

Printing

The procedure PROC PRINT will display the SAS data set at the terminal. If the data set is large, the process will be time consuming. If the number of variables is large, observations probably will "wrap around" the screen. This can be avoided if the user creates a temporary data set containing only the observations of interest before executing PROC PRINT.

Prompt	Command/Explanation
?	PROC PRINT DATA=D3.BYMONTH;RUN; Print all observations and all variables.
?	PROC PRINT DATA=D3.BYMONTH; VAR MON MLOAD MQAFT MTDS;RUN; Print all observations, and selected variables.
?	DATA DDDD; SET D3.MLOAD;
?	IF WY NE 1968 THEN DELETE;RUN;
?	PROC PRINT DATA=DDDD;
?	VAR MTDS M915 M945 MNAK MCO3;RUN; Print a restricted set of observations, and selected variables. Note the use of temporary data sets. Using the DATA statement, the user can create any desired subset of observations.
?	PROC CONTENTS DATA=D3._ALL_ NOSOURCE;RUN; List contents of the data set. This includes the space occupied, the number of observations, and a list of variable names for each subset of the data set.

Plots and Graphs

SAS can produce plots and graphs on any interactive terminal, using the same procedures that create plots and graphs on a line printer. In addition, the SAS/GRAPH option can produce publication-quality plots and graphs on a graphics terminal or a plotter. Its use, however is beyond the scope of this report. Before attempting to produce interactive plots or graphs, the user needs to allocate the temporary data set F(USER). (See Attachment A-1.2.)

Prompt	Command/Explanation
?	PROC PLOT DATA=D2.QW;
?	PLOT TDS*DIS;RUN;
	A simple plot of TDS versus DIS
?	PROC PLOT DATA=D3.ALOAD;
?	PLOT M925*WY='M' / VAXIS= 1 TO 10 BY 1; RUN;
	Specify the plotting symbol 'M' and specify the tick marks on the vertical axis.
?	PROC PLOT DATA=D3.BYMONTH;
?	PLOT MCO3*MONTH='C' M945*MONTH='S' / OVERLAY; RUN;
	Display several variables on the same plot.
?	DATA JJJJ; SET D3.MLOAD;
?	TIME=YEAR+(MONTH-.5)*12; RUN;
?	PROC PLOT DATA=JJJJ;
?	PLOT MQAFT*TIME / VAXIS 1000 10000 100000; RUN;
	Produce a logarithmic vertical scale. The scale VAXIS 1 3 10 30 100 also produces logarithmic plots. Note the use of a temporary data set, which contains the user-created variable TIME.
?	PROC CHART DATA=D2.DV;
?	VBAR DCOND / TYPE=PERCENT; RUN;
	Produce a vertical bar chart showing the percent frequency distribution of the variable DCOND.

ATTACHMENT A-2. -- LISTING OF PROGRAMS
1 -- FLAGIT

```
//JOB##### JOB (PASSWORD#,FLAG,5,40),'YOUR NAME',
//  CLASS=F
//*
//*****  USER'S MANUAL VERSION OF FLAGIT  *****    (TDL 10-15-84)
//*    THIS PROGRAM IS A PRE-PROCESSOR FOR THE SALTLOADS PROGRAM.
//*    * RETRIEVE DATA FROM WATSTORE DV & QW FILES, PLACE ON SAS DATA
//*    * SETS, MASSAGE DATA INTO MORE USABLE FORM, FLAG POSSIBLE ERRORS,
//*    * DISPLAY THE DATA SET, AND GIVE A FEW BASIC PLOTS & REGRESSIONS.
//*
//*    * ALLOWS USER TO SET NON-DEFAULT VALUES FOR FLAGGING COEFFICIENTS.
//*
//* USER INPUT:  XXXX =BEGINNING WATER YEAR,
//*              YYYY =ENDING WATER YEAR
//*              ZZZZ =BEGINNING CALENDAR YEAR
//*              FFFF =NAME OF DATA FILE
//*              VVVVVV =VOLUME NAME OF DAILY VALUES FILE
//*              WWWWWW =VOLUME NAME OF WATER-QUALITY FILE
//*              SSSSSSSS =STATION IDENTIFIER NUMBER
//* USER INPUT:  CHANGE VALUES OF FLAGGING COEFFICIENTS, IF DESIRED
//* USER INPUT:  CHANGE DISPOSITION OF OUTPUT FILE, IF NECESSARY
//*
/*SETUP    VVVVVV/H,WWWWWW/H
//PROCLIB DD DSN=WRD.PROCLIB,DISP=SHR
//  EXEC QWRETR,VOL1=WWWWWW
//HDR.SYSIN DD *
M3  XXXX    YYYY        X
XQWSAS
000060000610009500915009250093000933
000935009400094500955703007030100410
0004409044095440004459041O
D SSSSSSSS
/*
//   EXEC  DVRETR,AGENCY=USGS,VOL1=VVVVVV
//HDR.SYSIN DD *
M3  ZZZZ10  YYYY09
R0006000095
F0000300011
D SSSSSSSS
/*
// EXEC WRDSAS,MACRO=DV,DSN='&&BKREC',TIME1=5,REGION=700K
//DISK DD DSN=USERID.SALT.FFFF,
//  UNIT=ONLINE,
//  DISP=(NEW,CATLG),SPACE=(TRK,(150,20),RLSE)
//* DISP=(OLD,KEEP)
//SYSIN DD *
PROC QWSAS DATE DECTIME;
DATA QW; SET;
DVINPUT _SNAME _STATCOD
DATA DV; SET;
```

```
PROC SORT DATA=DV; BY PARMCODE DATE;
DATA FLAGS;
  INPUT LABEL $CHAR40. ;
**---------------------------;
**DEFINITION OF BASIC TERMS   ;
**---------------------------;
* DV       = DAILY-VALUES INFORMATION;
* QW       = WATER-QUALITY INFORMATION;
* TDS      = TOTAL DISSOLVED SOLIDS, MG/L;
* SOC      = P70301 = TDS, SUM OF CONSTITUENTS;
* ROE      = P70300 = TDS, RESIDUE ON EVAPORATION;
* CTDS     = TDS, SUM OF CONSTITUENTS AS CALCULATED IN THIS PROGRAM;
* Q        = DISCHARGE:  DV= MEAN DAILY,  QW= P00060 OR P00061;
* COND.    = SPECIFIC CONDUCTANCE:  DV= MEAN DAILY,  QW= P00095;
**------------------------------------------------------;
**USER DEFINABLE FLAGGING COEFFICIENTS                   ;
**VALUES LISTED HERE ARE DEFAULT, CHANGE AS DESIRED      ;
**------------------------------------------------------;
*****MAKE CHANGES TO FLAGGING COEFFICIENTS HERE*****;
  FL1 = 100    /*  % DIFF. BETWEEN DV Q AND PREVIOUS DV Q */ ;
  FL2 =  50    /*  % DIFF. BETWEEN DV Q AND QW Q */ ;
  FL3 =  50    /*  % DIFF. BETWEEN DV COND. AND PREVIOUS DV COND. */ ;
  FL4 =  50    /*  % DIFF. BETWEEN DV COND. AND QW COND. */ ;
  FL5 =   .55  /*  LOWER BOUND FOR  RATIO OF TDS TO QW COND. */ ;
  FL6 =   .75  /*  UPPER BOUND FOR RATIO OF TDS TO QW COND. */ ;
  FL7 =  10    /*  % DIFF. BETWEEN TDS AND ROE */ ;
  FL8 =  10    /*  % DIFF. BETWEEN CTDS AND SOC */ ;
  FL9 =   5    /*  % ERROR IN CHARGE BALANCE */ ;
  FL10=  2.    /*  # OF STD DEV. IN CHARGE BALANCE */ ;
  COUNT=  0;
  CARDS        /*  NEXT LINE IS A LABEL LINE */  ;
DEFAULT COEFFICIENTS
;
DATA DVQ; SET DV;
  IF DATE EQ LAG(DATE) AND STATCODE NE LAG(STATCODE) THEN DELETE;
  IF PARMCODE NE 00060 THEN DELETE;
  DISCHARG=VALUE;
DATA DVC; SET DV;
  IF DATE EQ LAG(DATE) AND STATCODE NE LAG(STATCODE) THEN DELETE;
  IF PARMCODE NE 00095 THEN DELETE;
  DCOND=VALUE;
DATA DV1; MERGE DVQ DVC; BY DATE;
  DROP PARMCODE VALUE;
PROC SORT DATA=QW; BY DATE;
DATA QW1; SET QW;
* COMPUTE CTDS;
* CALCIUM, MAGNESIUM, CHLORIDE, SULFATE, & SILICA;
  IF P00915 NE. AND P00925 NE. AND P00940 NE. AND P00945 NE.
      AND P00955 NE.   THEN
      SUM1=P00915+P00925+P00940+P00945+P00955;
    ELSE SUM1=.;
```

```
* SODIUM,POTASSIUM;
  NA=0; K=0; NAK=P00930;
  IF P00933 NE. THEN DO;
    NA=P00933; NAK=P00933; END;
  IF P00930 NE. AND P00935 NE. THEN  NAK=P00930+P00935;
  IF P00930 NE. THEN NA=P00930;
  IF P00935 NE. THEN K =P00935;
* CARBONATE EQUIVALENT;
  IF P00440 EQ. THEN DO;
    IF P90440 NE. THEN P00440=P90440;
    ELSE IF P95440 NE. THEN P00440=P95440;
   END;
  IF P00445 NE. AND P00440 NE. THEN CO3=P00445 + P00440/2.03;
    ELSE IF P00440 NE. THEN CO3= P00440/2.03;
    ELSE IF P00410 NE. THEN CO3= P00410*.6;
    ELSE IF P90410 NE. THEN CO3= P90410*.6;
    ELSE CO3=.;
  IF SUM1 NE. AND NAK NE. AND CO3 NE.  THEN
      CTDS= SUM1 + NAK + CO3;
  DROP P00930 P00933 P00935 P00410 P00445 P00440 P90440 P95440 P90410;
*****DEFINE TDS HERE*****;
** DEFAULT PRIORITY   CTDS>P70301>P70300;
  IF CTDS NE. THEN DO;
     TDS=CTDS; FLTDS='CTDS';     END;
   ELSE IF P70301 NE. THEN DO;
     TDS=P70301; FLTDS='SOC';    END;
   ELSE IF P70300 NE. THEN DO;
     TDS=P70300; FLTDS='ROE';    END;
* DEFINE DIS (i.e. DISCHARGE);
  IF P00061 NE. THEN DO;
     DIS=P00061; FLQ='61';       END;
   ELSE IF P00060 NE. THEN DO;
     DIS=P00060; FLQ='60';       END;
  DROP P00061 P00060;
DATA QW2 QWBAD; SET QW1;
* DELETE USELESS OBSERVATIONS FROM QW FILE;
  IF TDS EQ. THEN DO;
     TEST='NOTDS';  OUTPUT QWBAD;     END;
   ELSE IF DIS EQ. THEN DO;
     TEST='NO Q';   OUTPUT QWBAD;     END;
   ELSE IF DATE EQ LAG(DATE) AND ABS(TDS-LAG(TDS)) LT .1  THEN DO;
     TEST='D,TDS';  OUTPUT QWBAD;     END;
* RUN LAG TESTS TO FIND DUPLICATE LISTINGS OF AN ANALYSIS;
   ELSE IF ABS(P00095-LAG1(P00095)) LT .1  AND  ABS(TDS-LAG1(TDS)) LT .1
     AND LAG1(TDS) NE. THEN DO;  TEST='LAG1';  OUTPUT QWBAD;      END;
   ELSE IF ABS(P00095-LAG2(P00095)) LT .1  AND  ABS(TDS-LAG2(TDS)) LT .1
     AND LAG2(TDS) NE. THEN DO;  TEST='LAG2';  OUTPUT QWBAD;      END;
   ELSE IF ABS(P00095-LAG3(P00095)) LT .1  AND  ABS(TDS-LAG3(TDS)) LT .1
     AND LAG3(TDS) NE. THEN DO;  TEST='LAG3';  OUTPUT QWBAD;      END;
```

```
   ELSE IF ABS(P00095-LAG4(P00095)) LT .1  AND  ABS(TDS-LAG4(TDS)) LT .1
     AND LAG4(TDS) NE. THEN DO;  TEST='LAG4';  OUTPUT QWBAD;      END;
   ELSE   OUTPUT QW2;
DATA DISK.QW; SET QW2;
  DROP TEST;
  RETAIN COUNT 0000; COUNT+1;
  WY=YEAR(DATE); IF MONTH(DATE) GT 9 THEN WY=WY+1;
  FORMAT DIS 9.2 TDS 8.1 CTDS 8.1 SUM1 7.1 NAK 7.1 CO3 7.1 P00095 5. ;
  FORMAT P00915 7.1 P00925 7.1 P00940 7.1 P00945 7.1 P00955 6.1 ;
  FORMAT P70300 5. P70301 5. ;
DATA DV2 DVBAD; SET DV1;
* DELETE USELESS OBSERVATIONS FROM DV FILE;
  IF DATE EQ LAG(DATE)  THEN DO;
     CHECK='DUPL';  OUTPUT DVBAD;     END;
   ELSE IF DISCHARG EQ. THEN DO;
     CHECK='NO Q';  OUTPUT DVBAD;     END;
   ELSE  OUTPUT DV2;
DATA DISK.DV; SET DV2;
  DROP CHECK;
  RETAIN COUNT 9000; COUNT+1;
  WY=YEAR(DATE); IF MONTH(DATE) GT 9 THEN WY=WY+1;
  SNAME=SUBSTR(SNAME,1,37);
  FORMAT  DISCHARG 9.2  DCOND 5. ;
PROC PRINT DATA=FLAGS; BY LABEL;
  TITLE 'LIST OF COEFFICIENTS USED IN FLAGGING ROUTINE';
  VAR FL1-FL10;
DATA FLAGGED; MERGE DISK.QW DISK.DV; BY DATE;
DATA FLAGGED FOUT; SET FLAGS FLAGGED;
**--------------------------------------------------------------------;
**               FLAG POTENTIALLY INCORRECT DATA                       ;
**--------------------------------------------------------------------;
* THESE FLAGS DIFFER SLIGHTLY FROM EARLIER VERSIONS;
*      '123456789012 '= FLAG                                   DEFAULT;
*                                                               VALUES;
*       D            = DUPLICATE DATE;
*       M            = MISSING DATE;
*FL1     Q          = DV Q AND PREVIOUS DV Q DIFFER BY >FL1      100% ;
*FL2      W         = DV Q AND QW Q DIFFER BY >FL2                50% ;
*FL3       C        = DCOND AND PREVIOUS DCOND DIFFER BY >FL3     50% ;
*FL4        I       = DCOND AND P00095 DIFFER BY >FL4             50% ;
*FL5,FL6     R      = TDS/P00095 RATIO IS <FL5 OR >FL6      .55, .75 ;
*FL7          T     = TDS AND ROE DIFFER BY >FL7                  10% ;
*FL8           Z    = CTDS AND SOC DIFFER BY >FL8                 10% ;
*               6   = P00060 SUBSTITUTED FOR P00061;
*                1  = P70301 SUBSTITUTED FOR CTDS;
*                0  = P70300 SUBSTITUTED FOR CTDS;
*                   CHARGE BALANCE:   ;
*FL9              % = OFF BY >FL9                                  5% ;
*FL10,FL9         s = OFF BY >FL10 STD. DEV., BUT <FL 9%      2.0, 5% ;
*                  + = CATIONS > ANIONS;
*                  - = ANIONS > CATIONS;
```

```
IF COUNT EQ 0 THEN DO;
  FLL1=FL1;FLL2=FL2;FLL3=FL3;FLL4=FL4;FLL5=FL5;FLL6=FL6;
  FLL7=FL7;FLL8=FL8;FLL9=FL9;FLL10=FL10;
  DELETE;
 END;
RETAIN FLL1-FLL10;
BAD=0;
FORMAT FLAG $CHAR12. ;
IF DATE EQ LAG(DATE) THEN SUBSTR(FLAG,1,1)='D';
IF LAG(DATE) NE. AND DATE GT LAG(DATE)+1  THEN DO;
   SUBSTR(FLAG,1,1)='M';  BAD=1;  END;
IF (ABS(DISCHARG-LAG(DISCHARG))/MIN(DISCHARG,LAG(DISCHARG))) GT FLL1/100
   AND LAG(DISCHARG) NE.
      THEN SUBSTR(FLAG,2,1) = 'Q';
IF DIS NE. THEN DO;
   IF (ABS(DISCHARG-DIS)/MIN(DISCHARG,DIS)) GT FLL2/100
      THEN SUBSTR(FLAG,3,1)='W';
 END;
IF DCOND NE. AND LAG(DCOND) NE.  AND
 (ABS(DCOND-LAG(DCOND))/MIN(DCOND,LAG(DCOND))) GT FLL3/100
   THEN SUBSTR(FLAG,4,1)='C';
IF DCOND NE. AND P00095 NE. THEN DO;
   IF (ABS(DCOND-P00095)/MIN(DCOND,P00095)) GT FLL4/100
      THEN SUBSTR(FLAG,5,1)='I';
 END;
IF P00095 NE. THEN DO;
   IF (TDS/P00095) LT FLL5  OR  (TDS/P00095) GT FLL6
      THEN DO;  SUBSTR(FLAG,6,1)='R';  BAD=1;  END;
 END;
IF P70300 NE. THEN DO;
   IF (ABS(TDS-P70300)/MIN(TDS,P70300)) GT FLL7/100
      THEN DO;  SUBSTR(FLAG,7,1)='T';  BAD=1;  END;
 END;
IF CTDS NE. AND P70301 NE. THEN DO;
   IF (ABS(CTDS-P70301)/MIN(CTDS,P70301)) GT FLL8/100
      THEN DO;  SUBSTR(FLAG,8,1)='Z';  BAD=1;  END;
 END;
IF FLTDS EQ 'SOC' THEN SUBSTR(FLAG,10,1)='1';
IF FLTDS EQ 'ROE' THEN SUBSTR(FLAG,10,1)='0';
IF FLQ EQ '60' THEN SUBSTR(FLAG,9,1)='6';
* CHARGE BALANCE;
IF CTDS NE.  THEN DO;
  SCAT = P00915*.04990 + P00925*.08229 + NA*.04350 + K*.02558;
  SAN  = P00940*.02821 + P00945*.02082 + CO3*.03333;
  SIONS = SAN + SCAT;
  IF (ABS(SAN-SCAT)/(SAN+SCAT)) GT FLL9/100  THEN DO;
     SUBSTR(FLAG,11,1)='%';  BAD=1;  END;
   ELSE IF (ABS(SAN-SCAT)/(.1065+.0155*SAN)) GT FLL10  THEN
     SUBSTR(FLAG,11,1)='s';
```

```
    IF SUBSTR(FLAG,11,1) NE ' '  THEN DO;
      IF SAN GT SCAT  THEN SUBSTR(FLAG,12,1)='-';
       ELSE SUBSTR(FLAG,12,1)='+';
    END;
  END;
  DROP NA K FL1-FL10 LABEL FLL1-FLL10 ;
* END OF FLAGGING SESSION;
  IF TDS GT 0 THEN LTDS=LOG(TDS);
  IF DIS GT 0 THEN LDIS=LOG(DIS);
  IF P00095 GT 0 THEN LCOND=LOG(P00095);
  FORMAT SIONS 5.1  ;
  IF BAD EQ 1  THEN OUTPUT FOUT;
  OUTPUT FLAGGED;
DATA DISK.QW; SET DISK.QW;
  DROP  NA K CTDS P70301 P70300 SUM1;
PROC PRINT DATA=FLAGGED UNIFORM SPLIT=*; BY STATION;
  TITLE 'COMBINED DATA SET, WITH POSSIBLE ERRORS FLAGGED';
  VAR FLAG DATE DISCHARG DCOND DIS P00095 CTDS P70301 P70300 SUM1
      NAK CO3 SIONS ;
  LABEL  DISCHARG ='  DV*DISCH.'
    DCOND     =' DV*COND.'
    DATE      ='DATE'
    P70301    =' SOC*P70301'
    P70300    =' ROE*P70300'
    CTDS      ='CALC.* TDS'
    DIS       ='  QW*DISCH.'
    P00095    =' QW*COND.'
    SUM1      ='Ca,Mg,Cl* SO4,Si'
    NAK       ='Na,K'
    CO3       ='Carbon.* equiv.'
    SIONS     ='Sum of*meq/L' ;
PROC PRINT DATA=QWBAD UNIFORM; BY STATION;
  TITLE 'DATA DISCARDED FROM QW FILE';
  VAR DATE DIS P00095 CTDS P70301 P70300 SUM1 NAK CO3 TEST;
DATA DISK.QWBAD; SET QWBAD;
  DROP NA K;
DATA DISK.DVBAD; SET DVBAD;
PROC PRINT DATA=DVBAD UNIFORM; BY STATION;
  TITLE 'DATA DISCARDED FROM DV FILE';
  VAR DATE DISCHARG DCOND CHECK STATCODE SNAME;
PROC PRINT DATA=FOUT  UNIFORM; BY STATION;
  TITLE 'QW OBSERVATIONS WITH FLAGS: M, R, T, Z, OR %';
  TITLE2 'MOST LIKELY TO DEGRADE THE ACCURACY OF ESTIMATED LOADS';
  VAR  DATE FLAG P00095 CTDS P70301 P70300 SIONS;
PROC GLM DATA=FLAGGED;
  TITLE 'LINEAR REGRESSION ON QW DATA:  TDS = a + b(CONDUCTANCE)';
  MODEL TDS=P00095;
PROC GLM DATA=FLAGGED;
  TITLE 'LOG-LOG REGRESSION ON QW DATA:  TDS = a * (DISCHARGE)**b';
  MODEL LTDS=LDIS;
```

```
PROC GLM DATA=FLAGGED;
  TITLE 'LOG-LOG REGRESSION ON QW DATA:  TDS = a * (DISCH.)**b * (COND)**C';
  MODEL LTDS=LDIS LCOND;
PROC PLOT DATA=FLAGGED;
  TITLE 'DAILY VALUES:  DCOND VS. DISCHARG';
  PLOT DCOND*DISCHARG;
PROC PLOT DATA=FLAGGED;
  TITLE 'CONDUCTANCE:  DAILY VS. QW';
  PLOT DCOND*P00095;
PROC PLOT DATA=FLAGGED;
  TITLE 'QW VALUES:  TDS  VS.  DISCHARGE';
  PLOT TDS*DIS;
PROC PLOT DATA=FLAGGED;
  TITLE 'CHARGE BALANCE:  SUM OF CATIONS  VS.  SUM OF ANIONS';
  PLOT SCAT*SAN  / HZERO VZERO ;
PROC PLOT DATA=FLAGGED;
  TITLE 'QW VALUES:  TDS VS. COND';
  PLOT TDS*P00095;
PROC CONTENTS DATA=DISK._ALL_ NOSOURCE;
  TITLE ' ';
/*
//
```

ATTACHMENT A-2. -- LISTING OF PROGRAMS
2 -- DVCOND

```
//JOB##### JOB (PASSWORD#,COND,1,10),'YOUR NAME',
// CLASS=C
//*
//*****  USER'S MANUAL VERISON OF DVCOND ***** (TDL 11-21-84)
//*    THIS PROGRAM FILLS IN MISSING DAILY CONDUCTANCE VALUES.
//*    NOTE: USE ONLY WHEN FLOW IS COMPLETELY REGULATED
//*    LOGIC:
//*     1)  IF <10 CONSECUTIVE MISSING DAYS, FILL IN
//*         BY INTERPOLATING FROM THE BOUNDARY DCOND VALUES.
//*     2)  OTHERWISE, FILL IN LARGE GAPS BY INSERTING QW P00095
//*         INTO DCOND, THEN INTERPOLATING BETWEEN VALUES.
//*    USER INPUT:   FFFF = FILE NAME
//*                  YYYY = YEAR THAT REGULATION BEGAN
//*                    ZZ = MONTH THAT REGULATION BEGAN
//*
//  EXEC SAS,TIME=5
//DISK DD DSN=USERID.SALT.FFFF,
//  DISP=(OLD,KEEP),UNIT=ONLINE
//SYSIN DD *
DATA DVPRE DVPOST; SET DISK.DV;
**SEPARATE DV RECORD INTO PRE-REGULATION AND POST-REG. PERIODS;
  MONTH=MONTH(DATE);  YEAR=YEAR(DATE);
  IF YEAR EQ YYYY AND MONTH GE ZZ THEN OUTPUT DVPOST;
  ELSE IF YEAR GT YYYY THEN OUTPUT DVPOST;
  ELSE OUTPUT DVPRE;
  DROP MONTH YEAR COUNT;
DATA D1; SET DVPOST;
**BEGIN PROCEDURE TO FILL IN SMALL GAPS, USING  ONLY DV COND VALUES;
  RETAIN COUNT 0000; COUNT+1;
  RETAIN EC1;  CHK=0;
  RETAIN N1 0000; N1+1;
  IF DCOND NE. THEN DO;
     EC1=DCOND; N1=1; CHK=1;
   END;
PROC SORT DATA=D1; BY DESCENDING COUNT;
DATA D1; SET D1;
  RETAIN EC3;
  IF EC1 NE. THEN EC3=EC1;
   ELSE EC1=EC3;
  RETAIN BCOUNT 0000; BCOUNT+1;
  IF COUNT EQ 1 OR BCOUNT EQ 1  THEN CHK=1;
  RETAIN EC2; IF CHK EQ 1  THEN EC2=EC1;
  RETAIN N2;
  IF BCOUNT EQ 1 THEN N2=N1;
   ELSE IF N1 GT LAG(N1)  THEN N2=N1;
PROC SORT DATA=D1; BY COUNT;
```

ATTACHMENT A-2. -- LISTING OF PROGRAMS--Continued
2 -- DVCOND--Continued

```
DATA D1; SET D1;
  IF CHK EQ 0   AND   N2 LE 10   THEN DO;
     DCOND= EC1 + (EC2-EC1)*(N1-1)/N2;
     FL1='EST';   FL2='ESTDV';
   END;
  DROP EC1 EC2 EC3 N1 N2 COUNT BCOUNT CHK;
  FLAG='KEEP';
DATA QW; SET DISK.QW;
**NOW FILL IN BIG GAPS BY INSERTING QW AND THEN INTERPOLATING;
  KEEP DATE P00095;
  IF DATE EQ LAG(DATE) THEN DELETE;
DATA D2; MERGE D1 QW;  BY DATE;
  IF FLAG NE 'KEEP' THEN DELETE;
  IF DCOND EQ. AND P00095 NE.  THEN DO;
     DCOND=P00095;
     FL1='EST';   FL2='00095';
   END;
  DROP P00095;
DATA D2; SET D2;
  RETAIN COUNT 0000; COUNT+1;
  RETAIN EC1;  CHK=0;
  RETAIN N1 0000; N1+1;
  IF DCOND NE. THEN DO;
     CHK=1; N1=1;  EC1=DCOND;
   END;
PROC SORT DATA=D2; BY DESCENDING COUNT;
DATA D2; SET D2;
  RETAIN EC3;
  IF EC1 NE. THEN EC3=EC1;
   ELSE EC1=EC3;
  RETAIN BCOUNT 0000; BCOUNT+1;
  IF COUNT EQ 1 OR BCOUNT EQ 1 THEN CHK=1;
  RETAIN EC2;   IF CHK EQ 1  THEN EC2=EC1;
  RETAIN N2;
  IF BCOUNT EQ 1  THEN N2=N1;
   ELSE IF N1 GT LAG(N1)  THEN N2=N1;
PROC SORT DATA=D2; BY COUNT;
DATA D2; SET D2;
  IF CHK EQ 0    THEN DO;
     DCOND= EC1 + (EC2-EC1)*(N1-1)/N2;
     FL1='EST';   FL2='ESTQW';
    END;
   ELSE IF DCOND EQ. THEN DO;
*   FIRST OR LAST OBSV.;
    DCOND=EC2; FL1='EST'; FL2='ESTQW';
    END;
```

```
  DROP FLAG EC1 EC2 EC3 N1 N2 COUNT BCOUNT CHK;
DATA DISK.DV; SET DVPRE D2;
**NOW REJOIN THE DATASET;
  RETAIN COUNT 9000; COUNT+1;
DATA DDD; SET DISK.DV;
  IF FL2 EQ 'ESTDV' THEN EDV=1;
  ELSE IF FL2 EQ '00095' THEN QW=1;
  ELSE IF FL2 EQ 'ESTQW' THEN EQW=1;
  ELSE IF DCOND NE. THEN DV=1;
  ELSE MISS=1;
  KEEP STATION DATE WY DV EDV QW EQW MISS;
PROC MEANS DATA=DDD NOPRINT;  BY WY;
  VAR DV EDV QW EQW MISS;
  OUTPUT OUT=DSUM SUM=SDV SEDV SQW SEQW SMISS;
PROC PRINT DATA=DSUM UNIFORM SPLIT=*;
  TITLE 'DAILY VALUES CONDUCTANCE: METHOD OF GENERATION OF DATA';
  VAR WY SDV SEDV SQW SEQW SMISS;
  LABEL WY='WATER*YEAR'
    SDV='ORIGINAL*DV COND'
    SEDV='ESTIMATED BY*DV COND INTERP.'
    SQW='ORIGINAL*QW COND'
    SEQW='ESTIMATED BY*QW COND INTERP.'
    SMISS='  MISSING*  DV COND*NOT REPLACED';
  SUM SDV SEDV SQW SEQW SMISS;
PROC CONTENTS DATA=DISK._ALL_ NOSOURCE;
/*
//
```

ATTACHMENT A-2. -- LISTING OF PROGRAMS
3 -- SLOAD

```
//JOB##### JOB (PASSWORD#,LOAD,5,20),'YOUR NAME',
// CLASS=E
//*
//*****  USER'S MANUAL VERSION OF SLOAD  *****    (TDL 10-22-84)
//*    THIS PROGRAM USES DATA SETS CREATED BY THE FLAGIT PROGRAM.
//*    * PERFORMS LOG-LOG REGRESSION TO PREDICT TDS & IONS LOADS
//*    * FROM DAILY VALUES DATA.  REGRESSION COEFFICIENTS, MONTHLY
//*    * AND ANNUAL LOADS ARE STORED ON OUTPUT FILE.
//*
//* USER INPUT:  FFFF = NAME OF DATA FILE
//* USER INPUT:  CHANGE DISPOSITION OF OUTPUT FILE, IF NECESSARY
//*
//  EXEC SAS,TIME=5,REGION=700K
//DISK  DD DSN=USERID.SALT.FFFF,
//  DISP=SHR,UNIT=ONLINE
//DISK2 DD DSN=USERID.SALT.SLOAD.FFFF,
//  UNIT=ONLINE,
//  DISP=(NEW,CATLG),SPACE=(TRK,(20,5),RLSE)
//* DISP=(OLD,KEEP)
//FT20F001 DD DSN=&&FT20,SPACE=(TRK,150),DISP=(,PASS),
//  UNIT=3350,VOL=SER=PUBT01
//FT21F001 DD DSN=&&FT21,SPACE=(TRK,150),DISP=(,PASS),
//  UNIT=3350,VOL=SER=PUBT01
//HEADR1   DD DSN=&&HEADR1,SPACE=(TRK,5),DISP=(,PASS),
//  UNIT=ONLINE
//HEADR2   DD DSN=&&HEADR2,SPACE=(TRK,5),DISP=(,PASS),
//  UNIT=ONLINE
//SYSIN DD *
DATA D1 H1; SET DISK.DV;
**CREATE HEADER CONTAINING STATION NAME & NUMBER;
  FORMAT STNAME $CHAR37.  ;
  RETAIN STNAME; IF COUNT EQ 9001 THEN DO;
    STNAME=SUBSTR(SNAME,1,37);
    OUTPUT H1;                          END;
  OUTPUT D1;
  DROP SNAME;
DATA _NULL_; SET H1;  FILE HEADR1;
  PUT @3 'TITLE STATION:' +2 STATION $CHAR9. +5 STNAME $CHAR37. +1 ';'  ;
DATA QW1; SET DISK.QW;
  KEEP STATION DATE WY COUNT LQ LCOND KLOD L915 L925 L940
       L945 LNAK LCO3 W1 WYST SROE NOSROE SQ NOSQ;
  SROE=0; NOSROE=0; SQ=0; NOSQ=0;
  RETAIN WYST;
  IF COUNT EQ 1 THEN WYST=WY;
  W1=WY;
  IF DIS GT 0  THEN DO;
    LQ=LOG(DIS);
    IF FLQ EQ '60'  THEN SQ=1;
     ELSE NOSQ=1;
   END;
```

```
  IF P00095 GT 0  THEN LCOND=LOG(P00095);
  IF TDS GT 0 AND DIS GT 0  THEN DO;
    KLOD=LOG(TDS*DIS*.0027)    /* tons/day */  ;
    IF FLTDS EQ 'ROE' THEN SROE=1;
     ELSE NOSROE=1;
   END;
  IF FLTDS EQ 'CTDS' THEN DO;
    IF P00915 LE 0 THEN P00915=.1;
    IF P00925 LE 0 THEN P00925=.1;
    IF P00940 LE 0 THEN P00940=.1;
    IF P00945 LE 0 THEN P00945=.1;
    IF NAK    LE 0 THEN    NAK=.1;
    IF CO3    LE 0 THEN    CO3=.1;
    L915=LOG(P00915);
    L925=LOG(P00925);
    L940=LOG(P00940);
    L945=LOG(P00945);
    LNAK=LOG(NAK);
    LCO3=LOG(CO3);
   END;
PROC SORT DATA=QW1; BY DESCENDING COUNT;
DATA QW1 H2; SET QW1;
  RETAIN BCOUNT 0000; BCOUNT+1;
  RETAIN WYEND;  IF BCOUNT EQ 1 THEN DO;
    WYEND=W1;
    OUTPUT H2;                     END;
  OUTPUT QW1;
  DROP W1 BCOUNT;
DATA _NULL_; SET H2;  FILE HEADR2;
  PUT @3 'TITLE3 FOR THE PERIOD:  WATER YEARS' +1 WYST 4. +1 'TO'
      +1 WYEND 4. ';'  ;
DATA GRUPZ; SET QW1;
** BREAK QW DATA INTO GROUPS FOR 3-YEAR SLIDING REGRESSION;
  DO  YR = WYST TO WYEND;
    IF YR EQ WYST  THEN DO;
      IF WY=YR OR WY=YR+1 OR WY=YR+2  THEN DO;
        GROUP=YR;  OUTPUT;
       END;
     END;
    ELSE IF YR EQ WYEND  THEN DO;
      IF WY=YR OR WY=YR-1 OR WY=YR-2  THEN DO;
        GROUP=YR;  OUTPUT;
       END;
     END;
    ELSE DO;
      IF WY=YR-1 OR WY=YR OR WY=YR+1  THEN DO;
        GROUP=YR;  OUTPUT;
       END;
     END;
   END;
```

```
PROC SORT DATA=GRUPZ; BY GROUP;
DATA GROUP1 GROUP2 GROUP3 GROUP4; SET GRUPZ;
  OUTPUT GROUP1;
  IF L915 NE. THEN OUTPUT GROUP2;
  IF LCOND NE. THEN OUTPUT GROUP3;
  IF L915 NE. AND LCOND NE. THEN OUTPUT GROUP4;
* ELIMINATE GROUPS THAT HAVE LESS THAN 3 OBSERVATIONS;
DATA GROUP1; SET GROUP1;
  RETAIN GCOUNT 0000; GCOUNT+1;  RETAIN C1;
  IF GROUP NE LAG(GROUP) OR GCOUNT EQ 1  THEN C1=1;
  ELSE  C1=C1+1;
PROC SORT DATA=GROUP1; BY DESCENDING GCOUNT;
DATA GROUP1; SET GROUP1;
  RETAIN BGCOUNT 0000; BGCOUNT+1;  RETAIN C2;
  IF C1 GE LAG(C1) OR BGCOUNT=1  THEN C2=C1;
PROC SORT DATA=GROUP1; BY GCOUNT;
DATA GROUP1; SET GROUP1;
  IF C2 LT 3  THEN DELETE;
  DROP C1 C2 GCOUNT BGCOUNT;
DATA GROUP2; SET GROUP2;
  RETAIN GCOUNT 0000; GCOUNT+1;  RETAIN C1;
  IF GROUP NE LAG(GROUP) OR GCOUNT EQ 1  THEN C1=1;
  ELSE  C1=C1+1;
PROC SORT DATA=GROUP2; BY DESCENDING GCOUNT;
DATA GROUP2; SET GROUP2;
  RETAIN BGCOUNT 0000; BGCOUNT+1;  RETAIN C2;
  IF C1 GE LAG(C1) OR BGCOUNT=1  THEN C2=C1;
PROC SORT DATA=GROUP2; BY GCOUNT;
DATA GROUP2; SET GROUP2;
  IF C2 LT 3  THEN DELETE;
  DROP C1 C2 GCOUNT BGCOUNT;
DATA GROUP3; SET GROUP3;
  RETAIN GCOUNT 0000; GCOUNT+1;  RETAIN C1;
  IF GROUP NE LAG(GROUP) OR GCOUNT EQ 1  THEN C1=1;
  ELSE  C1=C1+1;
PROC SORT DATA=GROUP3; BY DESCENDING GCOUNT;
DATA GROUP3; SET GROUP3;
  RETAIN BGCOUNT 0000; BGCOUNT+1;  RETAIN C2;
  IF C1 GE LAG(C1) OR BGCOUNT=1  THEN C2=C1;
PROC SORT DATA=GROUP3; BY GCOUNT;
DATA GROUP3; SET GROUP3;
  IF C2 LT 3  THEN DELETE;
  DROP C1 C2 GCOUNT BGCOUNT;
DATA GROUP4; SET GROUP4;
  RETAIN GCOUNT 0000; GCOUNT+1;  RETAIN C1;
  IF GROUP NE LAG(GROUP) OR GCOUNT EQ 1  THEN C1=1;
  ELSE  C1=C1+1;
```

```
PROC SORT DATA=GROUP4; BY DESCENDING GCOUNT;
DATA GROUP4; SET GROUP4;
  RETAIN BGCOUNT 0000; BGCOUNT+1;  RETAIN C2;
  IF C1 GE LAG(C1) OR BGCOUNT=1  THEN C2=C1;
PROC SORT DATA=GROUP4; BY GCOUNT;
DATA GROUP4; SET GROUP4;
  IF C2 LT 3  THEN DELETE;
  DROP C1 C2 GCOUNT BGCOUNT;
PROC PRINTTO UNIT=20 NEW;
** DERIVE REGRESSION STATISTICS;
** IT IS MORE EFFICIENT TO USE 'PROC REG....OUTEST=...' TO STORE THE     ;
** REGRESSION COEFFICIENTS, BUT THAT DOES NOT STORE R-SQUARE, ETC.       ;
PROC GLM DATA=GROUP1; BY GROUP;
  MODEL KLOD = LQ;
PROC GLM DATA=GROUP2; BY GROUP;
  MODEL L915 L925 L940 L945 LNAK LCO3 = LQ;
PROC PRINTTO;
PROC PRINTTO UNIT=21 NEW;
PROC GLM DATA=GROUP3; BY GROUP;
  MODEL KLOD = LQ LCOND;
PROC GLM DATA=GROUP4; BY GROUP;
  MODEL L915 L925 L940 L945 LNAK LCO3 = LQ LCOND;
PROC PRINTTO;
DATA REGR1; INFILE FT20F001  EOF=NEXT;
  FORMAT VARNAME $4.;
  INPUT #2  GROUP=4.;
  INPUT #6  S1 $ S2 $ VARNAME $     /* e.g. L915  */  ;
  INPUT #10 S1 $ DUM1 DUM2 DUM3 DUM4 DUM5 RSQR1;
  INPUT #14 S1$ S2 $ N1 DUM1 SE1;
  INPUT #25 S1 $ A;
  INPUT #26 S1 $ B;
  OUTPUT;
  KEEP GROUP VARNAME N1 RSQR1 SE1 A B;
  FORMAT RSQR1 7.5   SE1 7.5  A 8.5  B 8.5  N1 4.  ;
NEXT:
DATA REGR2; INFILE FT21F001  EOF=NEXT2;
  FORMAT VARNAME $4.;
  INPUT #2  GROUP=4.;
  INPUT #6  S1 $ S2 $ VARNAME $;
  INPUT #10 S1 $ DUM1 DUM2 DUM3 DUM4 DUM5 RSQR2;
  INPUT #14 S1 $ S2 $ N2 DUM1 SE2;
  INPUT #26 S1 $ C;
  INPUT #27 S1 $ D;
  INPUT #28 S1 $ E;
  OUTPUT;
  KEEP GROUP VARNAME N2 RSQR2 SE2 C D E;
  FORMAT RSQR2 7.5  SE2 7.5  C 8.5  D 8.5  E 8.5  N2 4.  ;
NEXT2:
```

```
PROC MEANS DATA=GRUPZ NOPRINT; BY GROUP;
** SUM THE NUMBER OF SUBSTITUTIONS;
  ID STATION GROUP;
  VAR  SROE NOSROE SQ NOSQ;
  OUTPUT OUT=SUBST  SUM= ROE NOROE Q NQ;
DATA DISK2.SUBST; SET SUBST;
  SUBR= ROE/(ROE+NOROE)*100;
  SUBQ= Q/(Q+NQ)*100;
  NQW=  Q+NQ;
  KEEP STATION GROUP NQW SUBR SUBQ;
  FORMAT NQW 3. SUBR 5.1 SUBQ 5.1;
PROC PRINT DATA=DISK2.SUBST SPLIT=*;
  %INCLUDE  HEADR1;
  TITLE2 'SUMMARY OF QW OBSERVATIONS, BY 3-YEAR SLIDING GROUP';
  VAR GROUP NQW SUBR SUBQ;
  LABEL  NQW  ='# OF QW* OBSV.'
         SUBR ='% P70300* SUBST.'
         SUBQ ='% P00060* SUBST.'
         GROUP='WATER* YEAR'       ;
PROC SORT DATA=REGR1; BY GROUP VARNAME;
PROC SORT DATA=REGR2; BY GROUP VARNAME;
DATA DISK2.REGR; MERGE REGR1 REGR2;  BY GROUP VARNAME;
  N1=N1+1;  N2=N2+1;
  FORMAT CNAME $CHAR9.  ;
  IF VARNAME EQ 'KLOD' THEN CNAME='SALT LOAD';
   ELSE IF VARNAME EQ 'L915' THEN CNAME='Calcium  ';
   ELSE IF VARNAME EQ 'L925' THEN CNAME='Magnesium';
   ELSE IF VARNAME EQ 'L940' THEN CNAME='Chloride ';
   ELSE IF VARNAME EQ 'L945' THEN CNAME='Sulfate  ';
   ELSE IF VARNAME EQ 'LNAK' THEN CNAME='Sodium +K';
   ELSE IF VARNAME EQ 'LCO3' THEN CNAME='Carbonate';
PROC PRINT DATA=DISK2.REGR  SPLIT=* UNIFORM;  BY GROUP;
  %INCLUDE  HEADR1;
  TITLE2 'REGRESSION STATISTICS, BY 3-YEAR SLIDING GROUPS';
  TITLE3 'REGRESSION #1:   VARIABLE = e**A * DISCHARGE**B              ';
  TITLE4 'REGRESSION #2:   VARIABLE = e**C * DISCHARGE**D * COND**E';
  TITLE5 'VARIABLE=(mg/L), except for SALT LOAD (tons/day)';
  TITLE6 'DISCHARGE= (cfs)  COND=(uMHOS/cm)';
  VAR  CNAME N1 RSQR1 SE1 A B N2 RSQR2 SE2 C D E;
  LABEL RSQR1 ='R-square*   #1'
        RSQR2 ='R-square*   #2'
        N1    ='  #1*obsv.'
        N2    ='  #2*obsv.'
        CNAME ='VARIABLE'
        SE1   =' Std.*Error'
        SE2   =' Std.*Error'  ;
** REGRESSION INFORMATION IS NOW COMPLETE,          ;
** SO PREDICT LOADS BASED ON DAILY VALUES,          ;
** BY ADDING ONE CONSTITUENT AT A TIME.             ;
```

```
DATA D1; SET D1;
  MONTH= MONTH(DATE);
  KEEP STATION STNAME DATE WY MONTH DISCHARG DCOND;
DATA RTDS R915 R925 R940 R945 RNAK RCO3;  SET DISK2.REGR;
  RENAME GROUP=WY;
  DROP RSQR1 RSQR2 SE1 SE2;
  IF VARNAME EQ 'KLOD' THEN OUTPUT RTDS;
   ELSE IF VARNAME EQ 'L915' THEN OUTPUT R915;
   ELSE IF VARNAME EQ 'L925' THEN OUTPUT R925;
   ELSE IF VARNAME EQ 'L940' THEN OUTPUT R940;
   ELSE IF VARNAME EQ 'L945' THEN OUTPUT R945;
   ELSE IF VARNAME EQ 'LNAK' THEN OUTPUT RNAK;
   ELSE IF VARNAME EQ 'LCO3' THEN OUTPUT RCO3;
DATA D1;  MERGE RTDS D1;  BY WY;
 DAYS=1; NOC=0;
  IF DCOND NE. AND C NE. THEN
    LOAD=EXP(C)*DISCHARG**D*DCOND**E      /* tons/day */  ;
  ELSE DO;
    LOAD=EXP(A)*DISCHARG**B;  NOC=1;
   END;
  DROP A B C D E;
DATA D1; MERGE D1 R915; BY WY;
  IF DCOND NE. AND C NE. THEN  L915=EXP(C)*DISCHARG**D*DCOND**E;
   ELSE L915=EXP(A)*DISCHARG**B;
  L915= L915*DISCHARG*.0027;
  DROP A B C D E;
DATA D1; MERGE D1 R925; BY WY;
  IF DCOND NE. AND C NE. THEN  L925=EXP(C)*DISCHARG**D*DCOND**E;
   ELSE L925=EXP(A)*DISCHARG**B;
  L925= L925*DISCHARG*.0027;
  DROP A B C D E;
DATA D1; MERGE D1 R940; BY WY;
  IF DCOND NE. AND C NE. THEN  L940=EXP(C)*DISCHARG**D*DCOND**E;
   ELSE L940=EXP(A)*DISCHARG**B;
  L940= L940*DISCHARG*.0027;
  DROP A B C D E;
DATA D1; MERGE D1 R945; BY WY;
  IF DCOND NE. AND C NE. THEN  L945=EXP(C)*DISCHARG**D*DCOND**E;
   ELSE L945=EXP(A)*DISCHARG**B;
  L945= L945*DISCHARG*.0027;
  DROP A B C D E;
DATA D1; MERGE D1 RNAK; BY WY;
  IF DCOND NE. AND C NE. THEN  LNAK=EXP(C)*DISCHARG**D*DCOND**E;
   ELSE LNAK=EXP(A)*DISCHARG**B;
  LNAK= LNAK*DISCHARG*.0027;
  DROP A B C D E;
DATA D1; MERGE D1 RCO3; BY WY;
  IF DCOND NE. AND C NE. THEN  LCO3=EXP(C)*DISCHARG**D*DCOND**E;
   ELSE LCO3=EXP(A)*DISCHARG**B;
  LCO3= LCO3*DISCHARG*.0027;
```

```
  DROP A B C D E;
PROC MEANS DATA=D1 NOPRINT; BY WY MONTH  NOTSORTED;
** DAILY PREDICTIONS ARE NOW COMPLETE, SO SUM BY MONTH;
  ID STATION STNAME WY MONTH;
  VAR DISCHARG LOAD DAYS NOC L915 L925 L940 L945 LNAK LCO3;
  OUTPUT OUT=MLOAD SUM=MQ MLOAD MD MNOC M915 M925 M940 M945 MNAK MCO3;
DATA DISK2.MLOAD; SET MLOAD;
**IONS ARE INPUT IN TONS, & THUS ARE FLOW-WEIGHTED;
  MQAFT=MQ*1.9835                               /* ACREFEET */    ;
  MLAFT=MLOAD/MQAFT                             /* TONS/ACREFOOT */    ;
  MTDS=MLAFT*735.29                             /* mg/L */    ;
  SUMT=SUM(M915,M925,M940,M945,MNAK,MCO3)       /* TONS */    ;
  SUMC=SUMT/MQAFT*735.29                        /* mg/L */    ;
  ESTERR= (SUMC-MTDS)/MTDS*100                  /* PERCENT */    ;
  M915=M915/SUMT*100                            /* PERCENT */    ;
  M925=M925/SUMT*100;
  M940=M940/SUMT*100;
  M945=M945/SUMT*100;
  MNAK=MNAK/SUMT*100;
  MCO3=MCO3/SUMT*100;
  YEAR=WY; IF MONTH GT 9  THEN YEAR=YEAR-1;
  DROP MQ SUMC SUMT;
  FORMAT MQAFT 9. MLAFT 6.3 MLOAD 9. MTDS 7.1 MD 3. MNOC 3. MONTH 2.
   M915 5.2 M925 5.2 M940 5.2 M945 5.2 MNAK 5.2 MCO3 5.2  ESTERR 6.1
    WY 4.  YEAR 4.   ;
PROC PRINT DATA=DISK2.MLOAD SPLIT=* UNIFORM;
  %INCLUDE  HEADR1;
  TITLE2 'MONTHLY DISSOLVED SOLIDS, PREDICTED BY REGRESSION';
  TITLE3 'IONS ARE EXPRESSED AS PERCENT OF TOTAL SALT LOAD, BY WEIGHT';
  VAR MONTH YEAR MLOAD MLAFT MQAFT MTDS M915 M925 M940 M945 MNAK MCO3
      ESTERR MD MNOC;
  LABEL MLOAD=' SALT* LOAD*(tons)' MLAFT='SALT LOAD*(tons per*acre foot)'
        MQAFT=' DISCHARGE*(acre feet)'  MTDS=' MEAN* TDS*(mg/L)'
        M915=' Ca*(%)' M925=' Mg*(%)' M940=' Cl*(%)' M945='SO4*(%)'
        MNAK='Na+K*(%)'
        MCO3=' CO3*equiv.* (%)'  ESTERR='  %*diff.'
        MD='# OF*DAYS'  MNOC=' W/O*COND.'  ;
PROC MEANS DATA=MLOAD NOPRINT; BY WY;
  ID STATION STNAME WY;
  VAR MQ MLOAD MD MNOC M915 M925 M940 M945 MNAK MCO3;
  OUTPUT OUT=ALOAD SUM=AQ ALOAD AD ANOC A915 A925 A940 A945 ANAK ACO3;
DATA DISK2.ALOAD; SET ALOAD;
  AQAFT=AQ*1.9835;
  ALAFT=ALOAD/AQAFT;
  ATDS=ALAFT*735.29;
  SUMT=SUM(A915,A925,A940,A945,ANAK,ACO3);
  SUMC=SUMT/AQAFT*735.29;
  ESTERR= (SUMC-ATDS)/ATDS*100;
  A915=A915/SUMT*100;
  A925=A925/SUMT*100;
```

```
  A940=A940/SUMT*100;
  A945=A945/SUMT*100;
  ANAK=ANAK/SUMT*100;
  ACO3=ACO3/SUMT*100;
  DROP AQ SUMT SUMC;
  FORMAT AQAFT 9. ALAFT 6.3 ALOAD 9. ATDS 7.1 AD 3. ANOC 3. WY 4.
   ESTERR 6.1 A915 5.2 A925 5.2 A940 5.2 A945 5.2 ANAK 5.2 ACO3 5.2 ;
PROC PRINT DATA=DISK2.ALOAD SPLIT=* UNIFORM;
  %INCLUDE  HEADR1;
  TITLE2 'ANNUAL DISSOLVED SOLIDS';
  TITLE3 'SUMMED BY WATER YEAR, PREDICTED BY REGRESSION';
  TITLE4 'IONS ARE EXPRESSED AS PERCENT OF TOTAL SALT LOAD, BY WEIGHT';
  VAR WY ALOAD ALAFT AQAFT ATDS A915 A925 A940 A945 ANAK ACO3 ESTERR
    AD ANOC;
  LABEL WY='Water* Year'  ALOAD=' SALT* LOAD*(tons)'
    ALAFT='SALT LOAD*(tons per*acre foot)' AQAFT=' DISCHARGE*(acre feet)'
    ATDS=' MEAN* TDS*(mg/L)' A915=' Ca*(%)' A925=' Mg*(%)' A940=' Cl*(%)'
    A945='SO4*(%)' ANAK='Na+K*(%)' ACO3=' CO3*equiv.* (%)'
    ESTERR='  %*diff.' AD='# of*days'
    ANOC=' w/o*Cond.'   ;
PROC SORT  OUT=BYMONTH  DATA=DISK2.MLOAD;  BY MONTH;
PROC MEANS DATA=BYMONTH NOPRINT; BY MONTH;
**GIVE SEASONAL VARIATIONS, BY MONTH;
** IONS ARE INPUT AS mg/L, & THUS ARE NOT FLOW-WEIGHTED;
  ID STATION STNAME MONTH;
  VAR MLOAD MQAFT M915 M925 M940 M945 MNAK MCO3;
  OUTPUT OUT=BYMONTH   MEAN=MLOAD MQAFT M915 M925 M940 M945 MNAK MCO3;
DATA DISK2.BYMONTH; SET BYMONTH;
  MLAFT=MLOAD/MQAFT;
  MTDS=MLAFT*735.29;
  D=11; Y=1999;
  FORMAT  MON WORDDATE9.  ;
  MON= MDY(MONTH,D,Y)  ;
  DROP D Y;
  FORMAT  MLOAD 9.  MQAFT 9.  MLAFT 6.3  MTDS 7.1  MONTH 2.  M915 6.2
          M925 6.2  M940 6.2  M945 6.2  MNAK 6.2  MCO3 6.2   ;
PROC PRINT DATA=DISK2.BYMONTH SPLIT=* UNIFORM;
  %INCLUDE  HEADR1;
  TITLE2 'SEASONAL MEANS: GROUPED BY MONTH';
  %INCLUDE  HEADR2;
  VAR MON MLOAD MLAFT MQAFT MTDS M915 M925 M940 M945 MNAK MCO3;
  LABEL  MON='Month'  MLOAD=' SALT* LOAD*(tons)'
    MLAFT='SALT LOAD*(tons per*acre foot)'  MQAFT=' DISCHARGE*(acre feet)'
    MTDS=' MEAN* TDS*(mg/L)'  MCO3=' CO3*equiv.* (%)'
   M915=' Ca*(%)'  M925=' Mg*(%)'  M940=' Cl*(%)'  M945='SO4*(%)'
   MNAK='Na+K*(%)' ;
PROC PLOT DATA=DISK2.ALOAD;
  %INCLUDE  HEADR1;
  TITLE2 'ANNUAL LOAD, DISSOLVED SOLIDS CONCENTRATION, AND DISCHARGE';
  TITLE3 'LOAD: L=tons    CONCENTRATION: C=mg/L    DISCHARGE: Q=acre feet';
```

```
  PLOT ALOAD*WY='L' ATDS*WY='C' AQAFT*WY='Q';
PROC PLOT DATA=DISK2.BYMONTH;
  %INCLUDE  HEADR1;
  TITLE2 'MEAN SEASONAL LOAD, CONCENTRATION, AND DISCHARGE: GROUPED BY MONTH';
  %INCLUDE  HEADR2;
  TITLE4 'LOAD: L=tons    CONCENTRATION: C=mg/L    DISCHARGE: Q=acre feet';
  TITLE5 'MONTH #1 = JANUARY, etc.';
  PLOT MLOAD*MONTH='L' MTDS*MONTH='C' MQAFT*MONTH='Q';
PROC CHART DATA=DISK2.MLOAD;
  %INCLUDE  HEADR1;
  TITLE2 'FREQUENCY DISTRIBUTION OF MONTHLY DISCHARGE';
  TITLE3 '(acre feet per month)';
  VBAR MQAFT / TYPE=PERCENT;
PROC CHART DATA=DISK2.MLOAD;
  %INCLUDE HEADR1;
  TITLE2 'FREQUENCY DISTRIBUTION OF MONTHLY TOTAL DISSOLVED SOLIDS';
  TITLE3 '(mean umhos/cm)';
  VBAR MTDS / TYPE=PERCENT;
PROC CHART DATA=DISK2.MLOAD;
  %INCLUDE  HEADR1;
  TITLE2 'FREQUENCY DISTRIBUTION OF MONTHLY SALT LOAD';
  TITLE3 '(tons per month)';
  VBAR MLOAD / TYPE=PERCENT;
PROC PLOT DATA=DISK2.MLOAD;
  %INCLUDE  HEADR1;
  TITLE2 'MONTHLY SALT LOAD vs. DISCHARGE';
  TITLE3 'tons vs. acre feet';
  PLOT MLOAD*MQAFT;
PROC PLOT DATA=DISK2.MLOAD;
  %INCLUDE HEADR1;
  TITLE2 'MONTHLY TOTAL DISSOLVED SOLIDS vs. DISCHARGE';
  TITLE3 'mg/L vs. acre feet';
  PLOT MTDS*MQAFT;
PROC PLOT DATA=DISK2.ALOAD;
  %INCLUDE  HEADR1;
  TITLE2 'ANNUAL BALANCE OF MAJOR IONS';
  TITLE3 'PERCENT COMPOSITION BY WEIGHT: BY WATER YEAR';
  TITLE4 'S =SO4     C =CO3     U =Ca     M =Mg     L =Cl     N =Na+K';
  PLOT A915*WY='U' A925*WY='M' A940*WY='L' A945*WY='S'
       ANAK*WY='N' ACO3*WY='C'  / OVERLAY  VAXIS= 1 3 10 30 100  ;
PROC PLOT DATA=DISK2.BYMONTH;
  %INCLUDE  HEADR1;
  TITLE2 'SEASONAL BALANCE OF MAJOR IONS';
  %INCLUDE  HEADR2;
  TITLE4 'PERCENT COMPOSITION BY WEIGHT: GROUPED BY MONTH';
  TITLE5 'S =SO4     C =CO3     U =Ca     M =Mg     L =Cl     N =Na+K' ;
  PLOT M915*MONTH='U' M925*MONTH='M' M940*MONTH='L' M945*MONTH='S'
       MNAK*MONTH='N' MCO3*MONTH='C'  / OVERLAY  VAXIS= 1 3 10 30 100  ;
PROC CONTENTS DATA=DISK2._ALL_ NOSOURCE;
  %INCLUDE  HEADR1;
/*
//
```

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS
1 -- FLAGIT: COMBINED DATA SET, WITH FLAGS

COMBINED DATA SET, WITH POSSIBLE ERRORS FLAGGED
STATION IDENTIFICATION NUMBER=09069000

OBS	FLAG	DATE	DV DISCH.	DV COND.	QW DISCH.	QW COND.	CALC. TDS	SOC P70301	ROE P70300	Ca,Mg,Cl SO4,Si	Na,K	Carbon. equiv.	Sum of meq/L
3164		68-05-20	480.00	323	.	.	.	.	.	.	.	.	.
3165		68-05-21	560.00	421	.	.	.	.	.	.	.	.	.
3166		68-05-22	870.00	327	.	.	.	.	.	.	.	.	.
3167		68-05-23	1090.00	325	.	.	.	.	.	.	.	.	.
3168	RT 6 %+	68-05-24	970.00	302	1061.00	291	369.6	370	188	305.3	9.1	55.2	15.7
3169		68-05-25	843.00	305	.	.	.	.	.	.	.	.	.
3170		68-05-26	798.00	295	.	.	.	.	.	.	.	.	.
3171		68-05-27	753.00	316	.	.	.	.	.	.	.	.	.
3172		68-05-28	807.00	244	.	.	.	.	.	.	.	.	.
3173		68-05-29	1170.00	317	.	.	.	.	.	.	.	.	.
3174		68-05-30	1430.00	242	.	.	.	.	.	.	.	.	.
3175		68-05-31	1720.00	229	.	.	.	.	.	.	.	.	.
3176	IRT 6	68-06-01	2010.00	229	2488.00	922	137.0	.	123	87.0	4.2	45.8	4.6
3177		68-06-02	2420.00	225	.	.	.	.	.	.	.	.	.
3178		68-06-03	2880.00	257	.	.	.	.	.	.	.	.	.
.													
.													
.													
3199		68-06-24	2480.00	195	.	.	.	.	.	.	.	.	.
3200		68-06-25	2260.00	201	.	.	.	.	.	.	.	.	.
3201	6	68-06-26	1910.00	251	1826.00	241	137.4	.	134	91.6	7.4	38.4	4.7
3202		68-06-27	1820.00	236	.	.	.	.	.	.	.	.	.
3203		68-06-28	1950.00	223	.	.	.	.	.	.	.	.	.
3204		68-06-29	1850.00	225	.	.	.	.	.	.	.	.	.
3205		68-06-30	1600.00	254	.	.	.	.	.	.	.	.	.
3206	6	68-07-01	1260.00	315	1083.00	359	215.3	.	225	154.0	14.0	47.3	7.2
3207		68-07-02	1060.00	345	.	.	.	.	.	.	.	.	.
3208		68-07-03	1090.00	333	.	.	.	.	.	.	.	.	.

This is an example of the listing of the data set retrieved from WATSTORE. Daily values and water-quality observations are merged into one temporary data set. There are two errors in the data on this page. First, calcium on 68-05-24 is reported as 230 mg/L instead of 32 mg/L, generating the flags "R", "T", and "%+". This error causes incorrect values to be computed for dissolved solids and the cation-anion balance. Secondly, the daily value of specific conductance on 68-06-01 is reported as 922 instead of 229, generating the flags "I" and "R". The flag "6" denotes substitution of parameter code 00061 for parameter code 00060.

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS--Continued

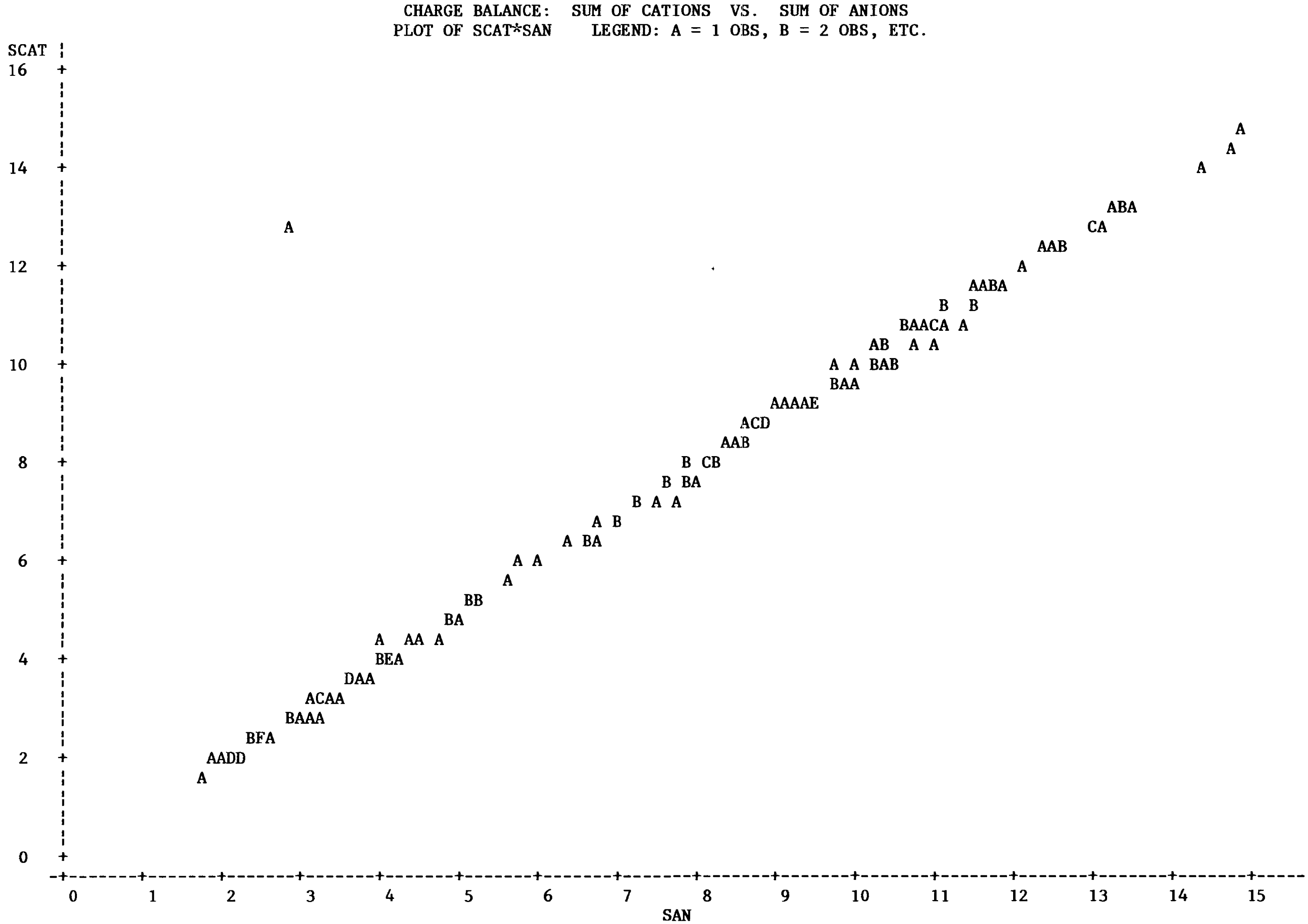
2 -- FLAGIT: WATER-QUALITY OBSERVATIONS WITH MAJOR FLAGS

QW OBSERVATIONS WITH THE FLAGS M, R, T, Z, OR %
MOST LIKELY TO DEGRADE THE ACCURACY OF ESTIMATED LOADS
--- STATION IDENTIFICATION NUMBER=09069000 ---

OBS	DATE	FLAG	P00095	CTDS	P70301	P70300	SIONS
1	60-05-19	T 6	250	177.1	.	158	6.0
2	61-05-01	IR 6	305	304.4	300	.	10.2
3	61-06-03	R 6	230	123.1	.	125	4.2
4	64-10-01	R 60	1210	.	.	948	.
5	66-04-30	R 60	261	.	.	198	.
6	66-05-27	T 6	210	116.6	120	133	4.1
7	67-06-14	R 60	264	.	.	145	.
8	68-03-01	T 6	861	552.2	552	608	18.3
9	68-05-24	RT 6 %+	291	369.6	370	188	15.7
10	68-06-01	IRT 6	922	137.0	.	123	4.6
11	68-06-13	T 6	193	113.7	.	100	3.9
12	69-04-01	T 6	756	463.1	.	515	15.6
13	69-05-01	W T 6	281	162.3	.	181	5.6
14	69-06-25	C T 6	707	470.2	.	534	15.9
15	69-09-01	T 6	815	506.0	.	563	16.8
16	70-01-26	T 6	1110	637.2	640	756	21.2
17	70-05-21	T 6	190	109.8	110	123	3.9
18	70-08-26	T 6	767	465.1	470	528	15.5

FLAGIT produces a compact list of water-quality observations that have generated major flags. This list enables the user to identify potential errors without having to examine the entire data set, which may exceed 200 pages of printed output. The variable P00095 is specific conductance. The variable SIONS is the sum of the absolute values of the sum of cations and sum of anions.

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS--Continued
3 -- FLAGIT: CATION-ANION BALANCE



This graph is useful for visually locating errors in the values of ionic constituents. SCAT is the sum of cations, SAN is the sum of anions. Note the obvious outlier representing the incorrect observation on 68-05-24 (see Attachment A-3.1), which contains the flag "%+". By using a straightedge to connect equal values on each axis, the outlier lies approximately on the line connecting the values 15.7, which equals the value of the variable SIONS for that outlier.

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS--Continued

4 -- FLAGIT: DISSOLVED-SOLIDS CONCENTRATIONS VERSUS SPECIFIC CONDUCTANCE

```
                                  QW VALUES:  TDS VS. COND
                          PLOT OF  DS*P00095    LEGEND: A = 1 OBS, B = 2 OBS, ETC.
  TDS I
800.0 +                                                                                              CA A AA
      I                                                                                           AA  BB B
      I                                                                                          BC  A
      I                                                                                     A AA AD A
      I                                                                                  A A  A  A
700.0 +                                                                              A   E  BABA A
      I                                                                              B BAC   A
      I                                                                              BBCAB   A
      I                                                                            AAAAAA       A
      I                                                                         BD  C    A
600.0 +                                                                     A  ABBA A
      I                                                                 A   A BABB
      I                                                                    ACCAB
      I                                                                A   AB  A
      I                                                              ACCBDB
500.0 +                                                             CA AB
      I                                                         DC  ACC
      I                                                       BABA BB
      I                                                      BAA
      I                                                    A  B
400.0 +                                                 ABCA A
      I                                               CA BA
      I                      A                 AA  B  B
      I                                          B ABA
      I                                       AAAB
300.0 +                       A             ABB
      I                                   AAE A
      I                              AA BAA
      I                            AACCCA
      I                           BCC
200.0 +                    A    BEDA
      I                   A AAGBB
      I                   DBDA
      I                CHFAA                                                     A
      I              BBFB
100.0 +            A B
      -+-------+-------+-------+-------+-------+-------+-------+-------+-------+-------+-------+-------+-------+-------+-------+-
       0      100     200     300     400     500     600     700     800     900    1000    1100    1200    1300    1400    1500
                                                SPECIFIC CONDUCTANCE (UMHOS)
```

This graph is the visual representation of equation 5. If the ratio of dissolved solids to specific conductance is outside the specified range, the flag "R" is generated. Note the three outliers, corresponding to the dates 61-05-01, 68-05-24, and 68-06-01 (see Attachments A-3.1 and A-3.2).

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS
5 -- SLOAD: MONTHLY DISSOLVED-SOLIDS LOADS

STATION: 09069000 EAGLE RIVER AT GYPSUM, CO.
MONTHLY DISSOLVED SOLIDS, PREDICTED BY REGRESSION
IONS ARE EXPRESSED AS PERCENT OF TOTAL SALT LOAD, BY WEIGHT

OBS	MONTH	YEAR	SALT LOAD (tons)	SALT LOAD (tons per acre foot)	DISCHARGE (acre feet)	MEAN TDS (mg/L)	Ca (%)	Mg (%)	Cl (%)	SO4 (%)	Na+K (%)	CO3 equiv. (%)	% diff.	# OF DAYS	W/O COND.
1	10	1959	14344	0.710	20208	521.9	19.63	3.58	12.94	38.10	9.99	15.77	-3.5	31	0
2	11	1959	12528	0.778	16094	572.4	19.05	3.56	13.70	38.57	10.33	14.80	-2.7	30	0
3	12	1959	10740	0.927	11582	681.8	17.96	3.52	15.15	39.34	10.95	13.08	-0.9	31	0
4	1	1960	10190	0.969	10513	712.7	17.67	3.51	15.56	39.50	11.11	12.65	-0.3	31	0
5	2	1960	8949	0.944	9479	694.2	17.58	3.54	15.70	39.36	11.14	12.68	-0.2	29	0
6	3	1960	11334	0.757	14969	556.7	18.76	3.60	14.11	38.43	10.46	14.64	-2.2	31	0
7	4	1960	12266	0.367	33446	269.7	21.06	3.86	10.89	34.54	8.75	20.90	-4.7	30	0
8	5	1960	15596	0.211	73854	155.3	22.74	3.89	8.25	30.55	7.18	27.39	-3.5	31	0
9	6	1960	26238	0.177	148624	129.8	24.21	3.66	6.27	28.20	6.06	31.61	-1.6	30	0
10	7	1960	16712	0.388	43024	285.6	21.63	3.74	10.24	34.61	8.50	21.29	-4.9	31	0
11	8	1960	11450	0.785	14595	576.9	18.62	3.58	14.28	38.65	10.55	14.33	-2.0	31	0
12	9	1960	11074	1.046	10584	769.3	17.71	3.44	15.44	39.87	11.13	12.42	-0.2	30	0
13	10	1960	12624	1.154	10939	848.5	17.65	3.35	15.46	40.33	11.20	12.02	0.2	31	0
14	11	1960	14578	1.091	13357	802.5	18.31	3.34	14.55	40.17	10.86	12.77	-1.0	30	0
15	12	1960	12785	1.076	11883	791.1	17.92	3.39	15.11	40.04	11.04	12.49	-0.4	31	0
16	1	1961	11070	1.082	10235	795.3	17.51	3.42	15.72	39.99	11.24	12.12	0.3	31	0
17	2	1961	9039	1.029	8785	756.6	17.41	3.48	15.90	39.74	11.26	12.21	0.3	28	0
18	3	1961	9378	0.949	9880	698.0	17.51	3.54	15.81	39.37	11.18	12.60	-0.1	31	0
19	4	1961	9150	0.785	11659	577.0	18.13	3.64	14.98	38.59	10.78	13.88	-1.4	30	0
20	5	1961	12141	0.205	59104	151.0	21.98	3.99	9.12	31.01	7.59	26.30	-3.2	31	0
21	6	1961	15913	0.189	84172	139.0	23.01	3.92	7.71	29.62	6.86	28.88	-4.6	30	7
22	7	1961	12644	0.553	22848	406.9	19.94	3.70	12.51	36.94	9.67	17.24	-3.8	31	0
23	8	1961	12687	0.745	17040	547.4	19.07	3.57	13.66	38.39	10.29	15.00	-2.7	31	1
24	9	1961	17136	0.479	35800	352.0	21.28	3.65	10.78	35.84	8.87	19.58	-4.9	30	0

This is an example of monthly output from SLOAD. Values given for ionic constituents represent the percent mass fraction of each. The value of percent difference represents the percent error between the dissolved-solids concentration and the sum of the ionic concentrations. The last column lists the number of days during the month that daily values of specific conductance were not available, that is, the number of days that estimates were based on discharge alone.

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS--Continued
6 -- SLOAD: ANNUAL DISSOLVED-SOLIDS LOADS

STATION: 09069000 EAGLE RIVER AT GYPSUM, CO.
ANNUAL DISSOLVED SOLIDS
SUMMED BY WATER YEAR, PREDICTED BY REGRESSION
IONS ARE EXPRESSED AS PERCENT OF TOTAL SALT LOAD, BY WEIGHT

OBS	Water Year	SALT LOAD (tons)	SALT LOAD (tons per acre foot)	DISCHARGE (acre feet)	MEAN DS (mg/L)	Ca (%)	Mg (%)	Cl (%)	SO4 (%)	Na+K (%)	CO3 equiv. (%)	% diff.	# of days	w/o Cond.
1	1960	161421	0.397	406971	291.6	20.32	3.64	11.86	35.61	9.22	19.36	-2.4	366	0
2	1961	149145	0.504	295702	370.9	19.36	3.59	13.14	37.25	9.93	16.74	-2.0	365	8
3	1962	192788	0.342	563762	251.4	21.30	3.50	11.23	34.41	8.82	20.73	-3.3	365	0
4	1963	143515	0.556	258129	408.8	20.07	3.54	13.03	37.02	9.81	16.53	-1.1	365	365
5	1964	144282	0.465	310112	342.1	19.79	3.83	12.58	36.70	9.64	17.45	-3.8	366	366
6	1965	183236	0.350	522944	257.6	21.72	4.01	9.66	36.10	7.75	20.75	-3.4	365	0
7	1966	141344	0.496	285110	364.5	20.01	4.93	10.17	37.20	8.45	19.24	-8.4	365	365
8	1967	142264	0.450	315946	331.1	19.63	4.46	11.58	37.32	8.19	18.82	-4.1	365	0
9	1968	147275	0.399	368947	293.5	20.73	4.52	9.79	37.47	7.12	20.37	-4.7	366	0
10	1969	145545	0.403	361493	296.0	20.63	4.53	9.79	37.69	7.20	20.15	-3.4	365	1
11	1970	162415	0.341	476958	250.4	21.23	4.45	9.19	36.68	6.83	21.61	-3.6	365	2

Annual dissolved-solids loads and discharge are summed by water year. Dissolved-solids concentration and percent mass fractions are flow-weighted averages.

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS--Continued

7 -- SLOAD: SEASONAL DISSOLVED-SOLIDS LOADS, BY MONTH

STATION: 09069000 EAGLE RIVER AT GYPSUM, CO.
SEASONAL MEANS: GROUPED BY MONTH
FOR THE PERIOD: WATER YEARS 1960 TO 1970

OBS	Month	SALT LOAD (tons)	SALT LOAD (tons per acre foot)	DISCHARGE (acre feet)	MEAN TDS (mg/L)	Ca (%)	Mg (%)	Cl (%)	SO4 (%)	Na+K (%)	CO3 equiv. (%)
1	JANUARY	9631	0.903	10660	664.3	17.88	4.14	13.94	40.49	10.02	13.52
2	FEBRUARY	8506	0.902	9435	662.9	17.75	4.16	14.11	40.40	10.09	13.48
3	MARCH	9398	0.854	11004	628.0	17.92	4.20	13.85	40.10	10.02	13.90
4	APRIL	10997	0.512	21469	376.6	19.68	4.36	11.56	37.76	8.87	17.77
5	MAY	17383	0.228	76378	167.3	23.04	4.32	7.44	31.25	6.51	27.46
6	JUNE	22106	0.194	113834	142.8	24.13	4.05	6.59	29.81	5.87	29.54
7	JULY	17249	0.331	52095	243.5	22.04	4.09	9.45	34.79	7.60	22.03
8	AUGUST	13461	0.582	23138	427.8	19.98	4.04	11.97	38.25	8.96	16.80
9	SEPTEMBER	12367	0.691	17909	507.8	19.21	4.00	12.88	39.12	9.41	15.37
10	OCTOBER	12521	0.739	16952	543.1	19.05	3.96	12.99	39.77	9.45	14.79
11	NOVEMBER	11668	0.822	14195	604.4	18.81	3.98	13.18	40.17	9.55	14.30
12	DECEMBER	10462	0.897	11665	659.5	18.13	4.05	13.80	40.53	9.91	13.57

Monthly means for the entire period of record are listed. At this station, a definite snowmelt peak dominates the hydrograph, with a June maximum in dissolved-solids load and a June minimum in dissolved-solids concentration. Also evident during the runoff peak are increased percent mass fractions of dissolved calcium and carbon, and decreased percent mass fractions of dissolved chloride, sulfate, and sodium. These means are saved in the subfile BYMONTH.

ATTACHMENT A-3. -- EXAMPLES OF OUTPUT FROM PROGRAMS
8 -- SLOAD: REGRESSION INFORMATION

STATION: 09069000 EAGLE RIVER AT GYPSUM, CO.
REGRESSION STATISTICS, BY 3-YEAR SLIDING GROUPS
REGRESSION #1: VARIABLE = e**A * DISCHARGE**B
REGRESSION #2: VARIABLE = e**C * DISCHARGE**D * COND**E
VARIABLE=(mg/L), except for SALT LOAD (tons/day)
DISCHARGE=(cfs) COND=(uMHOS/cm)

GROUP=1961

OBS	VARIABLE	#1 obsv.	R-square #1	Std. Error	A	B	#2 obsv.	R-square #2	Std. Error	C	D	E
8	SALT LOAD	106	0.66535	0.18357	4.29125	0.29810	106	0.99138	0.02961	-6.85693	1.00593	1.06809
9	Carbonate	82	0.76063	0.17837	6.50536	-0.38303	82	0.86426	0.13517	-1.45043	0.14634	0.74194
10	Sodium +K	82	0.92785	0.23180	9.57767	-1.00134	82	0.97520	0.13676	-3.15171	-0.15435	1.18711
11	Calcium	82	0.89777	0.18020	8.19365	-0.64332	82	0.98683	0.06508	-3.20846	0.11536	1.06332
12	Magnesium	82	0.91437	0.18297	6.96198	-0.72024	82	0.96130	0.12377	-2.22055	-0.10925	0.85634
13	Chloride	82	0.94377	0.22464	10.46313	-1.10860	82	0.97991	0.13510	-1.74614	-0.29622	1.13860
14	Sulfate	82	0.92811	0.20927	10.35698	-0.90583	82	0.99066	0.07589	-2.87651	-0.02530	1.23412

GROUP=1962

OBS	VARIABLE	#1 obsv.	R-square #1	Std. Error	A	B	#2 obsv.	R-square #2	Std. Error	C	D	E
15	SALT LOAD	92	0.45105	0.28039	4.17175	0.31323	92	0.99540	0.02582	-6.63385	0.98560	1.05254
16	Carbonate	41	0.84851	0.15558	6.98007	-0.46631	41	0.96440	0.07640	-1.00101	0.08501	0.72761
17	Sodium +K	41	0.90396	0.26630	9.75790	-1.03467	41	0.98222	0.11606	-4.34149	-0.06070	1.28539
18	Calcium	41	0.88508	0.20434	8.63033	-0.71815	41	0.98950	0.06258	-2.79352	0.07098	1.04147
19	Magnesium	41	0.89653	0.20114	7.06489	-0.74983	41	0.96877	0.11194	-2.79262	-0.06889	0.89867
20	Chloride	41	0.91352	0.27115	10.50931	-1.11610	41	0.98476	0.11530	-3.92493	-0.11900	1.31592
21	Sulfate	41	0.90872	0.23679	10.56710	-0.94622	41	0.99157	0.07290	-2.66412	-0.03223	1.20624

Regression statistics are based on 3-year moving groups. Seven dependent variables are modeled for each group. The regression on SALT LOAD uses dissolved-solids load as the dependent variable; the other regressions use dissolved-solids concentration as the dependent variable. Two regressions are performed on each variable. The first regression fits the variable as a function of discharge alone, and calculates the coefficients a and b used in equation 10. The second regression fits the variable as a function of discharge and specific conductance, and calculates the coefficients c, d, and e used in equation 11. For each regression, the number of observations, correlation coefficient (R-square), and the standard error (based on natural logarithms) are also shown.

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