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THE NUMERICAL COMPUTATION OF STREAMFLOW AND ITS ERROR USING THE CONSTANT RATE INJECTION METHOD OF DILUTION GAUGING

BY

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ABSTRACT

This report describes an efficient procedure for computing the flow value and its error when using the constant rate injection technique of dilution gauging. The computation method proposed, by describing the error contribution from each part of the flow value calculation and revealing where such errors are systematic, allows the user to assess the validity of the gauging.

CONTENTS

INTRODUCTION

This report describes the methods and programs that have been written for use with dilution gauging using the results from constant rate injection techniques. As such, it supplements an internal report (Greenland 1975) on the field work aspect of dilution gauging and should be thought of as continuing the discussion of the computation of the flow value and its error.

Constant rate dilution gauging is based on the process of continuously injecting a chemical tracer of a known concentration and at a known constant rate into a stream reach. Stream samples are collected further down the reach after a plateau concentration has been obtained. Since the stream sample concentration can be determined, the flow value of the stream can also be found. This simplified description begs many questions (eg. adsorption of tracer, gauging whilst the flow is changing, etc.) answers to which are beyond the scope of this report. However, much work has been done on these questions at the Institute, notably by Gilman (1972, 1975 & 1976) and Neal and Truesdale (1976 and recourse to some of this work is required in interpreting systematic variation in the results in section 4.

The first three sections of this report are concerned with the methods behind different aspects of the numerical calculation of the flow value. Programs have been written in Fortran V for these methods and they appear in Appendices A-D along with representative data sets and output. Use has also been made of the statistical package ASCOP (1972) available on the Univac 1108 computer at the Institute. A guide on how to use the programs, along with the order of their execution, for a typical gauging, is given in section 4. The reader who is only interested in using the programs need only refer to this section.

The comments made throughout the Report are relevant to all tracers with the exception of Section 3 which is concerned only with the catalytic procedure for the determination of (10-80 μg/l) total iodine after the injection of the tracer sodium iodide (Truesdale and Smith 1975). Sodium iodide has given good results for a number of gaugings and is the only tracer in regular use by the Institute. The iterative method developed for the calibration of this procedure with standards of known concentration of iodide is given in appendix E.

1. INJECTION OF TRACER

Injection of tracer at a constant rate is achieved by using a Mariotte vessel, which is an airtight container that has a nozzle near its base. The tracer flows through the nozzle and air enters the vessel through a tube at a fixed height above the nozzle maintaining atmospheric pressure at the lower end of the tube. Thus the head of tracer at the nozzle and consequently the injection rate remains constant, independent of the level of liquid in the vessel. On most of the Mariotte vessels used at the Institute a sight tube has been fitted to the side of the vessel. This sight tube is graduated so that readings of the level in the Mariotte vessel can be taken at different times during the injection. There is no necessity to make field measurements of the injection rate when a previously calibrated Mariotte is being used. However, Institute experience has been that by making field measurements errors in the injection arising from effects such as blocked nozzles, changes in solution density and its viscosity can be avoided. An extra operative is not necessarily required to read the sight tube of the Mariotte vessel since the readings can be made in two groups with a gap in the middle so that river samples can be collected. This will give a slightly greater error in the determination of the injection rate and thus in the estimation of streamflow although the error in streamflow is likely to be small. However, care must be taken to ensure that faults in the injection do not occur when the river samples are being collected.

1.1 Mariotte vessel calibration

Before a Mariotte vessel can be used for dilution gauging it is necessary not only to calibrate readings taken from the sight tube with volumes of liquid discharged but also to verify that the resulting relationship is linear. A Mariotte vessel is calibrated by first filling it with water and then as amounts of water are discharged and weighed, taking readings from the sight tube. The calibration is repeated a number of times to give the co-ordinate pairs $(S_k, M_k)_l$, $k = 1, \ldots, m; l = 1, \ldots, n$ where S_k is the sight tube reading in cms. M_k is the total mass of water discharged in kgms, m is the number of pairs for a particular calibration and n is the number of replications of the calibration (usually n = 3).

Method

The program .MARIOTTE, together with the density of water (ρ) at ambient temperature, fits the n best straight lines to the n calibrations and computes the grouped best estimate for the slope $\hat{\alpha}$ ($l\ cm^{-1}$) and its variance var($\hat{\alpha}$) ($l^2 cm^{-2}$). The method is as follows:

Let the $(S_k, M_k)_l$ be rewritten as (X_{ij}, Y_{ij})

where X_{ij} is the jth replicate of the i^{th} scale reading

and Y_{ij} is the jth replicate of the i^{th} measured volume (M_k/ρ)

and $i = 1, \ldots, m_j$ and $j = 1, \ldots, n$. Using this notation the linear model is

$$Y_{ij} = C^j + B^j X_{ij} + \varepsilon_i$$

where B^j and C^j are the slope and intercept for the j^{th} replicate calibrations and the errors ε_i satisfy the usual normality and independence conditions. Then the least square estimates for the slope and intercept are respectively:

$$\hat{B}^j = S^j_{xy}/S^j_{xx}$$

$$\hat{C}^j = \left(\sum_{i=1}^{m_j} Y_{ij} - \hat{B}^j \sum_{i=1}^{m_j} X_{ij}\right)/m_j$$

and the residual sums of squares are

$$R^j = S_{yy}^{\ j} - (S^j_{xy})^2/S^j_{xx}$$

where $$S_{xx}^{\ j} = \sum_{i=1}^{m_j} X_{ij}^2 - \left(\sum_{i=1}^{m_j} X_{ij}\right)^2/m_j$$

$$S_{yy}^{\ j} = \sum_{i=1}^{m_j} Y_{ij}^2 - \left(\sum_{i=1}^{m_j} Y_{ij}\right)^2/m_j$$

$$S_{xy}^{\ j} = \sum_{i=1}^{m_j} X_{ij}\, Y_{ij} - \left(\sum_{i=1}^{m_j} X_{ij} \sum_{i=1}^{m_j} Y_{ij}\right)/m_j \quad \text{for } j = 1, \ldots, m_j$$

The grouped estimate for the slope is then

$$\hat{\alpha} = \sum_{j=1}^{n} S^j_{xy} / \sum_{j=1}^{n} S_{xx}^{\ j}$$

and the variance of the slope is

$$\text{Var}(\hat{\alpha}) = \left[\sum_{j=1}^{n} R^j / \sum_{j=1}^{n} (m_j - 2)\right] / \sum_{j=1}^{n} S_{xx}^{\ j} .$$

with $\sum_{j=1}^{n} (m_j-2)$ degrees of freedom.

The program .MARIOTTE produces the results in the form of a graph. This graph has a title, volume in litres as the ordinate axis and scale readings in cms as the abscissae axis. The n replicate calibrations are shown, together with the readings represented as asterisks and lines representing the best fit to the readings. The grouped estimate of the slope and its variance are also shown on this graph.

This method of calibrating the Mariotte has been shown to be reproducible with only extremely small variations in the slope and its variance recorded by repeated calibrations. Unless the performance of the Mariotte or the results of a particular gauging are questioned, only periodic check calibrations of the Mariottes will be necessary.

The complete set of graphs for all the Institute's Mariotte bottles are given by Greenland (1975). Appendix A gives examples of a typical data set, graphical output and the Fortran code of the program.

1.2 Determining the injection rate

The discharge of tracer solution into the river during a continuous dilution gauging is monitored by noting the sight tube readings. With a previously calibrated Mariotte this enables the relationship between sight tube readings and time to be transformed into one of volume and time. Thus continuing with the notation used in 1., data is collected in the form (t_k, S_k), $k = 1, \ldots, m$ where t_k is the time from the start of the gauging in seconds and S_k is the sight tube reading in cms. This data is then used in the program .INJECT along with $\hat{\alpha}$ and var$(\hat{\alpha})$ found using the method described in 1.1 to give the injection rate $\hat{q}$ $(1\ s^{-1})$ and var $(\hat{q})$ $(1^2 s^{-2})$.

Method

The program .INJECT determines the best straight line for the pairs (t_k, S_k), $k = 1, \ldots, m$ by choosing the model,

$$S_k = \gamma + \beta t_k + \varepsilon_k \quad , \quad k = 1, \ldots, m$$

the least square estimate for gradient and intercept are respectively

$$\hat{\beta} = \left(\sum_{k=1}^{m} S_k t_k - \left(\sum_{k=1}^{m} S_k \sum_{k=1}^{m} t_k\right)/m\right) / \left(\sum_{k=1}^{n} t_k{}^2 - \left(\sum_{k=1}^{m} t_k\right)^2/m\right)$$

$$\hat{\gamma} = \left(\sum_{k=1}^{m} S_k - \hat{\beta} \sum_{k=1}^{m} t_k\right)/m$$

and the variance of $\hat{\beta}$ is

$$\text{var}\ (\hat{\beta}) = \frac{(\sum_{k=1}^{m} s_k^{\,2} - (\sum_{k=1}^{m} s_k)^2/m) - \hat{\beta}(\sum_{k=1}^{m} s_k t_k - (\sum_{k=1}^{m} s_k \sum_{k=1}^{m} t_k)/m)}{(m-2)\ (\sum_{k=1}^{m} t_k^2 - (\sum_{k=1}^{m} t_k)^2/m)}$$

The injection rate q and its variance var $(\hat{q})$ are estimated by

$$\hat{q} = \hat{\alpha}\ .\hat{\beta} \qquad (1\ s^{-1})$$

and $\text{var}\ (\hat{q}) = \hat{\beta}^2\ \text{Var}\ (\hat{\alpha}) + \hat{\alpha}^2\ \text{Var}\ (\hat{\beta}) \qquad (1\ s^{-2})$

covariance terms being zero because α,β are estimated independent data sets.

The results are produced in the form of a graph. The graph has a title, the Mariotte number, the jet number, the date of injection, the time injection started and finished, scale readings in cms as the ordinate axis and time in seconds as the abscissae axis. The sight tube readings are plotted on the graph against time along with the calculated straight line. An additional graph is also drawn of the residual error of the actual reading from that of the predicted reading. This graph is a useful check on whether any systematic errors have occurred in the injection caused, for instance, by a jet becoming progressively blocked. The values of the best estimate of slope, the variance of the slope, the correlation coefficient, the injection rate (ls^{-1} and its variance (l^2s^{-2}) are also shown on the graph. In Appendix B there are examples of a typical data set, graphical output and the Fortran code of the program.

2. CALIBRATING THE AUTO-ANALYSER

Truesdale and Smith (1975) have described the setting up of a catalytic procedure, in which a Technicon Auto Analyser (I) is used for determining the amount of iodide or iodate which is added to river water during dilution gauging. The calibration curve was shown to be of the form:

$$T = e^{-Z}\ \exp\{Z(1 - e^{-I\omega t})\} - 1 \qquad \dots\ (1)$$

where $Z = D_1 \ln 10$

T is the transmission (Vogel (1939))

D_1 is the transmission that defines the base line

I is the concentration of iodide in $\mu g l^{-1}$
ω is the sensitivity of the reaction to iodide in $1\ \mu g^{-1}\ sec^{-1}$
and t is the reaction time in secs.

To minimize inconsistencies in the flow measurement the standard error of transmission relative to the iodide concentration was made constant over the range of iodide concentrations considered. This criterion implied that the calibration curve (1) should be a logarithmic curve; by visually matching logarithmic curves with (1), values of 1.00 and 0.0417 were found for D_1 and ωt respectively. Using these two values it was possible to set up the catalytic procedure. With this procedure it is necessary to construct an empirical calibration curve. Standards prepared from river water containing known concentrations of iodide produce a response on the chart recorder which when plotted against concentration gives the calibration curve for the particular gauging.

A least squares technique (Appendix E) can be used to estimate the parameters of the model for a particular set of standards. The advantages of this approach over drawing the calibration curve freehand are that:

(i) any error introduced by drawing the calibration curve and taking readings from it is eliminated,

(ii) the standard error for every iodide concentration can be estimated,

(iii) the results can be presented not only in the form of a calibration curve on the plotter, but also as a table containing the iodide concentration and its variance corresponding to a particular transmission of a river sample,

(iv) the long-term behaviour of the procedure can be studied using the estimates of the parameters.

The modified model

During chemical analysis the standard solutions are prepared from river water which may have a background iodide coloration relative to distilled water, because of background iodide and/or inert material present in the river water. It is convenient to use distilled water as a wash solution in the Auto-Analyser not only because less river water is needed but also because changes in the behaviour of the analytical equipment can be observed as deviations away from the constant Z value. The use of distilled water in this way necessitates the modification of model (1) to include a parameter D as a measure of the background coloration. Thus (1) becomes

$$T = e^{-Ze^{-I\theta}} - e^{-Z} + D \qquad \ldots. (2)$$

by simplifying and considering $\omega t = \theta$ as one compound variable.

Obtaining the calibration curve from a set of standards

The calibration curve, for a particular set of standards, is found by estimating the parameters (θ, Z and D) for the non-linear model (2). The estimation of these parameters is achieved by reducing the square of the deviations of the transmission of the standards for given iodide concentrations from those predicted by the model (2) at the same iodide concentrations. The approach is outlined in Appendix E with particular reference to the difficulties encountered with a non-linear model such as (2).

The data for the calibration curve is of the form (I_i', T_{ij}'), i = 1, ..., n and j = 1, ..., m, where the T_{ij}' are replicated observations of transmission for a particular iodide concentration I_i'. If $k = (i - 1)*m + j$ the T_{ij}' map into T_k and I_k' map into I_k where $I_k = I_j$, $j = (k - 1)/m + 1$, $k = 1, \ldots, N$ and $N = nm$. Thus,

$$T_k = e^{-Ze^{-I_k\theta}} - e^{-Z} + D + \rho_k \qquad \ldots.\ (3)$$

where ρ_k is the k^{th} error, $k = 1, \ldots, N$. Let $a = e^{-I_k\theta}$, $b = e^{-Za}$ and $c = e^{-Z}$, so that (3) becomes

$$T_k = b - c + D + \rho_k \qquad \ldots.\ (4)$$

If $\underline{\beta} = (\theta, z, D)'$ and $\sum = \sum_{k=1}^{N}$, equation (E.6) of Appendix E becomes

$$\underline{\delta\beta} = \begin{bmatrix} \delta\theta \\ \delta z \\ \delta D \end{bmatrix} = \begin{bmatrix} \Sigma\alpha_k^2 & \Sigma\alpha_k\gamma_m & \Sigma-\alpha_k \\ \Sigma\alpha_k\gamma_k & \Sigma\gamma_k^{\ 2} & \Sigma-\gamma_k \\ \Sigma-\alpha_k & \Sigma-\gamma_k & N \end{bmatrix}^{-1} \cdot \begin{bmatrix} -\Sigma\rho_k\alpha_k \\ -\Sigma\rho_k\gamma_k \\ -\Sigma-\rho_k \end{bmatrix} \qquad \ldots.\ (5)$$

where
$$\alpha_k = -ZI_k ab = -ZI_k e^{-I_k\theta} e^{-Ze^{-I_k\theta}}$$
$$\gamma_k = ab - c = e^{-I_k\theta} e^{-Ze^{-I_k\theta}} - e^{-Z}$$
$$\rho_k = T_k - b + c - D = T_k - e^{-Ze^{-I_k\theta}} + e^{-Z} - D.$$

Thus taking the initial estimate of $\underline{\beta}$ as

$$\underline{\beta}_o = \begin{bmatrix} \theta_o \\ Z_o \\ D_o \end{bmatrix} = \begin{bmatrix} -\ln(-\ln(T_{k*} + T_N)/Z_o)/I_{k*} \\ -\ln(1 - T_N) \\ T_1 - \exp(-Z_o \exp(-I_1\theta_o)) + \exp(-Z_o) \end{bmatrix}$$

where $k^* = (N + 3)/2$ (found to be suitable by trial and error) and using (5) to obtain $\underline{\delta\beta}_j$ the iterative method defined by equation 7 converges to the least squares estimate of the parameters and is terminated using the criterion described in Appendix E. Thus using this method the estimates $\hat{\theta}$ and $\hat{D}$ can be found such that the error sums of squares is minimized and the predicted transmissivity T, given an iodide concentration I, is therefore

$$T = e^{-\hat{Z}e^{-I\hat{\theta}}} - e^{-\hat{Z}} + \hat{D}. \qquad \ldots . \quad (7)$$

Estimating the errors

Reverting back to the original form of the data and removing the primes (I_i, T_{ij}), $i = 1, \ldots, n$ and $j = 1, \ldots, m$, where T_{ij} are replicated observations of transmission for iodide concentrations I_i. The standard error of $\bar{T}_i$ is given by

$$S_i = \Big(\sum_{j=1}^{m} (T_{ij} - \bar{T}_i)^2/m(m-1)\Big)^{\frac{1}{2}}$$

where $\bar{T}_i = \sum_{j=1}^{m} T_{ij}/m$ and $i = 1, \ldots, n$. Using a cubic spline to fit a smooth curve through the points $(\bar{T}_i, S_i)$, it is possible to estimate the standard error for a particular transmission T_o, say S_{T_o} since

$$S_{I_o} \simeq S_{T_o}/\Big[\frac{dT}{dI}\Big]_{I=I_o}$$

where S_{I_o} is an approximate value of the standard error of iodide concentration and $\big[dT/dI\big]_{I=I_o}$ is the derivative of (7) with $I = I_o$.

In this way a table is constructed with the correct iodide concentration and estimated variance for a range of transmission values, say, 0.1 (0.001) 0.95. The program .CALIBRATE plots the calibration curve for a set of standards using this method.

Also plotted on the graph are the axes, iodide in $\mu g l^{-1}$ (0, 100 $\mu g l^{-1}$) and transmission (0,1), the title read from the input data, the data points as asterisks and the estimated parameter values $\hat{D}_1 = \hat{Z}/\ln 10$, $\hat{\omega} = \hat{\theta}$ and $\hat{D}$. The results are also given in tabular form for transmission values from .1 (.001) .95 with the iodide concentration and its variance. The cubic spline routine used to interpolate between the known standard errors is in the mathematics package IHLIBS*MATHSTAT. The Fortran code for this program, along with a typical data set and graphical output, is given in Appendix C.

3. EVALUATING THE FLOW VALUE AND ITS ERROR

It is usual in dilution gauging with the constant rate injection method to take samples across the stream (to check that mixing is adequate) and further sets of samples in time (to check that a plateau concentration has been reached). Figure 1 gives a schematic view of the tracer concentration at the injection and the sampling sites in a stream with crosses representing sample positions. Using the method described in Section 2, each sample will be replicated. Thus before a mean sample concentration can be calculated, the significance of the variation across the stream, with time and between replicates, should be determined. A suitable method for studying this variation is by using a two-way analysis of variance such as Fisher (1946). At the Institute the statistical package ASCOP can be used for this purpose.

Before describing the methods for dealing with significant variation in gauging results, it should be stressed that the only sure way of obtaining an accurate gauging result is to repeat the gauging, using the results to alter the experimental procedure to eliminate the cause of significant variation. This second gauging should have a longer mixing length if there is significant variation across the stream.

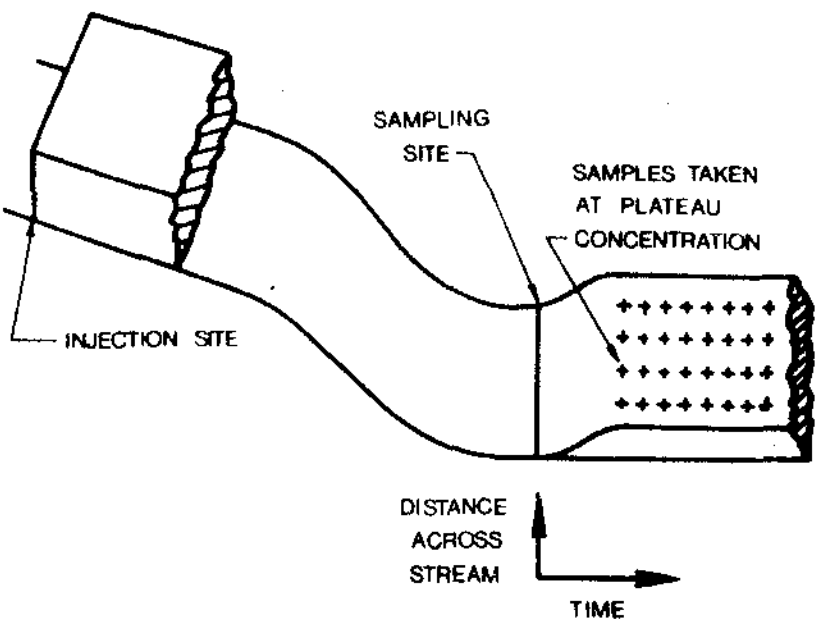

FIGURE 1

Schematic view of a river during dilution gauging.

Alternatively the time of injection should be longer if there is significant variation in time. If there is a significant variation between the replicates the stream samples can be reanalysed and checks carried out for possible causes of contamination.

Variation across the stream is the simplest of the possible variations to explain, and there is little doubt that, in the absence of tributary streams, a longer reach will eliminate this fault. However, if it is impossible to repeat the gauging there are two methods that can be used. One method, used by Smith and Greenland (1977) for a gauging on the River Avon was to use a defined velocity distribution from current metering results to weight the concentration distribution across the river and therefore find the weighted mean sample concentration. An alternative approach (Gilman, 1972) is to use the harmonic mean of the sample concentrations, and then to use an estimated flow distribution across the stream to assess the systematic error involved in calculating the flow figure from this mean.

Variation in the concentration of tracer with time is more difficult to explain, since there are two obvious causes. Either the plateau concentration has not been reached or the flow of the stream is varying and therefore information about how the stage varies during the gauging is required before one of these two possible causes can be eliminated.

If the stage readings are reasonably constant and the concentration of tracer is rising asymptotically then it can be assumed that a plateau concentration has not been reached. A limiting procedure, assuming the rise to be roughly exponential near the plateau concentration, would give a concentration limit to evaluate the flow, but this obviously limits the confidence that can be placed on its value.

An example of failure to reach plateau concentration is shown in Figure 2. The calculated flow values from the dilution gauging results approach the calculated flow values from the stage readings.

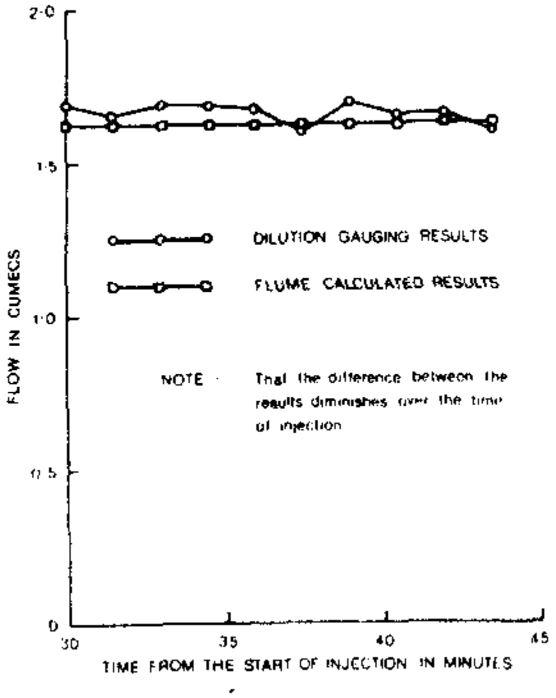

FIGURE 2

Gauging No 4 at the Tanllwyth flume on 23.1.75

These stage readings were read with an electric contact gauge in the stilling well of the flume and the flow values calculated from the flume calibration. If any part of the concentration profile is falling with time and the stage readings are constant, this would be indicative of a "stuck" stage recorder and the gauging should be discarded. If the stage is rising, the rate of rise will be important to the error in the gauging, (Gilman, 1975). If the stage is falling and if the concentration is rising then it is possible to compare the flows measured by the flume with those measured by dilution gauging. This will determine whether the concentration is on plateau thus giving several measurements of the flow for the gauging. An example of a gauging undertaken when the stage was falling and plateau concentration had been reached is shown in Figure 3. The difference between the calculated flow values from the dilution gauging from those calculated by the stage recordings remains fairly constant. Again the stage readings were read using the electric contact gauge in the stilling well of the flume and the streamflow calculated from the flume calibration.

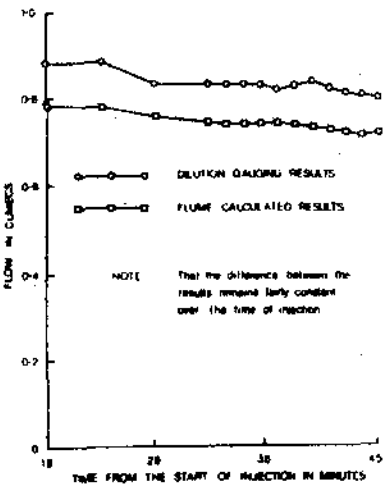

FIGURE 3

Gauging No 6 at the Cyff flume on 31.1.75

When the significance of the variations have been resolved it is only necessary to calculate the streamflow and its confidence level. This can be calculated by .FLOVAR which is based on the following method:

$$Q = \frac{q \bar{C}_1 D}{\bar{C}_2 d} \pm 2\sqrt{\text{Var } Q} \qquad (1/s)$$

where

$$\text{Var } Q = \left[\frac{\bar{C}_1 D}{\bar{C}_2 d}\right]^2 \text{var } q + \left[\frac{qD}{\bar{C}_2 d}\right]^2 \text{var } \bar{C}_1 + \left[\frac{q\bar{C}_1}{\bar{C}_2 d}\right]^2 \text{var } D$$

$$+ \left[\frac{q\bar{C}_1}{\bar{C}_2^2 d}\right]^2 \text{var } \bar{C}_2 \qquad (1^2/s^2)$$

and Q flow in ls^{-1}

q injection rate ls^{-1}

D dilution factor of the injection sample

d dilution factor of the stream sample

$\bar{C}_1$ mean injection concentration μgl^{-1}

$\bar{C}_2$ mean stream concentration μgl^{-1}

var Q variance of Q l^2s^{-2}

var q variance of q l^2s^{-2}

var $\bar{C}_1$ variance of the mean $\bar{C}_1$ $\mu g^2 l^{-2}$

var $\bar{C}_2$ variance of the mean $\bar{C}_2$ $\mu g^2 l^{-2}$

Notes 1) In the calculation for the $\bar{C}_1$ and $\bar{C}_2$ the variance of the mean is required. Therefore divide the sample variance by the number in the samples.

2) The var d is neglected since it is extremely small and only required if the estimated final stream sample concentration is outside the chemical analytical limits of (10-80 µg/l).

4. A GUIDE TO USING THE PROGRAMS

This section describes the form of data set for each program; actual examples are given in the relevant appendices together with the output the program produces. The complete runstreams are also given. (All the programs are in the file GAUGE*RIVER).

The program .MARIOTTE (Appendix A)

The program using the method described in Section 1.1 estimates the grouped best estimate of the slope and its variance and plots a graph of scale readings against volume. The program data has the following form, with all the numbers in free format and using the standard method of names starting with the letter I-N denoting integer numbers.

TITLE one card long

N,RHO (where N is the number of replicate calibrations and RHO is the density of water at ambient temperature)

M1 (where M1 is the number of points of the first calibration)

S_1, AM_1 (Enter the data, one point to a card with S_i value first, and AM_i second, separated by a comma.

S_2, AM_2 (Where S_i and AM_i is the i^{th} scale reading and the i^{th} mass of water discharged respectively).

. .

. .

. .

S_{M1}, AM_{M1}

M2

S_1, AM_1

S_2, AM_2 Second block of data with M2 points continue in this fashion for N blocks.

. .

. .

. .

S_{M2}, AM_{M2}

etc.

The following runstream will execute the program .MARIOTTE. on the Univac 1108 computer at the Institute

```
@RUN runid, accid, GAUGE
@ASG,AX   RIVER

@MSG  PLEASE KEEP A 7 TRACK TAPE FOR PLOTTING

@ASG,TJ  GRAPHTAPE,8C
@USE  8,GRAPHTAPE
@XQT  RIVER.MARIOTTE
(data set)
@FIN
```

The program .INJECT (Appendix B)

The program using the method described in Section 1.2 estimates the injection rate and its variance given the scale and time readings measured in the field. Graphs are plotted of scale reading against time and of the residual error against time.

Input data to the program is of the form:

TITLE (one card long)		Card 1	cols 1-80
MNO JET CALF VCALF IVCEXP			
where MNO is the Mariotte number	(I3)	Card 2	cols 1-3
JET is the jet number	(I3)	Card 2	cols 4-6
CALF is the Mariotte calibration factors	(F8.5)	Card 2	cols 7-14

VCALF is the mantissa of the variance of CALF (F8.5)		Card 2	cols 15-22
and IVCEXP is its exponent (I3)		Card 2	cols 23-25

ID IM IY IST1 IST2 IFIN1 IFIN2 N

where ID IM IY	is the date of injection (3I3)	Card 3	cols 1-9
IST1 IST2	is the start time: hours, minutes (2I3)	Card 3	cols 10-15
IFIN1 IFIN2	is the finish time: hours, minutes (2I3)	Card 3	cols 16-21
N	is the number of readings (I3)	Card 3	cols 22-24

IMIN1	ISEC1	SR1	where IMIN and ISEC is the time	Card 4	cols 1-12
IMIN2	ISEC2	SR2	in minutes and seconds from the	Card 5	cols 1-12
.	.	.	start of injection (2I4)	:	
.	.	.	and SR is the scale reading in		
			cms. (F4.1)	Card N+3	cols 1-12
IMINN	ISECN	SRN			

TITLE or @EOF — If another injection rate is required the next set of data starts here with the TITLE, if no more data, then put @EOF

The following runstream will execute the program .INJECT on the Univac 1108 computer at the Institute.

```
@RUN   run id, accid, GAUGE
@ASG,AX    RIVER
@MSG   PLEASE KEEP A 7 TRACK TAPE FOR PLOTTING
@ASG,TJ   GRAPHTAPE,8C
@USE      8,GRAPHTAPE
@XQT      RIVER.INJECT
(data set)
@EOF
@FIN.
```

<u>The program .CALIBRATE (Appendix C)</u>

The program using the method described in Section 2 estimates the values of $\hat{\theta}$, $\hat{Z}$ and $\hat{D}$ in (7) and plots the curve. The iodide concentrations and its variance are also produced in tabular form for transmission values .1(.001).95.

Input data to the program is of the form:

TITLE (one card long)
N,M (where N is the number of standards and M the number of replicates)
AI_1, T_{11}, ..., T_{1M} where AI_i is the iodide concentration in $\mu g l^{-1}$ and T_{ij} is the transmission of the standards

$AI_2, T_{21}, \ldots, T_{2M}$ (both numbers are real and are read in free format)

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.

.

.

$AI_N, T_{N1}, \ldots, T_{NM}$

Followed by the next set of data, if there is any; if there is none then put ∂EOF.

The following runstream will execute the program .CALIBRATE on the Univac 1108 computer at the Institute.

```
@RUN   runid, accid, GAUGE
@ASG,AX    RIVER
@MSG       PLEASE KEEP A 7 TRACK TAPE FOR PLOTTING
@ASG,TJ    GRAPHTAPE,8C
@USE       8,GRAPHTAPE
@XQT       RIVER.CALIBRATE
(data set)

@FIN
```

<u>Two-way classification Analysis of Variance using ASCOP (Appendix D)</u>

An integral part of calculation of the flow value from a gauging is the determination of the errors. It is important, using the sampling technique described in Section 3, to ensure that no significant systematic variation is occurring either across the stream or with time. One method to determine whether the variation is significant is to use the analysis variance technique. How to interpret the results is discussed in Appendix D, whilst the following typical runstream will produce ANOVA results for this problem on the Univac 1108 computer.

```
@RUN   runid, accid, GAUGE,100,100
@ASG,AX IHLIBS*STATS
@XQT    IHLIBS*STATS.ASCOP
TITLE   FLUME CALIBRATION
CUSTOMER G. TAME

READ DATA MATRIX SAMPLES VARIABLES CONC ACROSS TIME REPLICATES CONC 2
FULL SUMMARY
```

C_{111} C_{112}	1	1	(where C_{ij1}, C_{ij2} are replicated
C_{211} C_{212}	2	1	
C_{311} C_{312}	3	1	sample concentrations and
C_{411} C_{412}	4	1	they are real numbers

```
C121  C122       1    2
 .     .         .    .
 .     .         .    .

C421  C422       4    2
 .     .         .    .
 .     .         .    .

etc.

LEVELS     ACROSS     1 2 3 4     TIME 1 2 3 4 5 6 7 8
ANOVA OF CONC DESIGN ACROSS*TIME
FINISH
@FIN
```

(The words underlined are ASCOP key words and must be written as they are here).

The program .FLOVAR (Appendix D)

The program calculates the flow value and its confidence interval using the method described in Section 3. It differs from the other programs described in this report by being principally orientated for execution at a terminal. The departure from previous programs is that there is a printout at each step of the input of the different variables so that they can be checked for authenticity.

Input data to the program is of the form:

TITLE (one card long)

AINJ,INJEXP,VINJ, INJVEXP

where AINJ is the mantissa of the injection rate (ls^{-1})
INJEXP is its exponent
VINJ is the mantissa at the variance of the injection rate (l^2s^{-2})
INJVEXP is its exponent

DFAC,DFACEXP,VDFAC,VDFACEXP

where DFAC is the mantissa of the dilution factor
DFACEXP is its exponent
VDFAC is the mantissa of the variance of the dilution factor
VDFACEXP is its exponent

(See Greenland (1975) for the variances of the dilution factor)

C1,VARC1

where C1 is the mean concentration of iodide injected $\mu g l^{-1}$) and

VARC1 is its variance

C2, VARC2, DILC2

where C2 is the mean concentration of the stream samples ($\mu g l^{-1}$) and VARC2 is its variance

DILC2 is the dilution factor for the stream samples

(all numbers are in free format)

The following runstream will execute the program .FLOVAR on the Univac 1108 computer at the Institute.

```
@RUN  runid,accid,GAUGE
@ASG,AX  RIVER
@XQT RIVER.FLOVAR

(data set)      )
(data set)      ) more than one data set can be used in the same
   .            ) execution of the program
   .            )
etc.
@FIN
```

The order of execution of the programs

.MARIOTTE	(only used for periodic check calibrations or if there is some doubt about the efficacy of the injection).
.INJECT	(calculate the injection rate).
.CALIBRATE	(calculate the concentration of both injection samples and stream samples).
ASCOP	(investigate the systematic variation in the stream samples)
.FLOVAR	(calculate the flow value and its confidence interval).

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APPENDIX A

MARIOTTE BOTTLE CALIBRATION

1. EXAMPLE DATA SET

   MARIOTTE NO 8

2. EXAMPLE GRAPHICAL OUTPUT

   MARIOTTE NO 8

3. LISTING OF PROGRAM .MARIOTTE

A.1

BELT, IL RIVER. MAR8
ELTOT7 RLI870 08/26-19:51:17-(,0)

000001	000	MARIOTTE CALIBRATION NO 8
000002	000	3,.9982
000003	000	40
000004	000	40.,0.
000005	000	39.,1.084
000006	000	38.,2.101
000007	000	37.,3.155
000008	000	36.,4.157
000009	000	35.,5.116
000010	000	34.,6.099
000011	000	33.,7.115
000012	000	32.,8.184
000013	000	31.,9.242
000014	000	30.,10.307
000015	000	29.,11.405
000016	000	28.,12.414
000017	000	27.,13.451
000018	000	26.,14.518
000019	000	25.,15.565
000020	000	24.,16.63
000021	000	23.,17.654
000022	000	22.,18.699
000023	000	21.,19.74
000024	000	20.,20.8
000025	000	19.,21.833
000026	000	18.,22.885
000027	000	17.,23.918
000028	000	16.,24.958
000029	000	15.,25.989
000030	000	14.,27.038
000031	000	13.,28.065
000032	000	12.,29.091
000033	000	11.,30.137
000034	000	10.,31.134
000035	000	9.,32.166
000036	000	8.,33.199
000037	000	7.,34.218
000038	000	6.,35.255
000039	000	5.,36.279
000040	000	4.,37.284
000041	000	3.,38.307
000042	000	2.,39.335
000043	000	1.,40.32
000044	000	40
000045	000	40.,0.
000046	000	39.,1.063
000047	000	38.,2.069
000048	000	37.,3.125
000049	000	36.,4.152
000050	000	35.,5.103
000051	000	34.,6.08

A.1 (contd)

000052	000	33.,7.081
000053	000	32.,8.138
000054	000	31.,9.216
000055	000	30.,10.26
000056	000	29.,11.367
000057	000	28.,12.389
000058	000	27.,13.416
000059	000	26.,14.459
000060	000	25.,15.507
000061	000	24.,16.552
000062	000	23.,17.605
000063	000	22.,18.651
000064	000	21.,19.681
000065	000	20.,20.743
000066	000	19.,21.807
000067	000	18.,22.829
000068	000	17.,23.87
000069	000	16.,24.918
000070	000	15.,25.933
000071	000	14.,27.002
000072	000	13.,28.019
000073	000	12.,29.045
000074	000	11.,30.099
000075	000	10.,31.119
000076	000	9.,32.144
000077	000	8.,33.158
000078	000	7.,34.194
000079	000	6.,35.207
000080	000	5.,36.22
000081	000	4.,37.258
000082	000	3.,38.262
000083	000	2.,39.32
000084	000	1.,40.389
000085	000	40
000086	000	40.,0.
000087	000	39.,0.996
000088	000	38.,2.053
000089	000	37.,3.076
000090	000	36.,4.065
000091	000	35.,5.036
000092	000	34.,6.007
000093	000	33.,7.026
000094	000	32.,8.066
000095	000	31.,9.141
000096	000	30.,10.227
000097	000	29.,11.33
000098	000	28.,12.325
000099	000	27.,13.349
000100	000	26.,14.406
000101	000	25.,15.465
000102	000	24.,16.519
000103	000	23.,17.579
000104	000	22.,18.616

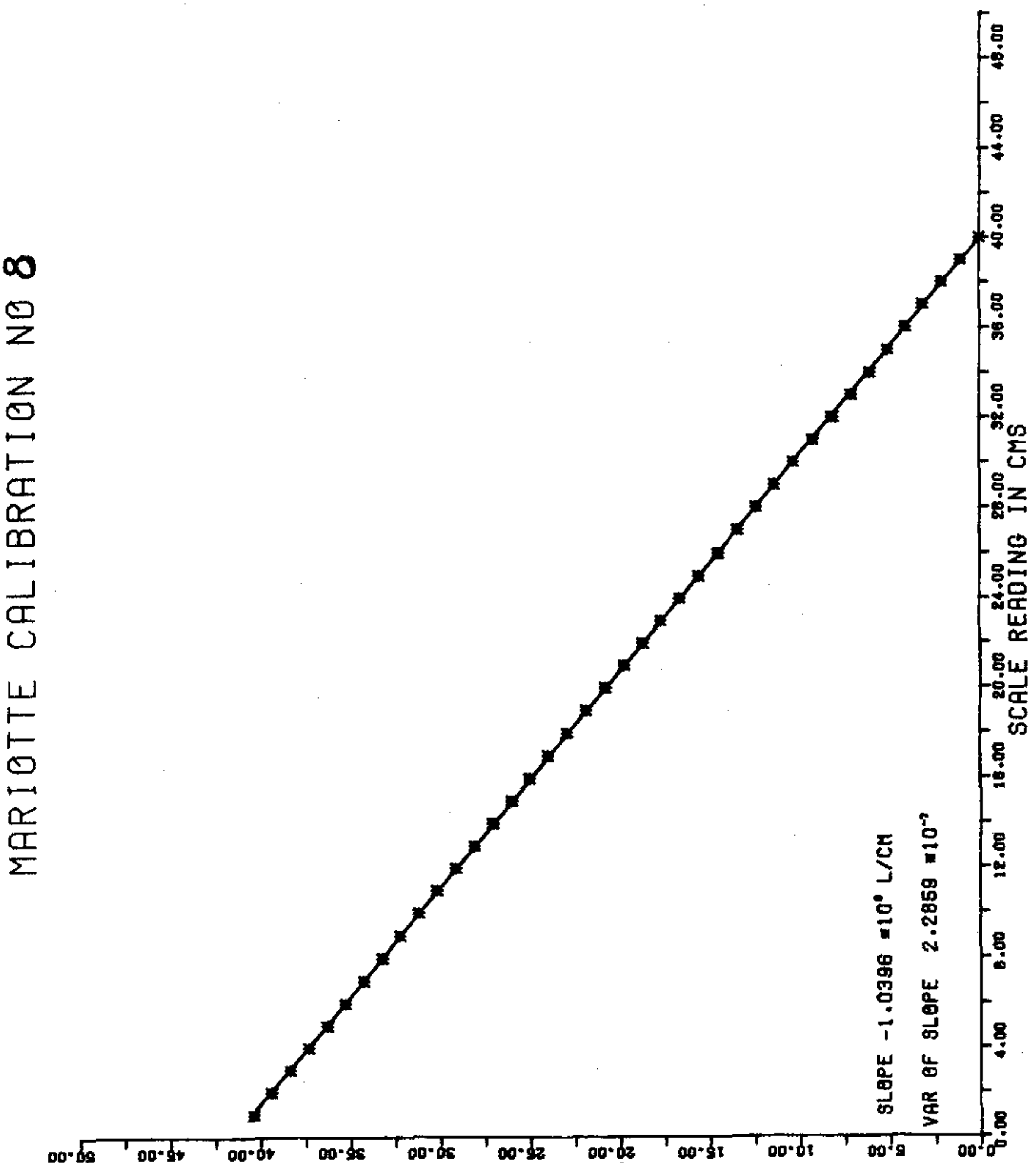
A.1 (contd)

```
000105      000    21.,19.638
000106      000    20.,20.696
000107      000    19.,21.756
000108      000    18.,22.78
000109      000    17.,23.824
000110      000    16.,24.868
000111      000    15.,25.898
000112      000    14.,26.938
000113      000    13.,27.966
000114      000    12.,29.01
000115      000    11.,30.058
000116      000    10.,31.063
000117      000    9.,32.109
000118      000    8.,33.121
000119      000    7.,34.153
000120      000    6.,35.18
000121      000    5.,36.181
000122      000    4.,37.226
000123      000    3.,38.26
000124      000    2.,39.26
000125      000    1.,40.267

END ELT.

@FIN
```

A.2



MARIOTTE CALIBRATION NO 8
SCALE READING IN CMS
0.00 4.00 8.00 12.00 16.00 20.00 24.00 28.00 32.00 36.00 40.00 44.00 48.00
VOLUME IN LITRES
0.00 5.00 10.00 15.00 20.00 25.00 30.00 35.00 40.00 45.00 50.00
SLOPE -1.0396 *10^0 L/CM
VAR OF SLOPE 2.2859 *10^-7

A.3

```
C
C       PROGRAM       .MARIOTTE
C                     ---------
C
C
C       USING LINEAR LEAST SQUARES THIS PROGRAM EVALUATES
C       THE GROUPED BEST ESTIMATE OF THE SLOPE AND VARIANCE
C       OF RESULTS OBTAINED FROM A MARIOTTE CALIBRATION.
C       THE PROGRAM PRODUCES THE RESULTS IN THE FORM OF A
                                   GRAPH.
C
C       P.SMITH MARCH 1975
C
C
           DIMENSION TITLE(13),X(10,90),Y(10,90),SC(6),
                                   B(10),C(10)
           DATA SC/.05,.1,.25,.5,1.,2.5/
C
C       READ IN TITLE,NUMBER N OF REPLICATE CALIBRATIONS
                                   AND ROE
C       THE DENSITY OF WATER AT AMBIENT TEMPERATURE
C
 98        READ(5,100,END=99)(TITLE(I),I=1,13)
 100       FORMAT(406)
           READ(5,101)N,ROE
 101       FORMAT( )
           RESID=0.
           DF=0.
           SUX=0.
           SUXY=0
C
C       READ IN THE NUMBER M(I) OF READINGS IN EACH
                                   CALIBRATION
C
           DO 1 I=1,N
           READ(5,101)M(I)
           MR=M(I)
           SX=0.
           SY=0.
           SSX=0.
           SSY=0.
           SSXY=0.
C
C       READ IN SCALE READINGS AND MASSES
C
           DO 2 J=1,MR
           READ(5,101)SP,AM
           V=AM/ROE
           Y(I,J)=V
           X(I,J)=SR
           SX=SX+SR
           SY=SY+V
           SSX=SSX+SR*SR
```

A.3 (contd)

```
      SSY=SSY+V*V
      SSXY=SSXY+SR*V
    2 CONTINUE
      SXX=SSX-(SX*SX)/MR
      SXY=SSXY-(SX*SY)/MR
      BB=SXY/SXX
      C(I)=(SY-BB*SX)/MR
      SYY=SSY-(SY*SY)/MR
      RESID=RESID+SYY-SXY*BB
      B(I)=BB
      DF=DF+MR-2
      SUX=SUX+SXX
      SUXY=SUXY+SXY
    1 CONTINUE
      S2=RESID/DF
C
C    EVALUATE BHAT AND VARB THE ESTIMATE OF THE SLOPE AND
                                  VARIANCE
C
      VARB=S2/SUX
```

APPENDIX B

DETERMINING THE INJECTION RATE

1. EXAMPLE DATA SET

   TANLLWYTH GAUGING NO 4

2. *EXAMPLE GRAPHICAL OUTPUT*

   (a) INJECTION RATE FOR TANLLWYTH GAUGING NO 4

   (b) THE RESIDUAL ERROR OF THE INJECTION

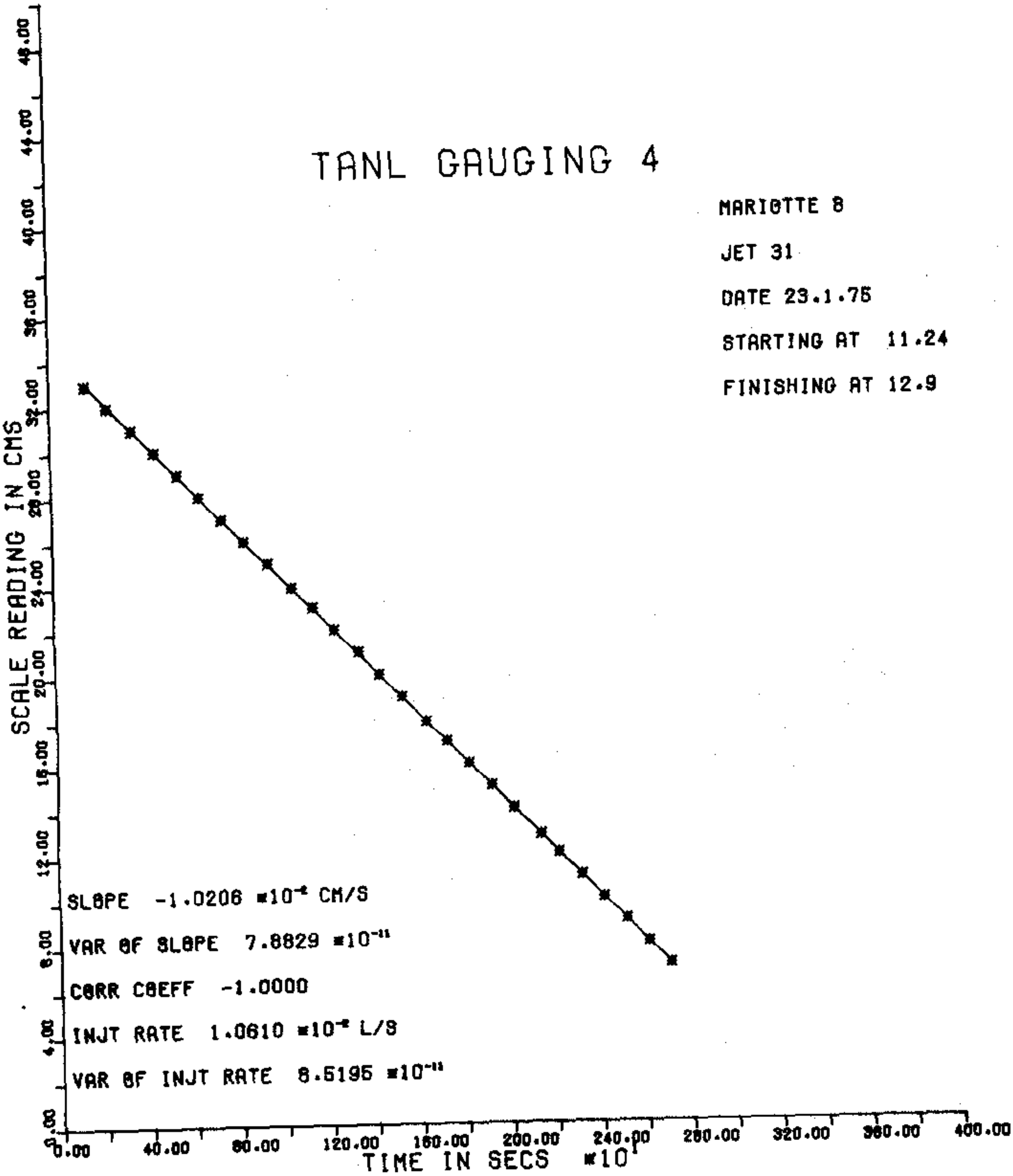
3. LISTING OF PROGRAM .INJECT

B.1

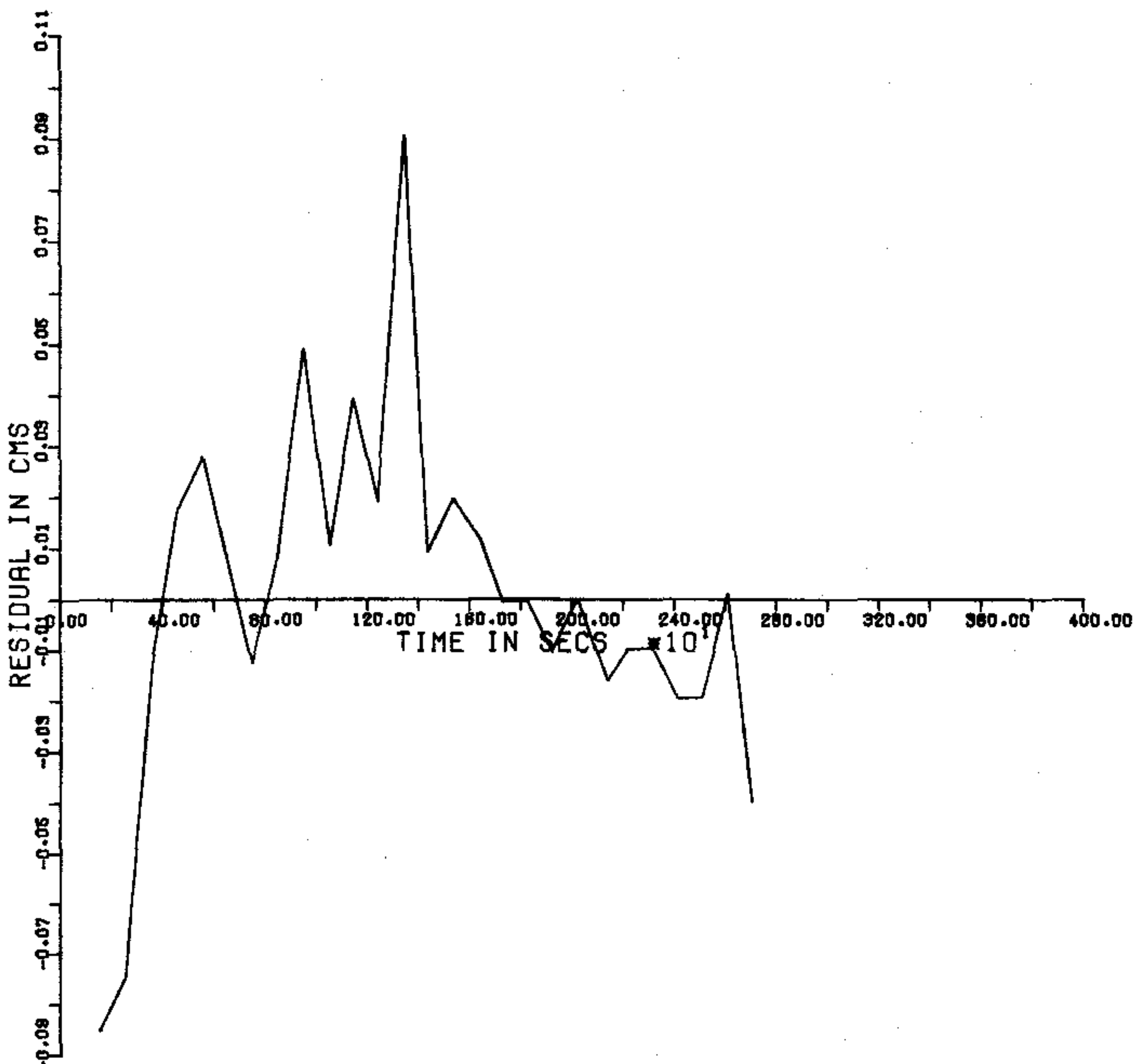
```
DELT,IL RIVER.INJTO4
ELTOT7 RLI870 08/26-19:51:51-(,0)
000001        000     TANL GAUGING 4
000002        000       8 31-1.0396  2.2859 -7
000003        000      23  1 75 11 24 12  9 27
000004        000       2  3533.0
000005        000       4  1432.0
000006        000       5  5831.0
000007        000       7  3930.0
000008        000       9  1829.0
000009        000      10  5428.0
000010        000      12  3027.0
000011        000      14  1026.0
000012        000      15  5225.0
000013        000      17  3623.9
000014        000      19  0723.0
000015        000      20  4322.0
000016        000      22  2821.0
000017        000      23  5820.0
000018        000      25  3719.0
000019        000      27  2417.9
000020        000      28  5117.0
000021        000      30  2916.0
000022        000      32  0615.0
000023        000      33  4514.0
000024        000      35  4112.8
000025        000      37  0012.0
000026        000      38  3811.0
000027        000      40  1510.0
000028        000      41  5309.0
000029        000      43  3308.0
000030        000      45  0707.0

END ELT.
```

B.2a


TANL GAUGING 4
MARIOTTE 8
JET 31
DATE 23.1.75
STARTING AT 11.24
FINISHING AT 12.9
SLOPE -1.0206 *10⁻² CM/S
VAR OF SLOPE 7.8829 *10⁻¹¹
CORR COEFF -1.0000
INJT RATE 1.0610 *10⁻² L/S
VAR OF INJT RATE 8.5195 *10⁻¹¹
SCALE READING IN CMS
TIME IN SECS *10
0.00
4.00
8.00
12.00
16.00
20.00
24.00
28.00
32.00
36.00
40.00
44.00
48.00
0.00
40.00
80.00
120.00
160.00
200.00
240.00
280.00
320.00
360.00
400.00

B.2b



RESIDUAL IN CMS
TIME IN SECS *10
0.00
40.00
80.00
120.00
160.00
200.00
240.00
280.00
320.00
360.00
400.00
0.11
0.09
0.07
0.05
0.03
0.01
-0.01
-0.03
-0.05
-0.07
-0.09

B.3

```
      C
      C        PROGRAM      .INJECT
      C                     -------
      C
      C        USING LINEAR LEAST SQUARES METHODS THIS PROGRAM
      C        ESTIMATES THE INJECTION RATE AND ITS VARIANCE GIVEN
      C        THE SLOPE AND VARIANCE FROM THE CALIBRATION OF THE
                                       MARIOTTE.
      C        THE PROGRAM PRODUCES THE RESULTS IN THE FORM OF
                                       A GRAPH
      C
      C        P.SMITH MARCH 1975
      C
               DIMENSION RESID(100),SC(7),IITLE(13),X(100),
                                       Y(100)
               DATA SC/0.,50.,100.,200.,500.,1000.,2000./
      C
      C        READ IN THE TITLE, MARIOTTE NO, JET NO AND CALB'N
                                       DETAILS
      C
       3       READ(5,100,END=2)(IITLE(I),I=1,13)
       100     FORMAT(3A6)
               READ(5.103)MNO,JET,CALF,VCALF,IVEXP
       103     FORMAT(213,2F8.5,13)
               VCALF=VCALF*10.**IVEXP
      C
      C        READ DATE,START AND FINISHING TIMES NUMBER OF
                                       READINGS
      C
               READ(5,101)ID,IM,IY,IST1,IST2,IFIN1,IFIN2,N
       101     FORMAT(813)
               SX=0.
               SY=0.
               SSX=0.
               SSY=0
               SSXY=0
      C
      C        READ IN DATA PAIRS TIME(MINS.,SECS) AND SCALE
                                       READINGS
      C
               DO 1 I=1,N
               READ(5,102)IT1,IT2,SR
               T=IT1*60.+IT2
       102     FORMAT(214,F4.1)
               X(I)=T
               Y(I)=SR
               SX=SX+T
               SY=SY+SR
               SSX=SSX+T*T
               SSY=SSY+SR*SR
               SSXY=SSXY+SR*T
       1       CONTINUE
               SXX=SSX-(SX*SX)/N
```

B.3 (contd)

```
            SYY=SSY-(SY*SY)/N
            SXY=SSXY-(SX*SY)/N
C
C     B AND VARB ARE THE SLOPE AND VARIANCE OF THE SLOPE
C
            B=SXY/SXX
            C=(SY-B*SX)/N
            R=SXY/SQRT(SXX*SYY)
            RSS=(SYY-SXY*B)/(N-2)
            VARB=RSS/SXX
C
C
C     PLOT THE INJECTION LINE AND OTHER DETAILS
C
C
            CALL PLOTS(0.,0.,8)
            CALL PLOT(0.,-100.,-3)
            CALL PLOT(0.,5.,-3)
            CALL FACTOR(.8)
            CALL AXIS(0.,0.,20HSCALE READING IN CMS.20,25.,
                                  90.,0.,2.)
            MAX=X(N)+1.
            SCALA=MAX/20.
            DO 4 JP=1,7
            IF(SCALA.LT.SC(JP))GOTO 6
4           CONTINUE
6           SCALA=SC(JP)
            CALL AXIS (0.,0.,12HTIME IN SECS,-12,20.,0.,
                                  0.,SCALA)
            XST=X(1)/SCALA
            YST=(B*X(1)+C)/2
            CALL PLOT(XST,YST,3)
            XFIN=X(N)/SCALA
            YFIN=(B*X(N)+C)/2
            CALL PLOT(XFIN,YFIN,2)
            IP1=1
            DO 5 J=1,N
            XA=X(J)/SCALA
            YA=Y(J)/2
              RRO=Y(J)-B*X(J)-C
              RESID(J)=RRO
            CALL SYMBOL(XA,YA,.21,11,0.,IP)
5           CONTINUE
            CALL SYMBOL(6.,21.,.56,ITTLE,0.,18)
            CALL SYMBOL(15.,20.,.28,9HMARIOTTE,0.,9)
            AMO=MNO
            CALL NUMBER (999.,999.,.28,AMO,0.,-1)
            CALL SYMBOL(15.,19.,.28,4HJET,0.,4)
            AJET=JET
            CALL NUMBER (999.,999.,.28,AJET,0.,-1)
            CALL SYMBOL(15.,18.,.28,5HDATE ,0.,5)
            AD=ID
            CALL NUMBER(999.,999.,28,AD,0.,0)
```

B.3 (contd)

```
      AM=IM
      CALL NUMBER (999.,999.,.28,AM,0.,0)
      AY=IY
      CALL NUMBER(999.,999.,.28,AY,0.,-1)
      CALL SYMBOL(15.,17.,.28,13HSTARTING AT ,0.,13)
      ST1=IST1
      CALL NUMBER(999.,999.,.28,ST1,0.,0)
      ST2=IST2
      CALL NUMBER(999.,999.,.28,ST2,0.,-1)
      CALL SYMBOL(15.,16.,.28,13HFINISHING AT ,0.,13)
      FIN1=IFIN1
      CALL NUMBER(999.,999.,.28,FIN1,0.,0)
      FIN2=IFIN2
      CALL NUMBER(999.,999.,.28,FIN2,0.,-1)
      CALL SYMBOL(.2,5.,.28,7HSLOPE ,0.,7)
        KP=0
 7      BE=B*10.**KP)
        IF(ABS(BE).GE.1.)GOTO 8
        KP=KP+1
        GOTO 7
 8    CALL NUMBER(999.,999.,.28,BE,0.,4)
        CALL SYMBOL(999.,999.,.28,4H *10,0.,4)
        AP=KP
        CALL NUMBER(999.,5.2,.14,AP,0.,-1)
      CALL SYMBOL(999.,5.,.28,5H CM/S,0.,5)
      CALL SYMBOL(.2,4.,.28,14HVAR OF SLOPE ,0.,14)
        KP=0
 11     BS=VARB*(10.**KP)
        IF(ABS(BS).GE.1.)GOTO 12
        KP=KP+1
        GOTO 11
 12   CALL NUMBER(999.,999.,.28,BS,0.,4)
          CALL SYMBOL(999.,999.,.28,4H *10,0.,4)
          AP=-KP
          CALL NUMBER(999.,4.2,.14,AP,0.,-1)
      CALL SYMBOL(.2,3.,.28,12HCORR COEFF ,0.,12)
      CALL NUMBER(999.,999.,.28,R,0.,4)
      RINJ=B*CALF
      CALL SYMBOL(.2,2.,.28,11HINJT RATE ,0.,11)
          KP=0
 9        BR=RINJ*(10.**KP)
          IF(ABS(BR).GE.1.)GOTO 10
          KP=KP+1
        GOTO 9
 10   CALL NUMBER(999.,999.,.28,BR,0.,4)
        CALL SYMBOL(999.,999.,.28,4H *10,0.,4)
        AP=-KP
        CALL NUMBER(999.,2.2,.14,AP,0.,-1)
      CALL SYMBOL(999.,2.,.28,4H L/S,0.,6)
        CALL SYMBOL(.2,1.,.28,18HVAR OF INJT RATE
                                ,0.,18)
        VARIN=CALF*CALF*VARB+B*BVCALF
```

B.3 (contd)

```
                 KP=0
      16         BV=VARIN*(10.**KP)
                 IF(ABS(BV).GE.1.)GOTO 17
                 KP=KP+1
                 GOTO 16
      17         CALL NUMBER(999.,999.,.28,BV,0.,4)
                 CALL SYMBOL(999.,999.,.28,4H *10,0.,4)
                 AP=-KP
                 CALL NUMBER(999.,1.2,.14,AP,0.,-1)
              CALL PLOT(25.,0.,-3)
                 CALL SCALE(RESID,20.,N,1)
                 FV=RESID(N+1)
                 DV=RESID(N+2)
                 CALL AXIS(0.,0.,15HRESIDUAL IN CMS,15,20.,90.,
                                           FV,DV)
                 YP=0
                 IF(FV.GE.0)GOTO 13
                 YP=-FV/DV
      13         CALL AXIS(0.,YP,12HTIME IN SECS,-12,20.,0.,0.,
                                           SCALA)
                 JO=3
                 DO 15 J=1,N
                 XA=X(J)/SCALA
                 YA=RESID(J)-FV)/DV
                 CALL PLOT(XA,YA,JO)
                 JO=2
      15         CONTINUE
                 CALL PLOT(25.,0.,-3)
              GOTO 3
      2       CALL PLOT(15.,0.,999)
              STOP
              END

END OF COMPILATION:       NO DIAGNOSTICS
```

APPENDIX C

CALIBRATING THE AUTO-ANALYSER

1. EXAMPLE DATA SET

   CALIBRATION FOR TANLLWYTH GAUGING NO 4

2. EXAMPLE OUTPUT

   (a) CALIBRATION CURVE FOR TANLLWYTH GAUGING NO 4

   (b) CALIBRATION LOOK-UP TABLE

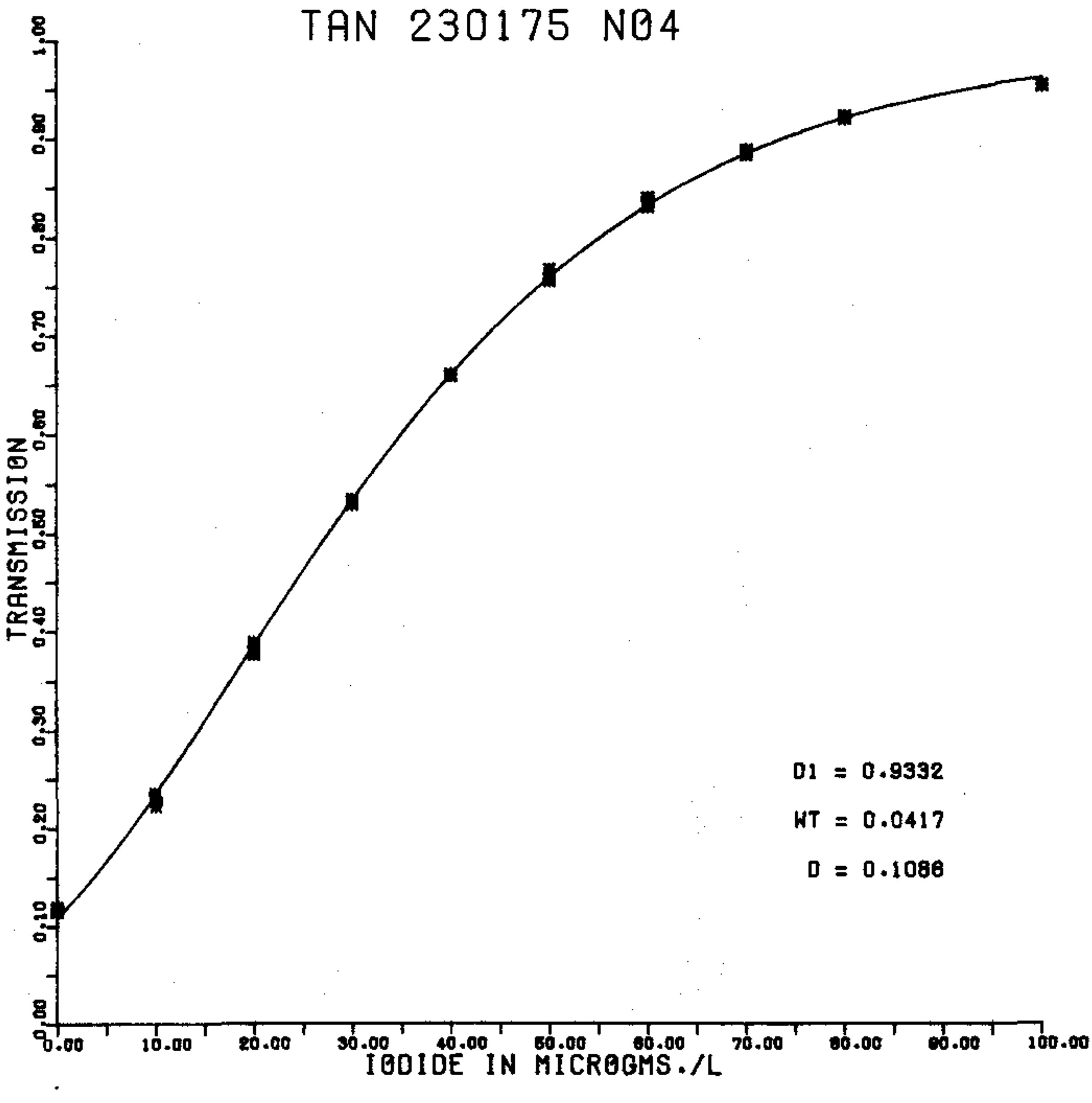
3. LISTING OF PROGRAM .CALIBRATE

C.1

```
DELT,IL RIVER.CAL664
ELTOT7 RLIB70 08/26-18:52:49-(,0)
000001        000      TAN230175 N04
000002        000      10,6
000003        000      0.,.116,.116,.116,.116,.118,.12
000004        000      10.,.222,.227,.229,.236,.231,.232
000005        000      20.,.384,.388,.388,.376,.378,.381
000006        000      30.,.534,.532,.53,.528,.531,.531
000007        000      40.,.658,.66,.66,.658,.658,.66
000008        000      50.,.761,.766,.766.,754,.757,.757
000009        000      60.,.835,.838,.829,.83,.833
000010        000      70.,.886,.886,.886,.882,.881,.884
000011        000      80.,.92,.92,.92,.917,.918,.918
000012        000      100.,.951,.952,.952,.951,.952,.951

END ELT.
```

C.2a


TAN 230175 N04
TRANSMISSION
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00
90.00
100.00
IODIDE IN MICROGMS./L
D1 = 0.9332
WT = 0.0417
D = 0.1086

C.2b

TAN 230175 N04

D1 = .9332 WT = .0417 D = .1085

PKHT	CONC	VAR	PKHT	CONC	VAR	PKHT	CONC	VAR	PKHT	CONC	VAR	PKHT	CONC	VAR
.150	3.66	.064	.151	3.74	.065	.152	3.82	.066	.153	3.90	.067	.154	3.98	.068
.155	4.06	.068	.156	4.15	.069	.157	4.23	.070	.158	4.31	.071	.159	4.39	.072
.160	4.47	.073	.161	4.55	.074	.162	4.63	.074	.163	4.71	.075	.164	4.79	.076
.165	4.86	.077	.166	4.94	.078	.167	5.02	.078	.168	5.10	.079	.169	5.18	.080
.170	5.26	.081	.171	5.34	.082	.172	5.41	.082	.173	5.49	.083	.174	5.57	.084
.175	5.65	.084	.176	5.72	.085	.177	5.81	.086	.178	5.88	.087	.179	5.95	.087
.180	6.03	.088	.181	6.11	.089	.182	6.18	.089	.183	6.26	.090	.184	6.33	.090
.185	6.41	.091	.186	6.48	.092	.187	6.56	.092	.188	6.64	.093	.189	6.71	.094
.190	6.79	.094	.191	6.86	.095	.192	6.93	.095	.193	7.01	.096	.194	7.08	.095
.195	7.16	.097	.196	7.23	.098	.197	7.31	.098	.198	7.38	.099	.199	7.45	.099
.200	7.53	.100	.201	7.60	.100	.202	7.67	.101	.203	7.75	.101	.204	7.82	.102
.205	7.80	.102	.206	7.95	.103	.207	8.04	.103	.208	8.11	.104	.209	8.18	.104
.210	8.25	.104	.211	8.33	.105	.212	8.40	.105	.213	8.47	.106	.214	8.54	.106
.215	8.61	.107	.216	8.69	.107	.217	8.76	.107	.218	8.83	.108	.219	8.90	.108
.220	8.97	.109	.221	9.04	.109	.222	9.11	.109	.223	9.18	.110	.224	9.26	.110
.225	9.33	.111	.226	9.40	.111	.227	9.47	.111	.228	9.54	.112	.229	9.61	.112
.230	9.68	.112	.231	9.75	.113	.232	9.82	.113	.233	9.89	.113	.234	9.96	.113
.235	10.66	.114	.236	10.10	.114	.237	10.17	.114	.238	10.24	.115	.239	10.31	.115
.240	10.38	.115	.241	10.45	.115	.242	10.52	.116	.243	10.58	.116	.244	10.65	.116
.245	10.72	.116	.246	10.79	.117	.247	10.86	.117	.248	10.93	.117	.249	11.00	.117
.250	11.07	.118	.251	11.14	.118	.252	11.20	.118	.253	11.27	.118	.254	11.34	.118
.255	11.41	.119	.256	11.48	.119	.257	11.55	.119	.258	11.61	.119	.259	11.68	.119
.260	11.75	.120	.261	11.82	.120	.262	11.89	.120	.263	11.95	.120	.264	12.02	.120
.265	12.09	.120	.266	12.16	.120	.267	12.22	.121	.268	12.29	.121	.269	12.36	.121

C.2b (contd)

.270	12.43	.121	.271	12.49	.121	.272	12.56	.121	.273	12.63	.121	.274	12.70	.121
.275	12.76	.122	.276	12.83	.122	.277	12.90	.122	.278	12.96	.122	.279	13.03	.122
.280	13.10	.122	.281	13.16	.122	.282	13.23	.122	.283	13.30	.122	.284	13.37	.122
.285	13.43	.122	.286	13.50	.122	.287	13.57	.122	.288	13.63	.122	.289	13.70	.122
.290	13.76	.123	.291	13.83	.123	.292	13.90	.123	.293	13.96	.123	.294	14.03	.123
.295	14.10	.123	.296	14.16	.123	.297	14.23	.123	.298	14.30	.123	.299	14.36	.123
.300	14.42	.123	.301	14.49	.123	.302	14.55	.123	.303	14.62	.123	.304	14.69	.123
.305	14.76	.123	.306	14.82	.123	.307	14.89	.123	.308	14.96	.123	.309	15.02	.123
.310	15.09	.122	.311	15.15	.122	.312	15.22	.122	.313	15.29	.122	.314	15.35	.122
.315	15.42	.122	.316	15.48	.122	.317	15.55	.122	.318	15.61	.122	.319	15.68	.122
.320	15.74	.122	.321	15.81	.122	.322	15.88	.122	.323	15.94	.122	.324	16.01	.121
.325	16.07	.121	.326	16.14	.121	.327	16.20	.121	.328	16.27	.121	.329	16.33	.121
.330	16.40	.121	.331	16.47	.121	.332	16.53	.121	.333	16.60	.120	.334	16.66	.120
.335	16.73	.120	.336	16.79	.120	.337	16.86	.120	.338	16.92	.120	.339	16.99	.120
.340	17.05	.119	.341	17.12	.119	.342	17.18	.119	.343	17.25	.119	.344	17.31	.119
.345	17.38	.119	.346	17.45	.118	.347	17.51	.118	.348	17.58	.118	.349	17.64	.118
.350	17.71	.118	.351	17.77	.117	.352	17.84	.117	.353	17.90	.117	.354	17.97	.117
.355	18.03	.117	.356	18.10	.116	.357	18.16	.116	.358	18.23	.116	.359	18.29	.116
.360	18.36	.115	.361	18.42	.115	.362	18.49	.115	.363	18.55	.115	.364	18.62	.114
.365	18.68	.114	.366	18.75	.114	.367	18.81	.114	.368	18.88	.113	.369	18.95	.113
.370	19.01	.113	.371	19.08	.112	.372	19.14	.112	.373	18.21	.112	.374	19.27	.112
.375	19.34	.111	.376	19.40	.111	.377	19.47	.111	.378	19.53	.110	.379	19.60	.110
.380	19.66	.110	.381	19.73	.109	.382	19.79	.109	.383	19.86	.109	.384	19.92	.108
.385	19.99	.108	.386	20.06	.108	.387	20.12	.107	.388	20.19	.107	.389	20.25	.107
.390	20.32	.106	.391	20.38	.106	.392	20.45	.105	.393	20.51	.105	.394	20.58	.105
.395	20.64	.104	.396	20.71	.104	.397	20.78	.103	.398	20.84	.103	.399	20.01	.103
.400	20.07	.102	.401	21.04	.102	.402	21.10	.101	.403	21.17	.101	.404	21.23	.100
.405	21.30	.100	.406	21.37	.100	.407	21.43	.099	.408	21.50	.099	.409	21.56	.098
.410	21.63	.098	.411	21.69	.097	.412	21.76	.097	.413	21.83	.096	.414	21.89	.096
.415	21.96	.095	.416	22.02	.095	.417	22.09	.094	.418	22.16	.094	.419	22.22	.093
.420	22.29	.093	.421	22.35	.092	.422	22.42	.092	.423	22.49	.091	.424	22.55	.091
.425	22.52	.090	.426	22.68	.090	.427	22.75	.089	.428	22.82	.089	.429	22.88	.088
.430	22.95	.088	.431	23.02	.087	.432	23.08	.087	.433	23.15	.086	.434	23.22	.086

C.2b (contd)

.435	23.28	.085	.436	23.35	.085	.437	23.41	.084	.438	23.48	.083	.439	23.55	.083
.440	23.51	.082	.441	23.68	.082	.442	23.75	.081	.443	23.81	.081	.444	23.88	.080
.445	23.95	.079	.446	24.02	.079	.447	24.08	.078	.448	24.15	.078	.449	24.22	.077
.450	24.28	.076	.451	24.35	.076	.452	24.42	.075	.453	24.48	.075	.454	24.55	.074
.455	24.62	.073	.456	24.69	.073	.457	24.75	.072	.458	24.82	.072	.459	24.88	.071
.460	24.96	.070	.461	25.02	.070	.462	25.09	.069	.463	25.16	.068	.464	25.23	.068
.465	25.29	.067	.456	25.36	.067	.467	25.43	.066	.468	25.50	.065	.469	25.57	.065
.470	25.63,	.064	.471	25.70	.063	.472	25.77	.063	.473	25.84	.062	.474	25.91	.061
.475	25.07	.061	.476	26.04	.060	.477	26.11	.059	.478	26.18	.059	.479	26.25	.058
.480	26.32	.057	.481	26.38	.057	.482	26.45	.056	.483	26.52	.055	.484	26.59	.055
.485	26.66	.054	.486	26.73	.053	.487	26.80	.053	.488	26.87	.052	.489	26.93	.051
.490	27.00	.050	.491	27.07	.050	.492	27.14	.049	.493	27.21	.048	.494	27.28	.048
.495	27.35	.047	.496	27.42	.046	.497	27.49	.045	.498	27.56	.045	.499	27.63	.044
.500	27.70	.043	.501	27.77	.043	.502	27.84	.042	.503	27.91	.041	.504	27.98	.041
.505	28.05	.040	.506	28.12	.039	.507	28.19	.038	.508	28.26	.038	.509	28.33	.041
.510	28.40	.036	.511	28.47	.035	.512	28.54	.035	.513	28.61	.034	.514	28.58	.033
.515	28.75	.033	.516	28.82	.032	.517	28.89	.031	.518	28.96	.030	.519	29.04	.030
.520	29.11	.029	.521	29.18	.028	.522	29.25	.027	.523	29.32	.027	.524	29.39	.026
.525	29.45	.025	.526	29.53	.024	.527	29.61	.024	.528	29.68	.023	.529	29.75	.022
.530	29.82	.022	.531	29.89	.021	.532	29.97	.020	.533	30.04	.019	.534	30.11	.019
.535	30.18	.018	.536	30.25	.017	.537	30.33	.016	.538	30.40	.016	.539	30.47	.015
.540	30.54	.014	.541	30.62	.013	.542	30.59	.013	.543	30.76	.012	.544	30.84	.011
.545	30.91	.010	.546	30.98	.010	.547	31.06	.009	.548	31.13	.008	.549	31.20	.007
.550	31.20	.007	.551	31.35	.005	.552	31.42	.005	.553	31.50	.005	.554	31.57	.004
.555	31.55	.003	.556	31.72	.003	.557	31.80	.002	.558	31.87	.001	.559	31.94	.000
.560	32.02	-.000	.561	32.09	-.001	.562	32.17	-.002	.563	32.24	-.002	.564	32.32	-.003
.565	32.30	-.004	.566	32.47	-.004	.567	32.54	-.006	.568	32.62	-.006	.569	32.69	-.006
.570	32.77	-.007	.571	32.85	-.007	.572	32.92	-.009	.573	33.00	-.009	.574	33.07	-.009
.575	33.18	-.010	.576	33.23	-.010	.577	33.30	-.011	.578	33.38	-.011	.579	33.46	-.012
.580	33.53	-.013	.581	33.61	-.013	.582	33.69	-.014	.583	33.76	-.014	.584	33.84	-.015
.585	33.92	-.015	.586	34.00	-.016	.587	34.07	-.016	.588	34.15	-.016	.589	34.23	-.017
.590	34.31	-.017	.591	34.39	-.018	.592	34.46	-.018	.593	34.54	-.019	.594	34.62	-.019

C.2b (contd)

.595	34.70	-.019	.596	34.78	-.020	.597	34.86	-.020	.598	34.94	-.020	.599	35.01	-.021
.600	35.09	-.021	.601	35.17	-.021	.602	35.25	-.021	.603	35.33	-.022	.604	35.41	-.022
.605	35.49	-.022	.606	35.57	-.022	.607	35.65	-.022	.608	35.73	-.022	.609	35.81	-.022
.610	35.89	-.023	.611	35.87	-.023	.612	36.05	-.023	.613	36.14	-.023	.614	36.22	-.023
.615	36.30	-.023	.616	36.38	-.023	.617	36.46	-.023	.618	36.54	-.022	.619	36.62	-.022
.620	36.71	-.022	.621	36.79	-.022	.622	36.87	-.022	.623	36.95	-.022	.624	37.04	-.021
.625	37.12	-.021	.626	37.20	-.021	.627	37.29	-.020	.628	37.37	-.020	.629	37.45	-.020
.630	37.54	-.019	.631	37.62	-.019	.632	37.70	-.018	.633	37.79	-.018	.634	37.87	-.017
.635	37.96	-.017	.636	38.04	-.016	.637	38.13	-.015	.638	38.21	-.016	.639	38.29	-.014
.640	38.38	-.013	.641	38.47	-.012	.642	38.55	-.012	.643	38.64	-.011	.644	38.72	-.010
.645	38.81	-.009	.646	38.90	-.008	.647	38.98	-.007	.648	39.07	-.006	.649	39.16	-.005
.650	39.24	-.003	.651	39.33	-.002	.652	39.42	-.001	.653	39.50	.000	.654	39.59	.002
.655	39.68	.003	.656	39.77	.005	.657	39.86	.006	.658	39.94	.008	.659	40.03	.009
.660	40.12	.011	.661	40.21	.013	.662	40.30	.015	.663	40.39	.016	.664	40.48	.018
.665	40.57	.020	.666	40.66	.022	.667	40.75	.024	.668	40.84	.027	.669	40.93	.029
.670	41.02	.031	.671	41.11	.033	.672	41.21	.035	.673	41.30	.038	.674	41.39	.040
.675	41.49	.043	.676	41.57	.045	.677	41.67	.048	.678	41.76	.050	.679	41.85	.053
.680	41.84	.056	.681	42.04	.058	.682	42.13	.061	.683	42.22	.064	.684	42.32	.067
.685	42.41	.070	.686	42.51	.073	.687	42.60	.076	.688	42.70	.079	.689	42.79	.082
.690	42.80	.085	.691	42.98	.088	.692	43.08	.092	.693	43.18	.095	.694	43.27	.098
.695	43.37	.101	.696	43.47	.105	.697	43.56	.108	.698	43.66	.112	.699	43.76	.115
.700	43.86	.119	.701	43.96	.122	.702	44.05	.126	.703	44.15	.130	.704	44.25	.133
.705	44.35	.137	.706	44.45	.141	.707	44.55	.144	.708	44.66	.148	.709	44.78	.152
.710	44.85	.156	.711	44.95	.160	.712	45.05	.164	.713	45.15	.168	.714	45.26	.172
.715	45.36	.175	.716	45.46	.179	.717	45.56	.184	.718	45.67	.188	.719	45.77	.192
.720	45.87	.196	.721	45.98	.200	.722	46.08	.204	.723	46.19	.208	.724	46.29	.212
.725	46.40	.216	.726	46.50	.220	.727	46.61	.225	.728	46.71	.229	.729	46.82	.233
.730	46.93	.237	.731	47.03	.241	.732	47.14	.245	.733	47.25	.250	.734	47.36	.254
.735	47.47	.258	.736	47.57	.262	.737	47.68	.266	.738	47.79	.270	.739	47.90	.275
.740	48.01	.279	.741	48.12	.283	.742	48.24	.287	.743	48.35	.291	.744	48.46	.295
.745	48.57	.299	.746	48.68	.303	.747	48.80	.307	-748	48.91	.311	.749	49.02	.315

C.2b (contd)

.750	49.14	.319	.751	49.25	.323	.752	49.37	.327	.753	49.48	.330	.754	49.60	.334
.755	49.71	.338	.756	49.83	.341	.757	49.95	.345	.758	50.06	.348	.759	50.18	.352
.760	50.30	.355	.761	50.42	.358	.762	50.54	.362	.763	50.66	.365	.764	50.78	.368
.765	50.00	.371	.766	51.12	.374	.767	51.14	.377	.768	51.26	.380	.769	51.38	.382
.770	51.60	.385	.771	51.63	.388	.772	51.75	.390	.773	51.87	.393	.774	52.00	.395
.775	52.12	.337	.776	52.25	.400	.777	52.38	.402	.778	52.50	.404	.779	52.63	.406
.780	52.76	.408	.781	52.88	.410	.782	53.01	.412	.783	53.14	.413	.784	53.27	.415
.785	53.40	.417	.786	53.53	.418	.787	53.66	.420	.788	53.80	.421	.789	53.93	.422
.790	54.06	.424	.791	54.19	.426	.792	54.33	.426	.793	54.56	.427	.794	54.60	.428
.795	54.73	.429	.796	54.87	.430	.797	55.01	.430	.798	55.14	.431	.799	55.28	.432
.800	55.42	.432	.801	55.56	.433	.802	55.70	.433	.803	55.84	.433	.804	55.98	.434
.805	56.13	.434	.806	56.27	.434	.807	56.41	.434	.808	56.56	.434	.809	56.70	.434
.810	56.85	.434	.811	56.99	.434	.812	57.14	.433	.813	57.29	.433	.814	57.44	.432
.815	57.59	.432	.816	57.74	.431	.817	57.89	.431	.818	58.04	.430	.819	58.19	.429
.820	58.34	.428	.821	58.50	.428	.822	58.65	.427	.823	58.81	.426	.824	58.96	.424
.825	59.12	.423	.826	59.28	.422	.827	59.44	.421	.828	59.60	.419	.829	59.76	.418
.830	59.92	.417	.831	60.08	.415	.832	60.25	.414	.833	60.41	.412	.834	60.57	.410
.835	50.74	.409	.836	60.91	.407	.837	61.08	.405	.838	61.24	.403	.839	61.42	.401
.840	61.59	.399	.841	61.76	.397	.842	61.93	.395	.843	62.11	.393	.844	62.28	.391
.845	62.46	.389	.846	62.63	.387	.847	62.81	.384	.848	62.99	.382	.849	63.17	.379
.850	63.35	.377	.851	63.54	.375	.852	63.72	.372	.853	63.91	.369	.854	64.09	.367
.855	64.28	.364	.856	64.47	.362	.857	64.66	.359	.858	64.85	.356	.859	65.05	.353
.860	65.24	.351	.861	65.44	.347	.862	65.63	.345	.863	65.83	.342	.864	66.03	.339
.865	66.23	.336	.866	66.44	.333	.867	66.64	.330	.868	66.85	.327	.869	67.06	.323
.870	67.27	.320	.871	67.48	.317	.872	67.69	.314	.873	67.90	.311	.874	68.12	.308
.875	68.34	.305	.876	68.55	.301	.877	68.78	.296	.878	69.00	.295	.879	69.22	.292
.880	69.45	.289	.881	69.68	.286	.882	69.91	.283	.883	70.14	.280	.884	70.37	.277
.885	70.61	.274	.886	70.85	.271	.887	71.09	.268	.888	71.33	.266	.889	71.58	.263
.890	71.82	.260	.891	72.07	.258	.892	72.32	.255	.893	72.58	.253	.894	72.83	.250
.895	73.09	.249	.896	73.36	.246	.897	73.62	.243	.898	73.89	.241	.899	74.16	.239
.900	74.44	.237	.901	74.72	.235	.902	74.99	.233	.903	75.27	.231	.904	75.55	.229
.905	75.83	.227	.906	76.12	.225	.907	76.42	.224	.908	76.71	.222	.909	77.01	.220

C.2b (contd)

.910	77.32	.219	.911	77.52	.217	.912	77.93	.216	.913	78.25	.214	.914	78.57	.213
.915	78.89	.211	.916	79.20	.210	.917	79.55	.208	.918	79.88	.207	.919	80.22	.206
.920	80.56	.204	.921	80.91	.203	.922	81.26	.202	.923	81.62	.200	.924	81.98	.199
.925	82.35	.198	.926	82.72	.196	.927	83.10	.195	.928	83.49	.194	.929	83.88	.192
.930	84.27	.191	.931	84.69	.189	.932	85.09	.188	.933	85.50	.186	.934	85.92	.184
.935	86.35	.182	.936	86.79	.180	.937	87.23	.178	.938	87.69	.176	.939	88.15	.174
.940	88.62	.171	.941	89.09	.169	.942	89.58	.166	.943	90.08	.163	.944	90.58	.159
.945	91.10	.155	.946	91.63	.151	.947	92.17	.146	.948	92.72	.141	.949	93.28	.135

```
      C                                                          C.3
      C       PROGRAM       .CALIBRATE
      C                     ----------
      C
      C       NON-LINEAR LEAST SQUARES FITTING OF THE IODIDE METHOD
      C       CALIBRATION EQUATION:
      C
      C                         R=EXP(-2)*(EXP(Z*(1-EXP(-I*W*T))-1)
      C
      C                         WHERE R IS TRANSMISSION(Y)
      C                               Z=DILNIO(0I IS THE BACKGROUND
                                                    LEVEL
      C                               I IS THE IODIDE CONCENTRATION
                                                    (X)
      C                               W*T=H A COMPOUND FITTING
                                                    PARAMETER
      C                           AND D IS AN ESTIMATE OF THE
                                                    COLOURATION
      C
      C       P.SMITH MARCH 1975
      C
              DIMENSION IITLE(13),P(20,6),PMN(20),CO(20),PSE(20),
                                                    X(200),Y(20
             1,CSP(27),WI(27),PI(5),C1(5),S2(5),VP(5),O20(2),NPT(3)
              O2D(1)=0.
              O2D(2)=0.
              NPT(1)=4
              NPT(2)=9
              NPT(3)=14
              EPS=.00001
      C
      C      READ IN TITLE,CONC OF STANDARDS AND THERE TRANSMISSION
      C
        500   READ(5,101,END=11)(IITLE(I),I=1,13)
        101   FORMAT(3A6)
              READ(5,100)M,NR
        100   FORMAT( )
              READ(5,100)(CO(I),(P(I,J),J=1,NP),I=1,M)
              N=M*NR
              DO 20 I=1,M
              CC=CO(I)
              DO 20 J=1,NR
              K=(I-1)*NR+J
              X(K)=CC
         20   Y(K)=P(I,J)
      C
      C      EVALUATE INITIAL VALUES FOR PARAM'S Z,H AND D
      C
              YN=1,-Y(N)
              ZM=ALOG(YN)
              Z=-ZM
              MP3=(N+3)/2
              H=-ALOG(ALOG(Y(MP3)+YN)/ZM)/X(MP3)
```

C.3 (contd)

```
            D=Y(1)-EXP(ZM*EXP(-X(1)*H))+EXP(ZM)
            L=D
            SSQ=0
            DO 2 I=1,N
            YA=Y(I)-EXP(ZM*EXP(-X(I)*H))+EXP(ZM)-D
      2     SSQ=SSQ+YA*YA
      3     L=L+1
            Z1=Z
            H1=H
            D1=0
            S1=SSQ
            C=EXP(-Z)
            E1=0
            E2=0
            E3=0
            D11=0
            D12=0
            D22=0
            D13=0
            D23=0
            D33=0
            DO 4 I=1,N
            XI=X(I)
            YI=Y(I)
            A=EXP(-H*XI)
            B=EXP(-Z*A)
            F1=-Z*XI*A*B
            F2=YI-B+C-D
            F3=A*B-C
      C
      C     EVALUATE THE 1ST AND 2ND DEIVATIVES OF THE LEAST SQUARES
      C     ERROR FUNCTION WITH RESPECT TO THE PARAM'S AND PLACE IN
      C     E1,... AND D11,... RESPECTIVELY
      C
            E1=E1+F2*F1
            E2=E2+F2*F3
            E3=E3-F2
            D11=D11+F1*F1
            D12=D12+F1*F3
            D22=D22+F3*F3
            D13=D13-F1
            D23=D23-F3
      4     CONTINUE
            D33=N
      C
      C     EVALUATE THE INVERSE OF THE MATRIX OF 2ND DERIV'S
                                            (HESSIAN)
      C
            T11=D22+D33-D23*D23
             T12=D13*D23-D12*D33
             T13=D12*D23-D13*D22
             T22=D11*D33-D13*D13
             T23=D12*D13-D11*D23
```

C.3 (contd)

```
      T33=D11*D22-D12*D12
      T  =D11*T11+D12*T12+D13*T13
      U=-(E1*T11+E2*T12+E3*T13)/T
      V=-(E1*T12+E2*T22+E3*T23)/T
      W=-(E1*T13+E2*T23+E3*T33)/T
      H=H+U
      Z=Z+V
      D=D+W
      SSQ=0
      DO 5 I=1,N
      YA=Y(I)-EXP(-Z*EXP(-X(I)*H))+EXP(-Z)-D
    5 SSQ=SSQ+YA*YA
      IF(L.GE.1000)GOTO 500
      IF(ABS(Z-Z1)-EPS)6,3,3
    6 IF(ABS(H-H1)-EPS)8,3,3
    8 IF(ABS(d-D1)-EPS)9,3,3
    9 IF(ABS(SSQ-S1)-EPS)10,3,3
   10 EZ=EXP(-Z)
C
C      PLOT CALIBRATION CURVE
C
      CALL PLOTS(D.,D.,8)
      CALL PLOT(0.,-100.,-3)
      CALL PLOT(0.,5.,-3)
      CALL FACTOR(.8)
      CALL AXIS(0.,0.,21HIODIDE IN MICROGMS./L,-21,20.,0.,
                                 0.,5.)
      CALL AXIS(0.,0.,12HTRANSMISSION,12,20.,90.,0.,.05)
      XA=0.
      IP=3
   12 XB=XA*5
      YA=(EXP(-Z*EXP(-XB*H))-EZ+D)*20.
      CALL PLOT(XA,YA,IP)
      XA=XA+.1
      IP=2
      IF(XA-20.)12,12,13
   13 IP=-1
      DO 14 j=1,N
      XA=X(J)/5
      YA=Y(J)*20.
      CALL SYMBOL(XA,YA,.21,11,0.,IP)
   14 CONTINUE
      CALL SYMBOL(5.,20.,.55,IITLE,0.,18)
      CALL SYMBOL(15.,5.,.28,5HD1 = ,0.,5)
      D1Z=Z/2.303
      CALL NUMBER(999.,999.,.28,D1Z,0.,4)
      CALL SYMBOL(15.,4.,.28,5HWT = ,0.,5)
      CALL NUMBER(999.,999.,.28,H,0.,4)
      CALL SYMBOL(15.,3.,.28,5H D = ,0.,5)
      CALL NUMBER(999.,999.,.28,D,0.,4)
      CALL PLOT(25.,0.,-3)
C
C      PRODUCE LOOK-UP TABLE FOR CALIBRATIO N
```

C.3 (contd)

```
C
          WRITE(6,202)(IITLE(I),I=1,3),01Z,H,D
  202     FORMAT(1H1//1X,316//5H 01 =,F7.4,5H WT =,F7.4,5H
                                        D =,F7.4//)
          WRITE(6,201)
          WRITE(6,203)
  203     FORMAT(5(2H I,18X),2H I/5(20H I PKHT CONC  VAR),
         12H I/5(2H I,18X),2H I)
          WRITE(6,201)
           DO 30 I=1,M
           SUM=0
           SUMSQ=C
           DO 40 J=1,NR
           PP=P(I,J)
           SUM=SUM+PP
  40       SUMSQ=SUMSQ+PP*PP
           PM=SUM/NR
           SDSQ=SUMSQ-PM*PM*NR
           PMN(I)=PM
          IF(SDSQ.GT..00000001)GOTO 31
          PSE(I)=0
          GOTO 30
  31        PSE(I)=SOSO/(NR-1)
  30      CONTINUE
C
C     USE THE SPLINE ROUTINE TO ESTIMATE THE VARIANCE OF CONC
C     FROM THAT OF TRANSMISSION
C
              CALL SPLNI(M,PNN,PSE,2,020,CSP,W1)
              VPA=.149
            NPP=1
             DO 50 NP=1,16
            DO 52 LPA=1,10
             DO 51 MP=1,5
             VPA=VPA+.001
             VP(1)=VPA
             CALL SPLN2(M,PMN,PSE,CSP,VP)
             P1(MP)=VPA
             C1(MP)=-ALOG(-ALOG(VPA+EZ-D)/Z)/H
             EHZ=EXP(-C1(MP)*H)
             DYX=H*Z*EHZ(-Z*EHZ)
             S2(MP)=VP(2)/(DYX*DYX)
  51        CONTINUE
  52         WRITE(6,200)(P1(J),C1(J),S2(J),J=1,5)
            WRITE(6,201)
  201       FORMAT(1X,101(1H-))
            IF(NP.NE.NPT(NPP))GOTO 50
            WRITE(6,204)
  204       FORMAT(1H1,101(1H-))
            NPP=NPP+1
  50         CONTINUE
  200       FORMAT(5(2H I,F6.3,F6.2,F6.3),2H I)
            GOTO 500
```

C.3 (contd)

```
205*    11      CALL PLOT(40.,0.,999)
206*            STOP
207*            END

END OF COMPILATION:          NO DIAGNOSTICS.
```

APPENDIX D

EVALUATING THE FLOW VALUE AND ITS ERROR

I EXAMPLES OF COMPONENTS OF VARIATION

1. NO SIGNIFICANT VARIATION EITHER ACROSS THE STREAM OR IN TIME
   - (a) ASCOP DATA FOR NANT IAGO GAUGING NO 22
   - (b) ASCOP OUTPUT AND INTERPRETATION
2. SIGNIFICANT VARIATION IN TIME BUT NOT ACROSS THE STREAM
   - (a) ASCOP DATA FOR CYFF GAUGING NO 6
   - (b) ASCOP OUTPUT AND INTERPRETATION
3. SIGNIFICANT VARIATION BOTH IN TIME AND ACROSS THE STREAM
   - (a) ASCOP DATA FOR HORE GAUGING NO 16
   - (b) ASCOP OUTPUT AND INTERPRETATION
4. SIGNIFICANT VARIATION IN TIME BUT NOT ACROSS THE STREAM
   - (a) ASCOP DATA FOR TANLLWYTH GAUGING NO 4
   - (b) ASCOP OUTPUT AND INTERPRETATION

II EXAMPLES OF FLOW AND ERROR EVALUATIONS

1. EXAMPLE DATA SET
   - (a) HORE GAUGING NO 16
   - (b) IAGO GAUGING NO 22
   - (c) TANLLWYTH GAUGING NO 4
2. EXAMPLE OUTPUT FOR a) to c) above
3. THE PROGRAM .FLOVAR

D.I 1a

DELT,IL RIVER.IAG022
ELTOT7 RLIB70 08/26-10:50:34-(,0)

000001	000	53.30	53.43	1	1
000002	000	53.56	53.56	2	1
000003	000	53.94	53.94	3	1
000004	000	53.94	53.94	4	1
000005	000	53.56	53.43	1	2
000006	000	53.30	53.30	2	2
000007	000	53.18	53.18	3	2
000008	000	53.18	53.18	4	2
000009	000	56.63	56.63	1	3
000010	000	52.80	52.80	2	3
000011	000	53.05	53.30	3	3
000012	000	53.30	53.43	4	3
000013	000	53.94	53.94	1	4
000014	000	53.94	53.94	2	4
000015	000	53.68	53.68	3	4
000016	000	53.68	53.68	4	4
000017	000	52.93	52.93	1	5
000018	000	52.80	53.18	2	5
000019	000	53.18	53.18	3	5
000020	000	53.43	53.56	4	5
000021	000	53.94	53.20	1	6
000022	000	54.59	54.59	2	6
000023	000	54.86	54.72	3	6
000024	000	54.46	54.59	4	6
000025	000	53.43	53.43	1	7
000026	000	53.30	53.18	2	7
000027	000	53.18	53.05	3	7
000028	000	53.18	53.18	4	7
000029	000	51.58	52.80	1	8
000030	000	53.43	53.43	2	8
000031	000	53.30	53.18	3	8
000032	000	53.94	53.94	4	8
000033	000	51.58	52.80	1	9
000034	000	53.43	53.43	2	9
000035	000	53.30	53.18	3	9
000036	000	53.94	53.94	4	9

END ELT.

TITLE APPENDIX EXAMPLE OF COMPONENTS OF VARIATION 1

DATA MATRIX SAMPLES THERE ARE 3 MAIN VARIABLES 36 POINTS AND 36 POINTS WITH NO MISSING VALUES

SUMMARY INCLUDING ALL POSSIBLE OBSERVATIONS

NO	NAME	REPS	POINTS	OBS	MINIMUM	MEAN	MAXIMUM	STD. DEV.	VARIANCE
1	CONC	2	36	72	.515800+002	.535501+002	.566300+002	.789158+000	.622771+000
2	ACROSS	1	36	36	.100000+001	.250000+001	.400000+001	.113389+001	.128571+000
3	TIME	11	36	36	.100000+001	.500000+001	.900000+001	.261861+001	.685714+000

CORRELATION MATRIX FOR DATA MATRIX SAMPLES

	CONC	ACROSS	TIME
CONC	1.000000	.078976	-.184202
ACROSS	.078976	1.000000	.000000
TIME	-.184202	.000000	1.000000

** LEVELS ACROSS 1 2 3 4 TIME 1 2 3 4 5 6 7 8 9
** ANOVA OF CONC DESIGN ACROSS*TIME

FACTORIAL ANALYSIS OF VARIANCE FOR VARIABLE CONC

SOURCE OF VARIATION	SUMS OF SQUARES	D F	MEAN SQUARES	F RATIO	PROB
ACROSS (1+)	.519582+000	3	.173194+000	3.20	.0347
TIME (1+)	.122097+002	8	.152621+001	28.21	.0000
ACROSS (1+)*TIME (1+)	.278883+002	24	.116201+001	21.48	.0000
RESIDUAL - REPLICATES	.194775+001	36	.541042-001		
TOTAL	.425653+002	71			

INSTEAD OF USING THE SUMS OF SQUARES GIVEN BY THE REPLICATION AS THE RESIDUAL WE SHALL USE THE ACROSS x TIME INTERACTION SUMS OF SQUARES, SINCE THE VARIATION OF THE REPLICATES IS REQUIRED TO BE TESTED FOR SIGNIFICANCE. THUS THE ANOVA TABLE BECOMES:

SOURCE	MEAN SQUARES	F RATIO	DEGRESS OF FREEDOM	SIGNIFICANCE
ACROSS	.1732	.1491	(3,24)	None
TIME	1.5262	1.3134	(6,24)	None
REPLICATE	.0541	.0466	(40,24)	None
ACROSS x TIME RESIDUAL	1.1620			

THERE IS NO SIGNIFICANT VARIATION IN ANY OF THE SOURCES OF VARIATION THUS THE MEAN AND THE VARIANCE ON THE PREVIOUS PAGE DI1b CAN BE USED AS THE MEAN SAMPLE CONCENTRATION AND SAMPLE VARIANCE.

```
DELT,IL  RIVER.CYFF06
ELTOT7 RL1B70 08/25-19:49:52-(,0)
000001        000    37.21   37.21   1   1
000002        000    36.80   36.80   2   1
000003        000    37.21   37.21   3   1
000004        000    37.21   37.21   4   1
000005        000    37.21   37.38   1   2
000006        000    37.38   37.38   2   2
000007        000    37.05   37.13   3   2
000008        000    36.88   36.88   4   2
000009        000    37.38   37.38   1   3
000010        000    37.13   37.90   2   3
000011        000    36.96   37.05   3   3
000012        000    37.38   37.21   4   3
000013        000    37.13   37.05   1   4
000014        000    37.63   37.30   2   4
000015        000    37.55   37.47   3   4
000016        000    37.30   37.38   4   4
000017        000    38.06   38.14   1   5
000018        000    38.23   38.23   2   5
000019        000    40.43   40.70   3   5
000020        000    37.13   37.30   4   5
000021        000    37.05   37.13   1   6
000022        000    37.05   37.05   2   6
000023        000    37.63   37.30   3   6
000024        000    37.38   37.38   4   6
000025        000    37.30   37.21   1   7
000026        000    36.39   37.13   2   7
000027        000    37.38   37.38   3   7
000028        000    37.30   37.13   4   7
000029        000    37.38   37.63   1   8
000030        000    37.68   37.63   2   8
000031        000    37.89   37.80   3   8
000032        000    37.88   38.06   4   8
000033        000    38.23   38.23   1   9
000034        000    38.23   38.23   2   9
000035        000    37.89   38.23   3   9
000036        000    37.72   37.80   4   9
000037        000    38.49   38.49   1  10
000038        000    38.14   38.23   2  10
000039        000    38.23   38.23   3  10
000040        000    38.57   38.49   4  10
000041        000    38.83   39.10   1  11
000042        000    39.10   39.18   2  11
000043        000    39.45   39.71   3  11
000044        000    39.01   38.92   4  11

END ELT.
```

TITLE APPENDIX EXAMPLE OF COMPONENTS OF VARIATION 2 D.I 2b

DATA MATRIX SAMPLES THERE ARE 3 MAIN VARIABLES 44 POINTS AND 44 POINTS WITH NO MISSING VALUES

SUMMARY INCLUDING ALL POSSIBLE OBSERVATIONS

NO	NAME	REPS	POINTS	OBS	MINIMUM	MEAN	MAXIMUM	STD. DEV.	VARIANCE
1	CONC	2	44	88	.363900+002	.377420+002	.407000+002	.814052+000	.662680+000
2	ACROSS	1	44	44	.100000+001	.250000+001	.400000+001	.113096+001	.127907+000
3	TIME	1	44	44	.100000+001	.600000+001	.110000+002	.319884+001	.102326+000

CORRELATION MATRIX FOR DATA MATRIX SAMPLES

	CONC	ACROSS	TIME
CONC	1.000000	.013912	.618407
ACROSS	.013912	1.000000	.000000
TIME	.618407	.000000	1.000000

** LEVELS ACROSS 1 2 3 4 TIME 1 2 3 4 5 6 7 8 9 10 11
** ANOVA OF CONC DESIGN ACROSS*TIME

FACTORIAL ANALYSIS OF VARIANCE FOR VARIABLE CONC

D.I 2b (contd)

SOURCE OF VARIATION	SUMS OF SQUARES	D F	MEAN SQUARES	F RATIO	PROB
ACROSS (1+)	.193773+001	3	.645911+000	30.75	.0000
TIME (1+)	.385307+002	10	.385307+001	183.44	.0000
ACROSS (1+)*TIME (1+)	.133098+002	30	.443660+000	21.12	.0000
RESIDUAL - REPLICATES	.924200+000	44	.210045-001		
TOTAL	.547024+002	87			

CONVERTING THE ANOVA TABLE ABOVE SO THAT ACROSS x TIME BECOMES THE RESIDUAL VARIATION:

SOURCE	MEAN SQUARES	F RATIO	DEGRESS OF FREEDOM	SIGNIFICANCE
ACROSS	.6459	1.4559	(3,30)	None
TIME	3.8531	8.6847	(10,30)	***(sig .1% level)
REPLICATE	.0210	0.0473	(40,30)	None
ACROSSxTIME RESIDUAL	.4437			

THERE IS SIGNIFICANT VARIATION IN THE TIME DIRECTION AT THE .1% LEVEL

D.I 3a

DELT,IL RIVER.HORE16
ELT017 RL1570 08/26-19:52:21-(,0)

000001	000	49.77	50.22	1	1
000002	000	52.35	52.47	2	1
000003	000	54.23	53.88	3	1
000004	000	56.22	56.78	4	1
000005	000	51.51	51.87	1	2
000006	000	54.36	54.36	2	2
000007	000	56.64	56.50	3	2
000008	000	58.94	59.09	4	2
000009	000	51.39	51.51	1	3
000010	000	53.09	53.09	2	3
000011	000	55.63	55,85	3	3
000012	000	58.35	58.20	4	3
000013	000	51.75	51.87	1	4
000014	000	54.75	55.28	2	4
000015	000	56.92	57.06	3	4
000016	000	53.98	53.09	4	4
000017	000	52.47	52.35	1	5
000018	000	54.10	53.85	2	5
000019	000	56.09	56.09	3	5
000020	000	58.35	58.49	4	5
000021	000	54.49	54.36	1	6
000022	000	53.22	54.23	2	6
000023	000	56.50	56.22	3	6
000024	000	57.91	57.77	4	6
000025	000	52.72	52.72	1	7
000026	000	54.23	54.52	2	7
000027	000	56.36	56.36	3	7
000028	000	58.94	58.94	4	7
000029	000	53.09	53.22	1	8
000030	000	55.01	54.88	2	8
000031	000	56.92	56.92	3	8
000032	000	58.94	58.64	4	8

END ELT.

TITLE APPENDIX EXAMPLE OF COMPONENTS OF VARIATION 3 D.I 3b

DATA MATRIX SAMPLES THERE ARE 3 MAIN VARIABLES 32 POINTS AND 32 POINTS WITH NO MISSING VALUES

SUMMARY INCLUDING ALL POSSIBLE OBSERVATIONS

NO	NAME	REPS	POINTS	OBS	MINIMUM	MEAN	MAXIMUM	STD. DEV.	VARIANCE
1	CONC	2	32	64	.497700+002	.550039+002	.590900+002	.244383+001	.597230+001
2	ACROSS	1	32	32	.100000+001	.250000+001	.400000+001	.113592+001	.129032+001
3	TIME	1	32	32	.100000+001	.450000+001	.800000+001	.232795+001	.541935+001

CORRELATION MATRIX FOR DATA MATRIX SAMPLES

	CONC	ACROSS	TIME
CONC	1.000000	.860362	.267203
ACROSS	.860362	1.000000	.000000
TIME	.267203	.000000	1.000000

** LEVELS ACROSS 1 2 3 4 TIME 1 2 3 4 5 6 7 8
** ANOVA OF CONC DESIGN ACROSS*TIME

FACTORIAL ANALYSIS OF VARIANCE FOR VARIABLE CONC

D.I 3b (contd)

SOURCE OF VARIATION	SUMS OF SQUARES	D F	MEAN SQUARES	F RATIO	PROB
ACROSS (1+)	.275833+003	3	.919443+002	1686.62	.0000
TIME (1+)	.436242+002	7	.623203+001	114.32	.0000
ACROSS (1+)*TIME (1+)	.515470+002	21	.245986+001	45.12	.0000
RESIDUAL - REPLICATES	.174445+001	32	.545141-001		
TOTAL	.372859+003	63			

CONVERTING THE ANOVA TABLE ABOVE SO THAT ACROSSxTIME BECOMES THE RESIDUAL VARIATION:

SOURCE	MEAN SQUARES	F RATIO	DEGREES OF FREEDOM	SIGNIFICANCE
ACROSS	91.9443	37.3773	(3,21)	***(sig .1% level)
TIME	6.2320	2.5335	(7,21)	* (sig 5% level)
REPLICATE	.0545	.0222	(32,21)	None
ACROSSxTIME RESIDUAL	2.4599			

THERE IS SIGNIFICANT VARIATION IN BOTH TIME AND ACROSS THE STREAM AT THE 5% LEVEL.

D.I 4a

```
DELT,IL  RIVER.TANLE4
ELT077 RLIB70 08/26-19;51:21-(,0)
000001      000   44.65  44.65  1  1
000002      000   44.45  44.35  2  1
000003      000   43.27  43.86  3  1
000004      000   43.86  44.45  4  1
000005      000   44.65  44.75  1  2
000006      000   44.65  43.47  2  2
000007      000   44.85  44.85  3  2
000008      000   44.65  44.45  4  2
000009      000   44.35  44.45  1  3
000010      000   43.86  43.86  2  3
000011      000   43.47  44.55  3  3
000012      000   43.66  43.86  4  3
000013      000   43.56  43.56  1  4
000014      000   44.26  44.35  2  4
000015      000   44.35  44.65  3  4
000016      000   44.45  44.25  4  4
000017      000   44.65  44.65  1  5
000018      000   44.35  44.55  2  5
000019      000   43.86  44.15  3  5
000020      000   43.86  43.86  4  5
000021      000   45.05  45.05  1  6
000022      000   45.56  45.05  2  6
000023      000   45.15  45.67  3  6
000024      000   45.35  45.36  4  6
000025      000   43.47  43.08  1  7
000026      000   43.08  43.66  2  7
000027      000   43.66  43.18  3  7
000028      000   44.05  43.66  4  7
000029      000   43.66  44.25  1  8
000030      000   44.85  44.85  2  8
000031      000   44.75  44.65  3  8
000032      000   44.95  44.65  4  8
000033      000   44.55  45.46  1  9
000034      000   44.45  44.35  2  9
000035      000   44.65  45.15  3  9
000036      000   44.35  44.15  4  9
000037      000   44.85  44.65  1 10
000038      000   45.98  44.55  2 10
000039      000   44.85  44.85  3 10
000040      000   45.05  45.05  4 10

END ELT.
```

D.I 4b

TITLE APPENDIX EXAMPLE OF COMPONENTS OF VARIATION 4

DATA MATRIX SAMPLES THERE ARE 3 MAIN VARIABLES 40 POINTS AND 40 POINTS WITH NO MISSING VALUES

SUMMARY INCLUDING ALL POSSIBLE OBSERVATIONS

NO	NAME	REPS	POINTS	OBS	MINIMUM	MEAN	MAXIMUM	STD. DEV.	VARIANCE
1	CONC	2	40	80	.430800+002	.444114+002	.459800+002	.661525+000	.437616+000
2	ACROSS	1	40	40	.100000+001	.250000+001	.400000+001	.113228+001	.128205+001
3	TIME	1	40	40	.100000+001	.550000+001	.100000+002	.290887+001	.846154+001

CORRELATION MATRIX FOR DATA MATRIX SAMPLES

	CONC	ACROSS	TIME
CONC	1.000000	-.001280	.293108
ACROSS	-.001280	1.000000	.000000
TIME	.293108	.000000	1.000000

** LEVELS ACROSS 1 2 3 4 TIME 1 2 3 4 5 6 7 8 9 10
** ANOVA OF CONC DESIGN ACROSS*TIME

FACTORIAL ANALYSIS OF VARIANCE FOR VARIABLE CONC

D.I 4b (contd)

SOURCE OF VARIATION	SUMS OF SQUARES	D F	MEAN SQUARES	F RATIO	PROB
ACROSS (1+)	.120137-001	3	.400458-002	.04	.9904
TIME (1+)	.186891+002	9	.207657+001	19.11	.0000
ACROSS (1+)*TIME (1+)	.708112+001	27	.262264+000	2.41	.0056
RESIDUAL - REPLICATES	.434585+001	40	.108646+000		
---------	------------	---			
TOTAL	.301281+002	79			

CONVERTING THE ANOVA TABLE ABOVE SO THAT ACROSSxTIME BECOMES THE RESIDUAL VARIATION:

SOURCE	MEAN SQUARES	F RATIO	DEGREES OF FREEDOM	SIGNIFICANCE
ACROSS	.0040	.0153	(3,27)	None
TIME	2.0766	7.918	(9,27)	***(sig.1%level)
REPLICATE	.2623	.414	(40,27)	None
ACROSSxTIME RESIDUAL				

THERE IS A SIGNIFICANT VARIATION IN TIME AT THE 1% LEVEL

D.II 1

(a)

```
DELT,IL RIVER.FLO16
ELTOT7 RLIB70 08/26-19:52:13-(,0)
000001       000            HORE GAUGING NO 16  210375
000002       000   1.0103,-2,2.55,-10
000003       000   33.33,2,4.,0
000004       000   52.93,.448
000005       000   55.004,2.414,1.

END ELT.
```

(b)

```
DELT,IL RIVER.FLO22
ELTOT7 RLIB70 08/26-19:52:14-(,0)
000001       000            IAGO GAUGING NO 22 240375
000002       000   I.0321,-2,3.8675,-10
000003       000   33.33,2,4.,0
000004       000   44.09,.299
000005       000   53.476,.579,1.

END ELT.
```

(c)

```
DELT,IL RIVER.FLO4
ELTOT7 RLIB70 08/26-19:52:12-(,0)
000001       000            TANLLWYTH GAUGING NO 4  230175
000002       000   1.061,-2,8.5195,-11
000003       000   4.,4,4.,0
000004       000   34.71,.0282
000005       000   44.409,.366,2.

END ELT.
```

TANLLWYTH GAUGING NO 4 230175 D.II 2

INJT RATE	.1061-01L/S	VAR INJT RATE	.8519-10L/S	(c)
DILTN FACT	.4000+05	VAR DILTN FACT	.4000+01	
INJT CONC	.3471+02 10-6G/L	VAR INJT CONC	.2820-01 10-6G/L	
STREAM CONC	.8882+02 10-6G/L	VAR STREAM CONC	.1464+01 10-6G/L	

FLOW .1659+83L/S 95% CONF INT .4804+01L/S

IAGO GAUGING NO 22 240375

INJT RATE	.1032-01L/S	VAR INJT RATE	.3857-09L/S	(b)
DILTN FACT	.3333+04	VAR DILTN FACT	.4000+01	
INJT CONC	.4409+02 10-6G/L	VAR INJT CONC	.2990+00 10-6G/L	
STREAM CONC	.5348+12 10-6G/L	VAR STREAM CONC	.5790+00 10-6G/L	

FLOW .2836+02L/S 95% CONF INT .1077+01L/S

HORE GAUGING NO 16 210375

INJT RATE	.1010-01L/S	VAR INJT RATE	.2550-09L/S	(a)
DILTN FACT	.3333+04	VAR DILTN FACT	.4000+01	
INJT CONC	.5293+02 10-6G/L	VAR INJT CONC	.4480+00 10-6G/L	
STREAM CONC	.5500+02 10-6G/L	VAR STREAM CONC	.2414+01 10-6G/L	

FLOW .3240+02L/S 95% CONF INT .2009+01L/S

```
C
C      PROGRAM        .FLOVAR
C                     -------
C
C      EVALUATE THE FLOW VALUE AND ITS VARIANCE
C
C      P.SMITH MARCH 1975
C
       DIMENSION TITLE(13)
C      READ IN TITLE
 1     READ(5,200,END=2)(TITLE(J),J=1,13)
 200   FORMAT(12A6)
       WRITE(6,300)(TITLE(J),J=1,12)
 300   FORMAT(////10X,12A6//)
C
C      READ IN INJECTION AND VARIANCE OF INJECTION
C
C
         READ(5,100,END=2)01,IEQ1,VARQ1,IVARQ1
 100     FORMAT()
         Q1=Q1*(10.**IEQI)
         VARQ1=VARQ1*(10.**IVARQ1)
        WRITE(6,500)Q1,VARQ1
 500    FORMAT(10X,'INJT RATE  ',E15.4,'L/S',6X,'VAR INJT
                            RATE  ',
      1E1S.4,'L/S'/)
C
C     READ IN DILUTION FACTOR AND VARIANCE
C
         READ(5,100)D,IED,VARD,IEVARD
         D=0*(60.**IED)
         VARD=VARD*(10.**IEVARD)
        WRITE(6,501)D,VARD
 501    FORMAT(10X,'DILTN FACT ',E15.4,9X,'VAR DILTN FACT ',
                            E15.4/)
C
C     READ IN INJT CONC AND VARIANCE OF INJT CONC
C
        READ(5,100)C1,VAR01
       WRITE(6,502)C1,VAR01
 502   FORMAT(10X,'INJT CONC ',E15.4,' 10-66/L ','VAR INJT
                            CONC  '
     1,E15.4,' 10-6G/L'/)
C
C    READ IN STREAM SAMPLE CONC AND VARIANCE
C
        READ(5,100)C2,VARC2,D1
      C2=C2*01
        VARC2=VARC2*D1*D1
       WRITE(6,504)C2,VARC2
 504   FORMAT(10X,'STREAM CONC',E15.4,' 10-6G/L '.
     1'VAR STREAM CONC',E15.4,' 10-66/L'//)
```

D.II 3 (contd)

```
              Q=(Q1*C1*D)/C2
              A1=Q/Q1
              A2=Q/Q1
              A3=Q/D
              A4=Q/Q2
              VARQ=A1*A1*VARQ1+A2*A2*VARC1+A3*A3*VARD+A4*A4*VARC2
             OI=SORT(VARQ)*2
      C
      C     WRITE OUT FLOW AND ITS CONFIDENCE INTERVAL
      C
              WRITE(6,101)Q,CI
       101    FORMAT(10X,'FLOW ',E15.4,'L/S'.5X,'95% CONF INT ',
                                        E15.4,'L/S
              GOTO
        2     STOP
              END

END OF COMPILATION:            NO DIAGNOSTICS.
```

APPENDIX E

ESTIMATING PARAMETERS OF A NON-LINEAR MODEL USING A LEAST SQUARES METHOD

Let the model to be fitted to the data be

$$y = f(x;\beta_1, \beta_2, \ldots, \beta_p) \qquad \ldots. \text{(E.1)}$$

where f is non-linear in the β's. Let $\underline{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)'$, (E.1) becomes

$$y = f(x, \underline{\beta}) \qquad \ldots. \text{(E.2)}$$

If there are n observations of the form (x_i, y_i) for i = 1, ..., n, (E.2) can be written

$$y_i = f(x_i, \underline{\beta}) + \varepsilon_i$$

where ε_i is the i^{th} error, i = 1,2, ..., n. Making the usual assumptions of normality and indpendence of the errors $\underline{\varepsilon} \sim N(\underline{O}, I\,\sigma^2)$ where $\underline{\varepsilon} = (\varepsilon_1, \varepsilon_2, \ldots \varepsilon_n)'$, $\underline{O}$ is the null vector and I is a unit matrix both of the correct dimensions.

The error sum of squares is defined for the non-linear model and the given data as

$$S(\underline{\beta}) = \sum_{i=1}^{n} \{y_i - f(x_i, \underline{\beta})\}^2. \qquad \ldots. \text{(E.3)}$$

$\hat{\underline{\beta}}$ denotes a least squares estimate of $\underline{\beta}$ (i.e. that value of $\underline{\beta}$ which minimizes $S(\underline{\beta})$). To find $\hat{\underline{\beta}}$ differentiate (3) with respect to $\underline{\beta}$ to give the p normal equations

$$\frac{\partial S}{\partial \beta_r} = \sum_{i=1}^{n} \{y_i - f(x_i, \hat{\underline{\beta}})\} \left[\frac{\partial f(x_i, \underline{\beta})}{\partial \beta_r}\right]_{\underline{\beta}=\hat{\underline{\beta}}} = 0, \qquad \text{(E.4)}$$

for r = 1, ..., p, which can be solved for $\hat{\underline{\beta}}$. When $f(x_i, \underline{\beta})$ is linear its derivative with respect to β_r is a function of x_i only and (E.4) can be solved as a set of p linear equations (linear regression). However, when f is non-linear (E.4) is a set of non-linear equations which require another method of solution such as the following.

Let $G(\beta_1) = \dfrac{\partial S}{\partial \beta_r}$, r=1,..., p, in (E.4), given an estimate $\hat{\underline{\beta}}$ of $\underline{\beta}$ then

$$G(\hat{\underline{\beta}} + (\underline{\beta} - \hat{\underline{\beta}})) = G(\hat{\underline{\beta}} + \delta\beta)$$

can be expanded, neglecting 2nd and higher order terms, as a Taylor series to give,

$$G(\hat{\underline{\beta}}) + \delta\underline{\beta} \left[\frac{\partial G(\beta)}{\partial \beta_r}\right]_{\beta=\hat{\underline{\beta}}} = \underline{0}. \qquad \ldots \qquad (E.5)$$

since $G(\underline{\beta} + \delta\underline{\beta}) = \underline{0}$ at the optimum value of $\underline{\beta}$.

Thus letting $A = \left[\dfrac{\partial G(\beta)}{\partial \beta_r}\right]_{\underline{\beta}=\hat{\underline{\beta}}} = \dfrac{\partial^2 S}{\partial \beta_r \, \partial \beta_s}\Bigg|_{\underline{\beta}=\hat{\underline{\beta}}}$

for r = 1, ..., p and s = 1, ..., p, where A is pxp Hessian matrix,

(E.5) becomes

$$\delta\underline{\beta} = A^{-1}. \left[-\frac{\partial S}{\partial \beta_r}\right]_{\underline{\beta}=\hat{\underline{\beta}}} \quad , r = 1, \ldots, p$$

$$\begin{bmatrix} \delta\beta_1 \\ \delta\beta_2 \\ \cdot \\ \cdot \\ \cdot \\ \delta\beta_p \end{bmatrix} = \begin{bmatrix} \partial^2 S/\partial\beta_1^2 & \partial^2 S/\beta_1\partial\beta_2 & \ldots & \partial^2 S/\partial\beta_1\partial\beta_p \\ \partial^2 S/\partial\beta_1\partial\beta_2 & \partial^2 S/\partial\beta_2^2 & \ldots & \partial^2 S/\partial\beta_2\partial\beta_p \\ \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot \\ \cdot & & \cdot & \\ \partial^2 S/\partial\beta_1\partial\beta_p & \partial^2 S/\partial\beta_2\partial\beta_p & & \partial^2 S/\partial\beta_p^2 \end{bmatrix}^{-1}_{\underline{\beta}=\hat{\underline{\beta}}} . \begin{bmatrix} -\partial S/\partial\beta_1 \\ -\partial S/\partial\beta_2 \\ \cdot \\ \cdot \\ \cdot \\ \partial S/\partial\beta_p \end{bmatrix}_{\underline{\beta}=\hat{\underline{\beta}}} \qquad (E.6)$$

Therefore given an initial approximation to $\hat{\underline{\beta}}$, $\hat{\underline{\beta}}^o$ and evaluating $\delta\underline{\beta}$ using (E.6) ie $\underline{\delta\beta}_{\beta=\hat{\beta}^o} = \underline{\delta\hat{\beta}}^o$ and defining $\hat{\underline{\beta}}^1 = \hat{\underline{\beta}}^o + \delta\hat{\underline{\beta}}^o$ we can obtain a better approximation to $\hat{\underline{\beta}}$. Thus for $j = 0, 1, \ldots, \lambda$ the iterative scheme:

$$\hat{\underline{\beta}}^{j+1} = \hat{\beta}^{j} + \delta\hat{\underline{\beta}}^{j} \qquad \ldots. \text{ (E.7)}$$

converges to $\hat{\beta}$, provided $\hat{\underline{\beta}}^{o}$ is in some sense close to $\hat{\underline{\beta}}$. The value of λ is determined by the stopping criterion: given a δ there exists a λ such that both

$$|\hat{\beta}_r^{\lambda} - \hat{\beta}_r^{\lambda^{-1}}| < \delta \text{ and } |S(\hat{\beta}_r^{\lambda}) - S(\hat{\beta}^{\lambda^{-1}})| < \delta,$$

for $r = 1, \ldots, p$.

APPENDIX F

GRAPH PLOTTING SPOOLING SYSTEM (level 4.0)

Since the original design and testing of the programs presented here, a spooling system has been implemented on the Univac computer at IH. This system has greatly simplified the procedure for running graph plotting jobs and should be used for small plotting jobs like .MARIOTTE, .INJECT and .CALIBRATE. The following typical runstream replaced that presented in the text (4.).

```
@RUN runid, accid, GAUGE

@ASG,AX RIVER

@PLDIR

15, 5, BIRO,BLACK        (5 copies on 15" paper drawn with a
CALIBRATION CURVE         black biro)
@XQT RIVER.CALIBRATE
(data set)
@FIN
```

Similarly for .INJECT and .MARIOTTE.

For further details, refer to the Computer Section's user note 16/77.