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INLAND WATERS BRANCH

DEPARTMENT OF ENERGY, MINES AND RESOURCES

*Computer Programs in Use in the
Water Quality Division, Vol. 2.*

A. DEMAYO

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A. DEMAYO

INLAND WATERS BRANCH
DEPARTMENT OF ENERGY, MINES AND RESOURCES
OTTAWA, CANADA, 1971

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Preface

Volume 2 of "Computer programs in use in Water Quality Division" describes the programs used to calculate the results of chemical analysis of water, the programs used to type-out a complete report of such an analysis and, finally, a program used for calculating concentrations from a digitized recorder chart. Volume 1 is described in the list inside the back cover.

Computer Programs in Use in the Water Quality Division, Vol. 2

A. DEMAYO

1. BALANCE CALCULATION

1.1. Programs AD0009 and AD0010

1.1.1. Abstract

These programs are used mainly to check the analytical results of chemical analysis of water. The checking is done by calculating the difference between the sum of anions and the sum of cations. They also calculate several other parameters, as described below in Section 1.1.3.

1.1.2. Input data

The input parameters are listed in Table 1.1. The order is that in which they must be entered in the computer, and it follows the order in which these parameters appear on laboratory form IWB-WQD-1600-3 (1). If one of the values is not available a zero is entered.

The different values in input are separated by a blank, or by a comma. An example of a set of input data is given at the top of Figure 1.1.

TABLE 1.1

Input Parameters

Number	Parameter	Symbol in the Program	Unit
1	Sample number	SP	integer number
2	Conductance (at 25°C)	C	micromhos/cm
3	Alkalinity-Phenol	AP	mg/l CaCO ₃
4	Alkalinity-Total	AT	mg/l CaCO ₃
5	Total hardness	TH	mg/l CaCO ₃
6	Calcium	CA	mg/l
7	Sulphate	SF	mg/l
8	Silica	SI	mg/l
9	Sodium	NA	mg/l
10	Temperature	T	°C
11	pH	PH	pH units
12	Chloride	CL	mg/l
13	Fluoride	LF	mg/l
14	Nitrate + Nitrite (as nitrogen)	NI	mg/l

1.1.3. Output data

The parameters appearing in the output, the symbols denoting them and the units in which they are expressed, are listed in Table 1.2. They are discussed individually below. To save memory space, some of the symbols used in the input are also used for output; in this way, some symbols may denote two or more different parameters. This is allowed as long as the calculation of the various parameters carrying the same symbol do not interfere with each other.

It should also be noted that the abbreviations used to represent various parameters on the typed output are not always identical to the symbols used in the program. The abbreviations on the typed output approximate the chemical symbols of the various parameters when possible.

A typical output from Program AD0009 is reproduced in Figure 1.1. An output from Program AD0010 is reproduced in Figure 1.2. The same input data have been used in both instances.

Sample number (SP). This is the same number which was entered as the first value of the input parameters and is used for identification purposes only.

Carbonate (CR), Bicarbonate (BI), Hydroxide (OH) are calculated from the values of phenolphthalein alkalinity (AP) and total alkalinity (AT) (2), (Statements no. 2.17, 2.20, and 2.22)

(i) When $AP \leq AT/2$: BI ($\text{mg/l } \text{HCO}_3^-$) = $1.219 (AT - 2AP)$
CR ($\text{mg/l } \text{CO}_3^{--}$) = $1.2 AP$
OH ($\text{mg/l } \text{OH}^-$) = 0

(ii) When $AP > AT/2$: BI = 0
CR = $1.2 (AT - AP)$
OH = $0.3399 (2AP - AT)$

The me/l (milliequivalents per litre) values are obtained for each parameter calculated above by multiplying by appropriate factors (3) in the formula:

$$\text{me/l} = \text{mg/l} \times f$$

where the factors f are:

BI	0.01639
CR	0.03333
OH	0.05880

Magnesium (MG) is calculated from the values of total hardness (TH) and calcium (CA), (Statement no. 2.07):

$$MG (\text{mg/l Mg}) = 12.16 (0.01988 TH - 0.0499 CA)$$

This method assumes that the total hardness results only from calcium and magnesium hardnesses.

To obtain the value in me/l, the value in mg/l obtained above is multiplied by 0.08226.

TABLE 1.2

Output Parameters

Number	Parameter	Symbol in the Program	Units
1	Sample number	SP	integer
2	Carbonate	CR	mg/l and me/l
3	Bicarbonate	BI	mg/l and me/l
4	Hydroxide	OH	mg/l and me/l
5	Magnesium	MG	mg/l and me/l
6	Sulphate	SF	me/l
7	Chloride	CL	me/l
8	Fluoride	LF	me/l
9	Nitrate + Nitrite	NI	me/l
10	Calcium	CA	me/l
11	Sodium, and per cent sodium	NA	me/l %
12	Potassium	K	me/l
13	Sum of cations	SI	me/l
14	Sum of anions	S2	me/l
15	Percent difference (see text)	DI	%
17	Non-carbonate hardness	H	mg/l CaCO ₃
18	Sodium absorption ratio, and	SA	-
19	Saturation index		pH units
20	Sum of constituents, and	SM	mg/l
21	Sum of constituents/con- ductance		-
22	Free carbon dioxide	CO	mg/l
23	Stability index	SB	pH units

NOTE: The abbreviation me/l stands for milliequivalents per litre. For dilute aqueous solutions at room temperature, me/l is approximately equal to epm (equivalents per million) i.e., gram-equivalents per 10^6 grams of solution.

Sulphate (SF), Chloride (CL), Fluoride (LF), Nitrate + Nitrite (NI), Calcium (CA), Sodium (NA), and Potassium (K). These parameters are obtained in terms of me/l from the respective values in mg/l multiplied by a factor f:

$$\text{me/l} = \text{mg/l} \times f$$

where f is (3) (Statements no. 2.30 to 2.33):

SF	0.02082
CL	0.02821
LF	0.05264
NI	0.07143
CA	0.04990
NA	0.04350
K	0.02557

Sum of Cations (S1) and Sum of Anions (S2) are calculated from the following relations. (Statement no. 2.40):

$$\begin{aligned} S1 &= CA + MG + K + NA \\ S2 &= CR + BI + SF + CL + LF + NI + OH \end{aligned}$$

where all parameters are in me/l.

Per Cent Difference (DI) is obtained from (Statement no. 2.42):

$$DI = 100 (S1 - S2) / (S1 + S2)$$

This parameter is the main check on the quality of the analysis. In the current practice of Water Quality Division, the analysis must be checked very closely for errors if the absolute value of DI is above 3; a special case occurs when not all of the parameters which enter in the calculation of DI are measured. Generally, if no special reason for a value above 3 is found, the analysis is repeated.

Non Carbonate Hardness (H) is calculated from the values of total alkalinity (AT) and total hardness (TH). (Statements no. 2.44 and 2.45).

- (i) if $TH < AT$ then $H = 0$
- (ii) if $TH \geq AT$ then $H = TH - AT$

Sodium Absorption Ratio (SA) is calculated using the formula (Statement no. 2.47)

$$SA = 1.41 NA / (CA + MG)^{\frac{1}{2}}$$

where NA, CA, and MG are in me/l.

Saturation (SA) and Stability (SB) Indexes. The saturation index is calculated from (4) (Statement no. 2.65):

$$\text{Saturation index} = pH - pH_s$$

or in terms of symbols used in the program:

$$SA = PH - K$$

K (or pH_s) is the hypothetical pH which a given water must have, without any other changes in composition, to be in equilibrium with calcium carbonate. If $K > PH$, it indicates that the water is undersaturated with CaCO_3 .

$$pH_s = pK_2 - pK_s - \log[\text{Ca}^{++}] - \log[\text{Alk}] + 9.30 + 2.5u^{\frac{1}{2}}(1+5.3u^{\frac{1}{2}}+5.5u)^{-1}$$

where: pK_2 (in the program represented by the symbol NA) is the negative logarithm (base 10) of the second dissociation constant of carbonic acid.

pK_s (K) is the negative logarithm of the solubility product constant of calcium carbonate.

$[\text{Ca}^{++}]$ (CA) is the calcium concentration expressed as mg/l (or ppm) Ca.

$[\text{Alk}]$ (AT) is the total alkalinity expressed as mg/l (ppm) CaCO_3 .

u (R) is the ionic strength of the solution.

The value of pK_2 is calculated from (6) (Statement no. 2.62):

$$pK_2 = 2902.39T^{-1} - 6.498 + 0.02379T$$

where T is the temperature of testing, in kelvins.

The value of pK_S is obtained from (4,7) (Statement no. 2.60):

$$pK_S = 8.37 - 2(830/T - 2.78)$$

where T is the temperature at testing, in kelvins.

The ionic strength, u , is calculated from (5) (Statement no. 2.54):

$$u = 0.000025 \text{ SM}$$

where SM is the sum of constituents, in mg/l.

The values of $[\text{Ca}^{++}]$ and $[\text{Alk}]$ are both input values as CA and AT , respectively.

The stability index (SB) is obtained from (8) (Statement no. 2.65):

$$\text{Stability index} = pH_S - pH$$

where the symbols have the same significance as before.

Sum of Constituents (SM) is calculated by using the following expressions, (Statement no. 2.24):

$$\text{SM} = \text{CA} + \text{MG} + \text{NA} + \text{K} + \text{CR} + \text{BI}/2.03 + \text{SF} + \text{CL} + \text{LF} + 4.429 \text{ NI} + \text{SI} + \text{OH}$$

where all the symbols represent the various ions in mg/l.

$$\text{Sum of Constituents/Conductance} = \text{SM/C}$$

is calculated in (Statement no. 2.54):

Carbon Dioxide Free is obtained from (9) (Statement no. 2.56):

$$\text{CO}_2 \text{ free} = 9.7 \times 10^{10} [\text{H}^+] \left[\frac{\text{Alk}}{50000} + [\text{H}^+] - 10^{-14} [\text{H}^+] \right] \times \\ \left[1 + 11.22 \times 10^{-11} / [\text{H}^+]^{-1} \right]$$

where $[\text{H}^+]$ is the molar concentration of hydrogen ions and $[\text{Alk}]$ is the total alkalinity.

1.1.4. The computer program

The listing of Program AD0009 is reproduced in Figure 1.3. The program is written in FOCAL-69 (10) and is used by Water Quality Division on a PDP-8/L computer with 8K of memory. Because the FOCAL language is compatible with all PDP-8 series computers, the program can be used with any of the computers belonging to this series. The computer time required to calculate one set of data will be the only thing which will differ from computer to computer.

Program AD0009 requires 8K of memory and the extended functions. On a PDP-8/L, 70 seconds is required for a complete calculation, i.e., from the time the last input value is entered until the value of the stability index (the last output value) is typed out.

In Figure 1.4, a similar program is given. This program, AD0010, can be used on a PDP-8 series with only 4K of memory and extended functions deleted. The time required to complete a calculation is again 70 seconds on a PDP-8/L.

The main difference between the program listed in Figure 1.3 and that of Figure 1.4 arises from the fact that the logarithm and exponential functions used in the calculation in the latter program are calculated by the program itself instead of being part of the compiler.

The logarithm function is calculated from (10) (Statements no. 5.05 to 5.50):

$$\text{LOG } (X) = \text{LOG } (2^N \cdot F) = N \cdot \text{LOG } (2) + \text{LOG } (F)$$

$$= 0.69315N + \sum_{i=1}^{6} A_i (F-1)^i$$

where $1 < F < 2$ and $X > 1$

When $0 < X < 1$ use the identity:

$$\text{LOG } (X) = - \text{LOG } (1/X)$$

$A_1 = 1; A_2 = 0.5; A_3 = 0.3317; A_4 = 0.2407; A_5 = 0.167654; A_6 = 0.09533.$

The exponential function is calculated from (10) (Statements no. 2.51 to 2.54):

$$e^x = 2^x \cdot \log_2 e = 2^{1.442695 x} = 2^{N+F} = 2^N \cdot 2^F$$

where N is an integer, $0 < F < 1$, and $x > 0$.

$$2^F = 1 + \frac{2^F}{A - F + BF^2 - \frac{C}{D + F^2}}$$

where $A = 9.9546; B = 0.03466; C = 617.972; D = 87.417$

When $x < 0$, the following identity is used:

$$e^{-x} = \frac{1}{e^x}$$

1.1.5. References

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9. Hirsch, A.A. 1942. A Slide Rule for Carbonate Equilibria and Alkalinity in Water Supplies, Ind. and Eng. Chemistry, 14, 943.
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Figure 1.1. Program AD0009 - Input and Output

*G
:2598 :1050 :0 :323 :497 :157 :102 :11.1 :1.2 :22.3 :8.1
:32 :0 :0 :0.4

SAMPLE NUMBER= 2598

CALCULATED VALUES (PPM) :

CO₃ = 0.0 MG= 25.5
HCO₃= 393.7
OH = 0.0

CONSTITUENTS (EPM) :

CO₃ = 0.0000 CA= 7.8343
HCO₃= 6.4534 MG= 2.0964
SO₄ = 2.1236 NA= 0.0522
CL = 0.9027 K = 0.0102
F = 0.0000
NO₃ = 0.0000
OH = 0.0000

SUM OF CATIONS = 9.9931
SUM OF ANIONS = 9.4797 DIFFERENCE = 2.64 %

NON CARBONATE HARDNESS = 174.0

SODIUM ABSORPTION RATIO (SAR) = 0.0
% SODIUM = 0.5
SUM OF CONSTITUENTS (PPM) = 523.2
CO₂ = 4.9
SUM OF CONSTITUENTS/CONDUCTANCE = 0.50
SATURATION INDEX = 1.3 STABILITY INDEX= 5.5

Figure 1.2. Program AD0010 - Input and Output

```
*G  
:2598 :1050 :0 :323 :497 :157 :102 :11.1 :1.2 :22.3 :8.1  
:32 :0 :0 :0.4  
  
SAMP.NO. = 2598  
  
CALC. VAL.-PPM :  
CO3 = 0.0 MG= 25.5  
HC03= 393.7  
OH = 0.0  
  
CONST.-EPM :  
CO3 = 0.0000 CA= 7.8343  
HC03= 6.4534 MG= 2.0964  
SO4 = 2.1236 NA= 0.0522  
CL = 0.9027 K = 0.0102  
F = 0.0000  
NO3 = 0.0000  
OH = 0.0000  
  
SC = 9.9931  
SA = 9.4797  
DIF.= 2.6363 %  
  
N-CARB-HRDN. = 174.00  
SUM CONST.-PPM = 523.14  
SUM CONST./COND.= 0.50  
  
SAR = 0.02  
% NA = 0.52  
  
CO2 = 4.91  
  
SAT.INDX. = 1.29  
STAB.INDX. = 5.52
```

Figure 1.3. Program AD0009 - Listing

```

*W
C-8K FOCAL @1969

02.04 E
02.05 A SP,C,AP,AT,TH,CA,SF,SI,NA,T,PH,CL,LF,NI,K
02.07 S MG=12.16*(TH*0.01998-CA*0.0499)
02.09 T !!"SAMPLE NUMBER",%4,SP,!!,"CALCULATED VALUES (PPM) :",!
02.11 T "
    MG",%6.01,MG
02.17 I (AP-AT/2)2.20,2.20,2.22
02.20 S BI=(AT-2*AP)*1.219;S CR=AP*1.2;S OH=0;G 2.24
02.22 S BI=0;S CR=1.2*(AT-AP);S OH=(2*AP-AT)*0.3399
02.24 S SM=CA+MG+NA+K+CR+BI/2.03+SF+CL+LF+NI*4.429+SI+OH
02.26 T #!"CO3",CR,!,"HC03",BI,!,"OH ",OH
02.30 S CA=CA*0.0499;S MG=MG*0.08226;S NA=NA*0.0435
02.31 S K=K*0.02557;S CR=CR*0.03333;S BI=BI*0.01639
02.32 S SF=SF*0.02082;S CL=CL*0.02821;S NI=NI*0.07143
02.33 S LF=LF*0.05264;S OH=OH*0.0588;T !!"CONSTITUENTS (PPM) :",!
02.36 T "CO3",%9.04,CR," CA",CA,!,"HC03",BI," MG",MG,!
02.37 T "SO4",SF," NA",NA,!,"CL ",CL," K ",K,!
02.38 T "F ",LF,!,"NO3",NI,!,"OH ",OH,!
02.40 S S1=CA+MG+K+NA;S S2=CR+BI+SF+CL+LF+NI+OH
02.42 S DI=(S1-S2)*100/(S1+S2);T !!"SUM OF CATIONS ",S1,!
02.43 T "SUM OF ANIONS ",S2," DIFFERENCE ",%4.02,DI,"%",!
02.44 S H=TH-AT;I (H)2.45,2.46,2.46
02.45 S H=0
02.46 T !"NON CARBONATE HARDNESS ",%4.01,H,!
02.47 S SA=1.41*NA/FSQT(CA+MG);S NA=100*NA/S1
02.48 T !"SODIUM ABSORPTION RATIO (SAR) ",%5.01,SA,!
02.50 T "% SODIUM ",%5.01,NA,!,"SUM OF CONSTITUENTS (PPM) ",SM
02.54 S H=FEXP(-PH/0.4343);S R=SM*25E-6;S SM=SM/C;S T=T+273.15
02.56 S CO=9.7E10*H*((AT/5E4+H-1E-14/H)/(1+11.22E-11/H))
02.58 T !"CO2 ",CO,!,"SUM OF CONSTITUENTS/CONDUCTANCE ",%6.02,SM
02.60 S K=-8.37+2*(830/T-2.78)
02.62 S NA=2902.39/T-6.498+0.02379*T
02.63 S K=K+NA-FLOG(CA/0.0499)/2.3026-FLOG(AT)/2.3026+9.3
02.64 S K=K+2.5*FSQT(R)/(1+5.3*FSQT(R)+5.5*R)
02.65 S SA=PH-K;S SB=2*K-PH
02.66 T !"SATURATION INDEX ",%4.01,SA," STABILITY INDEX",SR,!!!!
02.70 G 2.04
*

```

Figure 1.4. Program AD0010 - Listing

```

*4
C-FOCAL, 1969

02.04 E
02.05 A SP,C,AP,AT,TH,CA,SF,SI,NA,T,PH,CL,LF,NI,K
02.07 S MG=12.16*(TH*0.01998-CA*0.0499)
02.09 T !!!"SAMP.NO.",%4,SP,!!,"CALC. VAL.-PPM :!",!
02.11 T " MG",%5.01,MG
02.17 I (AP-AT/2)2.20,2.20,2.22
02.20 S BI=(AT-2*AP)*1.219;S CR=AP*1.2;S OH=0;G 2.24
02.22 S BI=0;S CR=1.2*(AT-AP);S OH=(2*AP-AT)*0.3399
02.24 S SM=CA+MG+NA+K+CR+BI/2.03+SF+CL+LF+NI*4.429+SI+OH
02.26 T #;"CO3 ",CR,!,"HC03",BI,!,"OH ",OH;S NI=NI*.07143
02.30 S CA=CA*.0499;S MG=MG*.08226;S NA=NA*.0435;S SF=SF*.02082
02.31 S K=K*.02557;S CR=CR*.03333;S BI=.01639*RI;S CL=CL*.02821
02.33 S LF=LF*.05264;S OH=.0588*OH;T !!!"CONST.-EPM :!",!
02.36 T "CO3 ",%8.04,CR," CA",CA,!,"HC03",BI," MG",MG,! 
02.37 T "SO4 ",SF," NA",NA,!,"CL ",CL," K ",K,! 
02.38 T "F ",LF,!,"NO3 ",NI,!,"OH ",OH,!;S S1=CA+MG+K+NA
02.40 S S2=CR+BI+SF+CL+LF+NI+OH;S DI=(S1-S2)*100/(S1+S2)
02.43 T !"SC ",S1,!,"SA ",S2,!,"DIF.",DI,"%"
02.44 S H=AT-TH;I (H)2.46;S H=0
02.46 T !!!"N-CARB-HRDN.",,%8.02,-H,!,"SUM CONST.-PPM ",SM,! 
02.47 S SP=SM/C;T "SUM CONST./COND.",SP,!;S SA=1.41*NA/FSQT(CA+MG)
02.50 S NA=100*NA/S1;T !!!"SAR ",SA,!,"% NA ",NA,! 
02.51 S K=PH/.4343;S S1=FITR(K*1.442695);S S2=K*1.442695-S1
02.52 S S2=1+2*S2/(9.9546-S2+.03466*S2^2-617.972/(87.417+S2^2))
02.54 S S2=S2*2+S1;S H=1/S2;S R=SM*25E-6;S SM=SM/C;S T=T+273.15
02.56 S SI=9.7E10*H*((AT/5E4+H-14/H)/(1+11.22E-11/H))
02.60 S K=-8.37+2*(830/T-2.78);S NA=2902.39/T-6.498+.02379*T
02.63 S T=CA/.0499;D 5;S CA=C;S T=AT;D 5;S AT=C
02.71 S K=K+NA-CA/2.3026-AT/2.3026+9.3;T !!!"CO2 ",SI
02.72 S K=K+2.5*FSQT(R)/(1+5.3*FSQT(R)+5.5*R);S SA=PH-K;S SR=2*K-PH
02.75 T !!!"SAT.INDX.",SA,!,"STAB.INDX.",SB,!!!;G 2.04

05.05 S A=1;I (1-T)5.10,5.50;S T=1/T;S A=-1
05.10 S C=0;S S2=2
05.15 I (T/S2-1)5.30,5.40;S S2=S2*2;S C=C+1;G 5.15
05.30 S LF=T/(2+C)-1;S T=LF-.5*LF^2+.3317*LF^3-.2407*LF^4
05.31 S T=T+.167654*LF^5-.09533*LF^6
05.35 S C=A*(C*.69315+T);R
05.40 S T=0;S C=C+1;G 5.35
05.50 S C=0;R
*

```

2. CALCULATION OF CONCENTRATION FROM AUTOANALYZER CHARTS.

2.1. Program AD0011

2.1.1. Abstract

This program calculates by the least squares method an expression which fits, within preset limits, a series of X-Y points (X = concentration; Y = peak height) corresponding to a series of standard solutions.

After having done this, the program calculates from this expression the respective concentration of water samples using the experimentally measured peak heights.

The program is useful for calculating the results of automated chemical analyses such as those from the AutoAnalyzer. The program requires that the X-Y values be entered in a digital form via Teletype key-board or punched paper tape.

2.1.2. Method

The points corresponding to the L1 standard solutions are fitted by the least squares method to an expression of the form:

$$Y = \sum_{i=0}^L B_i [\ln (X+1)]^i \quad \dots \quad (1)$$

L = 1,2,3, or 4

where Y is the peak height and X is the concentration in mg/l.

The standard deviation is calculated from:

$$SD = \left[\sum_{j=1}^{L1} [(Y_j(\text{obs}) - Y_j(\text{calc}))^2 / (L1-L)] \right]^{\frac{1}{2}} \quad \dots \quad (2)$$

The relative standard deviation is obtained from:

$$RSD = SD \times L1 \times 100 \sqrt{\sum_{j=1}^{L1} Y_j(\text{obs})} \quad \dots \quad (3)$$

RSD is then compared to L5; L5 is an input variable which sets the level for the desired "Precision of fitting" in per cent.

Notice in Expression 1 that relations with up to five adjustable coefficients are tried to fit the standard points. If any of these expressions fails to fit the data within the preset limit, i.e., $RSD > L5$, then the program offers two options: the first option is to use as the standard curve the last calculated expression, i.e., the one with five adjustable coefficients; the second option is to abandon the calculation entirely. The choice is made by answering with the proper number (1 or 2), via Teletype keyboard, to the program query (see Figure 2.3).

The number of standard points, L_1 , the corresponding concentrations, X_i , and the corresponding peak heights, Y_i , are all input values. This gives the program a certain degree of flexibility since it can be used with any sets of standards.

After the standard curve has been calculated, the program goes on to calculate the concentration of the unknown samples. In this step, Y , the peak height, is entered. The corresponding concentration is found by first solving an equation of the form (for $L=4$):

$$B_0 + B_1Z + B_2Z^2 + B_3Z^3 + B_4Z^4 - Y = 0 \quad \dots (4)$$

where $Z = \ln(X+1)$

The largest real positive root is assumed to correspond to the concentration being sought. Only concentration values which fall within the range of the standard solutions are typed out. For those values which fall outside these limits, explanatory messages are typed out.

Various expressions have been considered in the present work for calculating the standard curve. Ideally, a plot of concentration vs peak height would give a straight line:

$$Y = B_0 + B_1X \quad \dots (5)$$

For various reasons this is not so, especially over a wide range of concentration values (1,2). Published papers use second and third degree polynomials (1,2,3,4):

$$Y = B_0 + B_1X + B_2X^2 \quad \dots (6)$$

$$Y = B_0 + B_1X + B_2X^2 + B_3X^3 \quad \dots (7)$$

to fit data obtained by atomic absorption.

In the present work, besides Expressions (5) to (7), the following Expressions have been tried for use as standard curves:

$$Y = B_0 + B_1X + B_2X^2 + B_3X^3 + B_4X^4 \quad \dots (8)$$

$$Y = B_0 + B_1X + B_2X^2 + B_3X^3 + B_4X^4 + B_5X^5 \quad \dots (9)$$

$$Y = B_0 + B_1\ln(X+1) + B_2\ln^2(X+1) \quad \dots (10)$$

$$Y = B_0 + B_1\ln(X+1) + B_2\ln^2(X+1) + B_3\ln^3(X+1) \quad \dots (11)$$

$$Y = B_0 + B_1\ln(X+1) + B_2\ln^2(X+1) + B_3\ln^3(X+1) + B_4\ln^4(X+1) \quad \dots (12)$$

$$\ln Y = B_0 + B_1X + B_2X^2 + B_3X^3 \quad \dots (13)$$

$$\ln Y = B_0 + B_1X + B_2X^2 + B_3X^3 + B_4X^4 \quad \dots (14)$$

$$\ln Y = B_0 + B_1\ln(X+1) + B_2\ln^2(X+1) + B_3\ln^3(X+1) \quad \dots (15)$$

$$\ln Y = B_0 + B_1\ln(X+1) + B_2\ln^2(X+1) + B_3\ln^3(X+1) + B_4\ln^4(X+1) \quad \dots (16)$$

Expressions (5) to (16) have been tested with actual experimental data obtained in a Water Quality Division Laboratory. Such a set of standard points is given in Table 2.1. These points correspond to a series of standard solutions for sodium analysis by flame photometry using Technicon AutoAnalyzer equipment. The points were fitted by the least square method to the above expressions. The computer programs used for this have already been described (5). The results obtained are given in Table 2.2. Expressions of the type (10) - (12) gave the best results and therefore they have been chosen for further use as standard curves.

The baseline is assumed to be a straight line:

$$Y = TT + SL \times V \quad \dots \quad (17)$$

The values of TT and SL are calculated by the computer from several Y,V input points.

TABLE 2.1

Concentration and Peak Height Values for Calculating the Standard Curve

No.	X mg Na/l sol'n.	Y Relative Units
1	1. $\times 10^{-6}$	2
2	1	96
3	2	180
4	4	342
5	8	616
6	10	739
7	15	989
8	25	1354
9	30	1517
10	40	1795
11	60	2175
12	80	2446
13	100	2642

TABLE 2.2

Results Obtained from Various Expressions used for the Standard Curves.

Expression No.	No. of Adjustable Coefficients	Y(obs) - Y(calc) Min	Y(obs) - Y(calc) Max	Standard Deviation (SD)
(5)	2	29	411	288
(6)	3	3.5	125	97
(7)	4	5.7	55	42
(8)	5	1.3	30	21.0
(9)	6	0.3	21	12.2
(10)	3	3	45	24.3
(11)	4	0	33	23.6
(12)	5	1.8	19	10.5
(13)	4	39	1375	833
(14)	5	23	1435	783
(15)	4	0.7	630	785
(16)	5	0.1	220	134

2.1.3. Input data

In the Water Quality Division, the recorder charts from the Technicon AutoAnalyzer are digitized at present by using a D-Mac Pencil Follower, essentially a table with a reading pencil and an electronic console. The X and Y origins of the reading table are set at its bottom left hand corner. The chart to be digitized is placed face-up on the reading surface. The desired points of the chart are digitized by placing the point of the reading pencil at the respective position followed by the depressing of a readout switch. These operations cause the co-ordinate location of the reading pencil to be passed from the electronic console to the output unit. In our case the output unit is a Teletype ASR-33. The data are punched onto a paper tape which is processed off-line by the present program.

On the paper tape, the first group of numbers represent baseline points. This group is identified by numeral "-1" (minus one) at the beginning and "-2" at the end. A minimum of two baseline points are necessary for the program to be able to calculate the baseline expression (17). Usually, four points are digitized on the base line.

The second group of numbers represents the peak heights of the standard solutions. This group of points is identified by a "-3" at the beginning and a "-4" at the end.

The third group of numbers is made up of the peak height of the water samples. This group of numbers is indicated by a "-5" in front and a "-6" at the very end. After this the input data can follow any pattern. For example, if a new set of standards follows the first set of samples, this new set is indicated by a "-3" followed by the actual points and a "-4" at the end. This new standard curve is used for the subsequent calculations until a new one is calculated. The same thing is valid for the baseline. At any point, the baseline can be reset by digitizing several points on the new baseline and indicating them by a "-1" and a "-2" at the beginning and end, respectively. The "indicators" are summarized in Table 2.3.

TABLE 2.3
Program AD0011 Indicators

Type of Reading	Indicator	
	Beginning	End
Baseline	-1	-2
Standards for standard curve	-3	-4
Samples	-5	-6
New chart	-7	

The contents of such a tape are reproduced in Figure 2.1.

Before the punched paper tape containing the digitized data from the recorder output starts to be read, the following input variables must be entered:

- (i) Recorder Chart Number (symbol RC). This variable has only an identification role; it is not used in any calculation.

- (ii) Number of standard solutions used for calculating the standard curve, including the zero concentration (symbol L1).
- (iii) The concentration of the standard solutions (in mg/l) in the same order in which they appear on the recorder chart (usually in the order of increasing concentration).
- (iv) The frequency of standards, i.e., how many samples are to be run before a standard is run (symbol J9).
- (v) The desired precision of fitting (symbol L5).

2.1.4. Output data

Typical outputs are reproduced in Figures 2.2 - 2.6.

The output consists of the coefficients of the standard curve, a table of Y(obs) and Y(calc) values for the standard solutions, the standard deviation and, finally, a table with the results for the unknown samples.

2.1.5. The Computer program

A listing of the computer program is reproduced in Figure 2.7.

The program is written in FOCAL-69 for a PDP-8/L-8K computer, and goes through the following sequence of operations:

- (i) Calculation of the base line. The points corresponding to the baseline readings are fitted to a straight line [Expression (17)]. (Statements no. 4 and 5).
- (ii) The calculation of the standard curve, (Statements no. 2, 3, and 6). The Y values (peak heights) after being read in, are corrected for the base line offset. This correction is done by subtracting from the actual Y reading the Y (same V value) calculated from Expression (17).

Then, the X (concentration), Y (corrected peak height) points are fitted to relations of type (1). The starting value of L is unity. This is increased a unit at a time until RSD [Expression (3)] becomes smaller or equal to "Precision of fitting" or, until L equals 4. If in this latter case, RSD is still greater than "Precision of fitting", the two options described in Section 2.1.2 are offered.

The coefficients of Expressions (17) and (1) are calculated by the least squares method. The subroutine solving the system of linear equations, which leads to these coefficients, is contained in Statements no. 14 and 15.

- (iii) The calculation of unknown concentrations. In this part of the program the V and Y values (peak height) corresponding to the actual samples analysed are read in, and corrected for the baseline offset. Then, an Expression of type (4) is formed, solved, and the concentration calculated from the largest positive root.

As explained in Section 2.1.2, only concentrations within the range of concentrations of the standard solutions are considered. If the values obtained fall outside this range, a warning message is typed out. Messages are also typed out when no real root, or when no positive real root is found. After calculating one sample, the program goes on to the next. In this way, any number of samples can be calculated without using a large-sized, computer memory.

After every J9 unknown sample (recall that J9 is an input parameter), a sample of known concentration is run for checking the analytical procedure. This sample is processed in the same way as the unknown samples. It is up to the analyst to compare the calculated result with the known value and to decide whether or not the analytical system works within specifications.

At any point, the baseline can be reset and/or the standard curve recalculated from a new set of standard solutions.

The program performs a series of check operations. These can be divided in two main groups. The first group, which includes the checks on how the calculation proceeds, were mentioned before:

- (i) Compare RSD with L5.
- (ii) Compare the calculated concentration with the two extreme concentrations of the standard solutions.
- (iii) Check for negative or imaginary results.

In any of these cases, if a calculated value is not as expected, a message is typed out and the calculation continues with the exception of (i) at which point the operator has the option to abandon the calculation altogether.

The second group contains the checks on the input data. The main difference between this group and the first one is that if something is found to be wrong by one of these check steps, then the calculation is abandoned entirely. This group contains:

- (iv) Check for the number of standard points entered. If this does not correspond to the expected number (L1), a message is typed out.
- (v) Check for the indicators. If the indicators are not in the right order (Table 2.3) a message is typed out.
- (vi) If, by mistake, J9 has been entered as a negative number, the calculation is stopped.
- (vii) Finally, a last and very important check is to see if the standard curve has its maxima or minima within the concentration range of the standard solutions. This check is done immediately after the standard curve has been calculated.

The 1st derivative of the standard curve [(Expression (1))] is calculated from:

$$Y_1 = \sum_{i=1}^L iB_i [\ln(X+1)]^{i-1} \quad \dots \quad (18)$$

and then equation

$$\sum_{i=1}^L iB_i [\ln(X+1)]^{i-1} = 0 \quad \dots (19)$$

is solved. If one or more of the L roots has a real value which is within the concentration range of the standard solutions, i.e., if

$$0 < X < X_{L1}$$

a message and the concentration value at which maxima (minima) are occurring are typed out and the calculation is abandoned (see Figure 2.5).

Patches to FOCAL-69 compiler. To obtain the outputs shown in Figures 2.2 - 2.6, series patches to the FOCAL-69 compiler are necessary (6,7). They are listed in Table 2.4.

TABLE 2.4

Patches to FOCAL-69 Compiler

No.	Scope	(Octal Numbers)		
		Location	Old Content	New Content
1	Suppress colon sign in input	1217	4551	7600
2	Suppress equal sign in output	6002	4551	7600
3	Suppress the typing of input data	2163	4551	7000
4	Read punched paper tapes (program, data) without creating an "input-buffer overflow"	0063 0064 2732 2762	2676 2666 6001 6046	1354 2414 5336 7000

2.1.6. References

1. De Galan, L. and G.F. Samaey, 1969. Some trivial causes for bending of analytical curves in atomic absorption spectrometry, Spectrochim. Acta 24B, 679.
2. Gabler, R.G. Jr., R.E. Brown and J.G. Haymes, 1970. A computer program for atomic absorption data processing, 21 Pittsburgh Conference on Analytical Chemistry and Spectroscopy.
3. Marshall, J.C. 1969. Computer Calculations vs the "eyeballing" of atomic absorption calibration curves, Atomic Absorption Newsletter, 8, 85.
4. Wendt, R.H. 1968. Computer calculations of atomic absorption data, Atomic Absorption Newsletter, 7, 28.
5. Demayo, A. 1971. Computer programs in use in Water Quality Division - Vol. 1, Report Series No. 11, Inland Waters Branch.
6. Digital Equipment Corporation, 1969. Advanced Focal Specifications, Publication No. Dec - 08 - AJBB - DL.
7. Digital Software News, May 1970.

Figure 2.1. Program AD0011 - Input

-01 8922 1371 7375 1391
4735 1427 1876 1466 -02 -03 8925 1370 8846 1405
8741 1432 8641 1483 8540 1537 8440 1581
8337 1635 8238 1900 8145 2397 -04 -05 7826 1394
7622 1665 7222 2089 7117 1816 6927 2690
6711 1754 6611 1937 6502 1457 6399 1414
5704 2585 5483 1444 5388 1744 5281 1620
5080 1532 4981 1864 4585 2600 4265 1635
4061 1452 3958 1507 3861 1497 3550 1459
3465 2566 3250 1741 3154 1987 3034 1470
2540 1854 2431 1487 2333 1572 2228 1552
2141 2563 1536 2784 -06 -01 8934 0803 7393 0777
5822 0753 2731 0705 1832 0689 -02 -05 7843 0792
7630 1058 7215 1469 7118 1194 6901 2064
6712 1122 6605 1301 6512 0816 6413 0769
5680 1922 5493 0772 5388 1070 5291 0944
5189 0748 5088 0848 4980 1180 4561 1899
4272 0927 4070 0737 3967 0788 3866 0780
3559 0730 3447 1839 3256 1001 3149 1244
3055 0726 2543 1094 2445 0728 2344 0809
2242 0786 2121 1795 1512 1993 -06
-01 8722 0699
2297 0585 0440 0551 5698 0642 -02 -03 8722 0696
8578 0833 8348 0940 8117 1142 7884 1454
7653 1587 7417 1855 7186 2241 6956 2404
6729 2651 -04 -05 2187 0806 1967 0735 1732 0872
1507 0817 1278 0724 1049 0717 0818 0752
0590 0716 -06 -01 2165 0914 0313 0898 0291 0897
2140 0914 -02 -05 2049 1136 1827 1067 1595 1204
1372 1149 1137 1064 0911 1059 0679 1095
0449 1063 -06

Figure 2.2. Program AD0011 - Output

RECORDER CHART NUMBER= 1

NUMBER OF STANDARDS = 9

CONCENTRATION OF STANDARDS :

1	0.00
2	0.01
3	0.02
4	0.04
5	0.06
6	0.08
7	0.10
8	0.20
9	0.40

A STANDARD SOLUTION IS RUN AFTER EVERY 5 SAMPLE(S)

PRECISION OF FITTING (%) = 3.0

CALCULATION OF THE STANDARD CURVE

COEFFICIENTS:

B(1) = 0.422562E+01

B(2) = 0.256872E+04

B(3) = 0.130811E+04

NO.	CONCENTRATION STANDARDS	HEIGHT MEASURED	HEIGHT CALCULATED	DIFFERENCE %
1	0.00	0.5	4.3	4.8 912.3
2	0.01	33.4	29.9	3.5 10.5
3	0.02	59.0	55.6	3.4 5.7
4	0.04	108.6	107.0	1.7 1.5
5	0.06	161.3	158.4	2.9 1.8
6	0.08	203.9	209.7	5.8 2.8
7	0.10	256.5	260.9	4.4 1.7
8	0.20	520.2	516.1	4.2 0.8
9	0.40	1015.9	1016.6	0.7 0.1

MEAN (MEASURED) PEAK HEIGHT = 262.1

STANDARD DEVIATION = 4.7

RELATIVE STANDARD DEVIATION (%)= 1.8

SAMPLE CALCULATION

NO.	STATUS	HEIGHT MEASURED	CONCENTRATION CALCULATED
1	UNKNOWN	9	0.00
2	UNKNOWN	277	0.11
3	UNKNOWN	696	0.27
4	UNKNOWN	421	0.16
5	UNKNOWN	1293	WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.
6	STANDARD	354	0.14
7	UNKNOWN	535	0.21
8	UNKNOWN	54	0.02
9	UNKNOWN	9	0.00
10	UNKNOWN	1171	WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.
11	UNKNOWN	27	0.01
12	STANDARD	326	0.13
13	UNKNOWN	200	0.08
14	UNKNOWN	110	0.04
15	UNKNOWN	440	0.17
16	UNKNOWN	1171	WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.
17	UNKNOWN	202	0.08
18	STANDARD	16	0.01
19	UNKNOWN	69	0.03
20	UNKNOWN	58	0.02
21	UNKNOWN	16	0.01
22	UNKNOWN	1122	WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.
23	UNKNOWN	294	0.11
24	STANDARD	539	0.21
25	UNKNOWN	20	0.01
26	UNKNOWN	397	0.15
27	UNKNOWN	29	0.01
28	UNKNOWN	112	0.04
29	UNKNOWN	91	0.03
30	STANDARD	1101	WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.
31	UNKNOWN	1314	WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.
32	UNKNOWN	7	0.00
33	UNKNOWN	276	0.11
34	UNKNOWN	694	0.27
35	UNKNOWN	421	0.16
36	STANDARD	1294	WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.

Figure 2.3. Program AD0011 - Output

RECORDER CHART NUMBER= 1

NUMBER OF STANDARDS = 9

CONCENTRATION OF STANDARDS :

1	0.00
2	0.01
3	0.02
4	0.04
5	0.06
6	0.08
7	0.10
8	0.20
9	0.40

A STANDARD SOLUTION IS RUN AFTER EVERY 4 SAMPLE(S)

PRECISION OF FITTING (%) = 0.5

CALCULATION OF THE STANDARD CURVE

THE STANDARD CURVE DID NOT FIT THE EXPERIMENTAL POINTS
WITHIN THE PRESET LIMITS WHEN USING 1ST-4TH DEGREE POLYNOMIALS.

OPTIONS :

1. USE THE RESULTS OBTAINED WITH THE 4TH DEGREE POLYNOMIAL TO CONTINUE
THE CALCULATION

2. STOP THE CALCULATION

OPTION CHOSEN ? 1

COEFFICIENTS:

B(1)	= 0.116440E+01
B(2)	= 0.307383E+04
B(3)	=-0.977927E+04
B(4)	= 0.684358E+05
B(5)	=-0.118534E+06

NO.	CONCENTRATION STANDARDS	HEIGHT MEASURED	HEIGHT CALCULATED	DIFFERENCE %
1	0.00	0.5	1.2	- 1.7 328.2
2	0.01	33.4	30.9	2.6 7.7
3	0.02	59.0	58.7	0.3 0.5
4	0.04	108.6	110.5	- 1.9 - 1.7
5	0.06	161.3	159.3	2.0 1.3
6	0.08	203.9	206.9	- 2.9 - 1.4
7	0.10	256.5	254.8	1.8 0.7
8	0.20	520.2	520.3	- 0.1 - 0.0
9	0.40	1015.9	1015.9	0.0 0.0

MEAN (MEASURED) PEAK HEIGHT = 262.1

STANDARD DEVIATION = 2.8

RELATIVE STANDARD DEVIATION (%) = 1.1

SAMPLE CALCULATION

NO.	STATUS	HEIGHT MEASURED	CONCENTRATION CALCULATED
1	UNKNOWN	9	0.00
2	UNKNOWN	277	0.11
3	UNKNOWN	696	0.26
4	UNKNOWN	421	0.17
5	STANDARD	1293	WARNING: IMAGINARY RESULTS!!
6	UNKNOWN	354	0.14
7	UNKNOWN	535	0.21
8	UNKNOWN	54	0.02
9	UNKNOWN	9	0.00
10	STANDARD	1171	WARNING: IMAGINARY RESULTS!!

Figure 2.4. Program AD0011 - Output

RECORDER CHART NUMBER= 3

NUMBER OF STANDARDS = 7

CONCENTRATION OF STANDARDS :

1	0.00
2	1.00
3	4.00
4	10.00
5	15.00
6	20.00
7	25.00

A STANDARD SOLUTION IS RUN AFTER EVERY 0 SAMPLE(S)

PRECISION OF FITTING (%) = 3.0

CALCULATION OF THE STANDARD CURVE

COEFFICIENTS:

B(1) = 0.272145E+02
 B(2) = 0.131950E+03
 B(3) = -0.534218E+02
 B(4) = 0.498476E+02

NO.	CONCENTRATION STANDARDS	HEIGHT MEASURED	HEIGHT CALCULATED	DIFFERENCE	%
1	0.00	30.8	27.2	3.6	11.5
2	1.00	99.3	109.6	- 10.3	- 10.4
3	4.00	320.6	309.0	11.6	3.6
4	10.00	726.0	723.7	2.3	0.3
5	15.00	1033.4	1044.8	- 11.5	- 1.1
6	20.00	1337.7	1340.5	- 2.7	- 0.2
7	25.00	1621.1	1614.0	7.1	0.4

MEAN (MEASURED) PEAK HEIGHT = 738.4

STANDARD DEVIATION = 12.4

RELATIVE STANDARD DEVIATION (%) = 1.7

SAMPLE CALCULATION

NO.	STATUS	HEIGHT MEASURED	CONCENTRATION CALCULATED
1	UNKNOWN	202	2.42
2	UNKNOWN	39	0.10
3	UNKNOWN	23	WARNING: AFTER BASELINE CORRECTION THE MEASURED HEIGHT IS BELOW THE BASELINE
4	UNKNOWN	564	7.65
5	UNKNOWN	226	2.79
6	UNKNOWN	527	7.12
7	UNKNOWN	224	2.76
8	UNKNOWN	750	10.40
9	UNKNOWN	257	3.24
10	UNKNOWN	111	1.02
11	UNKNOWN	149	1.62
12	UNKNOWN	780	10.84
13	UNKNOWN	100	0.85

Figure 2.5. Program AD0011 - Output

RECORDER CHART NUMBER= 4

NUMBER OF STANDARDS = 9

CONCENTRATION OF STANDARDS :

1	0.00
2	0.03
3	0.10
4	0.20
5	0.40
6	0.60
7	0.80
8	1.00
9	2.00

A STANDARD SOLUTION IS RUN AFTER EVERY 10 SAMPLE(S)

PRECISION OF FITTING (%) = 3.0

CALCULATION OF THE STANDARD CURVE

COEFFICIENTS:

BC 1D = -0.219239E+02
BC 2D = 0.182671E+04
BC 3D = 0.130481E+04
BC 4D = -0.160769E+04

NO.	CONCENTRATION STANDARDS	HEIGHT MEASURED	HEIGHT CALCULATED	DIFFERENCE %
1	0.00	10.7	21.9	11.2 - 104.3
2	0.03	113.9	131.1	17.2 - 15.1
3	0.10	174.5	169.3	5.2 3.0
4	0.20	352.2	357.5	5.4 - 1.5
5	0.40	693.9	702.8	3.9 - 0.6
6	0.60	1005.5	990.9	14.7 1.5
7	0.80	1229.2	1217.3	11.9 - 1.0
8	1.00	1365.8	1384.3	18.4 - 1.4
9	2.00	1506.7	1504.9	1.8 0.1

MEAN (MEASURED) PEAK HEIGHT = 715.1

STANDARD DEVIATION = 15.6

RELATIVE STANDARD DEVIATION (%) = 2.2

WARNING: STANDARD CURVE CALCULATED ABOVE SHOWS 1 MAXIMA (MINIMA)
IN THE CONCENTRATION RANGE OF STANDARD SOLUTIONS :

1 CONCENTRATION= 1.60 HEIGHT CALCULATED= 1579.19

THE CALCULATION IS STOPPED

*

Figure 2.6. Program AD0011 - Output

RECORDER CHART NUMBER= 1

NUMBER OF STANDARDS = 9

CONCENTRATION OF STANDARDS :

1	0.00
2	0.01
3	0.02
4	0.04
5	0.06
6	0.08
7	0.10
8	0.20
9	0.40

A STANDARD SOLUTION IS RUN AFTER EVERY 5 SAMPLE(S)

PRECISION OF FITTING (%) = 3.0

INDICATOR MISSING

THE CALCULATION IS STOPPED

*

Figure 2.7. Program AD0011 - Listina

```

C-8K FOCAL #1969

01.02 E
01.03 T !!!!RECORDER CHART NUMBER="JA RCJT ZS,RC
01.06 S J7=0;S X(I)=1E-5;T !!"NUMBER OF STANDARDS ="JA LIST L1
01.08 T !!!CONCENTRATION OF STANDARDS :"!
01.09 T " 1 ",%3.02,X(I);J=2;LIST !,%3,J," "JA X(J)JT %5.02,X(J)
01.12 T !!!A STANDARD SOLUTION IS RUN AFTER EVERY"JA J9JT Z2,J9
01.21 T " SAMPLE(S)"!!!PRECISION OF FITTING (%) = "JA LSJT %3.01,L5
01.22 F J2=1,L1;S X(J2)=FLOG(X(J2)+1)
01.25 G 13.10

02.05 S L=2
02.17 S N2=2*L-1
02.20 F J1=1,N2;S SX(J1)=0
02.22 F J1=1,L1;S YX(J1)=0
02.25 F J2=1,N2;F J1=1,L1;S SX(J2)=SX(J2)+X(J1)*(J2-1)
02.27 F J2=1,L1;F J1=1,L1;S YX(J2)=YX(J2)+Y(J1)*(X(J1)*(J2-1))
02.30 F J2=1,L1;F J1=1,L1;S A(J2+J1*L)=SX(J1+(J2-1))
02.35 D 15.0;S SD=0;F J1=1,L1;S YY=B(1);D 8
02.36 S SD=FSQRT(SD/(L1-L))J1 (SD-SY*L5/L1*100)2.99,2.99;S L=L+1
02.37 I (L->)2.17,2.17,2.90
02.90 T !!!THE STANDARD CURVE DID NOT FIT THE EXPERIMENTAL POINTS"
02.91 T !!!WITHIN THE PRESET LIMITS WHEN USING 1ST-4TH DEGREE "
02.92 T "POLYNOMIALS.",!"OPTIONS :"! 1.USE THE RESULTS"
02.93 T " OBTAINED WITH THE 4TH DEGREE POLYNOMIAL TO CONTINUE"
02.94 T !!!THE CALCULATION!" 2-STOP THE CALCULATION"
02.95 T !!!OPTION CHOSEN ?"JA RJT %3,R,!!I (R-1)6.47,2.98,6.47
02.98 S L=L-1
02.99 R

03.08 D 4;D 5;G 13.10
03.15 T !!!CALCULATION OF THE STANDARD CURVE!"S J=0;S SY=0;G 6.10
03.18 S LT=0;T !"COEFFICIENTS:";F K=i,L;T !"B(K",%2,K,") =",%3,B(K)
03.22 T !!!NO. CONCENTRATION HEIGHT HEIGHT DIFFERENCE"
03.23 T !" STANDARDS MEASURED CALCULATED %
03.24 F J1=1,L1;S YY=B(1);D 8;T !,%2,J1,X9.02,FEXP(X(J1))-1;D 16
03.25 S SD=FSQRT(SD/(L1-L))
03.26 T !!!MEAN (MEASURED) PEAK HEIGHT =",%5.01,SY/L1
03.27 T !!!STANDARD DEVIATION =",SD
03.28 T !!!RELATIVE STANDARD DEVIATION (%) =",SD*L1*100/SY
03.29 I (L->)6.47,13.10;D 10;G 13.10
03.35 S LT=1;S JS=0;S J6=0;T !!!SAMPLE CALCULATION"
03.37 T !!! NO. STATUS HEIGHT CONCENTRATION"
03.38 T !!! MEASURED CALCULATED"
03.40 G 9.05;G 13.10
03.97 T !!!INDICATOR MISSING"JG 6.47

04.05 S SW=0;S ST=0;S WT=0;S W2=0;S J=0
04.10 A WJI (W)4.30;A T;S J=J+1
04.20 S SW+SW;S ST=ST+T;S WT=WT+W*T;S W2=W2+W*W;G 4.10
04.30 I (W+2)4.40,4.90,4.40
04.40 T !!!THE INDICATORS ARE IN THE WRONG ORDER"JG 6.47
04.90 R

05.10 S P=SW*SW-J*W2;S TT=(SW*WT-ST*W2)/P;S SL=(SW*ST-J*WT)/P;R

06.10 A WJI (W)6.20;A T;G 6.99
06.20 I (W+4)4.40,6.40,4.40
06.40 I (L1-J)6.45,6.50,6.45
06.45 T !!!WARNING: STANDARD VALUES ENTERED: ",%2,J
06.46 T !!! STANDARD VALUES EXPECTED:",L1
06.47 T !!!THE CALCULATION IS STOPPED"!;Q
06.50 D 2;G 3.18
06.99 S J=J+1;S Y(J)=T-TT-SL*W;S SY=SY+Y(J);G 6.10

07.05 I (FABS(RI(J2))-1E-6)7.07,7.07;R
07.07 I (FABS(RC(J2))-1E-6)11.80,11.80;R

08.10 F J2=2;L1;S YY=YY+B(J2)*(X(J1)+(J2-1))
08.15 S D=Y(J1)-YY;S SD=SD*D*D;R

09.05 A WJI (W)9.10;S J6=J6+1;G 9.25
09.10 I (W+5)13.10,4.40,4.40
09.25 S JS=J5+1;A T;S T=T-TT-SL*W;G 22.10
09.28 S C(L)=B(1)-T
09.31 D 9.99;D 11;G 9.35
09.32 D 9.64;T !!! WARNING: AFTER BASELINE CORRECTION THE"
09.33 T !!!MEASURED HEIGHT IS BELOW THE BASELINE"JG 9.96
09.34 D 9.64;S C0=0;G 9.75
09.35 S IJ=0;S IK=0;S MX=1E100;S MI=0;S CO=0
09.40 F J2=1,L2;D 10
09.64 I (J9)6.47,9.67,9.65
09.65 I (J7-J9)9.67,9.70,6.47
09.67 T !,%3,J5," UNKNOWN ",%2,T;S J7=J7+1
09.68 G 9.80
09.70 T !,%3,J5," STANDARD ",%2,T;S J7=0
09.71 G 9.80
09.75 T %11.02,C0;G 9.96
09.80 I (C0)9.83,9.83,9.75
09.82 T !!! WARNING: IMAGINARY RESULTS!"JG 9.96
09.83 I (MX-1E100)9.90,9.94,9.90
09.84 I (MI)9.92,9.86,9.92
09.85 I (C0-FEXP(X(I))+1)*9.92,9.87,9.87
09.86 I (IK-L)9.88,9.94,9.88
09.87 I (FEXP(X(L1))-1-C0)9.90,9.75,9.75
09.88 I (IJ-L)9.89,9.82,9.89
09.89 T !!! WARNING: IMAGINARY AND NEGATIVE RESULTS !!"JG 9.96

```

09.90 T " WARNING: CONC. VAL. HIGHER THAN HIGHEST STAND.";G 9.96
 09.92 T " WARNING: CONC. VAL. SMALLER THAN SMALLEST STAND.";G 9.96
 09.94 T " WARNING: NEGATIVE RESULTS!!"
 09.96 I (J6-5)9.95,9.98,6.47
 09.98 T !JS J6=01G 9.05
 09.99 S L2=L-1;F J2=1,L2JS MT=L-J2+1JS C(J2)=B(MT)

 10.10 I (RI(J2))10.85,10.25,10.85
 10.25 I (RR(J2))10.80,10.27,10.27
 10.27 I (RRC(J2)-XL(1))10.32,10.32,10.29
 10.29 I (MX-RRC(J2))10.90,10.90;S MX=RRC(J2);R
 10.30 I (RRC(J2)-X(1))10.35,10.35,10.50
 10.35 I (RRC(J2)-M1)10.90;S M1=RRC(J2);R
 10.50 S C1=FEXP(RR(J2))-1;I (C1-C0)10.90;S C0=C1;R
 10.80 S IK=IK+1;R
 10.85 S IJ=IJ+1
 10.90 R

 11.07 S IS=0;S I=1;S P=1/C(1);F J2=1,L2;S C(J2)=P*C(J2+1)
 11.11 S P=C(L2-1)*1E-6;S Q=C(L2);J1 (I-L2+1)11.16,11.54,11.13
 11.13 S RRC(I)=-QJS RI(I)=0;R
 11.16 S IC=1;S B1=C(L2-2);J1 (B1)11.19,11.90,11.19
 11.19 S BI=1;B1JS P=P/B1JS Q=Q*B1
 11.21 S BI=1;S B3=1;JS B2=0;S B4=0;F J2=1,L2;D 12
 11.26 S RI(L2-1)=RI(L2-1)-RR(L2-1);S B2=1;S B3=RI(L2-1)
 11.28 S B4=RI(L2-2);J1 (I-L2+2)11.30,11.32,11.30
 11.30 S B2=RI(L2-3)
 11.32 S B1=B4*B4-B3*B2;S B1=1/B1;S B3=(RR(L2-1)*B3-RR(L2)*B4)*B1
 11.35 S B2=(RR(L2-1)*B4-RR(L2)*B2)*B1
 11.38 I (FABS(B2)/(FABS(P)+1)-SE-6)11.40,11.40,11.42
 11.40 I (FABS(CB3)/(FABS(Q)+1)-SE-6)11.84,11.84,11.42
 11.42 S P=P+B2;S Q=Q-B3;S IC=IC+1;I (IC-50)11.21,11.21,11.44
 11.44 I (IS)11.46;R
 11.46 S IS=1;S IN=1-I;S J3=L2;S L2=L2+1;S C(L2)=0
 11.48 S CJ3+1)=C(J3+1)+C(J3);JS J3=J3-1
 11.50 I (J3)11.52,11.52,11.48
 11.52 S C(1)=C(1)+1;G 11.11
 11.54 I (P)11.56,11.61,11.56
 11.56 S B4=4*(P+P);J1 (FABS(B4)-1E-6)11.59,11.59,11.61
 11.59 S RRC(I)=-P;S RRC(I+1)=-Q/P;G 11.69
 11.61 S RRC(I)=-.5*P;S RRC(I+1)=RRC(I);JS BI=P*P-4*Q
 11.63 I (B1)11.65,11.65,11.67
 11.65 S RIC(I)=-.5*FSQT(-B1);S RI(I+1)=-RIC(I);JG 11.70
 11.67 S BI=-.5*FSQT(B1);S RRC(I)=RRC(I)+B1;S RR(I+1)=RR(I+1)-B1
 11.69 S RIC(I)=0;S RI(I+1)=0
 11.70 S I=1+2;J1 (I-L2)11.11,11.11,11.72
 11.72 I (-IS)11.74;R
 11.74 S K2=IN+1;F J2=K2,L2;D 7
 11.76 R
 11.80 F J2=J3,L2;S RR(J2)=RR(J2+1);S RI(J2)=RI(J2+1)
 11.82 S IN=L2-1;R
 11.84 F J2=1,L2;S C(J2)=RR(J2-2)
 11.86 G 11.54
 11.90 S P=QJG 11.21

 12.05 S RR(J2)=C(J2)-P*B1-Q*B2;J1 (J2-L2)12.10;R
 12.10 S RI(J2)=RR(J2)-P*B3-Q*B4;S B2=B1;S B4=B3
 12.15 S BI=RR(J2);S B3=RI(J2)

 13.10 A N1;I (N1)13.20,3.97,3.97
 13.20 I (N1+2)13.30,4.40,3.08
 13.30 I (N1+4)13.40,4.40,3.15
 13.40 I (N1+6)13.50,4.40;I (LT)16.47,3.35;G 3.40
 13.50 I (N1+8)4.40,4.40;G

 14.05 S N=K+1;S DD=A(N+II*L)/A(II+II*L)
 14.10 F J=II,L;S A(N+J*L)=A(N+J*L)-A(II+J*L)*DD
 14.15 S Y(X(N)=YX(N)-YX(II)*DD; R

 15.10 S MM=L-1;F II=1,MM; F K=II,MM; D 14+0
 15.15 S B(L)=YX(L)/AC(L+L*L)
 15.20 F M=2;L;S N=L+1;M;S KK=N+1;JS B(N)=YX(N)/A(N+N*L);D 15.25;R
 15.25 F K=KK,L;S B(N)=B(N)-A(N+K*L)*B(K)/A(N+N*L)

 16.10 T " ,Z9.01,Y(J1),", " ,Z7.01,YY
 16.20 T " ,%,4.01,D," ,D*100/Y(J1)

 20.10 F J2=1,L-1;S C(J2)=B(L-J2+1)*(L-J2)
 20.15 S L2=L-2;D 11;S IM=0;F J2=1,L2;D 2;
 20.30 I (IM)20.40,20.90,20.40
 20.40 T !!WARNING: STANDARD CURVE CALCULATED ABOVE SHOWS",%2,IM
 20.41 T " MAXIMA (MINIMA)"!IN THE CONCENTRATION RANGE OF STANDARD"
 20.42 T " SOLUTIONS "!
 20.45 F J1=1,IM;S YY(J1)=B(1);F J2=2,L;D 20.8
 20.50 F J1=1,IM;T 1,%3,J1," CONCENTRATION=";D 20.60
 20.55 T !!G 6.47
 20.60 T Z7.02,FEXP(R2(J1))-1," HEIGHT CALCULATED=",YY(J1)
 20.80 S YY(J1)=YY(J1)+B(J2)*(R2(J1)+(J2-1))
 20.90 R

 21.10 I (RI(J2))=21.20,21.30,21.20
 21.20 R
 21.30 I (RR(J2))21.20,21.20,21.40
 21.40 I (RRC(J2)-X(L1))21.50;R
 21.50 S IN=IM+1;S R2(IM)=RR(J2)

 22.10 I (Y(1))22.20;J1 (T)9.32;I (T-Y(1))9.32,9.34,9.28
 22.20 I (T)22.30,9.28,9.28
 22.30 I (Y(1)-T)9.28,9.34,9.32

3. REPORT ON ANALYSIS

3.1. Program AD0012

3.1.1. Abstract

This program generates a typed report on a chemical analysis of water. At the same time the program calculates and types out a series of calculated parameters.

3.1.2. Input data

The input parameters are listed in Table 3.1. The order in which they appear in the table is identical to the order in which they must be entered in the computer. This order facilitates the input operation when using the new laboratory forms (1).

For parameters 1 to 50, only numerical values must be entered. There is only one exception to this rule; when a particular parameter is not available, then "-N" must be entered.

For parameters 51 and 52, any combination of letters and numbers is allowed. Three words are allowed in each instance (one word in this case is defined as being any combination of letters and/or numbers terminated by a space, comma, period, or hyphen). If the "Location" or the "Source" has less than three words then the missing words can be made up from the combination ". ." (i.e., period and space) or ", ." (comma and space) or "- ." (hyphen and space). Any of these combinations replaces one word.

Examples of input data can be seen in Figure 3.1.

3.1.3. Output data

A typical report is reproduced in Figure 3.2. The numerical value entered for each test appears in the output. For those parameters entered as "-N", the words "NOT AVAILABLE" are typed out as shown in Figure 3.2.

In the case of calculated parameters, if one of the parameters entering the calculation is "NOT AVAILABLE", the calculation is not performed and a hyphen appears in the output.

The "Sum of constituents (mg/l)" is calculated only when all of the following parameters are present: Calcium - dissolved, Magnesium - dissolved, Potassium - dissolved, Sodium - dissolved, Alkalinity - total, Alkalinity - Phenolphthalein, Chloride, Fluoride, Silica - Reactive, Sulphate. If any of these has not been determined, i.e., if it was entered as "-N", then the "Sum of constituents" is not calculated; in this case also, the "Saturation and Stability indices" are not calculated because their calculation requires the "Sum of constituents" value.

If any of the cations listed above has not been analysed, then "Sodium per cent" cannot be calculated.

Other ions listed in the output and not mentioned above are included in the "Sum of constituents" when present. These ions are: Copper - dissolved, Iron - dissolved, Lead - dissolved, Manganese - dissolved, Zinc - dissolved, Phosphate - dissolved, ortho.

The length of the printout is approximately 13 inches; therefore it will fit in a sheet of paper of 8 1/2 x 14 inches if it must be xeroxed.

3.1.4. The Computer program

The program is written in FOCAL-69. In Water Quality Division, a PDP-8/L, 8K computer is used to run the program. The listing is reproduced in Figure 3.4.

The time required to type out one report is approximately five minutes. The limiting factor is the speed of the Teletype. With a faster printer this time can be reduced to one minute or less.

3.1.5. References

- Demayo, A. 1970. A storage and retrieval system for water quality data, Inland Waters Branch, Report Series No. 9.

TABLE 3.1
Program AD0012 - Input Parameters

No.	Symbol	Parameter	Unit
1	A (1)	Laboratory number	Integer
2	A (2)	Field number	Integer
3	A (3)	Day of sampling	Integer
4	A (4)	Month of sampling	Integer
5	A (5)	Year of sampling	Integer
6	A (6)	Day of testing	Integer
7	A (7)	Month of testing	Integer
8	A (8)	Year of testing	Integer
9	A (9)	Turbidity	
10	A (10)	Temperature at testing	°C
11	A (11)	Colour	Hazen units
12	A (12)	pH	pH units
13	A (13)	Carbon: Total, Organic	mg/l
14	A (14)	Chloride: Dissolved	mg/l
15	A (15)	Copper: Total	mg/l
16	A (16)	Copper: Dissolved	mg/l
17	A (17)	Fluoride: Dissolved	mg/l
18	A (18)	Iron: Total	mg/l
19	A (19)	Iron: Dissolved	mg/l
20	A (20)	Lead: Total	mg/l
21	A (21)	Lead: Dissolved	mg/l
22	A (22)	Magnesium: Dissolved	mg/l
23	A (23)	Manganese: Total	mg/l
24	A (24)	Manganese: Dissolved	mg/l
25	A (25)	Nitrogen: Total Kjeldahl	mg/l
26	A (26)	Nitrogen: Nitrate + Nitrite	mg/l
27	A (27)	Nitrogen: Dissolved Ammonia	mg/l
28	A (28)	Oxygen: Total Chemical Demand	mg/l
29	A (29)	Phosphate: Dissolved, Ortho	mg/l
30	A (30)	Phosphate: Dissolved, Inorganic	mg/l
31	A (31)	Phosphate: Total	mg/l
32	A (32)	Potassium: Dissolved	mg/l
33	A (33)	Residue: Nonfilterable (105°C)	mg/l
34	A (34)	Residue: Filterable (105°C)	mg/l
35	A (35)	Residue: Fixed, Nonfilterable (550°C)	mg/l
36	A (36)	Residue: Fixed, Filterable (550°C)	mg/l
37	A (37)	Silica: Reactive	mg/l
38	A (38)	Sodium: Dissolved	mg/l
39	A (39)	Zinc: Total	mg/l
40	A (40)	Zinc: Dissolved	mg/l
41	A (41)	Carbon: Dissolved, Organic	mg/l
42	A (42)	Specific conductance	µmho/cm
43	A (43)	Alkalinity: Phenolphthalein	mg/l CaCO ₃
44	A (44)	Alkalinity: Total	mg/l CaCO ₃
45	A (45)	Acidity: pH 4.5	mg/l CaCO ₃
46	A (46)	Acidity: pH 8.3	mg/l CaCO ₃
47	A (47)	Hardness: Total	mg/l CaCO ₃
48	A (48)	Calcium: Dissolved	mg/l
49	A (49)	Oxygen: Consumed	mg/l
50	A (50)	Sulphate: Dissolved	mg/l
51	D	Location (3 words)	Alphabetic
52	D	Source (3 words)	Alphabetic

3.2. Program AD0013

This program is very similar to Program AD0012. The only difference is the fact that if a certain parameter was entered as "-N", it will not be listed in the typed output. Similarly, if a certain value cannot be calculated because some of the parameters entering its calculation are absent, then it is not listed in the typed output.

The input data are identical to those for Program AD0012 (see Table 3.1 and Figure 3.1). A typical output is shown in Figure 3.5. A listing of the program is reproduced in Figure 3.6. The program requires 8K of memory. The time required to type out one report depends on the number of parameters present. The report reproduced in Figure 3.5 required 2 minutes on a PDP-8/L.

3.3. Program AD0014

This program is another variation of Program AD0012. The following calculated parameters have been added to the typed output: "Sum of cations" (me/l), "Sum of anions" (me/l) and the "Difference" between them in per cent.

The "Sum of cations" is not calculated if one of the following ions has not been determined: Calcium - dissolved, Magnesium - dissolved, Potassium - dissolved, Sodium - dissolved. When present, the following ions are added to the "Sum of cations": Copper - dissolved, Iron - dissolved, Lead - dissolved, Manganese - dissolved, Zinc - dissolved.

The "Sum of anions" is not calculated if one of the following parameters has not been measured: Alkalinity - phenolphthalein, Alkalinity - total, Chloride - dissolved, Fluoride - dissolved, Sulphate - dissolved. If Phosphate - dissolved, ortho is present, then it is included in the "Sum of anions".

If either the "Sum of cations" or the "Sum of anions" could not be calculated, then the "Difference" (per cent) is not calculated.

The input data are identical to those for Program AD0012 or Program AD0013 (see Figure 3.1 and Table 3.1).

The output appears on two pages. A typical output is reproduced in Figure 3.7.

The program is written in FOCAL-69 and requires the whole 8K of memory of a PDP-8/L computer. A listing of the program is reproduced in Figure 3.8.

Approximately five minutes are required to type out a report.

Figure 3.1. Programs AD0012 - AD0014 - Input

```
3329 -N 13 7 1970 3 9 1970 .38 20.5 5 7.7 -N .5 -N -N .19 -N .02
-N -N -N -N 0 -N .17 -N -N .186 -N .7 -N 92 -N 65.6 4.4 1.2
-N -N -N 142 0 52.1 -N -N 67.3 22.9 -N 13.7 A B C X1 Y1 Z1
3330 123 23 9 1970 4 10 1970 .40 21 4 7.5 -N .5 -N -N .19 FINISH
A1 B1 C1 X Y Z
2972 -N 6 8 1970 27 8 1970 3.2 25.8 80 7.1 -N 15 0 -N .28
-N 0 -N -N -N .85 0 -N 1.2 -N -N .55 -N 26.8 -N -N -N -N .9
6.2 .08 -N -N 380 0 166 -N -N 146 52.7 -N 1.3
MELFORT, SASK • POTHOLE G-23 .
```

Figure 3.2. Program AD0012 - Output

ANALYSIS OF WATER SAMPLE

LOCATION : A B C
 SOURCE : X1 Y1 Z1

LABORATORY NUMBER= 3329
 FIELD NUMBER = NOT AVAILABLE
 DATE OF SAMPLING :
 DAY = 13 MONTH = 7 YEAR = 1970
 DATE OF TESTING :
 DAY = 3 MONTH = 9 YEAR = 1970

COLOUR (HAZEN UNITS) = 5.00
 SPECIFIC CONDUCTANCE (UMHO/CM) = 142.00
 TEMPERATURE OF TESTING (DEG.C.)= 20.50
 TURBIDITY = 0.38

PH (PH UNITS)= 7.70
 ACIDITY-PH 4.5 (MG/L CACO3)= NOT AVAILABLE
 ACIDITY-PH 8.3 (MG/L CACO3)= NOT AVAILABLE
 ALKALINITY-PHENOLPHTHALEIN (MG/L CACO3)= 0.00
 ALKALINITY-TOTAL (MG/L CACO3)= 52.10
 HARDNESS-TOTAL (MG/L CACO3)= 67.30

RESIDUE-NONFILTERABLE (105 DEG.C.) (MG/L)= NOT AVAILABLE
 RESIDUE-FILTERABLE (105 DEG.C.) (MG/L)= 92.00
 RESIDUE-FIXED,NONFILTERABLE (550 DEG.C.) (MG/L)= NOT AVAILABLE
 RESIDUE-FIXED,FILTERABLE (550 DEG.C.) (MG/L)= 65.60

CARBON- TOTAL ORGANIC, C (MG/L)= NOT AVAILABLE
 CARBON-DISSOLVED ORGANIC, C (MG/L)= NOT AVAILABLE
 NITROGEN-TOTAL, KJELDAHL, N (MG/L)= NOT AVAILABLE
 NITROGEN-DISSOLVED AMMONIA, N (MG/L)= NOT AVAILABLE
 OXYGEN-TOTAL CHEMICAL DEMAND (MG/L)= NOT AVAILABLE
 OXYGEN-CONSUMED (MG/L)= NOT AVAILABLE

CATIONS (MG/L) :
 CALCIUM-DISSOLVED, CA = 22.90
 COOPER-TOTAL, CU = NOT AVAILABLE
 COOPER-DISSOLVED, CU = NOT AVAILABLE
 IRON-TOTAL, FE = NOT AVAILABLE
 IRON-DISSOLVED, FE = 0.02
 LEAD-TOTAL, PB = NOT AVAILABLE
 LEAD-DISSOLVED, PB = NOT AVAILABLE
 MAGNESIUM DISSOLVED, MG= 2.46 (CALCULATED)
 MANGANESE-TOTAL, MN = NOT AVAILABLE
 MANGANESE-DISSOLVED, MN= 0.00
 POTASSIUM-DISSOLVED, K = 0.70
 SODIUM-DISSOLVED, NA = 1.20
 ZINC-TOTAL, ZN = NOT AVAILABLE
 ZINC-DISSOLVED, ZN = NOT AVAILABLE

ANIONS (MG/L) :
 BICARBONATE, HC03 = 63.51 (CALCULATED)
 CARBONATE, CO3 = 0.00 (CALCULATED)
 CHLORIDE-DISSOLVED, CL = 0.50
 FLUORIDE-DISSOLVED, F = 0.19
 HYDROXIDE, OH = 0.00 (CALCULATED)
 NITROGEN-NITRATE+NITRITE, N = 0.17
 PHOSPHATE-DISSOLVED, ORTHO, PO4 = NOT AVAILABLE
 PHOSPHATE-DISSOLVED, INORGANIC, PO4= 0.19
 PHOSPHATE-TOTAL, PO4 = NOT AVAILABLE
 SILICA-REACTIVE, SI02 = 4.40
 SULPHATE-DISSOLVED, SO4 = 13.70

OTHER CALCULATED PARAMETERS :
 SUM OF CONSTITUENTS (MG/L)= 78.11
 SODIUM ABSORPTION RATIO = 0.06
 SODIUM PER CENT = 3.69

NONCARBONATE HARDNESS (MG/L CACO3)= 15.20
 CO2 (MG/L)= 2.01
 SATURATION INDEX (PH UNITS)=- 0.71
 STABILITY INDEX (PH UNITS)= 9.11

Figure 3.3. Program AD0012 - Output

ANALYSIS OF WATER SAMPLE

LOCATION :A1 B1 C1
SOURCE :X Y Z

LABORATORY NUMBER= 3330
FIELD NUMBER = 123
DATE OF SAMPLING :
DAY = 23 MONTH = 9 YEAR = 1970
DATE OF TESTING :
DAY = 4 MONTH = 10 YEAR = 1970

COLOUR (HAZEN UNITS) = 4.00
SPECIFIC CONDUCTANCE (MHO/CM) = NOT AVAILABLE
TEMPERATURE OF TESTING (DEG.C.)= 21.00
TURBIDITY = 0.40

PH (PH UNITS)= 7.50
ACIDITY-PH 4.5 (MG/L CACO3)= NOT AVAILABLE
ACIDITY-PH 8.3 (MG/L CACO3)= NOT AVAILABLE
ALKALINITY-PHENOLPHTHALEIN (MG/L CACO3)= NOT AVAILABLE
ALKALINITY-TOTAL (MG/L CACO3)= NOT AVAILABLE
HARDNESS-TOTAL (MG/L CACO3)= NOT AVAILABLE

RESIDUE-NONFILTERABLE (105 DEG.C.) (MG/L)= NOT AVAILABLE
RESIDUE-FILTERABLE (105 DEG.C.) (MG/L)= NOT AVAILABLE
RESIDUE-FIXED,NONFILTERABLE (550 DEG.C.) (MG/L)= NOT AVAILABLE
RESIDUE-FIXED,FILTERABLE (550 DEG.C.) (MG/L)= NOT AVAILABLE

CARBON- TOTAL ORGANIC, C (MG/L)= NOT AVAILABLE
CARBON-DISSOLVED ORGANIC, C (MG/L)= NOT AVAILABLE
NITROGEN-TOTAL, KJELDAHL, N (MG/L)= NOT AVAILABLE
NITROGEN-DISSOLVED AMMONIA, N (MG/L)= NOT AVAILABLE
OXYGEN-TOTAL CHEMICAL DEMAND (MG/L)= NOT AVAILABLE
OXYGEN-CONSUMED (MG/L)= NOT AVAILABLE

CATIONS (MG/L) :
CALCIUM-DISSOLVED, CA = NOT AVAILABLE
COOPER-TOTAL, CU = NOT AVAILABLE
COOPER-DISSOLVED, CU = NOT AVAILABLE
IRON-TOTAL, FE = NOT AVAILABLE
IRON-DISSOLVED, FE = NOT AVAILABLE
LEAD-TOTAL, PB = NOT AVAILABLE
LEAD-DISSOLVED, PB = NOT AVAILABLE
MAGNESIUM DISSOLVED, MG= NOT AVAILABLE
MANGANESE-TOTAL, MN = NOT AVAILABLE
MANGANESE-DISSOLVED, MN= NOT AVAILABLE
POTASSIUM-DISSOLVED, K = NOT AVAILABLE
SODIUM-DISSOLVED, NA = NOT AVAILABLE
ZINC-TOTAL, ZN = NOT AVAILABLE
ZINC-DISSOLVED, ZN = NOT AVAILABLE

ANIONS (MG/L) :
BICARBONATE, HC03 = -
CARBONATE, CO3 = -
CHLORIDE-DISSOLVED, CL = 0.50
FLUORIDE-DISSOLVED, F = 0.19
HYDROXIDE, OH = -
NITROGEN-NITRATE+NITRITE, N = NOT AVAILABLE
PHOSPHATE-DISSOLVED, ORTHO, PO4 = NOT AVAILABLE
PHOSPHATE-DISSOLVED, INORGANIC, PO4= NOT AVAILABLE
PHOSPHATE-TOTAL, PO4 = NOT AVAILABLE
SILICA-REACTIVE, SIO2 = NOT AVAILABLE
SULPHATE-DISSOLVED, SO4 = NOT AVAILABLE

OTHER CALCULATED PARAMETERS :
SUM OF CONSTITUENTS (MG/L)= -
SODIUM ABSORPTION RATIO = -
SODIUM PER CENT = -

NONCARBONATE HARDNESS (MG/L CACO3)= -
CO2 (MG/L)= -
SATURATION INDEX (PH UNITS)= -
STABILITY INDEX (PH UNITS)= -

Figure 3.4. Program AD0012 - Listing

```

*W
C-8K FOCAL 01969

01.02 E
01.03 S Y=-0NJF J=1,53JS A(J)=Y
01.05 F J=1,50IA A(J)JI (0FINISH-A(J))1.06,1.06JC
01.06 S AKJ=YJS J=60
01.07 T !!!!!!!DEPARTMENT OF FISHERIES AND FORESTRY!!
01.08 T "INLAND WATERS BRANCH"!WATER QUALITY DIVISION!!
01.09 T "ANALYSIS OF WATER SAMPLE"!
01.10 T "LOCATION :"JA D1,D2,D3
01.12 T !"SOURCE :"JA D1,D2,D3
01.14 T !"LABORATORY NUMBER"JI (Y-A(1))1.15JD 6JG 1.17
01.15 T ,X10,A(1)
01.17 T !"FIELD NUMBER" JI (Y-A(2))1.18JD 6JG 1.20
01.18 T X10,AC2)
01.20 D 26.1JT "SAMPLING :"JS I=3JD 3
01.21 D 26.1JT "TESTING :"JS I=6JD 3
01.22 T !!"COLOUR (HAZEN UNITS)"JD 30.3JI (Y-A(11))1.45JD 6JG 1.48
01.45 T Z7.02,A(11)
01.48 T !"SPECIFIC CONDUCTANCE (UMHO/CM)"JI (Y-A(42))1.49JD 6JG 1.50
01.49 T A(42)
01.50 T !"TEMPERATURE OF TESTING (DEG.C.)"JI (Y-A(10))1.51JD 6JG 1.52
01.51 T A(10)
01.52 T !"TURBIDITY"JD 30.2JI (Y-A(9))1.53JD 6JG 1.55
01.53 T A(9)
01.55 T !!"PH"JD 30.4JD 26.92JI (Y-A(12))1.58JD 6JG 1.61
01.58 T A(12)
01.61 D 24.4JT "4.5"JD 30.5JD 27JI (Y-A(45))1.63JD 6JG 1.65
01.63 T A(45)
01.65 D 24.4JT "B+3"JD 30.5JD 27JI (Y-A(46))1.67JD 6JG 1.70
01.67 T A(46)
01.70 D 24.5JT "PHENOLPHTHALEIN"JD 27JI (Y-A(43))1.72JD 6JG 1.75
01.72 T A(43)
01.75 D 24.5JT "TOTAL"JD 30.8JD 27JI (Y-A(44))1.76JD 6JG 1.77
01.76 T A(44)
01.77 T !"HARDNESS-TOTAL"JD 30.5JD 27JI (Y-A(47))1.78JD 6JG 1.79
01.78 T A(47)
01.79 D 2
01.82 D 4
01.84 D 5
01.86 D 7
01.88 D 8
01.90 D 9
01.92 T !!!!!JD 1

02.05 T !JD 26.4JT "NON"JD 26.5JD 30.96JD 25JI (Y-A(33))2.07JD 6JG 2.10
02.07 T A(33)
02.10 D 26.4JD 26.5JD 30.6JD 25JI (Y-A(34))2.12JD 6JG 2.15
02.12 T A(34)
02.15 D 26.7JT "NON"JD 26.6JD 25JI (Y-A(35))2.17JD 6JG 2.20
02.17 T A(35)
02.20 D 26.7JD 26.6JT " "JD 25JI (Y-A(36))2.22JD 6JG 1.82
02.22 T A(36)

03.10 T !" DAY "JI (Y-A(1))3.18JD 6JG 3.20
03.18 T X2,AC1)
03.20 T !" MONTH "JI (Y-A(I+1))3.28JD 6JG 3.30
03.28 T A(I+1)
03.30 T !" YEAR "JI (Y-A(I+2))3.38JD 6JG 3.99
03.38 T X4,A(I+2)
03.99 R

04.15 T !JD 26.8JT " "JD 28JD 26.9JI (Y-A(13))4.17JD 6JG 4.20
04.17 T A(13)
04.20 D 26.8JD 29JD 26.9JI (Y-A(41))4.22JD 6JG 4.30
04.22 T A(41)
04.30 D 26.91JD 28JT ", KJELDAHL, N"JD 25
04.31 I (Y-A(25))4.32JD 6JG 4.35
04.32 T A(25)
04.35 D 26.91JD 29JT " AMMONIA, N"JD 25JI (Y-A(27))4.37JD 6JG 4.40
04.37 T A(27)
04.40 T !"OXYGEN-TOTAL CHEMICAL DEMAND "JD 25
04.41 I (Y-A(28))4.42JD 6JG 4.45
04.42 T A(28)
04.45 T !"OXYGEN-CONSUMED"JD 30.91JD 25JI (Y-A(49))4.47JD 6JG 1.84
04.47 T A(49)

05.05 T !!"CATIONS (MG/L) :"JS B=0JS D=0
05.07 T !"CALCIUM-DISSOLVED, CA "JI (Y-A(48))5.08JD 24.1JD 5.10
05.08 T A(48)JS B=B+A(48)*.0499JS D=D+A(48)
05.10 T !"COOPER-TOTAL, CU"JD 30.93JI (Y-A(15))5.12JD 6JG 5.15
05.12 T A(15)
05.15 T !"COOPER-DISSOLVED, CU "JI (Y-A(16))5.17JD 6JG 5.20
05.17 T A(16)JS B=B+A(16)*.03148JS D=D+A(16)
05.20 T !"IRON-TOTAL, FE"JD 30.6JI (Y-A(18))5.22JD 6JG 5.25
05.22 T A(18)
05.25 T !"IRON-DISSOLVED, FE "JI (Y-A(19))5.27JD 6JG 5.30
05.27 T A(19)JS B=B+A(19)*.05372JS D=D+A(19)
05.30 T !"LEAD-TOTAL, PB"JD 30.6JI (Y-A(20))5.32JD 6JG 5.35
05.32 T A(20)
05.35 T !"LEAD-DISSOLVED, PB "JI (Y-A(21))5.37JD 6JG 5.40
05.37 T A(21)JS B=B+A(21)*.009653JS D=D+A(21)
05.40 T !"MAGNESIUM DISSOLVED, MG"JI (Y-A(22))5.45,5.42,5.45
05.42 I (Y-A(47))5.43JD 24.1JD 5.46
05.43 I (Y-A(48))5.44JD 24.1JD 5.46
05.44 S A(22)=12.16*(A(47)*.01998-A(48)*.0499)JD 5.45JD 26.2JD 5.46
05.45 T A(22)JS B=B+A(22)*.08226JS D=D+A(22)
05.46 T !"MANGANESE-TOTAL, MN "JI (Y-A(23))5.47JD 6JG 5.50
05.47 T A(23)
05.50 T !"MANGANESE-DISSOLVED, MN"JI (Y-A(24))5.52JD 6JG 5.55
05.52 T A(24)JS B=B+A(24)*.03641JS D=D+A(24)
05.55 T !"POTASSIUM-DISSOLVED, K "JI (Y-A(32))5.57JD 24.1JD 5.60
05.57 T A(32)JS B=B+A(32)*.02557JS D=D+A(32)
05.60 T !"SODIUM-DISSOLVED, NA "JI (Y-A(38))5.62JD 24.1JD 5.65
05.62 T A(38)JS B=B+A(38)*.0435JS D=D+A(38)
05.65 T !"ZINC-TOTAL, ZN"JD 30.6JI (Y-A(39))5.67JD 6JG 5.70
05.67 T A(39)
05.70 T !"ZINC-DISSOLVED, ZN "JI (Y-A(40))5.72JD 6JG 1.86
05.72 T A(40)JS B=B+A(40)*.0306JS D=D+A(40)

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06.10 T == NOT AVAILABLE"; T 7.02
 07.05 T !!"ANIONS (MG/L) :" ; I (Y-A(43))7.12,7.29,7.12
 07.12 I (Y-A(44))7.20,7.29,7.20
 07.20 I (A(43)-A(44)/2)7.25,7.25,7.23
 07.23 S A(53)=0; S A(51)=1.2*(A(44)-A(43)); S A(52)=(2*A(43)-A(44))*3.399
 07.24 G 7.38
 07.25 S A(53)=(A(44)-2*A(43))+1.219; S A(51)=A(43)*1.215; S A(52)=0; G 7.38
 07.29 S D=Y; S C=Y
 07.30 T !"BICARBONATE, HC03"JD 30.94; I (Y-A(53))7.32; JD 24.91G 7.35
 07.32 T A(53); JD 26.2
 07.35 T !"CARBONATE, CO3"JD 30.95; I (Y-A(51))7.37; JD 24.91G 7.40
 07.37 T A(51); JD 26.2
 07.40 T !"CHLORIDE-DISSOLVED, CL"JD 30.90; I (Y-A(14))7.42; JD 24.21G 7.45
 07.42 T A(14)
 07.45 T !"FLUORIDE-DISSOLVED, F"JD 30.91; I (Y-A(17))7.47; JD 24.21G 7.50
 07.47 T A(17)
 07.50 T !"HYDROXIDE, OH"JD 30.23; I (Y-A(52))7.52; JD 24.91G 7.55
 07.52 T A(52); JD 26.2
 07.55 T !"NITROGEN-NITRATE+NITRITE, N"JD 30.93
 07.56 I (Y-A(26)); JD 7.57; JD 24.21G 7.60
 07.57 T A(26)
 07.60 D 26.3; T "DISSOLVED, ORTHO, PO4" ; I (Y-A(29))7.62; JD 6; G 7.65
 07.62 T A(29)
 07.65 D 26.3; T "DISSOLVED, INORGANIC, PO4" ; I (Y-A(30))7.67; JD 6; G 7.70
 07.67 T A(30)
 07.70 D 26.3; T "TOTAL, PO4" ; JD 30.91; I (Y-A(31))7.72; JD 6; G 7.73
 07.72 T A(31)
 07.73 T !"SILICA-REACTIVE, SiO2" ; JD 30.91; I (Y-A(37))7.74; JD 24.21G 7.78
 07.74 T A(37)
 07.75 T !"SULPHATE-DISSOLVED, SO4" ; JD 30.5; I (Y-A(50))7.81; JD 24.21G 1.88
 07.81 T A(50); JD 7.84; G 1.88
 07.84 S D=D*(A(50)+A(51)+A(52)+A(53))/2.03+A(14)+A(17)+A(37)+A(26)*4.429
 07.90 I (Y-A(29))7.92; G 1.88
 07.92 S D =D+A(29); G 1.88
 08.05 T !!"OTHER CALCULATED PARAMETERS :" ; S L=2.3026
 08.07 D 24.3; T " " ; JD 25; I (Y-D)8.50; JD 24.91G 8.75
 08.50 T D
 08.75 T !"SODIUM ABSORPTION RATIO" ; JD 30.6; I (Y-A(38))8.77; JD 24.91G 8.83
 08.77 I (Y-A(48))8.79; JD 24.91G 8.83
 08.79 I (Y-A(22))8.81; JD 24.91G 8.83
 08.81 T 1.41+A(38)*.0435/FSQT(A(22)*.08226+A(48)*.0499)
 08.83 T !"SODIUM PER CENT" ; JD 30.92; I (Y-B)8.87; JD 24.91G 8.89
 08.87 T 4.35*A(38)/B
 08.89 T !"NONCARBONATE HARDNESS" ; JD 27; I (Y-A(47))8.90; JD 24.91G 8.99
 08.90 I (Y-A(44))8.91; JD 24.91G 8.99
 08.91 S B=A(44)-A(47); I (B)8.92; S B=0
 08.92 T -B
 08.99 G 1.90
 09.03 T !"CO2" ; JD 30.2; JD 25; I (Y-A(12))9.04; JD 24.91G 9.44
 09.04 I (Y-A(44))9.05; JD 24.91G 9.44
 09.05 S B=FEXP(-A(12)/.4343)
 09.10 S B=9.7E10*B*(A(44)/5E4+B-1E-14/B)/(1+1.22E-11/B)
 09.12 T B
 09.15 T !"SATURATION INDEX" ; JD 30.93; JD 26.92
 09.17 I (Y-D)9.19; JD 24.91G 9.45
 09.19 I (Y-A(10))9.27; JD 24.91G 9.45
 09.27 S R=25E-6; S D=A(10)+273.15; S B=-8.37+2*(830/D-2.78)
 09.29 S C=2902.39/D-6.498+.02379*D; S B=B+C*FLOG(A(48))/L-FLOG(A(44))/L
 09.31 S B=B+9.3*2.5*FSQT(R)/(1+5.3*FSQT(R)+5.5*R); T A(12); B
 09.40 D 26.93; T 2*B-A(12); G 1.92
 09.44 D 9.15; JD 24.9
 09.45 D 26.93; JD 24.91G 1.92
 24.10 D 6; S B=Y; S D=Y
 24.20 D 6; S D=Y
 24.30 T !"SUM OF CONSTITUENTS"
 24.40 T !"ACIDITY-PH"
 24.50 T !"ALKALINITY-"
 24.60 T "
 25.10 T "(MG/L)"
 26.10 T !"DATE OF"
 26.20 T "(CALCULATED)"
 26.30 T !"PHOSPHATE-"
 26.40 T !"RESIDUE-"
 26.50 T "FILTERABLE (105 DEG.C.)"
 26.60 T "FILTERABLE (550 DEG.C.)"
 26.70 T !"RESIDUE-FIXED."
 26.80 T !"CARBON-"
 26.90 T "ORGANIC, C" ; JD 25
 26.91 T !"NITROGEN-"
 26.92 T "(PH UNITS)"
 26.93 T !"STABILITY INDEX" ; JD 30.93; JD 26.92
 27.10 T "(MG/L CACO3)"
 28.10 T "TOTAL"
 29.10 T "DISSOLVED"
 30.10 F K=1,M1T " "
 30.20 S M=22; JD 30.1
 30.30 S M=11; JD 30.1
 30.40 S M=25; JD 30.1
 30.50 S M=12; JD 30.1
 30.60 S M=9; JD 30.1
 30.70 S M=8; JD 30.1
 30.80 S M=10; JD 30.1
 30.90 S M=13; JD 30.1
 30.91 S M=14; JD 30.1
 30.92 S M=16; JD 30.1
 30.93 S M=7; JD 30.1
 30.94 S M=18; JD 30.1
 30.95 S M=21; JD 30.1
 30.96 S M=6; JD 30.1

Figure 3.5. Program AD0013 - Output

ANALYSIS OF WATER SAMPLE

LOCATION : A B C
SOURCE : X1 Y1 Z1

LABORATORY NUMBER= 3329
DATE OF SAMPLING :
DAY = 13 MONTH = 7 YEAR = 1970
DATE OF TESTING :
DAY = 3 MONTH = 9 YEAR = 1970

COLOUR	(HAZEN UNITS)=	5.00
SPECIFIC CONDUCTANCE	(MUMHO/CM)=	142.00
TEMPERATURE OF TESTING	(DEG.C.)=	20.50
TURBIDITY	=	0.38
PH	(PH UNITS)=	7.70
ALKALINITY-PHENOLPHTHALEIN	(MG/L CACO3)=	0.00
ALKALINITY-TOTAL	(MG/L CACO3)=	52.10
HARDNESS-TOTAL	(MG/L CACO3)=	67.30
RESIDUE-FILTERABLE (105 DEG.C.)	(MG/L)=	92.00
RESIDUE-FIXED, FILTERABLE (550 DEG.C.)	(MG/L)=	65.60
CALCIUM-DISSOLVED, CA	(MG/L)=	22.90
IRON-DISSOLVED, FE	(MG/L)=	0.02
MAGNESIUM-DISSOLVED, MG	(MG/L)=	2.46 (CALCULATED)
MANGANESE-DISSOLVED, MN	(MG/L)=	0.00
POTASSIUM-DISSOLVED, K	(MG/L)=	0.70
SODIUM-DISSOLVED, NA	(MG/L)=	1.20
BICARBONATE, HC03	(MG/L)=	63.51 (CALCULATED)
CARBONATE, CO3	(MG/L)=	0.00 (CALCULATED)
CHLORIDE-DISSOLVED, CL	(MG/L)=	0.50
FLUORIDE-DISSOLVED, F	(MG/L)=	0.19
HYDROXIDE, OH	(MG/L)=	0.00 (CALCULATED)
NITROGEN-NITRATE+NITRITE, N	(MG/L)=	0.17
PHOSPHATE-DISSOLVED, INORGANIC, PO4	(MG/L)=	0.19
SILICA-REACTIVE, SI02	(MG/L)=	4.40
SULPHATE-DISSOLVED, SO4	(MG/L)=	13.70
SUM OF CONSTITUENTS	(MG/L)=	78.11 (CALCULATED)
SUM OF CATIONS	(ME/L)=	1.4159 (CALCULATED)
SUM OF ANIONS	(ME/L)=	1.3624 (CALCULATED)
DIFFERENCE PER CENT	=	1.93 (CALCULATED)
SODIUM ABSORPTION RATIO	=	0.06 (CALCULATED)
SODIUM PER CENT	=	3.69 (CALCULATED)
NONCARBONATE HARDNESS	(MG/L CACO3)=	15.20 (CALCULATED)
CO2	(MG/L)=	2.01 (CALCULATED)
SATURATION INDEX	(PH UNITS)=	0.71 (CALCULATED)
STABILITY INDEX	(PH UNITS)=	9.11 (CALCULATED)

Figure 3.6. Program AD0013 - Listing

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*W
C-BK FOCAL 01969

01.02 E
01.03 T %10JS Y=-0N;F J=1,53JS A(J)=Y
01.05 F J=1,50JA A(J)SI (0FINISH-A(J))1.06.1.06JC
01.06 S A(J)=YJS J=60
01.07 T !!!!!!!!!"DEPARTMENT OF FISHERIES AND FORESTRY"!
01.08 T "INLAND WATERS BRANCH" "WATER QUALITY DIVISION"!
01.09 T "ANALYSIS OF WATER SAMPLE"!
01.10 T "LOCATION :"!A D,D,D
01.12 T !"SOURCE :"!A D,D,D
01.13 T !J (Y-A(1))1.14JG 1.16
01.14 T !"LABORATORY NUMBER"!A(1)
01.16 I (Y-A(2))1.17JG 1.21
01.17 T !"FIELD NUMBER"!A(2)
01.21 F I=3.3.6JD 3
01.35 T !,ZT.02JI (Y-A(11))1.4JG 1.47
01.40 T !"COLOUR"!D 36.98JT "(HAZEN UNITS)"!A(11)
01.47 I (Y-A(42))1.48JG 1.49
01.48 T !"SPECIFIC CONDUCTANCE"!D 30.94JT "(UMHO/CM)"!A(42)
01.49 I (Y-A(18))1.50JG 1.51
01.50 T !"TEMPERATURE OF TESTING"!D 30.92JT "(DEG.C.)"!A(18)
01.51 I (Y-A(9))1.52JG 1.54
01.52 T !"TURBIDITY"!D 30.2JT A(9)
01.54 I (Y-A(12))1.55JG 1.60
01.55 T !"PH"!D 30.97JD 26.92JT A(12)
01.60 I (Y-A(45))1.61JG 1.64
01.61 D 24.4T "4.5"!D 30.5JD 27JT A(45)
01.64 I (Y-A(46))1.65JG 1.69
01.65 D 24.4T "6.3"!D 30.5JD 27JT A(46)
01.69 I (Y-A(43))1.70JG 1.74
01.70 D 24.5T "PHENOLPHTHALEIN"!D 30.7JD 27JT A(43)
01.74 I (Y-A(44))1.75JG 1.76
01.75 D 24.5T "TOTAL"!D 30.94JD 27JT A(44)
01.76 I (Y-A(47))1.77JG 1.79
01.77 T !"HARDNESS-TOTAL"!D 30.5JD 27JT A(47)
01.79 D 2JD 4JD 5JD 7JD 8JD 9
01.92 T !!!!!!JD 1

02.04 I (Y-A(33))2.05JG 2.09
02.05 D 26.4T "NON"!D 26.5JT " "!D 25JT A(33)
02.09 I (Y-A(34))2.10JG 2.14
02.10 D 26.4JD 26.5JD 30.7JT " "!D 25JT A(34)
02.14 I (Y-A(35))2.15JG 2.19
02.15 D 26.7JT "NON"!D 26.6JD 25JT A(35)
02.19 I (Y-A(36))2.20JG
02.20 D 26.7JD 26.6JT " "!D 25JT A(36)

03.06 S H=-1JI (Y-A(1))3.3.3.12.3.3
03.12 I (Y-A(I+1))3.32.3.14.3.32
03.14 I (Y-A(I+2))3.36JR
03.30 I (I-6)3.4.3.5.3.4
03.32 I (H)3.33JG 3.64
03.33 I (I-6)3.42.3.52.3.52
03.36 I (H)3.37JG 3.96
03.37 I (I-6)3.44.3.54.3.54
03.40 D 3.91JG 3.61
03.42 D 3.91JG 3.64
03.44 D 3.91JG 3.96
03.50 D 3.91JG 3.61
03.52 D 3.91JG 3.64
03.54 D 3.91JG 3.96
03.61 D 3.94JG 3.12
03.64 D 3.95JG 3.14
03.90 S H=0JT !"DATE OF SAMPLING"!
03.91 S H=0JT !"DATE OF TESTING"!
03.94 T " DAY ",%2,A(1+1)
03.95 T " MONTH ",%2,A(1+2)
03.96 T " YEAR ",%4,A(1+2)

04.14 I (Y-A(13))4.15JG 4.19
04.15 D 26.8JT " "!D 28JD 26.9JT A(13)
04.19 I (Y-A(41))4.2016 4.29
04.20 D 26.8JD 29JD 26.9JT A(41)
04.29 I (Y-A(25))4.3016 4.34
04.30 D 26.9JD 28JT ", KJELDAHL, N"!D 30.3JD 25JT A(25)
04.31 I (Y-A(25))4.3416 4.35
04.34 I (Y-A(27))4.3516 4.39
04.35 D 26.9JD 29JT " AMMONIA, N"!D 30.3JD 25JT A(27)
04.39 I (Y-A(28))4.4016 4.44
04.40 T !"OXYGEN-TOTAL CHEMICAL DEMAND"!D 30.3JD 25JT A(28)
04.44 I (Y-A(49))4.45JR
04.45 T !"OXYGEN-CONSUMED"!D 30.95JD 25JT A(49)

05.06 S B=0JS C=0JS D=0JS G=0JS H=0JI (Y-A(48))5.07JD 24.1JG 5.09
05.07 T !"CALCIUM-DISSOLVED, CA"!D 30.94JD 25JT A(48)
05.09 I (Y-A(15))5.1016 5.14
05.10 T !"COOPER-TOTAL, CU"!D 30.95JD 25JT A(15)
05.14 I (Y-A(16))5.15JG 5.19
05.15 T !"COOPER-DISSOLVED, CU"!D 30.5JD 25JT A(16)
05.16 S G=G+A(16)*.03148JS H=H+A(16)
05.19 I (Y-A(18))5.20JG 5.24
05.20 T !"IRON-TOTAL, FE"!D 30.98JD 25JT A(18)
05.24 I (Y-A(19))5.25JG 5.29
05.25 T !"IRON-DISSOLVED, FE"!D 30.95JD 25JT A(19)
05.26 S G=G+A(19)*.05372JS H=H+A(19)
05.29 I (Y-A(20))5.30JG 5.34
05.30 T !"LEAD-TOTAL, PB"!D 30.98JD 25JT A(20)
05.34 I (Y-A(21))5.35JG 5.39
05.35 T !"LEAD-DISSOLVED, PB"!D 30.95JD 25JT A(21)
05.36 S G=G+A(21)*.009653JS H=H+A(21)
05.39 I (Y-A(22))5.45.5.42.5.45
05.42 I (Y-A(47))5.43JD 24.11G 5.46
05.43 I (Y-A(48))5.44JD 24.11G 5.46
05.44 S A(22)=12.16*(A(47)*.01998-A(48)*.04999)!D 5.45JD 26.2JG 5.46
05.45 T !"MAGNESIUM-DISSOLVED, MG"!D 30.92JD 25JT A(22)
05.46 I (Y-A(23))5.47JG 5.49
05.47 T !"MANGANESE-TOTAL, MN"!D 30.5JD 25JT A(23)
05.49 I (Y-A(24))5.50JG 5.54
05.50 T !"MANGANESE-DISSOLVED, MN"!D 30.92JD 25JT A(24)
05.51 S G=G+A(24)*.0364JS H=H+A(24)
05.54 I (Y-A(32))5.55JD 24.11G 5.59
05.55 T !"POTASSIUM-DISSOLVED, K"!D 30.94JD 25JT A(32)

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05.59 I (Y-A(3B))S.60JD 24.1JG 5.64
 05.60 T !"SODIUM-DISSOLVED, NA"JD 30.5JD 25JT A(3B)
 05.64 I (Y-A(39))S.65JG 5.69
 05.65 T !"ZINC-TOTAL, ZN"JD 30.98JD 25JT A(39)
 05.69 I (Y-A(40))S.70JG 5.72
 05.70 T !"ZINC-DISSOLVED, ZN"JD 30.95JD 25JT A(40)
 05.71 S G=D+A(40)*.0306JS D=D+A(40)
 05.72 I (Y-B)S.74JR
 05.74 S B=B+A(48)*.0499+A(22)*.08226+A(32)*.02557+A(38)*.0435+G
 05.75 S D=D+A(48)+A(22)+A(32)+A(38)+H

 07.05 I (Y-A(43))7.12,7.14,7.12
 07.12 I (Y-A(44))7.20,7.14,7.20
 07.14 D 24.2JG 7.39
 07.20 I (A(43)-A(44))/27.25,7.25,7.23
 07.23 S A(53)=01S A(51)=1.2*(A(44)-A(43))JS A(52)=(2*A(43)-A(44))*.3399
 07.24 G 7.30
 07.25 S A(53)*(A(44)-2*(A(43)))1.219JS A(51)=A(43)*1.2JS A(52)=0
 07.30 T !"BICARBONATE, HCO₃"JD 30.95JD 25JT A(53)JD 26.2
 07.35 T !"CARBONATE, CO₃"JD 30.98JD 25JT A(51)JD 26.2
 07.39 I (Y-A(14))7.40JG 7.44
 07.40 T !"CHLORIDE-DISSOLVED, CL"JD 30.94JD 25JT A(14)
 07.44 I (Y-A(17))7.45JD 24.2JG 7.49
 07.45 T !"FLUORIDE-DISSOLVED, F"JD 30.94JD 25JT A(17)
 07.49 I (Y-A(52))7.50JG 7.54
 07.50 T !"HYDROXIDE, OH"JD 30.98JD 25JT A(52)JD 26.2
 07.54 I (Y-A(26))7.55JD 24.2JG 7.59
 07.55 T !"NITROGEN-NITRATE-NITRITE, N"JD 30.3JD 25JT A(26)
 07.59 I (Y-A(29))7.60JG 7.64
 07.60 D 26.3JT "DISSOLVED, ORTHO, PO4"JD 30.7JD 25JT A(29)
 07.64 I (Y-A(30))7.65JG 7.69
 07.65 D 26.3JT "DISSOLVED, INORGANIC, PO4"JD 25JT A(30)
 07.69 I (Y-A(31))7.70JG 7.72
 07.70 D 26.3JT "TOTAL, PO4"JD 30.92JD 25JT A(31)
 07.72 I (Y-A(37))7.73JS D=YJG 7.74
 07.73 T !"SILICA-REACTIVE, SiO₂"JD 30.94JD 25JT A(37)
 07.74 I (Y-A(58))7.78JD 24.2JR
 07.78 T !"SULPHATE-DISSOLVED, SO₄"JD 30.92JD 25JT A(58)
 07.81 I (Y-C)7.82JR
 07.82 I (Y-D)7.84JG 7.87
 07.84 S D=D+A(50)*+A(51)*+A(52)*+A(53)*+A(14)*+A(17)*+A(26)*+4.429
 07.87 S C=C+A(50)*.02082+A(51)*.03333+A(52)*.0588+A(53)*.01639
 07.88 S C=C+A(14)*.02821+A(17)*.05264+A(26)*.07143
 07.90 I (Y-A(29))7.92JR
 07.92 I (D-Y).88,1.88JS D=D+A(29)JS C=C+A(29)*.03159

 08.06 S L=2.30263I (Y-D)8.07JG 8.66
 08.07 D 24.3JD 30.5JT "JD 25JT DJD 26.2
 08.52 I (Y-B)8.53JG 8.59
 08.53 T !"SUM OF CATIONS"JD 30.98JT "(ME/L)",%9.04,BJD 26.2
 08.59 I (Y-C)8.60JG 8.66
 08.60 T !"SUM OF ANIONS"JD 30.98JT "(ME/L)"CJD 26.2
 08.61 I (Y-B)8.65JG 8.66
 08.65 T !"DIFFERENCE PER CENT"JD 30.98JT %7.02,(R-C)*100/(B+C)JD 26.2
 08.66 I (Y-A(38))8.67JG 8.86
 08.67 I (Y-A(48))8.69JG 8.86
 08.69 I (Y-A(22))8.75JG 8.86
 08.75 T !"SODIUM ABSORPTION RATIO"JD 30.95
 08.81 T %7.02*1.41*(A(38)*.0435/FSOT(A(22))+.08226+A(48)*.0499)JD 26.2
 08.84 I (Y-B)8.85JG 8.86
 08.85 T !"SODIUM PER CENT"JD 30.97JT 4.35*A(38)/BJD 26.2
 08.86 I (Y-A(44))8.87JG 1.92
 08.87 I (Y-A(47))8.88JR
 08.88 S B=A(44)-A(47)JS (B)8.89JS B=0
 08.89 T !"NONCARBONATE HARDNESS"JD 30.3JD 27JT -BJD 26.2

 09.01 I (Y-A(12))9.05JG 9.17
 09.05 S B=FEXP(-A(12)/.4343)
 09.10 S B=9.7E10*B*(A(44)/5E4+B-1E-14/B)/(1+1.22E-11/B)
 09.12 T !"CO2"JD 30.2JD 25JT BJD 26.2
 09.17 I (Y-D)9.19JG 1.92
 09.19 I (Y-A(10))9.27JS 1.92
 09.27 S R=D*25E-6JS D=A(10)+273.15JS B=-8.37+2*(B30/D-2.76)
 09.29 S C=2902.39/D-6.498+.02379*DJJS B=B+C-FLOG(A(48))/L-FLOG(A(44))/L
 09.31 S B=9.3+2.5*FSOT(R)/(1+5.3*FSOT(R)+5.5*R)
 09.35 T !"SATURATION INDEX"JD 30.5JD 26.92JT A(12)-BJD 26.2
 09.36 T !"STABILITY INDEX"JD 30.5JD 26.92JT 2*B-A(12)JD 26.2

 24.10 S B=YJS D=Y
 24.20 S C=YJS D=Y
 24.30 T !"SUM OF CONSTITUENTS"
 24.40 T !"ACIDITY-PH"
 24.50 T !"ALKALINITY"
 24.90 T "="

 25.10 T "(MG/L)"

 26.20 T "(CALCULATED)"
 26.30 T !"PHOSPHATE"
 26.40 T !"RESIDUE"
 26.50 T "FILTERABLE (105 DEG.C.)"
 26.60 T "FILTERABLE (550 DEG.C.)"
 26.70 T !"RESIDUE-FIXED"
 26.80 T !"CARBON"
 26.90 T "ORGANIC, C"JD 30.3JD 25
 26.91 T !"NITROGEN"
 26.92 T "(PH UNITS)"

 27.10 T "(MG/L CACO₃)"

 28.10 T "TOTAL"

 29.10 T "DISSOLVED"

 30.10 F K=1,M;T=""
 30.20 S M=37JD 30.1
 30.30 S M=11JD 30.1
 30.50 S M=20JD 30.1
 30.70 S M=8JD 30.1
 30.92 S M=16JD 30.1
 30.93 S M=24JD 30.1
 30.94 S M=18JD 30.1
 30.95 S M=22JD 30.1
 30.97 S M=32JD 30.1
 30.98 S M=26JD 30.1
 *

Figure 3.7. Program AD0014 - Output

ANALYSIS OF WATER SAMPLE

LOCATION : A B C
SOURCE : X1 Y1 Z1

LABORATORY NUMBER= 3329
FIELD NUMBER = NOT AVAILABLE
DATE OF SAMPLING :
DAY = 13 MONTH = 7 YEAR = 1970
DATE OF TESTING :
DAY = 3 MONTH = 9 YEAR = 1970

COLOUR (HAZEN UNITS) = 5.00
SPECIFIC CONDUCTANCE (UMHO/CM) = 142.00
TEMPERATURE OF TESTING (DEG.C.) = 20.50
TURBIDITY = 0.38

pH (PH UNITS)= 7.70
ACIDITY-PH 4.5 (MG/L CACO3)= NOT AVAILABLE
ACIDITY-PH 8.3 (MG/L CACO3)= NOT AVAILABLE
ALKALINITY-PHENOLPHTHALEIN (MG/L CACO3)= 0.00
ALKALINITY-TOTAL (MG/L CACO3)= 52.10
HARDNESS-TOTAL (MG/L CACO3)= 67.30

RESIDUE-NONFILTERABLE (105 DEG.C.) (MG/L)= NOT AVAILABLE
RESIDUE-FILTERABLE (105 DEG.C.) (MG/L)= 92.00
RESIDUE-FIXED,NONFILTERABLE (550 DEG.C.) (MG/L)= NOT AVAILABLE
RESIDUE-FIXED,FILTERABLE (550 DEG.C.) (MG/L)= 65.60

CARBON- TOTAL ORGANIC, C (MG/L)= NOT AVAILABLE
CARBON-DISSOLVED ORGANIC, C (MG/L)= NOT AVAILABLE
NITROGEN-TOTAL, KJELDAHL, N (MG/L)= NOT AVAILABLE
NITROGEN-DISSOLVED AMMONIA, N (MG/L)= NOT AVAILABLE
OXYGEN-TOTAL CHEMICAL DEMAND (MG/L)= NOT AVAILABLE
OXYGEN-CONSUMED (MG/L)= NOT AVAILABLE

CATIONS (MG/L) :
CALCIUM-DISSOLVED, CA = 22.90
COOPER-TOTAL, CU = NOT AVAILABLE
COOPER-DISSOLVED, CU = NOT AVAILABLE
IRON-TOTAL, FE = NOT AVAILABLE
IRON-DISSOLVED, FE = 0.02
LEAD-TOTAL, PB = NOT AVAILABLE
LEAD-DISSOLVED, PB = NOT AVAILABLE
MAGNESIUM DISSOLVED, MG= 2.46 (CALCULATED)
MANGANESE-TOTAL, MN = NOT AVAILABLE
MANCANESE-DISSOLVED, MN= 0.00
POTASSIUM-DISSOLVED, K = 0.70
SODIUM-DISSOLVED, NA = 1.20
ZINC-TOTAL, ZN = NOT AVAILABLE
ZINC-DISSOLVED, ZN = NOT AVAILABLE

ANIONS (MG/L) :
BICARBONATE, HC03 = 63.51 (CALCULATED)
CARBONATE, CO3 = 0.00 (CALCULATED)
CHLORIDE-DISSOLVED, CL = 0.50
FLUORIDE-DISSOLVED, F = 0.19
HYDROXIDE, OH = 0.00 (CALCULATED)
NITROGEN-NITRATE+NITRITE, N = 0.17
PHOSPHATE-DISSOLVED, ORTHO, PO4 = NOT AVAILABLE
PHOSPHATE-DISSOLVED, INORGANIC, PO4= 0.19
PHOSPHATE-TOTAL, PO4 = NOT AVAILABLE
SILICA-REACTIVE, SIO2 = 4.40
SULPHATE-DISSOLVED, SO4 = 13.70

OTHER CALCULATED PARAMETERS :
SUM OF CONSTITUENTS (MG/L)= 78.11
SUM OF CATIONS (ME/L)= 1.4159
SUM OF ANIONS (ME/L)= 1.3624
DIFFERENCE PER CENT = 1.93
SODIUM ABSORPTION RATIO = 0.06
SODIUM PER CENT = 3.69

NONCARBONATE HARDNESS (MG/L CACO3)= 15.20
CO2 (MG/L)= 2.01
SATURATION INDEX (PH UNITS)=- 0.71
STABILITY INDEX (PH UNITS)= 9.11

Figure 3.8. Program AD0014 - Listing

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*W
C-BK FOCAL 01969

01.02 E
01.03 S Y=-0NIF J=1,53JS A(J)=Y
01.05 F J=1,50JA A(J)JI (0FINISH-A(J))1.06,1.06JC
01.06 S A(J)=YIS J=69JD 30.97J T "1"
01.07 T !!!DEPARTMENT OF FISHERIES AND FORESTRY!!!
01.08 T "INLAND WATERS BRANCH"!WATER QUALITY DIVISION!!!
01.09 T "ANALYSIS OF WATER SAMPLE"!!
01.10 T "LOCATION :"IA D1,D2,D3
01.12 T !"SOURCE :"IA D1,D2,D3
01.14 T !!!LABORATORY NUMBER"JI (Y-A(1))1.15JD 6JG 1.17
01.15 T #10,A(1)
01.17 T !"FIELD NUMBER" "JI (Y-A(2))1.18JD 6JG 1.20
01.18 T #10,A(2)
01.20 D 26.1JT "SAMPLING :"JS I=3JD 3
01.21 D 26.1JT "TESTING :"JS I=6JD 3
01.40 T !!!COLOUR (HAZEN UNITS) "JD 30.6JI (Y-A(11))1.45JD 6JG 1.48
01.45 T #7.02A(1)
01.48 T !!!SPECIFIC CONDUCTANCE (UMHO/CM) "JI (Y-A(42))1.49JD 6JG 1.50
01.49 T A(42)
01.50 T !!!TEMPERATURE OF TESTING (DEG.C.)"JI (Y-A(10))1.51JD 6JG 1.52
01.51 T A(10)
01.52 T !!!TURBIDITY "JD 30.2JI (Y-A(9))1.53JD 6JG 1.55
01.53 T A(9)
01.55 T !!!PH "JD 30.2JD 26.29JI (Y-A(12))1.58JD 6JG 1.61
01.56 T A(12)
01.61 D 24.4JT "4.5"JD 30.5JD 27JI (Y-A(45))1.63JD 6JG 1.65
01.63 T A(45)
01.65 D 24.4JT "8.3"JD 30.5JD 27JI (Y-A(46))1.67JD 6JG 1.70
01.67 T A(46)
01.76 D 24.5JT "PHENOLPHTHALEIN"JD 27JI (Y-A(43))1.72JD 6JG 1.75
01.78 T A(43)
01.75 D 24.5JT "TOTAL "JD 30.6JD 27JI (Y-A(44))1.76JD 6JG 1.77
01.76 T A(44)
01.77 T !!!HARDNESS-TOTAL"JD 30.5JD 27JI (Y-A(47))1.78JD 6JG 1.79
01.78 T A(47)
01.79 D 2JD 4JD 5JD 7JD 8JD 9
01.92 T !!!!!!!JD 1

02.05 T !JD 26.4JT "NON"JD 26.5JD 30.93JD 25JI (Y-A(33))2.07JD 6JG 2.10
02.07 T A(33)
02.10 D 26.4JD 26.5JD 30.6JD 25JI (Y-A(34))2.12JD 6JG 2.15
02.12 T A(34)
02.15 D 26.7JT "NON"JD 26.6JD 25JI (Y-A(35))2.17JD 6JG 2.20
02.17 T A(35)
02.20 D 26.7JD 26.6JT " "JD 25JI (Y-A(36))2.22JD 6JR
02.22 T A(36)

03.10 T !" DAY "JI (Y-A(1))3.18JD 6JG 3.20
03.16 T #2,A(1)
03.20 T " MONTH "JI (Y-A(1+1))3.28JD 6JG 3.30
03.28 T A(1+1)
03.30 T " YEAR "JI (Y-A(1+2))3.38JD 6JG 3.99
03.38 T #4,A(1+2)
03.99 R

04.15 T !JD 26.8JT " "JD 28JD 26.9JI (Y-A(13))4.17JD 6JG 4.20
04.17 T A(13)
04.20 D 26.8JD 29JD 26.9JI (Y-A(41))4.22JD 6JG 4.30
04.22 T A(41)
04.30 D 26.91JD 28JT ", KJELDAHL, N"JD 25
04.31 I (Y-A(25))4.32JD 6JG 4.35
04.32 T A(25)
04.35 D 26.91JD 29JT " AMMONIA, N"JD 25JI (Y-A(27))4.37JD 6JG 4.40
04.37 T A(27)
04.40 T !!!OXYGEN-TOTAL CHEMICAL DEMAND "JD 25
04.41 I (Y-A(28))4.42JD 6JG 4.45
04.42 T A(28)
04.45 T !!!OXYGEN-CONSUMED"JD 30.91JD 25JI (Y-A(49))4.47JD 6JR
04.47 T A(49)

05.03 D 30.97JT "2"
05.05 T !!!CATIONS (MG/L) :"JS B=0JS D=0JS C=0
05.07 T !!!CALCIUM-DISSOLVED, CA "JI (Y-A(48))5.08JD 24.1JD 5.10
05.08 T (A(48))JS B=B+A(48)*.0499JS D=D+A(48)
05.10 T !!!COOPER-TOTAL, CU "JD 30.93JI (Y-A(15))5.12JD 6JG 5.15
05.12 T A(15)
05.15 T !!!COOPER-DISSOLVED, CU "JI (Y-A(16))5.17JD 6JG 5.20
05.17 T A(16)JS B=B+A(16)*.03148JS D=D+A(16)
05.20 T !!!IRON-TOTAL, FE"JD 30.6JI (Y-A(18))5.22JD 6JG 5.25
05.22 T A(18)
05.25 T !!!IRON-DISSOLVED, FE "JI (Y-A(19))5.27JD 6JG 5.30
05.27 T A(19)JS B=B+A(19)*.05372JS D=D+A(19)
05.30 T !!!LEAD-TOTAL, PB"JD 30.6JI (Y-A(20))5.32JD 6JG 5.35
05.32 T A(20)
05.35 T !!!LEAD-DISSOLVED, PB "JI (Y-A(21))5.37JD 6JG 5.40
05.37 T A(21)JS B=B+A(21)*.009653JS D=D+A(21)
05.40 T !!!MAGNESIUM DISSOLVED, MG"JI (Y-A(22))5.45,5.42,5.45
05.42 I (Y-A(47))5.43JD 24.1JD 5.46
05.43 I (Y-A(48))5.44JD 24.1JD 5.46
05.44 S A(22)=12.16*(A(47)*.01998-A(48)*.0499)JD 5.45JD 26.2JD 5.46
05.45 T A(22)JS B=B+A(22)*.08226JS D=D+A(22)
05.46 T !!!MANGANESE-TOTAL, MN "JI (Y-A(23))5.47JD 6JG 5.50
05.47 T A(23)
05.50 T !!!MANGANESE-DISSOLVED, MN"JI (Y-A(24))5.52JD 6JG 5.55
05.52 T A(24)JS B=B+A(24)*.0364JS D=D+A(24)
05.55 T !!!POTASSIUM-DISSOLVED, K "JI (Y-A(32))5.57JD 24.1JD 5.60
05.57 T A(32)JS B=B+A(32)*.02557JS D=D+A(32)
05.60 T !!!SODIUM-DISSOLVED, NA "JI (Y-A(38))5.62JD 24.1JD 5.65
05.62 T A(38)JS B=B+A(38)*.0435JS D=D+A(38)
05.65 T !!!ZINC-TOTAL, ZN"JD 30.6JI (Y-A(39))5.67JD 6JG 5.70
05.67 T A(39)
05.70 T !!!ZINC-DISSOLVED, ZN "JI (Y-A(40))5.72JD 6JR
05.72 T A(40)JS B=R+A(40)*.0306JS D=D+A(40)

06.10 T =" NOT AVAILABLE"ST #7.02

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07.05 T !!ANIONS (MG/L) I;"J1 (Y-A(43))7.12+7.29+7.12
 07.12 I (Y-A(44))7.20,7.29,7.20
 07.20 I (A(43)-A(44)/2)7.25,7.25,7.23
 07.23 S A(S3)=0JS A(S1)=1.0*(A(44)-A(43))/JS A(S2)=(2*A(43)-A(44))*0.3399
 07.24 G 7.30
 07.25 S A(S3)=(A(44)-2*(A(43))/I+219JS A(S1)=A(43)*1.2JS A(S2)=0JS 7.30
 07.29 S D=YJS C=Y
 07.30 T !"BICARBONATE, HC03 "JD 30.92JI (Y-A(53))7.32JD 24.91G 7.35
 07.32 T A(S3)JD 26.2
 07.33 T !"CARBONATE, CO3"JD 30.2JI (Y-A(51))7.37JD 24.91G 7.40
 07.37 T A(S1)JD 26.2
 07.40 T !"CHLORIDE-DISSOLVED, CL "JD 30.5JI (Y-A(14))7.42JD 24.21G 7.45
 07.42 T A(14)
 07.45 T !"FLUORIDE-DISSOLVED, F"JD 30.91JI (Y-A(17))7.47JD 24.21G 7.50
 07.47 T A(17)
 07.50 T !"HYDROXIDE, OH "JD 30.2JI (Y-A(52))7.52JD 24.91G 7.55
 07.52 T A(S2)JD 26.2
 07.55 T !"NITROGEN-NITRATE+NITRITE, N "JD 30.93
 07.56 I (Y-A(26))7.57JD 24.21G 7.60
 07.57 T A(26)
 07.60 D 26.3JT "DISSOLVED, ORTHO, PO4 "JI (Y-A(29))7.62JD 61G 7.65
 07.62 T A(29)
 07.65 D 26.3JT "DISSOLVED, INORGANIC, PO4"JI (Y-A(30))7.67JD 61G 7.70
 07.67 T A(30)
 07.70 D 26.3JT "TOTAL, PO4"JD 30.91JI (Y-A(31))7.72JD 61G 7.73
 07.72 T A(31)
 07.73 T !"SILICA-REACTIVE, SiO2"JD 30.91JI (Y-A(37))7.74JS D=YJS 7.78
 07.74 T A(37)
 07.78 T !"SULPHATE-DISSOLVED, SO4"JD 30.5JI (Y-A(50))7.81JD 24.21R
 07.81 T A(S0)JI (Y-C7.82JR
 07.82 I (Y-D7.84JR 7.87
 07.84 S D=D*(A(50)+A(51)+A(52)+A(53)/2.03+A(14)+A(17)+A(37)+A(26)*4.429
 07.87 S C=C*(A(50)+0.2882*A(51)+0.3333+A(52)+0.588+A(53)*+0.1639
 07.88 S C=C*(A(14)+0.2821+A(17)+0.5264+A(26)*+0.7143
 07.90 I (Y-A(29))7.91JR
 07.91 I (D-Y)7.92,7.92JS D=D+A(29)
 07.92 S C=C*(A(29)*+0.3159

08.05 T !!OTHER CALCULATED PARAMETERS :"JS L=2.3026
 08.07 D 24.31T " "JD 25JI (Y-D)8.50JD 24.91G 8.53
 08.50 T D
 08.53 T !"SUM OF CATIONS"JD 30.98JI (Y-B)8.55JD 24.91G 8.60
 08.55 T 29.84,B
 08.60 T !"SUM OF ANIONS "JD 30.98JI (Y-C)8.63JD 24.91G 8.65
 08.63 T C
 08.65 T !"DIFFERENCE PER CENT."JD 30.5JI (Y-B)8.66JD 24.91G 8.75
 08.66 I (Y-C)8.67JD 24.91G 8.75
 08.67 T 27.02*(B-C)*100/(B+C)
 08.75 T !"SODIUM ABSORPTION RATIO"JD 30.6JI (Y-A(38))8.77JD 24.91G 8.83
 08.77 I (Y-A(48))8.79JD 24.91G 8.83
 08.79 I (Y-A(22))8.81JD 24.91G 8.83
 08.81 T 27.02+1.41*(38)+0.435/FSQT(A(22))+0.88226+A(48)*+0.4999
 08.83 T !"SODIUM PER CENT"JD 30.92JI (Y-B)8.87JD 24.91G 8.89
 08.87 T 4.35*A(38)/B
 08.89 T !!NONCARBONATE HARDNESS"JD 27JI (Y-A(47))B.90JD 24.91R
 08.90 I (Y-A(44))B.91JD 24.91R
 08.91 S B=A(44)-A(47)JI (B)8.92JS B=0
 08.92 T -B

09.03 T !"CO2 "JD 30.2JD 25JI (Y-A(12))9.04JD 24.91G 9.44
 09.04 I (Y-A(44))9.05JD 24.91G 9.44
 09.05 S B=FEXP(-A(12))/4343
 09.10 S B=9.7E10*B*(A(44)/5E4+B-1E-14/B)/(1+11.22E-11/B)
 09.12 T B
 09.15 T !"SATURATION INDEX "JD 30.93JD 26.92
 09.17 I (Y-D9.19)I 24.91G 9.45
 09.19 I (Y-A(10))9.27JD 24.91G 9.45
 09.27 S R=D*25E-6JS D=(A(10)+273.15JS B=-8.37+2*(830/D-2.78)
 09.29 S C=29002.39/D-6.498+0.0379*DIS B=B+C*FLOG(A(48))/L-FLOG(A(44))/L
 09.31 S B=B+9.32*5*FSQT(R)/(1+5.3*FSQT(R)+5.5*R)JT A(12)-B.
 09.40 D 26.93JT 2*B-A(12)JR 1.92
 09.44 D 9.15JD 24.9
 09.45 D 26.93JD 24.91G 1.92

24.10 D 6JS B=YJS D=Y
 24.20 D 6JS D=YJS C=Y
 24.30 T !"SUM OF CONSTITUENTS"
 24.40 T !"ACIDITY-PH "
 24.50 T !"ALKALINITY-"
 24.90 T "E" -

25.10 T " (MG/L)"
 26.10 T !"DATE OF "
 26.20 T " (CALCULATED)"
 26.30 T !"PHOSPHATE-"
 26.40 T !"RESIDUE-"
 26.50 T "FILTERABLE (105 DEG.C.)"
 26.60 T "FILTERABLE (550 DEG.C.)"
 26.70 T !"RESIDUE-FIXED,"
 26.80 T !"CARBON-"
 26.90 T " ORGANIC, C"JD 25
 26.91 T !"NITROGEN-"
 26.92 T " (PH UNITS)"
 26.93 T !"STABILITY INDEX "JD 30.93JD 26.92

27.10 T " (MG/L CACO3)"
 28.10 T "TOTAL"
 29.10 T "DISSOLVED"

30.10 F K=1,MJ1 " "
 30.20 S M=21JD 30.1
 30.50 S M=12JD 30.1
 30.60 S M=9JD 30.1
 30.91 S M=14JD 30.1
 30.92 S M=17JD 30.1
 30.93 S M=6JD 30.1
 30.97 T !!!!!!!JS M=50JD 30.1JT "PAGE "
 30.98 D 30.5JT "(ME/L)"

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