LA-8957-MS

UC-15 and UC-32
Issued: August 1981

A User's Guide to the Hydrogen Monitor

M. M. Meier*
E. L. Adams

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of 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. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

*National Bureau of Standards, Washington, DC 20234.

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

A USER'S GUIDE TO THE HYDROGEN MONITOR

by

M. M. Meier and E. L. Adams

ABSTRACT

A protocol for calibration of the hydrogen monitor and for its use as an assay instrument is presented. A statistical analysis for the system, including effects of deadtime and pile-up loss, is developed, and the software that supports the system is described.

I. INTRODUCTION

The software developed and the procedures to be used for calibration and running of the ^{252}Cf hydrogen monitor (HM) are documented in this guide. Computer software was developed for use with the Digital Equipment Corporation (DEC) LSI-11 using the Version 3 operating system. Potential users are also referred to Refs. 1 and 2, which describe the ^{252}Cf -based HM.

II. EXPERIMENTAL

Design details of the HM are given in Ref. 1. Figure 1 shows the electronics block diagram used in the assay of High-Temperature Gas-cooled Reactor (HTGR) "green" rods, December 1979. The data were accumulated in a multi-channel analyzer (MCA) for constant live time. The spectrum of Fig. 2 is

Fig. 1.
Hydrogen monitor electronics.

Fig. 2.
Typical pulse-height spectrum from the hydrogen monitor. The data of interest are the integrated regions N, B1, P, and B2, as discussed in the text.

representative for a live time of 800 s. Summations for the spectrum intervals indicated were printed out for each run. They represent, respectively, events in the thermal peak, N ; low pulse height background for the pulser peak, $B1$; pulser peak plus background, P ; and high pulse height background for the pulser peak, $B2$. Intervals for pulser peak and background are selected so that net pulser peak area, P_0 , equals $P - (B1 + B2)$. The four indicated sums were printed out at the end of each run and comprised the raw data.

III. REDUCTION OF DATA TO RELATIVE RESPONSES

Relative responses, defined as the ratio of the true counts in the thermal peak for an unknown or standard sample to counts for an empty chamber ("background"), were the necessary data for calibration and use of the HM.

The thermal peak is used as a reference amplitude for the gain stabilization circuitry indicated in Fig. 1. Thus, when bias voltage drifts occur, the thermal peak amplitude remains constant, but the pulser peak may exhibit some drift. For this reason, as well as the inherent decay of the ^{252}Cf , the background for each sample is a function of time. Therefore, for a series of runs that include several background runs, and for which pulser peak drift is not so large as to necessitate changing the $B1$, $B2$, and P windows, the backgrounds are fit to a linear function of time.

The procedure followed was to treat the first background run as a reference for normalization. The reduced pulser peak, P_0 , for each background run was calculated and the ratio of each to the first was determined. Then the true rate for the i th background run was proportional to

$$N_0(i) = N(i)/[P_0(i)/P_0(1)] \quad . \quad (1)$$

The relative uncertainty is

$$\left[\frac{\Delta N_0(i)}{N_0(i)} \right]^2 = \left[\frac{\Delta N(i)}{N(i)} \right]^2 + \left[\frac{\Delta P_0(i)}{P_0(i)} \right]^2 + \left[\frac{\Delta P_0(1)}{P_0(1)} \right]^2 \quad (2)$$

and

$$[\Delta P_0(i)]^2 = [\Delta P(i)]^2 + [\Delta B1(i)]^2 + [\Delta B2(i)]^2 , \quad (3)$$

with

$$\Delta B1(i) = \sqrt{B1(i)} ,$$

and

$$\Delta B2(i) = \sqrt{B2(i)} ,$$

as usual, but the statistical uncertainty in $P(i)$ is only dependent on the number of lost counts that would have appeared in the peak. For example, consider the loss rate determination as an experiment in which a random source is counted only when the periodic pulse is present. The number of events counted in such an experiment is exactly the lost number in ours, and it is this quantity on which the statistical uncertainty depends. Therefore, even though only relative loss rates enter the calculation of relative response, knowledge of absolute loss rate is needed for calculation of the uncertainty.*

Each run was assigned a sequential identification number that was approximately proportional to time after the first run. This identification number was used as the time parameter for the linear least squares fit of the response to a straight line.

The program LSQMK1 was used for the fitting procedure. This program requires input responses, uncertainties, and time parameters on the DEC default file device (DK:), which can be conveniently created using the DEC-supplied editor, TECO.** The output of LSQMK1 are best values for the parameters A1 and A2 of the background parameterization

$$BK(T) = A1 + A2 \cdot T , \quad (4)$$

*We determined the absolute loss rate by measuring the pulser rate on an oscilloscope as $(1040 \pm 40 \mu s)^{-1} = 960$ cts/s. The total number of counts in 800 "live" seconds (890 true seconds) was then 850 000. Observed pulser counts were 625 000 and total loss was 225 000 counts. Therefore $\Delta P = 470$; $\Delta P_0/P_0 = 0.08$ per cent.

**As an aid in preparing the input file and interpreting the results, the introductory commentary for LSQMK1 and a typical output page are reproduced and annotated in Appendix A.

the estimate of the three-parameter variance-covariance matrix that describes the uncertainty in the background,

$$\begin{bmatrix} A_3 & A_4 \\ A_4 & A_5 \end{bmatrix},$$

where

$$[\Delta BK(T)]^2 = A_3 + 2A_4 T + A_5 T^2, \quad (5)$$

and $\chi^2/\text{degree of freedom}$ (χ^2/deg). For $\chi^2/\text{deg} \approx 1.0$, the fit is considered reasonable. When χ^2/deg exceeds 1.0 significantly, it is reasonable to multiply the variance-covariance matrix by χ^2/deg to obtain a more realistic estimate of $\Delta BK(T)$. A preferable course of action, of course, is to find and eliminate the systematic error that is responsible for the effect. If the assumption of linearity of the function is not valid, though, the former course of action may be the only one practical.

The relative response, $R(T)$, for a sample with run identification T (time = T) is then

$$R(T) = [N(T)/BK(T)] [P_0(1)/P_0(T)], \quad (6)$$

$$\begin{aligned} [\Delta P(T)/R(T)]^2 &= 1/N(T) + [\Delta BK(T)/BK(T)]^2 + [\Delta P_0(T)/P_0(T)]^2 \\ &+ [\Delta P_0(1)/P_0(1)]^2. \end{aligned} \quad (7)$$

As before,

$$[\Delta P_0(T)]^2 = b_1(T) + b_2(T) + N_{\text{Lost}}, \quad (8)$$

where N_{Lost} is the number of lost pulser pulses.

A program, "H Monitor Response," has been written and recorded on magnetic card for calculation of response and uncertainty from the linear background

function BK(T) using the HP-67 calculator. This program assumes that an LSQMK1 fit for BK(T) has already been done and that the parameter estimates $A_1 \dots A_5$ are available. This program is described in Appendix B.

When drifts occurred such that the pulser peak and background windows needed to be changed, the run sequence was restarted with a new background and reference run. Confidence in the technique was bolstered by reproducing responses within more than one sequence.

IV. RELATIVE MEASUREMENT FORMALISM

In the region of interest, the response of the hydrogen monitor can be represented by the expression

$$R = \sum_{i=1}^n A_i X_i \quad , \quad (9)$$

where $X_1 = 1.0$ and the remaining X_i 's are the contents of a sample, including hydrogen, which perturb the response. The calibration problem lies in deciding which sample characteristics (X_i) produce the largest perturbations, fabricating standards with these characteristics accurately known, and determining the A_i s by accurate measurement of the standards responses and least squares fitting of them. In principle, the instrument can then be used to measure hydrogen in unknowns through the relation

$$H^U = (R^U - \sum_{\substack{i=1 \\ i \neq H}}^N A_i X_i^U) / A_H \quad , \quad (10)$$

as long as the perturbing constituents X_i^U are closely enough matched to the constituents of the standards that their respective effects on the response are approximated by the assumed linear relationship. The uncertainty in the result of such an assay is

$$\begin{aligned}
\sigma(H^U)^2 = & A_H^{-2} \left[\sigma(R^U)^2 + \sum_{i \neq H} A_i^2 \sigma(X_i^U)^2 \right. \\
& + \sum_{i \neq H} \sum_{j \neq H} X_i^U X_j^U \text{cov}(A_i, A_j) \\
& + 2H^U \sum_{i \neq H} X_i^U \text{cov}(A_i, A_H) \\
& \left. + (H^U)^2 \sigma(A_H)^2 \right], \quad (11)
\end{aligned}$$

where $\sigma(Y)$ is the standard deviation (1 sigma) associated with the variable Y , and $\text{cov}(A_i, A_j)$ is the element of the variance-covariance matrix corresponding to the covariance of parameters A_i and A_j ($\text{cov}(A_i, A_i) = \sigma(A_i)^2$). The uncertainty is written in the above form to show its explicit dependence on $\sigma(A_H)^2$ and $\text{cov}(A_i, A_H)$.

A second technique for determining hydrogen with this instrument is to run standards along with unknown samples. In this case

$$H^U = H^S (R^U - \sum_{i \neq H} A_i X_i^U) / (R^S - \sum_{i \neq H} A_i X_i^S), \quad (12)$$

where H^S is the hydrogen content of the standard, R^S is its response, and X_i^S its perturbing constituents. For this case, the uncertainty is

$$\begin{aligned}
\sigma(H^U)^2 = & \left[(H^S)^2 / D(S)^2 \right] \left[\sigma(R^U)^2 + \sum_{i \neq H} A_i^2 \sigma(X_i^U)^2 + (H_U/H_S)^2 \sigma(R^S)^2 \right. \\
& + (H_U/H_S)^2 \sum_{i \neq H} A_i^2 \sigma(X_i^S)^2 \left. \right] + \left[D(U)/D(S) \right]^2 \sigma(H^S)^2 \\
& + \sum_{i \neq H} \sum_{j \neq H} \left[X_i^U/D(U) - X_i^S/D(S) \right] \left[X_j^U/D(U) - X_j^S/D(S) \right] \text{cov}(A_i, A_j), \quad (13)
\end{aligned}$$

with $D(T) = R^T - \sum_{i \neq H} A_i X_i^T$. Note the absence of dependence on variances or co-

variances of A_H and that for well-matched unknowns and samples ($X_i^U = X_i^S$) the coefficient of cov (A_i, A_j) tends to vanish.

V. CALIBRATION

A. General

From preceding and preliminary work it is necessary to determine which sample characteristics can be expected to perturb the response of the HM. These considerations then lead to the design and fabrication of standards in which the major characteristics are varied over the ranges to be expected of the unknowns. The standards then are assayed with high precision in the HM, and the responses, uncertainties, and quantitative characteristics of the standards form the data base for least squares fitting to produce the calibration constants.

The calibration of the HM for the 1979 assay of HTGR rods serves as an example of this procedure. Earlier work,¹ indicated a dependence of the HM response on ^{235}U content and a nonlinear dependence on hydrogen content. In addition, preliminary work showed a strong sensitivity to the sample position. For these reasons, standards were fabricated with the variable hydrogen, ^{235}U , and fill height, each in the range of interest of the HTGR rods. They are listed in Table I.

TABLE I
CALIBRATION STANDARDS FOR HYDROGEN MONITOR

Standard ID	H Contents (g)	Cap	Sample Height (cm)	^{235}U Contents (g)	Comments	Average Response	χ^2
1	0.5768	1.0	4.31	0.1036	CMB-1 analytic chemistry samples encapsulated in polyethylene vials.	1.5004 ± 0.0012	28.10
2	0.6420	1.0	4.31	0.0920		1.5839 ± 0.0013	4.81
3	0.5713	1.0	4.31	0.1873		1.4991 ± 0.0012	1.36
4	0.6467	1.0	4.31	0.1916		1.5855 ± 0.0013	0.73
5	0.5696	1.0	4.31	0.2930		1.4972 ± 0.0012	1.25
6	0.6306	1.0	4.31	0.2782		1.5719 ± 0.0012	9.26
P-1	0.4396	0.0	5.00	0.0	Weighed polyethylene vials.	1.3115 ± 0.0011	0.06
P-2	0.5004	0.0	5.00	0.0		1.3712 ± 0.0011	0.07
P + Cap	0.4983	1.0	5.00	0.0	Encapsulation for CMB-1 standards	1.4238 ± 0.0014	16.19

B. Standards

Standards 1 through 6 were fabricated by the Los Alamos Analytical Chemistry Group (CMB-1) and are comprised of U_3O_8 mixed with dextrose and graphite. The ^{235}U content was nominally 100, 200, and 300 mg with quoted accuracies of ± 0.01 per cent and the hydrogen content was 100 and 150 mg ± 0.01 per cent. The mixture's primary encapsulation was a glass "1-dram" vial with a Bakelite cap. Sufficient graphite was added to each standard to give it a constant (20 ± 1 mm) fill height. To make the resemblance to HTGR rods closer, a secondary encapsulation of a "2-dram" polyethylene vial, similar to those that provide primary encapsulation for the HTGR rods, was provided for each standard. The hydrogen content for each of these vials was determined by weighing and multiplying by the stoichiometric mass ratio, which was taken to be 0.1437. The mass determination by weighing was done on a calibrated commercial scale and has an accuracy of ± 0.2 mg (0.03 mg hydrogen). The hydrogen content in the table is the sum of the polyethylene hydrogen and dextrose hydrogen. The uncertainty was taken to be ± 0.1 mg, an estimate of our uncertainty in the stoichiometry.

The Bakelite cap contains hydrogen that is not uniformly distributed in the sample and that does not appear in the HTGR rods. To account for this characteristic we assign to these standards a parameter that is equal to 1.0 when the cap is present and 0 when it is not. A random sample of ten caps was weighed and found to have a relative standard deviation in mass of 0.87 per cent. The uncertainty in this parameter was therefore assigned the value 1.0 per cent. The height of the "2-dram" vials was about 5.0 cm with nominal contents of 450 mg H, and the fill height of the glass vials was 2.0 cm with nominal contents of 150 mg H. The fill height listed in the table is the weighted average for the encapsulated sample and is assigned an uncertainty of 0.1 cm.

Standards P-1 and P-2 are simply weighed polyethylene vials. Standard "P + Cap" is an empty glass vial with a cap and polyethylene encapsulation.

C. Experimental Procedure

Each standard of Table I was assayed three times over one continuous period and their responses were calculated as described above. Weighted averages were calculated for the response of each standard using either AVERAGE or LSQMK1. AVERAGE is a program designed to take teletype input values and uncertainties and calculate their weighted average, standard deviation of the mean, relative

standard deviation, and χ^2/deg . It was interesting to record relative responses, uncertainties, and time parameter on floppy disk for LSQMK1 input. In this way, the above information was generated by doing a single (constant) parameter fit to the data. One could then look for residual time dependence of the response (which was not removed by the BK(T) technique) indicating a systematic source of error by attempting a fit to a linear function of time. No residual time dependence was found in instances where this technique was used. The weighted averages for each response are listed in the table. A measure of the reproducibility of the system is $\chi^2/\text{degree of freedom}$ (χ^2/deg) for these averages. They ranged from a low of 0.10 to a high of 1.34 with a simple average of 0.71, giving confidence that the experimental variations were statistical.

D. Fitting of Data

Linear least squares fits were done to obtain best values for the parameters A_i , the associated variance-covariance matrix, and the value of χ^2/deg for each fit. LSQMK1 was used for this operation, the responses, uncertainties, and perturbing constituents of the standards having been recorded on disk with TECO. Parameters that were considered to represent the characteristics of the samples were hydrogen content, fill height, Bakelite cap, and ^{235}U contents. Although not strictly correct from a statistics point of view, a term for hydrogen-squared content was included as an independent parameter. Such a procedure is certainly not valid for situations where this term becomes comparable to, or larger than, the linear term but may be a reasonable way to include such effects if they are small perturbations on the response.

The fitting procedure of LSQMK1 assumes negligible uncertainties in the specification of the perturbing constituents. This is not always the case, and the uncertainty in the response can be enlarged to take account of this to first order. After obtaining a fit with the unmodified response, the functional form of the response is

$$R = \sum_{i=1}^N A_i X_i, \quad X_1 = 1.0 \quad . \quad (14)$$

For uncertainties, ΔX_i , in the X_i 's that are not negligible, the response uncertainty for a given standard can be expressed

$$\begin{aligned}\sigma(R^S)^2 &= \sigma_{\text{Stat}}(R^S)^2 + \sum_{i=1}^N \left(\frac{\delta R}{\delta X_i^S} \right)^2 \sigma(X_i^S)^2 \\ &= \sigma_{\text{Stat}}(R^S)^2 + \sum_{i=2}^N A_i^2 \sigma(X_i^S)^2, \quad (15)\end{aligned}$$

where $\sigma_{\text{Stat}}(R^S)^2$ is the unmodified variance dependent only on the counting statistics of the response.

The nine standards' responses were the data to be fit, and the parameter sets were varied to see the effect on χ^2/deg , reasonableness of parameters, and resulting assay accuracy. Table II gives a list of parameter sets obtained with χ^2/deg less than 30. Trial assays were done with each of the sets to find overall uncertainties that result from their use. In order to have the assay uncertainties reflect the imperfect fit of the linear model to the calibration data, the variance-covariance matrix associated with each set was multiplied by χ^2/deg . Two objections to using the set with the smallest χ^2/deg arise. First, the sign of the coefficient of fill height is physically unreasonable. One experimentally observes the response of the instrument to decrease as the hydrogen is moved from its central, optimum position. Hence a decrease in response is expected as the height of the sample is increased, which would give a negative sign to the coefficient of fill height. A second problem is the increase in the assay uncertainty, probably caused by the addition of a quantity that has a relatively large variance itself. To reduce the height uncertainty much below its 1-mm level would involve careful consideration of the weighted averaging of polyethylene and dextrose heights. For these

TABLE II
HYDROGEN MONITOR CALIBRATION PARAMETERS

Set	χ^2/deg	A_1	$A_2(\text{H}, \text{g}^{-1})$	$A_3(\text{Cap})$	$A_4(\text{H}^2, \text{g}^{-2})$	$A_5(\text{Ht}, \text{cm}^{-1})$	H(mg)
H8M309	16.3	0.818	1.114	0.047	--	--	3.4
H8M409	12.4	0.833	1.046	0.045	0.078	--	3.5
H8M509	6.2	0.719	1.078	0.049	0.103	0.019	4.2

reasons, the set H8M409 was chosen as representing the best parameters and variance-covariance matrix.

VI. UNKNOWN ASSAY AND ANALYSIS

To obtain the hydrogen content of the HTGR rods, they were assayed in the hydrogen monitor along with two standards for each blend. The sequence was chamber empty, first standard, four sequential rods, second standard. The standards associated with the various blends were blend 12, standards 2 and 4; blend 13, standards 2 and 4; and blend 14, standards 4 and 6. This procedure gave four to seven replicate assays of each standard for each day, permitting an assessment of system stability. Average responses,* their uncertainties, and χ^2/deg for each standard were calculated for each continuous running period. χ^2/deg greater than 2.0 occurred for 40 per cent of the cases, and for these the uncertainty of the average response was increased by a factor of $\sqrt{\chi^2/\text{deg}}$. Using as input the parameters and variance-covariance matrix of set H8M409, the average responses of the standards, and the response** of each unknown, the hydrogen content of each of the latter was computed relative to the two standards. The program used for the calculation was LINREL, which computes the hydrogen contents of the rod by Eq. (12). LINREL requires three floppy disk files for input. The first is the set of best parameters and associated variance-covariance matrix produced by the calibration procedure. These were dumped during the LSQMK1 runs for the satisfactory calibration sets. A slight modification of these dumps with TECO makes them compatible with the LINREL input. The second file includes average responses and characteristics of the standards that were run in conjunction with the unknown samples. This file must be generated to be consistent with the order of variables in the LSQMK1 output and includes, explicitly, the uncertainties in these perturbing constituents. Finally a file including unknowns' responses, uncertainties, and constituents' values (in the LSQMK1 order) is input. The introductory comments for LINREL are reproduced in Appendix C in order to elucidate the structure of the input files. A typical output is also included to

*Average values and χ^2/deg were computed using AVERAGE.

**Responses were calculated using the technique discussed above, i.e., generation of a function BK(T) with LSQMK1 and calculation with the HP-67 program.

aid in the interpretation of the results. The constituents of the standards and their uncertainties are discussed in Sec. III. The constituents of the rods were taken to be $\text{Cap} = 0.0 \pm 0.01$, $\text{H}^2 = 0.400 \pm 0.010 \text{ g}^2$, and $\text{Height} = 5.00 \pm 0.100 \text{ cm}$. The values for hydrogen were the weighted averages of the two determinations relative to the standards. These differed from the values obtained relative to each standard by about 3 mg, which was also the statistical accuracy of the determination. Since the nominal H^2 value was valid only for total hydrogen contents of 0.6325 g, an analytic expression was used to correct the hydrogen with an H^2 correction based on the initial assay results. Several cases were run using an iterative procedure to arrive at self-consistent values of H and H^2 . These agreed with the analytically generated correction to better than 0.3 mg.

VII. CONCLUSIONS

The hydrogen monitor has been calibrated for measurements in the vicinity of 600-mg hydrogen. With the current calibration and standards, the estimated accuracy is $\pm 4.5 \text{ mg}$, which is based on the difference in assay results for the same unknown for two different standards and measurement precisions. Before proceeding with work that improves the precision of the monitor, more work will need to be done to remove this $\pm 3\text{-mg}$ discrepancy. Likely candidates for investigation are the exact form of the response, which is likely to be more complex than the simple linear response assumed here, and use of calibration standards, which more closely match the rods (perhaps by elimination of the Bakelite cap).

Another matter of concern is the high position sensitivity of the HM. It would be convenient to redesign the instrument for more uniform irradiation of the sample, especially over its vertical dimension. Currently a 1-mm shift in position alters the response by 5 per cent, inducing one to believe that fill height must be an important parameter.

There may be correlations in the calibration data and the standards' responses that we have not properly treated. To take account of the constituents' uncertainties in the calibration, it was necessary to expand the response uncertainty by the additional term

$$\sum_{i=1}^N \left(\frac{\delta R}{\delta X_i} \right)^2 \Delta X_i^2 .$$

If the same standards are used in the relative measurements, then the uncertainties for these two measurements are not independent, although the framework presented here treats them as such.

REFERENCES

1. D. A. Close, R. C. Bearse, and H. O. Menlove, "²⁵²Cf-Based Hydrogen Analyzer," Nucl. Inst. Meth. 136, 131-135 (1976).
2. M. M. Meier and E. L. Adams, "HTGR 'Green' Rods Intercomparison: I. Hydrogen Assay," Los Alamos National Laboratory report (to be published).

APPENDIX A

PROGRAM LSQMK1 AND TYPICAL OUTPUT

FORTRAN IV V02.1-4 SAT 17-MAR-79 08:23:53 PAGE 001

```

C
C   LINEAR LEAST SQUARES FITTING PROGRAM      M.M.MEIER 30-AUG-79
C
C   MODIFIED 10-31-79 FOR DISC OUTPUT OF VAR-COV MATRIX AND BEST PARAMS.
C
C   MODIFIED 6-MGV-79 FOR NAMED INPUT FILE
C
C   MODIFIED 14-MAR-80 FOR OUTPUT OF SIGMAY,UMASS AND EXPANDED
C   COMMENTARY
C
C   DESIGNED TO OBTAIN BLST VALUES AND UNCERTAINTIES FOR THE NPKMP1
C   COEFFICIENTS ALFA(I) IN THE EXPRESSION:
C
C       Y = UMASS(ALFA(1) + ALFA(2)*X(2) + ALFA(3)*X(3) + ... + ALFA(NPKMP1)
C         *X(NPKMP1))
C
C   THE PROGRAM REQUESTS THE FILENAME OF THE DISKFILE ON WHICH THE
C   INPUT DATA RESIDES. THE FILENAM IS SPECIFIED BY 6 CHARACTERS
C   'ABCDEF' AND THE FILESPEC IS THEN DK:ABCDEF.DAT. THE INPUT FILE IS
C   READ FROM DISC.  FORMAT IS:
C
C   NPTS                                (15)
C   Y,SIGMAY,UMASS,X(2),X(3),...,X(NPKMP1)  (23F16.3)      (1)
C   Y,SIGMAY,UMASS,X(2),X(3),...,X(NPKMP1)  (23F16.3)      (2)
C   .
C   .
C   Y,SIGMAY,UMASS,X(2),X(3),...,X(NPKMP1)  (23F16.3)      (NLOW)
C   .
C   .
C   Y,SIGMAY,UMASS,X(2),X(3),...,X(NPKMP1)  (23F16.3)      (NHIGH)
C   .
C   .
C   Y,SIGMAY,UMASS,X(2),X(3),...,X(NPKMP1)  (23F16.3)      (NPTS)
C
C   USER IS THEN PROMPTED FOR POINTS TO BE CONSIDERED IN THE FIT,
C   SPECIFIED BY NLOW AND NHIGH.  NEXT PROMPT IS FOR THE NUMBER OF
C   PARAMETERS TO BE CONSIDERED, NPARMS, 1 .LE. NPARMS .LE. NPKMP1.
C   FIT PROCEEDS BY MATRIX INVERSION WITH INTERMEDIATE OUTPUT ON TT
C   AND LP.  AFTER THE FIT THE BLST VALUE COEFFICIENTS ('ALFA'S')
C   AND THE VARIANCE-COVARIANCE MATRIX ARE OUTPUT TO DISK AT USER
C   OPTION IN A FORMAT WHICH IS COMPATIBLE WITH LINKEL, LINKMS AND
C   URMAS INPUT.  USER CAN ALSO OBTAIN THE SAME OUTPUT WITH THE
C   VAR-COV MATRIX MULTIPLIED BY CHI-SQUARED/DEGREE OF FREEDOM.
C
C   NOTE THAT THE USE OF VARIABLE DIMENSIONED ARRAYS NECESSITATES THE
C   EXTENSIVE USE OF SUBROUTINES.
C
C

```

Y VALUES FROM INPUT FILE:

```

1
1 1.31154
2 1.37120
3 1.50040
4 1.58390
5 1.49913
6 1.58545
7 1.49723
8 1.57189
9 1.42381

```


SIGMA VALUES FROM INPUT FILE:

```

1
1 0.105000E-02
2 0.114000E-02
3 0.120000E-02
4 0.126000E-02
5 0.119000E-02
6 0.125000E-02
7 0.121000E-02
8 0.125000E-02
9 0.142000E-02

```

X VALUES FROM INPUT FILE:

	1	2	3	X(1),X(2),X(3)
1	1.00000	0.439600	0.000000	
2	1.00000	0.500400	0.000000	
3	1.00000	0.576800	1.00000	
4	1.00000	0.642000	1.00000	
5	1.00000	0.571300	1.00000	
6	1.00000	0.646700	1.00000	
7	1.00000	0.569600	1.00000	
8	1.00000	0.630600	1.00000	
9	1.00000	0.498300	1.00000	

MATRIX #1.000E+00

	1	2	3
1	0.616593E+07	0.344578E+07	0.448944E+07
2	0.344578E+07	0.195600E+07	0.266201E+07
3	0.448944E+07	0.266201E+07	0.448944E+07

INVERTED MATRIX # 1.000E+00

	1	2	3
1	0.202196E-04	-0.419741E-04	0.466892E-05
2	-0.419741E-04	0.897830E-04	-0.112628E-04
3	0.466892E-05	-0.112628E-04	0.223208E-05

Variance-covariance matrix

PRODUCT OF MATRIX AND INVERSE

MAXIMUM DIAGONAL ELEMENT = 1.00000
 MINIMUM DIAGONAL ELEMENT = 1.00000
 MAXIMUM OFF DIAGONAL ELEMENT = 0.111022E-14

Matrix inversion test

PARAMETER VALUES

	1	
1	0.818304	A(1)
2	1.11361	A(2)
3	0.466703E-01	A(3)

SUM OF RESIDUALS FOR EACH MEASUREMENT

	1
1	12.3738
2	14.5860
3	33.0991
4	10.0225
5	2.96469
6	0.595299E-01
7	2.88675
8	13.9821
9	7.63785

SUM OF ALL RESIDUALS = 97.6122
 CHI**2/DEG OF FREEDOM =

16.2687

APPENDIX B

H MONITOR RESPONSE—A PROGRAM FOR THE HP-67

After entering the program from magnetic card, begin loading the necessary constants into the HP-67 registers.

Enter

$$\begin{aligned}(\Delta DT/DT)^2 &= [\Delta P_0(T)/P_0(T)]^2 + [\Delta P_0(1)/P_0(1)]^2 \\ &= 2[B1(T) + B2(T) + N_{\text{Lost}}]/[P_0(T)]^2\end{aligned}$$

into register 3. Enter A1 and A2 into registers 4 and 5; A3, 2*A4 and A5 into registers 6, 7, and 8; $P_0(1)$, the net pulser area of the reference run, into register E. Enter N(T), "ENTER". Then begin the program by pressing Label "A"; N(T) remains in the display. Enter T; "R/S"; T remains in the display. Enter P(T); "R/S"; P(T) remains in the display. Enter B1(T); "R/S"; the difference $P(T) - B1(T)$ is displayed. Enter B2(T); "R/S"; B2(T) remains in display. "R/S"; program runs, then R(T) is displayed. "R/S"; then R(T) is displayed. "R/S"; then $R(T)/R(T)$ is displayed. At this time R(T), R(T), and $R(T)/R(T)$ are stored in registers A, B, and C and can be recalled for recording. Calculations for $R(T + 1)$ are done by repeating the instructions, beginning with Enter N(T + 1), "ENTER".

APPENDIX C

PROGRAM LINREL AND TYPICAL OUTPUT

FORTRAN IV

VO2.1-4

WED 21-MAY-79 00:54:00

PAGE 001

```

C
C*****      LINREL      *****
C
C      PROGRAM TO DETERMINE VALUES OF UNKNOWN FROM A RESPONSE
C      WHICH HAS THE FORM:
C
C       $R = A(1) + A(2)X(2) + \dots + A(NVAR)X(NVAR)$ 
C
C      THE RESPONSE OF A STANDARD HAS THE SAME FORM:
C
C       $RSTD = A(1) + A(2)XSTD(2) + \dots + A(NVAR)XSTD(NVAR)$ 
C
C      THE A(I)'S ARE INPUT FROM A FILE ON DK ALONG WITH THEIR
C      APPROPRIATE VARIANCE COVARIANCE MATRIX. FORM OF THIS FILE IS:
C
C      NVAR                                NUMBER OF A(I) COEFFS.
C      A(1),A(2),...A(1),...A(NVAR)        CORRECTION COEFFICIENTS
C      VARCOV(1,1),VARCOV(1,2)...VARCOV(1,NVAR)
C      VARCOV(2,1),VARCOV(2,2)...VARCOV(2,NVAR)
C      ,                                VARIANCE-COV. MATRIXSTD
C      ,
C      ,
C      VARCOV(NVAR,1),...,VARCOV(NVAR,NVAR)
C
C      'KUNK' A NUMBER BETWEEN 2 AND NVAR IS INPUT TO SELECT THE UNKNOWN
C      VARIABLE. DATA ON THE STANDARDS, THEIR RESPONSES, UNCERTAINTIES, PER-
C      TURBING CONSTITUENTS (XSTD(I)'S) AND UNCERTAINTIES ARE READ FROM ANOTHER
C      DK FILE WITH THE FOLLOWING FORMAT (SUBROUTINE RDRSTD):
C      NSTD
C      STDID(1),RSTD(1),DELXST(1),XSTD(1,1),DELXST(1,1),XSTD(1,2),DELXST(1,2)...
C      XSTD(1,NVAR),DELXST(1,NVAR)
C      ,
C      ,      (MASS IDENTIFICATION, RESPONSE AND UNCERTAINTY AND PERTURBATIONS
C      ,      AND THEIR UNCERTAINTIES)
C      ,
C      STDID(I),RSTD(I),DELXST(I),XSTD(I,1),DELXST(I,1),XSTD(I,2),DELXST(I,2)...
C      XSTD(I,NVAR),DELXST(I,NVAR)
C      ,
C      ,
C      ,
C      STDID(NSTD),RSTD(NSTD) ETC.
C
C      DATA ON THE SAMPLES, THEIR RESPONSES, UNCERTAINTIES, PER-
C      TURBING CONSTITUENTS (X(I)'S) AND UNCERTAINTIES ARE READ FROM ANOTHER
C      DK FILE WITH THE FOLLOWING FORMAT (RDKUNK):
C      NPTS
C      MASSID(1),RES(1),RES(1),X(1,1),DELX(1,1),X(1,2),DELX(1,2)...
C      X(1,KUNK-1),DELX(1,KUNK-1),X(1,KUNK+1),DELX(1,KUNK+1)...
C      X(1,NVAR-1),DELX(1,NVAR-1)
C      ,
C      ,      (MASS IDENTIFICATION, RESPONSE AND UNCERTAINTY AND PERTURBATIONS
C      ,      AND THEIR UNCERTAINTIES)
C      ,
C      ,
C      MASSID(I),RES(I),DELRES(I),X(I,1),DELX(I,1),X(I,2),DELX(I,2)...
C      X(I,KUNK-1),DELX(I,KUNK-1),X(I,KUNK+1),DELX(I,KUNK+1)...
C      X(I,NVAR-1),DELX(I,NVAR-1)
C      ,
C      ,
C      ,
C      MASSID(NPTS),RES(NPTS) ETC.
C
C      'NLOW' AND 'NHIGH' ARE IF INPUT AND SAMPLES WITH INDICES
C      BETWEEN THEM ARE CALCULATED:

```

```

C      UNKNOWN = UNSSTD*(RES - A(1) + A(2)*X(2) + ... + A(KUNA-1)*X(KUNK-1)
C      + A(KUNK+1)*X(KUNK+1) + ... + A(NVAK-1)*X(NVAK-1))/(RESSTD - A(1)
C      + A(2)*XSTD(2) + ... + A(KUNK-1)*XSTD(KUNK-1) + A(KUNK+1)*XSTD(KUNK+1)
C      + ... + A(NVAR-1)*XSTD(NVAR-1)
C
C*****

```

```

*****      PROGRAM LINKML      *****
PROGRAM TO DETERMINE UNKNOWN VALUES RELATIVE TO STANDARDS.
VERSION MAR11-20-79

```

COEFF AND VAR-COV DATA READ FROM BKTEMPN1.DAT

3 VARIABLES IN CORRECTION TERM

CORRECTION COEFFICIENTS:

```

1  0.8183E+00
2  0.1114E+01
3  0.4667E-01

```

LSQMK1

```

          VARIANCE-COVARIANCE MATRIX
I/J  1      2      3      4      5      6      7
1  0.329E-03 -0.463E-03  0.740E-04
2 -0.463E-03  0.146E-02 -0.163E-03
3  0.740E-04 -0.163E-03  0.363E-04

```

Output

UNKNOWN VARIABLE IS 2TH IN LIST

STANDARDS DATA READ FROM BKST1206.DAT

2 STANDARDS IN THIS FILE.

STD. ID	RESPONSE	XSTD(2)	XSTD(3)	XSTD(4)	XSTD(5)
1004	1.58812+ 0.00072	0.44470+ 0.00040	1.00000+ 0.01000		
1005	1.57412+ 0.00106	0.43040+ 0.00040	1.00000+ 0.01000		

UNKNOWN DATA READ FROM BKUN1206.DAT

FOR RUN ID 1244

RESPONSE AND UNCERTAINTY	PERCENTAGES AND UNCERTAINTY
1.53910 + 0.00148	2 0.00000 + 0.00000
	3 0.00000 + 0.01000

UNKNOWN IS 0.44371 + 0.00841(1.30/0 %) RELATIVE TO STANDARD 1004

CORRECTION FOR STANDARD = 0.72315
 CORRECTION FOR UNKNOWN = 0.71980
 RATIO = 1.00463

$$R = \sum_{i=1}^N A_i X_i$$

CONTRIBUTIONS TO (DELTA/U)SS2

RESPONSE OF STANDARD = (0.994E-03)SS2

RESPONSE OF UNKNOWN = (0.206E-02)SS2

PERTURBATION UNCERTAINTIES

I	X(I)	XSTD(I)
2	(0.000E+00)SS2	(0.619E-03)SS2
3	(0.648E-03)SS2	(0.645E-03)SS2

$$\sigma(R^S)/D(S)$$

$$\sigma(R^U) H^S / [D(S) H^U]$$

$$\sigma(X_1^U) A_1 H^S / [D(S) H^U], \quad \sigma(X_1^S) A_1 / D(S)$$

VARIANCE-COVARIANCE MATRIX FOR COEFF. UNCER.

```

I/J  1      2      3      4      5      6      7
1  0.328E-07  0.000E+00 -0.163E-05
2  0.000E+00  0.000E+00  0.000E+00
3 -0.163E-05  0.000E+00  0.166E-03
          Varcov(A1,Aj) [X1^U/D(U) - X1^S/D(S)]
VARIANCE-COVARIANCE SUM FOR COEFF 1= -0.160E-05
VARIANCE-COVARIANCE SUM FOR COEFF 2= 0.000E+00
VARIANCE-COVARIANCE SUM FOR COEFF 3= 0.166E-03
SUM OF MATRIX = 0.166E-03
          [X1^U/D(U) - X1^S/D(S)]

```

UNKNOWN IS 0.44007 + 0.00895(1.376 %) RELATIVE TO STANDARD 1004

CORRECTION FOR STANDARD = 0.70915
 CORRECTION FOR UNKNOWN = 0.71980
 RATIO = 0.98520

CONTRIBUTIONS TO (DELTA/U)002
 RESPONSE OF STANDARD = (0.152E-07)002
 RESPONSE OF UNKNOWN = (0.204E-02)002
 PERTURBATION UNCERTAINTIES
 1 X(I) XSTD(I)
 2 (0.000E+00)002 (0.434E-03)002
 3 (0.646E-03)002 (0.450E-03)002
 VARIANCE-COVARIANCE MATRIX FOR COEFF. UNCERT.
 I/J 1 2 3 4 5 6 7
 1 0.350E-04 0.000E+00 0.544E-05
 2 0.000E+00 0.000E+00 0.000E+00
 3 0.544E-05 0.000E+00 0.174E-03
 VARIANCE-COVARIANCE SUM FOR COEFF 1= 0.501E-05
 VARIANCE-COVARIANCE SUM FOR COEFF 2= 0.000E+00
 VARIANCE-COVARIANCE SUM FOR COEFF 3= 0.182E-03
 SUM OF MATRIX = 0.182E-03

AVERAGE VALUE FOR UNKNOWN = 0.64200073 +0.61284599E-02