197
5/15/79

MASTER

DR. 2581

UCRL-52532 Vol. 4 Part 3

COMPUTER AUTOMATION OF CONTINUOUS-FLOW ANALYZERS FOR TRACE CONSTITUENTS IN WATER

Volume 4 Description of Program Segments Part 3. TAASTART

R. W. Crawford

Work performed under the auspices of the U.S. Department of
Energy by the UCLLL under contract number W-7405-ENG-48.

**LAWRENCE
LIVERMORE
LABORATORY**
University of California / Livermore

LAWRENCE LIVERMORE LABORATORY
University of California Livermore, California 94550

UCRL-52532 Vol. 4 Part 3

**COMPUTER AUTOMATION OF
CONTINUOUS-FLOW ANALYZERS
FOR TRACE CONSTITUENTS IN WATER
Volume 4 Description of Program Segments
Part 3. TAASTART**

R. W. Crawford
MS. Date: January 18, 1979

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.

Handwritten signature or initials.

FOREWORD

There are 13 programs used in the computer automation of continuous-flow analyzers for trace constituents in water. Each program segment is published separately as a part of this volume:

- Part 1. TAAIN
- Part 2. TAAINRE
- Part 3. TAASTART
- Part 4. TAAACAL
- Part 5. TAA
- Part 6. TAAQCOP
- Part 7. TAA01
- Part 8. TAA02
- Part 9. TAA03
- Part 10. TAA04
- Part 11. TAARESTART
- Part 12. Utility Programs (TAAPRINT, TAAPEAK, TAAFILE)
- Part 13. Assembly Language Code

CONTENTS

Foreword	ii
Abstract	1
Program Description	1
Appendix A. Program Sections and Subroutines	5
Appendix B. Variables	6
Appendix C. Arrays	7
Appendix D. Strings	8
Appendix E. Program Listing	9
Appendix F. Symbol Table Listing	12

COMPUTER AUTOMATION OF CONTINUOUS-FLOW ANALYZERS FOR TRACE CONSTITUENTS IN WATER

Volume 4 Description of Program Segments

Part 3. TAASTART

ABSTRACT

This report describes TAASTART, the third program in the series of programs necessary in automating the Technicon AutoAnalyzer. Included is a flow chart that illustrates the program logic and a description of each section and subroutine. In addition, all arrays, variables and strings are listed and defined, and a sample program listing with a complete list of symbols and references is provided.

PROGRAM DESCRIPTION

The purpose of program TAASTART is to ensure that the mechanical and electrical components of the Technicon AutoAnalyzer are operating properly for accurate sample analysis. Using this program, the operator can test the electrical connection from the colorimeters to the analog to digital converter (A/D), establish the full-scale and baseline A/D readings, and initialize the real-time data taking. In addition, several counters can be adjusted, especially when restarting with Calibration Standards.

The electrical tests are run after initializing the first record number, the total number of runs, and the number of repeats. These tests have the following purposes (See Fig. 1):

- Ensure that the A/D is on and functioning.
- Ensure that the analog conditioner is on and functioning.
- Ensure that all electrical connections are made.
- Ensure that the correct A/D channel numbers were assigned.
- Ensure that the colorimeter is functioning.
- Ensure that the full-scale output of the colorimeter is 5V.
- Ensure that the baseline is electrically offset approximately 0.5V to allow for negative drift.

- Record the full-scale and baseline data so the recorder and computer read the same. In the case of the AutoAnalyzer I systems (TAA-I), this data is essential for calculating absorbance.

Three different calls to assembly language patches are made in this program: CALL 6, CALL 16, and CALL 20. CALL 6, used to read the A/D converter, has three arguments: the A/D channel number; the number of readings to be averaged together (15 is used); and the variable in which the answer is stored. The operator is instructed to turn the colorimeter to full-scale (insert shutters in TAA-I) and record the full-scale. The polarity of the TAA-I output is reversed and offset 5V so that the output looks electrically like the TAA-II.

The operator then sets the instrument to read the normal baseline and records the A/D reading. The difference between the full-scale and baseline is tested to see if it is at least 7000 counts (8192 counts is 5V). If not, an error message is printed. The baseline is then checked to see if it reads above 350 counts. The instruments are set up with an electrical offset of ~800 counts to allow for negative drift because the A/D is unipolar (reads positive voltage only).

Fig. 1. Program logic flow of TAASTART.

When the above tests are satisfactorily completed, a prompt is issued allowing the Set-Standard threshold to be modified. The threshold is set at 39% of full-scale, which works very well with half-scale Set Standards. If other than half-scale Set Standards are used, different threshold values should be entered. For example, for a full-scale Set Standard, a threshold of 85 to 90% is suggested.

The threshold is critical to establishing correct timing for the run, therefore, the first Set Standard must be reliably detected. When the threshold value is crossed in the positive direction, the real-time data system assumes it has found the first Set Standard and begins storing data at the operator-established data rate. When the threshold is crossed in the negative direction, the real-time data system assumes the first Set Standard has just passed. It then looks for the inflection point or "knee" of the peak (see Notes to the Computer Coordinator for the Technician Auto Analyzer Programs Vol 3, Fig. 2).

There are two extremely important points to check when setting the threshold. First, the threshold should not be set too close to the top of the Set Standard because a small amount of noise or CAL adjustment can cause the threshold to be detected on the negative side too soon. Second, the threshold should not be set so low that it cannot be reached on the negative side before the next Set Standard comes through. On chemistries with very little drop between peaks, it is a good idea to use a Blank or a low concentration for the second Set Standard.

Figure 2 illustrates the important parameters to consider when selecting a threshold, using six possible threshold settings. (The asterisk indicates the point at which the upslope and downslope are detected.) Setting 2a (~90%) is too high, and manually adjusting the CAL pot has triggered the downslope detector too early. Setting 2c (~60%) is too low and the rinse between peaks does not bring the signal down to the threshold. Setting 2b (~75%) is correct.

Figures 2d-2f illustrate the problem that arises when there is very little separation between adjacent peaks. As seen in Figs. 2d and 2e, there is no correct threshold. In situations like this, the second Set Standard should be a blank (Fig. 2f), which allows the selection of a satisfactory threshold.

After the threshold is established, the program sets up the arguments for CALL 16. This CALL establishes the necessary parameters for the real-time data algorithm. CALL 16 has two arguments (also called arrays). The first argument contains the A/D channel number for each analyte, followed by a -1. The second argument contains the timing and threshold data. (See the detailed description of C and P in Appendix C.)

Fig. 2. Threshold settings for Set Standards: (a) Too high; (b) Correct; (c) Too low; (d) Too high; (e) Too low; (f) Correct.

A CALL 20 with no arguments is issued immediately after CALL 16. This CALL starts the real-time data algorithm in the search mode, where it is continuously looking for data that exceeds the threshold on any channel. The program then chains to TAACAL.

No unusual algorithms are used in this program. There is another version of TAASTART, called TAA1START. The major difference between the two is the prompt to get full-scale and baseline, and the CHAIN. Differences are listed below:

```
THIS FILE CONTAINS THOSE LINES IN TAASTART WHICH ARE NOT IN TAA1START
0010 PRINT "TAASTART 2809 05/25/77 13:20 800 DC"
0270 INPUT "SET COLORIMETERS TO FULL SCALE, HIT RETURN",BS
0330 INPUT "SET COLORIMETER TO NORMAL OR PROPER DAMPING, HIT RETURN",BS
0790 CHAIN "TAACAL"
```

```
THIS FILE CONTAINS THOSE LINES IN TAA1START WHICH ARE NOT IN TAASTART
0010 REM *****TAA1START*****
0016 REM REGULAR PROGRAM AT MERL FOR TAA-1
0270 INPUT "PUT IN SHUTTERS, HIT RETURN",BS
0330 INPUT "REMOVE SHUTTERS, HIT RETURN",BS
0790 CHAIN "TAA1CAL"
```


APPENDIX A.

PROGRAM SECTIONS AND SUBROUTINES

10 - 192 Dimension strings and arrays, set up counters A9, A2, N9, and R1.
195 - 220 Set up string of analyte names.
250 - 408 Check full scale and baseline readings.
410 - 480 Set up correct threshold for first Set Standard.
490 Store* counters in the file SCRATCH.
500 - 700 Set up parameters to initialize the real-time data taking.
720 Issue CALL 16 which passes parameters to real-time algorithm.
730 - 750 Issue CALL 20 which starts the real-time data algorithm in the peak search mode.
780 - 790 CHAIN to program TAACAL.

•

*The term *enter* means to type in a value on the terminal. It does not indicate what happens to the data. *Get* applies to memory and *retrieve* applies to disk files. The term *write* is used with memory. *Write file* and *store* are used with disk files. *Save* is reserved for storing a program on disk.

APPENDIX B.

VARIABLES

A2	First record number in run. This number is set to one less than the first record number, and stored for use in TAACAL where it is incremented before use.
A4	Scratch variable used to retrieve from a file.
A9	The total number of samples and standards in the run.
F3	This variable is always set to 0 at present. It is added to the record number when reading and writing file TAAINF. This variable could be used in the future to allow two or more standard sets of parameters for a directory by offsetting everything by 100 or 200, etc.
F4	The threshold for detecting the first Set Standard. Initially set at 39% of full scale but can be modified in response to prompts.
I	Counter used for loops.
J	Counter used for a loop.
M0	Scratch variable used to retrieve and store data on a file.
M1	Scratch variable used to retrieve from a file.
N0	Number of analytes in this run.
N1 to N9	Scratch variables used to retrieve and store data on a file.
Q	Used in writing data in V array when reading full-scale and baseline A/D data. Q is 2 for full-scale, 3 for baseline.
R1	The number of samples that need to be repeated due to faulty data (noisy, off scale), set at 0.
R2	The separation in number of 2/15-second intervals between successive peaks (See P{4}).
V	The number of A/D readings averaged together when reading the full-scale and baseline values; set at 15.
Y	The data rate in data points per minute. See P{5}.

APPENDIX C.

ARRAYS

- C[X] The A/D channel number for each analyte. A -1 is written in the next element of the array after the last channel number.
- G[X] Scratch array used in retrieving and storing data from a file.
- P[X] Arguments passed to CALL 16 needed to initiate the real-time data taking properly. There are five arguments for each analyte and the arguments are entered in the P array sequentially. For example, P[1] to P[5] contain the arguments for the first analyte; P[6] to P[10] contain the arguments for the second analyte, etc. The arguments are calculated as follows:
- P[1] The amount (in A/D counts) of separation between data points required before the data is considered to be decreasing. This number is set at 15 using a DATA statement and was chosen based on experience.
- P[2] The number of data pairs that must be found consecutively, satisfying the decreasing criterion (P[1]) before the slope of a curve is considered down. This is set at 3 using a DATA statement based on experience, and cannot be larger than 6.
- P[3] The threshold in A/D counts above which a Set Standard is considered to occur, and below which a peak is considered to terminate. The threshold is normally 39% (see F4) but can be modified in response to prompts. The percentage is calculated using the following formula:
- $$P[3] = ((\text{threshold}/100) * \text{full-scale range in A/D counts}) + \text{baseline A/D counts}$$
- P[4] The separation in number of 2/15-second intervals between successive peaks. This number is calculated (in TAAIN) from the number of samples per hour:
- $$P[4] = (15/2 \text{ tick/sec} * 60 \text{ s/min} * 60 \text{ min/hour}) / \text{samples/hour.}$$
- P[5] The sampling period in 2/15-second intervals between the successive data points taken in the window of 35 data points used for each peak. This number is calculated from the answer to the question DATA RATE (data points per minute) in TAAIN:
- $$P[5] = \text{integer value of } ((15/2 \text{ ticks/s} * 60 \text{ s/min}) / \text{data rate} + 0.5)$$
- V[X,Y] The arguments for CALL 6 which read the A/D to get the full-scale and baseline data. The X portion of the array is 1, 2, or 3 and is defined below (where the Y is the successive analyte number).
- V[1,Y] The A/D channel number for each analyte.
- V[2,Y] The full-scale A/D reading for each analyte.
- V[3,Y] The baseline A/D reading for each analyte.

APPENDIX D.

STRINGS

- A\$** A string with the first six characters of each analyte name concatenated together.
- B\$** A scratch string used for retrieving and storing data from files, and entering answers to prompts.
- C\$** A scratch string used to pad out analyte names to six characters, and to retrieve and store data on files.

APPENDIX E.
PROGRAM LISTING

LISTING OF FILE TAASTART

15:53 FEB 1 1979

PAGE 1

```

0010 PRINT "TAASTART 2609 05/24/77 13:20 800 DC"
0015 REM ***** 8/10/78 *****
0030 REM ROUTINE TO START PEAK TAKING FOR TAA
0040 REM WRITTEN 2/11/76 AT LAWRENCE LIVERMORE LABORATORY
0050 REM ASSEMBLY PROGRAM-HENRY AMES,BASIC PROGRAM-RICHARD CRAWFORD
0060 REM CHAINED FROM TAAINRE AND CHAINS TO TAACAL
0065 CLOSE
0070 OPEN FILE(2,0),"TAAINF"
0080 OPEN FILE(3,0),"TAAPASS"
0090 DIM G$(5),B$(10),C$(10)
0100 READ FILE(2,7),A4,A2,M1,A9
0120 LET A9=A9-A2+1
0130 LET A2=A2-1
0140 LET F3=0
0150 REM F3 IS USED IN ALL READS OF TAAINF FILE, COULD BE CHANGED
    TO READ
0160 REM VARIOUS PORTIONS OF THE FILE SUCH AS FROM 100 TO 199,ETC.
0165 LET R1=0
0170 READ FILE(2,6+F3),N0,N1,N2,N3,N4,N5,N6,N7,N8,N9,M0
0180 WRITE FILE(2,6+F3),N0,N1,N2,N3,N4,N5,N6,N7,N8,A9,M0,R1
0190 DIM P(N0*5),C(N0+1),V(3,N0)
0192 DIM A$(6*N0)
0195 LET C$=" "
0200 FOR I=1 TO N0
0210   READ FILE(2,10+1+F3),B$,V(1,1)
0215   LET A$((I*6)-5,I*6)=B$,C$
0220 NEXT I
0230 CALL 17
0240 REM IN CASE PEAK TAKING STILL RUNNING
0250 LET V=15
0260 LET Q=2
0270 INPUT "SET COLORIMETERS TO FULL SCALE,HIT RETURN",B$
0280 FOR I=1 TO N0
0290   CALL 6,V(1,1),V,V(0,1)
0300 NEXT I
0310 IF Q=3 THEN GOTO 0350
0320 LET Q=3
0330 INPUT "SET COLORIMETER TO NORMAL OR PROPER DAMPING, HIT RETURN",B$
0340 GOTO 0280
0350 FOR I=1 TO N0
0360   IF V(2,1)-V(3,1)>7000 THEN GOTO 0400
0370   PRINT "DIFF BETWEEN F.S. & NORMAL OF CHANN, ";V(1,1);",
";A$((I*6)-5,I*6);
0380   PRINT " , READS LOW, ";(V(2,1)-V(3,1))/81.92;" % F.S."
0382   PRINT "SHOULD READ 100% + OR - 10%, CHECK THAT INTERFACE IS ON,"
0384   PRINT "COLORIMETER CONNECTED AND TURNED ON"
0390   GOTO 0260
0400   IF V(3,1)>350 THEN GOTO 0408
0402   PRINT "NOT ENOUGH 0 OFFSET ON CHANNEL ";V(1,1)

```

```

0404 PRINT "READS ";V(3,1); " A/D COUNTS, SHOULD BE AT LEAST 400"
0406 GOTO 0260
0408 NEXT I
0410 LET F4=30
0420 PRINT "THRESHOLD ON SET STND, OTHER THAN ";F4;" X";
0425 INPUT B$
0430 FOR I=1 TO N0
0440 IF B$(I,1)="N" THEN GOTO 0470
0450 PRINT "THRESHOLD FOR ";A$(I*6)-5,I*6); " ";
0460 INPUT F4
0470 LET P((I-1)*5+3)=((F4/100)*(V(2,I)-V(3,1)))+V(3,1)
0480 NEXT I
0490 WRITE FILE(3,9),A,F3,0
0500 INPUT "HIT RETURN WHEN READY TO RUN ",A$
0510 REM WAIT FOR OPERATOR
0520 DATA 15,3
0530 REM DSCND,PTSDW
0540 READ FILE(2,50+F3),R2
0550 FOR I=1 TO N0
0560 FOR J=1 TO 2
0570 READ P((I-1)*5+J)
0580 NEXT J
0590 LET P((I-1)*5+4)=R2
0600 REM TIME BETWEEN SAMPLES IN 2/15 SEC, TICKS, DELTA
0610 RESTORE
0620 READ FILE(2,10+1+F3),A$,C(1),B$,G(1),G(2),C$,Y,G(3),G(4),G(5)
0630 REM C(1) IS A/D NO, FOR EACH CHANNEL
0640 LET V(2,1)=V(2,1)-V(3,1)
0650 WRITE FILE(2,10+1+F3),A$,C(1),B$,G(1),G(2),C$,Y,G(3),G(4),
G(5),V(2,1),V(3,1)
0660 REM V(2,1) IS F.S , V(3,1) IS ZERO
0670 LET P((I-1)*5+5)=INT(450/Y+.5)
0680 REM Y IS RATE IN PTS/MIN, P((I-1)*5+5) IS C OF 2/15 SEC TICKS/PT,
0690 NEXT I
0700 LET C(ND+1)=-1
0720 CALL 16,C(1),P(1)
0730 CALL 20
0740 REM START PEAK SEARCH
0750 PRINT "PEAK SEARCH BEGUN"
0780 CLOSE
0790 CHAIN "TAACAL"
0800 END

```

APPENDIX F.
SYMBOL TABLE LISTING

REFERENCES AND SYMBOLS IN TAASART

14:32 FEB 8 1979

PAGE 1

0260 IS REFERENCED ON LINES:
0390 0406

0280 IS REFERENCED ON LINES:
0340

0350 IS REFERENCED ON LINES:
0310

0400 IS REFERENCED ON LINES:
0360

0408 IS REFERENCED ON LINES:
0400

0470 IS REFERENCED ON LINES:
0440

A5 OCCURS ON LINES:
0132 0215 0370 0450 0500
0520 0650

A2 OCCURS ON LINES:
0100 0120 0130 0490

A4 OCCURS ON LINES:
0100

A9 OCCURS ON LINES:
0100 0120 0180

B5 OCCURS ON LINES:
0090 0210 0215 0270 0330
0425 0440 0620 0650

C3 OCCURS ON LINES:
0090 0195 0215 0620 0650

C1 OCCURS ON LINES:
0190 0620 0650 0700 0720

F3 OCCURS ON LINES:
0140 0170 0180 0210 0490
0540 0620 0650

REFERENCES AND SYMBOLS IN TAASTART

14:32 FEB 8 1979

PAGE 2

F4 OCCURS ON LINES:

0410 0420 0460 0470

G1 OCCURS ON LINES:

0090 0620 0650

I OCCURS ON LINES:

0200 0210 0215 0220 0280
0290 0300 0350 0360 0370
0380 0400 0402 0404 0408
0430 0450 0470 0480 0550
0570 0590 0620 0640 0650
0670 0690

J OCCURS ON LINES:

0560 0570 0580

M0 OCCURS ON LINES:

0170 0180

M1 OCCURS ON LINES:

0100

N0 OCCURS ON LINES:

0170 0180 0190 0192 0200
0280 0350 0430 0550 0700

N1 OCCURS ON LINES:

0170 0180

N2 OCCURS ON LINES:

0170 0180

N3 OCCURS ON LINES:

0170 0180

N4 OCCURS ON LINES:

0170 0180

N5 OCCURS ON LINES:

0170 0180

N6 OCCURS ON LINES:

0170 0180

REFERENCES AND SYMBOLS IN TAASART

14:32 FEB 8 1979

PAGE 3

N7 OCCURS ON LINES:
0170 0180

N8 OCCURS ON LINES:
0170 0180

N9 OCCURS ON LINES:
0170

PI OCCURS ON LINES:
0190 0470 0570 0590 0670
0720

Q OCCURS ON LINES:
0260 0290 03 0 0320

R1 OCCURS ON LINES:
0165 0180

R2 OCCURS ON LINES:
0540 0590

V OCCURS ON LINES:
0250 0290

VI OCCURS ON LINES:
0190 0210 0230 0360 0370
0380 0400 0402 0404 0470
0640 0650

Y OCCURS ON LINES:
0620 0650 0670