350
11/28/66

MASTER

DATA EDITING AND PROCESSING COMPUTER PROGRAM
FOR ULTRACENTRIFUGE MOVING BOUNDARY
SCHLIEREN PATTERN CALCULATIONS

RODES TRAUTMAN

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

June 1966

BROOKHAVEN NATIONAL LABORATORY
ASSOCIATED UNIVERSITIES, INC.

under contract with the
UNITED STATES ATOMIC ENERGY COMMISSION

DISCLAIMER

This report 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.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

DATA EDITING AND PROCESSING COMPUTER PROGRAM FOR ULTRACENTRIFUGE MOVING BOUNDARY SCHLIEREN PATTERN CALCULATIONS*

CFSTI PRICES

RODES TRAUTMAN

H.C. \$ 4.00 MN ~~1.00~~

Biophysicist, Plum Island Animal Disease Laboratory, Agricultural Research Service,
U.S. Department of Agriculture, Greenport, New York

and

Research Collaborator, Medical Department, Brookhaven National Laboratory, Upton, New York

June 1966

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

*Research supported, in part, by the U.S. Atomic Energy Commission.

BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

PRINTED IN USA
PRICE \$4.00

Available from the
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards
U.S. Department of Commerce
Springfield, Virginia

September 1966

650 copies

C O N T E N T S

I.	Introduction.	1
II.	General Features of the Program.	3
	A. Scope.	3
	B. Computation sequence for s-rate and concentration.	5
	C. Computation sequence for polynomial least squares curve fitting.	7
	D. Data editing notes.	8
	E. Output.	15
III.	Instructions for Input.	21
	A. Arrangement of deck.	21
	B. Constants and options used on centrifuge "run control card".	24
	C. Constants and options used on centrifuge "frame control card".	26
	D. Format for centrifuge coordinates and reading codes for comparator data.	27
	E. Constants and options used on polynomial "options card".	30
	F. Format for coordinates for polynomial curve fitting.	33
	G. Relaxation of key punching requirements and compromises.	33
IV.	Formula Summary.	37
	A. Introduction.	37
	B. Centrifuge theory.	38
	C. Standard errors.	42
V.	Description of Main Program.	43
VI.	Description of Subroutines.	43
	A. D1-CS2 SUBROUTINE MAIN2.	43

C O N T E N T S

B. D2-CS2 SUBROUTINE DATA1.	44
C. D3-CS2 SUBROUTINE DATA3.	45
D. D4-CS2 SUBROUTINE CKDATA.	48
E. D5-CS2 SUBROUTINE SRATE2.	49
F. D6-CS2 SUBROUTINE CFLS2.	51
G. D7-CS2 SUBROUTINE PLOT.	59
H. D8-CS2 SUBROUTINE CONC.	61
I. D9-CS2 SUBROUTINE FTEST.	63
J. D10CS2 SUBROUTINE LSPOLY.	64
K. D11CS2 SUBROUTINE MATINV.	74
VII. Acknowledgements and Disclaimer.	76
VIII. References.	79
IX. Appendix.	
A. Source program listing in FORTRAN IV.	A 1
B. Test input data listing.	A34
C. Output of s-rate and concentration processing of test data.	A36
D. Output of polynomial least squares curve fitting of test data.	A49

* Footnote to Page 1.

This program has been converted to the Chippewa Operating System FORTRAN for use on the Control Data 6600 Computer using single precision throughout since it has precision of approximately 14-1/2 decimal digits (in contrast to the 8 of FORTRAN IV on the IBM 7094).

I. Introduction.

Electronic digital computers can process ultracentrifugation data many times faster than is possible by hand or by desk calculators. Their enormous speed makes it feasible to perform calculations heretofore considered too laborious on even selected experiments. Now the researcher may make very sophisticated analyses of all his data, and the large memory of the "32K" computers currently used permits labeling of all output quantities, as well as inclusion of many tests to screen and interpret data. Such programs make it possible for data from experiments performed by occasional users of the centrifuge to be processed and evaluated as would those obtained by the specialist.

This report describes data editing and processing for schlieren optical moving boundary ultracentrifugation using a FORTRAN IV computer program.* The program has been added to and modified over several years. At present, it can process two-dimensional comparator data for sedimentation rate and concentration determination as well as perform least squares polynomial curve fitting of any data. It is hoped that it can be extended to cover all the computational aspects described in detail previously (Trautman, 1956, 1963). Not only is it designed for semiautomatic comparator measurements, which soon will be generally available (Bartulovich and Ward, 1965), but it also can process existing data obtained by manual comparison. It is not necessary to reread old plates, but merely to transcribe the raw data on appropriate key punch forms. Only a few estimates of the baseline position are necessary if double sector cells were not used.

Procedures for facilitating comparison and computation by using a radius cubed scale (Trautman, 1956) are essentially made obsolete by this computer program. However, the simplifying plate alignment and reading procedures are still very useful for obtaining the data for hand computation that may be required for immediate experimental analysis on a day-to-day basis. The data obtained in this way can still be submitted for this program at a later date for the more refined calculations.

The program embodies features for research in computational methods, while permitting routine data processing. Thus, the standard procedure for s-rate determination is by linear least squares reduction of boundary positions measured at several times during the run ("log r vs. t method"). This program extends that procedure by using, in addition, quadratic least squares in order to give both the initial s-rate and the s-rate at the mean time of the data. The advantage of the tangent to the parabola at a given time is that computation is made internal to the data rather than by extrapolation to one end or outside, and that the s-rate refers to a definite position in the cell. This gives a very small standard error for the s-rate and permits specification of the applicable concentration and pressure. Initial concentrations are obtained by square law correction and summation of measured ordinates of the schlieren pattern. Novel features include numerous data editing comments as well as two line-printer plots ("log r vs. t" and "g*(s*)"), determination of zero time corrections, tests for cell leaks, and sufficient capacity to handle two simultaneous centrifuge runs with up to four components in each. Internal standard errors of almost all quantities are computed.

II. General Features of the Program.

A. Scope.

This program, CS2, is written completely in FORTRAN IV using about 1900 cards with 11 subroutines. It requires a 32K memory, all purpose digital computer. It can be used for centrifuge data processing or for weighted least squares polynomial curve fitting of any data.

The program accommodates double cell runs with up to 4 components in each. Either or both cells may be the synthetic boundary type and either or both may be a flotation instead of a sedimentation run. Both menisci and all components in both cells need not be read in every frame. Up to 29 frames may be entered for s-rate with up to 8 replicate measurements of each one-dimensional position. For concentration, up to 50 pairs of two-dimensional solution readings and 50 solvent (or baseline) readings in up to 10 frames out of the 29 may be entered. No individual replicates are permitted, but entire frames may be reread.

The one-dimensional data represent the positions of the maximum gradient $r_{\max}$ at selected timer values t but may be equivalent boundary positions $\bar{r}$ from previous processing or theoretical studies. The two-dimensional data represent points on the schlieren pattern, typically a series of bell shaped "peaks", but may be upper or lower meniscus regions for preliminary processing prior to Archibald method molecular weight calculations. The program gives concentrations and "observed" s-rates, neither corrected to standard conditions (20 °C, water) nor to infinite dilution.

The points need not be equally spaced either in time for s-rate or in distance for concentration. The program counts the number of cells, frames, components, number of one-dimensional replicates, and the number of two-dimensional coordinates from the data supplied. If the baseline is not measured for each point on the solution pattern, a least squares polynomial through the given points is computed to interpolate baseline values. The program starts with a quartic and successively reduces the degree until the last term is significant by F-test at the 5% level. Peaks do not have to be completely separated from the meniscus or from each other if the starting and stopping points (e.g. the meniscus or valley between peaks) are identified.

The operator of a semiautomatic comparator is permitted great flexibility in the sequence of plate reading by coding each coordinate. The program sorts the measurements and checks for certain omissions. The plate must be aligned so that the x-axis of the comparator is parallel to the centrifuge radial direction of the cell, but as long as reference (fiducial) edges are measured, the comparator scale can be arbitrary. Four choices of reference marks are permitted to correspond to centrifuge runs using a counter balance in which either or both reference edges are measured or to runs using a rotor reference hole for which either one of its edges, both, or its center are measured.

Blocks of data for least squares polynomial curve fitting can be processed with blocks of centrifuge data for s-rate and concentration. Up to 30 points are permitted which may be weighted; a) identically, b) according to the given weight, c) its reciprocal, or d) the square of its

reciprocal, as selected by options. The program counts the data. It can a) scale either or both abscissa or ordinate values, b) subtract a constant from all abscissas, and c) take the logarithm of the ordinates before fitting. The curve fitting is done for any range or polynomial degrees between zero and six, selected by the user.

The polynomial curve fitting feature allows the user to recycle edited centrifuge data: a) for processing the true boundary positions as $\log \bar{r}$ vs. t , b) for higher than quadratic fitting of $\log r_{\max}$ vs. t , or c) for obtaining weighted means of concentration data.

B. Computation sequence for s-rate and concentration.

1. Raw comparator data are sorted, averaged, and converted to a standard comparator reference. The baseline is interpolated, if necessary.

2. The meniscus positions are checked for a significant trend which would indicate a cell leak. If there is a leak (at the 5% level by the F-test), the position at the timer zero is calculated and then the equivalent s-rate of the leak and its standard error are determined using linear least squares of $\log r_{\text{meniscus}}$ vs. t data.

3. Quadratic and linear least squares curve fitting of $\log r_{\max}$ vs. t are made and the significance of a nonzero quadratic term tested.

4a. For conventional runs, the zero time correction and its standard error are determined from the time at which the fitted curve would pass through the average meniscus position. The linear fit is used only if the quadratic term is nonsignificant.

4b. For synthetic boundary cell runs, the starting level and its error are determined from the least squares intercept at the timer zero using the linear fit only if the quadratic term is nonsignificant.

5. All the components are treated as in 3 and 4 above.

6a. For conventional runs, the weighted zero time and its error are determined for all the components using the reciprocal of the square of the standard error as the weight. The timer values are corrected by this weighted zero time.

6b. For synthetic boundary cell runs, the weighted starting position and its error are similarly determined at the timer zero.

7. Both quadratic and linear least squares are made with the corrected data for all components. An additional zero time correction and its error are determined for each component using the quadratic fit regardless of both the significance of the curvature and the type of run. These are given for editing purposes.

8. The tangent to the quadratic at the mean time is computed (along with its standard error) and called the internal s-rate. The quadratic term itself is divided by the square of the linear term to give a "concentration-pressure dependence coefficient". Its standard error is also computed.

9. A line-printer plot is made of $\log r_{\max}$ vs. t which, for rough editing purposes, also displays the weighted zero time and starting level and their standard errors as well as the timer zero.

10. The converted data and the average s-rate ($\underline{s^*}$) computed from the weighted zero time to each point are listed to aid in identifying bad points.

11. Concentration calculations are made from the two-dimensional comparator readings component-by-component, frame-by-frame. Both the plateau concentration and the initial concentration together with their errors are computed. The boundary position is determined from these concentrations for comparison with the input position of the maximum ordinate.

12. Each ordinate value is converted to the distribution function g^* and the corresponding abscissa value converted to s^* using the corrected time and starting position as determined from the s-rate analysis. A line-printer plot is made of the $g^*(s^*)$ values superimposed for all frames which, for rough editing purposes, displays the internal s-rates of all components from the s-rate analysis.

13. For double cell runs of the conventional type, a weighted zero time correction is determined using both cells, and the s-rate analysis repeated.

C. Computation sequence for polynomial least squares curve fitting.

1. The x, y data are read from cards, counted, transformed, and proper weights assigned.

2. Powers of x are formed for the highest degree requested.

3. Sums of squares of powers of x and cross products with y are set up.

4. The normal equations are solved by matrix inversion.

5. Residuals are computed; the residual random error computed.

6. Significance of a nonzero last term coefficient of each polynomial is tested at the 5% level.

7. Additional cycles at other degrees are made as requested.

8. A summary of the input data and the residuals for each degree fit is made.

D. Data editing notes.

Cautionary notes are printed if the data reveal any of several types of anomalies and to indicate decisions made in the program. The dashes in the following are given the appropriate specific numbers. The deck names in parenthesis are given for reference to Section VI and to the FORTRAN listing in the appendix.

1. Input data (D3-CS2).

a. ~~**CAUTION**~~ FRAME -- DELETED.

Results if the reference is not given, the one-dimensional data are missing when two-dimensional data are given, or a special delete end code is given (Card D3 205).

b. ~~** CAUTION**~~ BASELINE ASSUMED = 0.0.

Results if no baseline values are given (Card D3 297).

c. ~~**CAUTION**~~ CELL -- POLYNOMIAL OF DEGREE -- PUT THROUGH -- BASELINE POINTS GIVING STANDARD ERROR OF COMPARATOR ORDINATE -----.

Given for run in which baseline points are read or estimated other than at each solution point. (If the standard error is too large, then the baseline is not adequately computed. The investigator should consider re-running the sample using a double sector cell.) The maximum degree is 4 and the minimum is zero (Card D3 318).

d. ~~**CAUTION**~~ CELL -- BASELINE NOT GIVEN FOR EACH POINT.

Occurs if solvent readings do not alternate with solution readings in

double sector cell runs. Concentration calculation for that cell in that frame is deleted (Card D3 327).

e. ****CAUTION**** CELL -- COMPONENT -- NUMBERED WRONG, CONC INCLUDES ALL SLOWER COMPONENTS READ IN THIS FRAME.

The components should be numbered from the fastest to the slowest and read from the slowest to the fastest. The x,y data corrected for baseline will be printed with the sequence code assumed by program to aid in locating the error. The concentration computed may be salvageable by the user depending on the actual error made in numbering (Card D3 408).

2. Time relationship of data (D4-CS2).

a. ****CAUTION**** INPUT TIMER VALUES REDUCED BY INPUT ZERO OF

-----.

The input value is subtracted from the given time of all frames (Card D4 030).

b. ****CAUTION**** CELL LEAK WITH S-RATE -- STD ERROR -- (SVED).

Occurs only if leak is significant at 5% level. The s-rate is determined and it may be either positive (cell distortion or leakage from another compartment) or negative (actual leakage) (Card D4 074).

3. One-dimensional data analysis (D5-CS2).

a. Kind of run.

1) ****CAUTION**** ZERO TIME DETERMINED BY STARTING PEAKS

AT MENISCUS.

Occurs for conventional run. The time intercept at which the least squares solution passes through average meniscus value is determined and called the zero time correction. In flotation, the bottom of the cell or lower

meniscus should be used as the "meniscus" (Card D5 040).

2) ~~**CAUTION** MENISCUS USED AS A POINT, ZERO TIME CORRECTION STILL MADE.~~

Special run in which the starting level is the meniscus at a known timer value (usually zero). The zero time correction is still computed as for a conventional run (Card D5 041).

3) ~~**CAUTION** STARTING LEVEL DETERMINED AS AVERAGE OF INTERCEPTS AT TIMER ZERO FOR SYNTHETIC BOUNDARY CELL.~~

Occurs for all synthetic boundary cell runs. The radial intercept at which the least squares solution passes through the timer zero is determined. If the timer is not correct, there is no effect on the internal s-rate computed, but there will be a slight error in the dilution factor. The additional zero time correction values and their standard errors should be scanned to see if they are significantly different from zero. If so, the data can be resubmitted with an input timer zero value given (Card D5 036).

b. Number of points for least squares analysis.

1) ~~**CAUTION** COMPONENT -- HAS LESS THAN 3 POINTS.~~

Linear least squares is done, but the standard error of the slope cannot be calculated. The listing of s* should be scanned to see how reasonable the points are (Card D5 052).

2) ~~**CAUTION** COMPONENT -- HAS JUST 3 POINTS, ONLY LINEAR FIT MADE.~~

Quadratic least squares with its error not possible because of too few data points. The linear least squares value of s-rate is given under

"internal s-rate" as well as under "linear" on output (Card D5 057).

c. Results of F-test on quadratic term.

1) ~~**CAUTION** COMPONENT~~ -- HAS LESS THAN 5 PERCENT CHANCE OF A CURVED LN R VS. T PLOT.

The "zero time" determination of conventional runs, and the "starting level" determination of synthetic boundary cell runs is determined from the linear fit since the error of extrapolating beyond the data is smaller if the lowest degree polynomial is used that significantly fits the data (Card D5 063).

2) ~~**CAUTION** COMPONENT~~ -- HAS SIGNIFICANTLY CURVED LN R VS. T PLOT AT 5 PERCENT LEVEL.

If the component is not one that should show a concentration or pressure dependence, then experimenter should check data or run for nonconstant temperature or speed. If sign of concentration-pressure dependence coefficient is positive, concentration dependence outweighs pressure dependence. If negative, and no pressure dependence is expected, then dissociation of an interacting system is possible (Card D5 071).

d. Check that starting conditions are reasonable.

1) ~~**CAUTION** STANDARD ERROR OF ZERO TIME TOO LARGE,~~
SET = 0.0 FOR PLOT.

The zero time correction can be any size depending on the timer values, but its error should be small. It is tested at a magnitude of 10 minutes for this cautionary note. Note that with too few points no zero time error can be computed and this note will occur normally (Card D5 119).

2) ~~**CAUTION**~~ STANDARD ERROR OF STARTING LEVEL TOO LARGE, SET = 0.0 FOR PLOT.

This tests the error of the meniscus values for conventional runs and the starting level intercept for synthetic boundary cell runs. The condition is that the error must be smaller than the depth of the standard centrifuge cell. With too few points, this note will occur normally (Card D5 125).

3) ~~**CAUTION**~~ COMPONENT -- HAS ERROR IN DATA, OR DID NOT START AT SAME TIME OR PLACE AS OTHERS.

Test of the sign of the initial s-rate and the internal s-rate is made on the second cycle after timer has been corrected by the weighted zero time for all components. If they are of different sign, the parabola is much too curved, or it is being extrapolated too far outside the data (Card D5 253)..

4) Further tests of the zero time correction are made in the least squares routine (D6-CS2).

e. Automatic addition of starting level as a point.

1) ~~**CAUTION**~~ SPECIAL CYCLE, WEIGHT -- USED FOR STARTING LEVEL, GENU ----.

If there is more than a single component, the weighted starting level from the first cycle of least squares is added as a point, with unit weight unless requested otherwise, and the s-rate redetermined. This may or may not effect a reduction in the standard error of the s-rate. It helps most with few points and imprecise data (Card D5 219).

2) ~~**CAUTION**~~ SPECIAL CYCLE FOR BOTH CELLS ADDING STARTING LEVEL AT WEIGHTED ZERO TIME.

Both cells are combined if both are conventional runs even if each has only a single component, since the zero time should be the same for both cells. The additional point may or may not improve the calculation depending on the data (Card D5 200).

4. Quadratic and linear least squares analysis (D6-CS2).

a. Zero time error

1) ~~**CAUTION** TOO LARGE ERROR IN DATA, ZERO TIME CANNOT BE CALCULATED.~~

This will result if the root of the quadratic is imaginary in calculating the intercept, i.e., the fitted parabola does not pass through the meniscus level (Card D6 213).

2) ~~**CAUTION** TOO LARGE ERROR IN DATA, ZERO TIME ERROR CANNOT BE COMPUTED.~~

This will happen if the variance and covariance of the constant and first degree terms of the quadratic result in an imaginary standard error (Card D6 222).

b. ~~**CAUTION** ALL WEIGHTS ARE ZERO, CCLS NOT DONE.~~

In the event that there are no points given, the curve fitting least squares subroutine is skipped. This can happen if the first component in a multicomponent run is not measured, for example (Card D6 266).

5. Concentration analysis (D8-CS2).

a. ~~**CAUTION** FRAME -- HAS ZERO CONC FACTOR.~~

No concentrations will be computed for this frame. This will result if the ordinate magnification is omitted on the run control card or if the phaseplate angle is either omitted or given as zero (Card D8 053).

b. ~~**CAUTION**~~ FRAME -- HAS ZERO TIME, S* CANNOT BE CALCULATED.

The concentrations will be computed, but the $g^*(s^*)$ editing calculations for that frame are omitted (Card D8 058).

c. ~~**CAUTION**~~ FRAME -- PEAK -- POINT -- IS OUT OF ORDER.

This results if the abscissas do not form a monotonic series. The concentration is computed, but will be in error, because the increment for the bad point is of opposite sign to the rest of the summation increments (Card D8 084).

d. ~~**CAUTION**~~ CONCENTRATION NOT CALCULATED.

This will normally appear if only one-dimensional data are given; or abnormally, if all two-dimensional input data were rejected for some reason (Card D8 155).

6. Polynomial least squares analysis (D10CS2).

~~**CAUTION**~~ LEAST SQUARES POLYNOMIAL NOT DONE.

Results when subroutine is called but all weights are zero (Card D10 255).

7. Compiler notes.

The FORTRAN IV monitor, instead of stopping computation, makes notes when certain irregularities occur. These are usually abnormal, although some overflow and underflow conditions can occur with limited or bad data and the cause will usually be apparent. The monitor supplies asterisks for output numbers which cannot fit the specified format. This is used for quantities that cannot be computed. Most format errors in input data will terminate the program, hence, blocks of data following which may be all

right are not processed. The user should not assume that a note will always be printed if something is wrong.

E. Output.

1. s-Rate and concentration data.

Several levels of output are possible and are controlled by the print option. The normal level (blank or zero) gives the output of key quantities indicated in the computation sequence above. Print out of the input data is suppressed by a -1, and all output except the cautionary notes is suppressed by a -2 (useful only if this entire program becomes part of a much larger centrifugation data processing system). Higher levels of the print option may be used on subsequent passes if the cautionary notes that are printed do not lead the investigator to find the error in the data. The print option set at 1 gives the input data corrected to a fixed comparator reference and for baseline. Levels from 2-6 give progressively more details from each of the subroutines and would be used only for debugging purposes or special investigations of computational methods when some of the intermediate computations are required.

Three levels are possible in the plot option and are independent of the print option. A negative deletes all line-printer plots; a blank or zero are normal and give the plot; and a 1 lists, in addition, the data plotted. A more refined or expanded plot can be made by hand from this listing.

Even with the large number of output options, all extraneous output is not deleted in the normal level (blank or zero). The full page width

has been used with important quantities put at the left. The extra space is used for additional values that may be of interest from a computational standpoint, or to aid in interpreting the run. They do not increase the number of lines of output. These features are included so that the program can be used for research in computational methods as well as for routine data processing.

2. Polynomial least squares curve fitting.

Several levels of output are possible as controlled by the print option. The normal level (blank or zero) gives the coefficients and their standard errors, the residual standard error of the y measurement, and the F-test value together with the results of the F-test. A negative suppresses all printed output. A 1 provides for the listing of the input data and all the residuals, whereas the higher levels (2 and 3) give details of the computation, such as the variance-covariance matrix, sums of squares, means and reinversions of matrices.

3. Description of sample test data input and output (see appendix).

a. RT TEST DATA 15 RECTANGULAR, ~~CONC~~-PRES, CONCENTRATION, AND LINEAR COMPS.

These 16 cards, ending in 999, illustrate one-dimensional data transcribed from a notebook onto a keypunch form with all control options set at blank on the second card. The peak positions of the four components and the meniscus appear across the card according to the format given in Section VI B 2, and show that the frame identification at the left of each card can be in any form and that all readings other than the reference do not have to be given for every frame.

The output lists the input data and the options selected, with the number of frames and components filled in by the program. The caution notes indicate a conventional run with the first three components exhibiting curvature on the s-rate plot (this is only barely detectable on the line-printer plot, but is of the order of magnitude found in practice). The components were selected as follows: component 1 was made to have constant velocity and the curvature results from the log function; component 2 was taken from Wales (1959) for an extreme case of concentration and pressure dependence (cf. Section IV B 2; $a = 1.0$, $b = 0.5$, $q = -0.25$), the latter strong enough to give a negative curvature; component 3 was taken from Lauffer (1944) for tobacco mosaic virus giving a positive curvature due to concentration dependence of the particle (axial ratio of 20:1); and component 4 was made to have constant s-rate.

b. TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT.

These 32 cards, ending in 999, illustrate two-dimensional data transcribed directly as read on the comparator to a keypunch form (input option 3, all others blank). The 6 minute and 12 minute frames were read for concentration, giving the baseline for each solution pattern point. The output lists the input data on the first page and the converted data on the second. The plot shows that the zero time is reasonably close to that expected since the timer was started at $2/3$ final speed during acceleration. The second cycle data page gives the internal s-rate and its error and the concentration data for the two frames. The standard error of the ordinate measurement was assumed by the program to $0.05 \text{ mm at } 45^\circ$

phaseplate angle and to increase as the cotangent for smaller angles. The line-printer plot of the distribution function shows that the peaks measured for concentration were the same as measured for s-rate and that the relative spread due to diffusion becomes narrower with time.

c. TEST DATA RT 20 SINGLE SECTOR CELL.

These 22 cards, ending in 999, illustrate two-dimensional data for a three component sample run in a single sector cell. The baseline is read only in the supernatant and in the plateau in the 64 minute frame, (baseline option 1). Component 1 was not read for concentration. The print option = 1 was selected so that details of the search for the best fitting polynomial to the baseline would be given.

The corrected data are given at the bottom of the first page. Component 3 includes point 1 through 11 and component 2, 11 through 21. Point 11 was actually coded as the minimum (a 9) and the first point (a zero) was supplied by the program. A leading zero was not supplied since the final input coordinate was coded also as a 9 (the minimum between components 2 and 1).

Two replicates were measured for the 48 minute frame and the print option = 1 gives the average comparator one-dimensional data summary at the top of the second page.

The second cycle output page shows the advantages of adding the common starting level on a special (third) cycle since now the fastest component has 3 points and an estimate of the standard error of the average can be made.

The concentration of the two components is given, and the distribution plot shows that the partition into components was all right, and that there was a fast component measured for s-rate but not concentration.

d. TRANSFER CARD.

This tells the computer that the following data are for polynomial least squares curve fitting.

e. ~~COMPONENT~~ 2 TEST DATA RT 15 (~~CONCENTRATION~~-PRESSURE DEPENDENCE).

These 13 cards, ending in 999, illustrate the data from Wales (1959) submitted for fitting from first through fourth degree. The remaining options on the second card are: Weight = 0 (all weights taken as unity); mean = 1 (take mean out of sums before matrix inversion); input = 1 (data are on cards); function = 1 (take log of ordinates); scale = 1 (convert all abscissas by the given factor in the middle of the card; and print = 1 (give residuals).

The output lists these options and shows that the relationship is significantly curved through the third degree. Note that the initial s-rate (the first of the successive terms to the right of ~~CONSTANT~~) does not change much, but that the second degree coefficient does. This means that no significant error is introduced in the s-rate by using the quadratic fit instead of the cubic for this highly pressure dependent sample. Computing by hand $q = b_2/b_1^2$ from the cubic fit gives -0.27 which agrees well with the theoretical -0.25, but shows that the highest degree that is significant must be used since q computed from the quadratic fit is -0.47.

FIG.1 ARRANGEMENT OF DECK

f. ~~COMPONENT~~ 3 TEST DATA RT 15 (~~CONCENTRATION~~ DEPENDENCE).

These 16 cards, ending in 999, illustrate resubmission of converted data from the first pass for more detailed study. The listing of r, t and the zero time correction on page 2 of the RT 15 TEST DATA given above was used. The ~~CONVERSION FACTOR~~ TIMER TO ~~QMSQT~~ was used as the XSCALE value. The output shows that the $\ln \underline{r}$ vs. t relationship is significantly curved up to the 3rd degree and that $q = b_2/b_1^2 = 0.63$, not the 0.35 computed from the quadratic fit. The output also shows that no significant error is introduced in the s-rate determination by using the quadratic fit in the s-rate program for this very concentration dependent aqueous sample.

III. Instructions for Input.

A. Arrangement of deck.

Figure 1 shows the general arrangement for the input deck which from front to back consists of the appropriate identification and control cards, the object program deck (machine language or "binary" deck), a data control card ("end of file" card at BNL), blocks of data, and the appropriate end control cards. Sample input data are given in the appendix. The data

PROBLEM CS2 Ultracentrifuge Moving Boundary Data Processing Program																																										CODER										DATE		PAGE 1 OF 1																																																	
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	COMMENT																															
Data for s-rate and concentration analysis (any number of runs)																																																																																																							
RUN IDENTITY CARD																																										Co's. 1-72										Aphanumeric Identification										Blank										Card 1																															
RUN CONTROL CARD																																										Speed										Rotor reference										X magnification										Options (integer)										Timer correction										Y magnification										Card 2	
																																																				Kind of run (upper cell)										Beginning weight										Kind of run (lower cell)																															
																																																				Output (Print)										Plot										Input																															
FRAME CONTROL CARD																																										Alphanumeric Identification										Time										Phaseplate angle										Baseline options										SE Y										Card 3											
																																																														Lower cell										Upper cell																															
ONE-DIMENSIONAL DATA CARDS (for frame indicated on card 3)																																																																																		Card 4 (30 cards maximum)																					
																																										Code (integer)										Code										X Coordinate										End Codes										777 Two-dimensional data follow 888 End of frame 999 End of run																					
TWO-DIMENSIONAL DATA CARDS (for frame indicated on card 3)																																																																																		Card 5 (30 cards maximum)																					
																																										Code (integer)										Code										Y Coordinate										End Codes										888 999																					
TRANSFER CARD (only one required no matter how many sets of data)																																																																																		Positive: Cols. 73-75																					
TITLE CARD																																										Cols. 1-72										Alphanumeric Identification										Blank										Card 1																															
																																																																																		Blank: Cols. 73-75																					
OPTIONS CARD																																										Control Options (integer)										E										E										E										Card 2																					
																																										Max Mean function Print										X Scale Factor										Y Scale Factor										X Zero Correction																															
																																										Min degree Weight Input Scale																																																													
WEIGHTED TWO-DIMENSIONAL DATA CARDS																																																																																		Card 3 (30 cards maximum)																					
																																										Alphanumeric Identification										X Coordinate										Y Coordinate										Weight										End Code 999																					

can be of mixed type. A transfer card is required both before and after the least squares polynomial data, except that the final transfer card may be omitted if the end of file and return to system cards are appropriate.

A general check list on the arrangement of cards of each data type is given below. The detailed format is described in Sections B, E and Fig. 2.

1. Sequence of cards for s-rate and concentration analysis.
 - a. Run identity card (first card) - alphanumeric identification, cols. 73, 74, 75 must be blank.
 - b. Run control card (second card) - constants and options.
 - c. Frame control card (third card) - alphanumeric identification, time, phaseplate angle, baseline options.
 - d. One-dimensional data cards - x data points consisting of fiducial or reference marks, menisci, peak positions with identifying code; last card must have end code 777 or 888.
 - e. Two-dimensional data cards - x,y data points on solution and baseline pattern with identifying code; last card must have end code 888.
 - f. Corresponding cards to 3, 4, 5 above for each succeeding frame; final card must have end code 999.
 - g. Corresponding cards to 1-6 for each centrifuge run.
2. Sequence of cards for polynomial least squares curve fitting.
 - a. Transfer card - 111 in cols. 73, 74, 75.
 - b. Title card - alphanumeric identification of data for curve fitting, cols. 73, 74, 75 must be blank.

- c. Options card - constants and options.
- d. Data cards - one for each point (not to exceed 30) giving x,y and the weight; last card must end with 999 in cols. 70, 71, 72.
- e. Corresponding cards to 2-4 for each set of data.
- f. Transfer card - lll in cols. 73, 74, 75 if return to s-rate and concentration desired.

B. Constants and options used on centrifuge "run control card".

See card 2 of upper portion of Fig. 2 for summary of format specifications. The decimal point assumed by the program (if not punched) is indicated.

Cols. 1-9 - Speed in R.P.M.

Cols. 10-19 - Rotor reference in cm. This is the actual reference corresponding to the fiducial mark measured as plate reference. If two different edges are measured, the rotor reference must correspond to the average of corresponding inner and outer edges of the counter balance or rotor reference hole at the speed used.

Cols. 20-29 = X-magnification. This includes the magnification of the objective lens and the magnification of the comparator including any dimensional changes, such as mm to cm.

Col. 33 - Kind of run:

Blank, 0,1: Conventional run in which boundaries start from meniscus, but starting time not known. ("Starting level known, starting time unknown".)

2: Boundaries start from meniscus at timer zero and this point is used as part of the data. ("Starting level and time known".)

3: Synthetic boundary cell run in which the starting level is not known, but timer is assumed to be true. ("Starting time known, starting level unknown".)

Cols. 34-35 - Output option:

Negative: caution notes only,

Blank, 0: normal (input data, caution notes, converted data, s* for each point, zero time and starting level, internal s-rate, initial s-rate, "linear" s-rate, and concentration-pressure dependence — all with their standard errors),

1: above and x, y data corrected for comparator reference and baseline,

2: above and implicit output of subroutines,

3-6: above and progressively more detailed output of subroutines.

Cols. 36-37 - Plot option:

Negative: no plot,

Blank, zero: plot is made,

1: plot and listing of data are made.

Col. 39 - Input option:

Blank, 0, 1: special input format for one-dimensional theoretical data not using automatic comparator (see description of SUBROUTINE DATA1),

2: special input format for one-dimensional comparator data using abbreviated reading codes, (see SUBROUTINE DATA3, card D3 097).

3: standard input format given in Fig. 2 for one- and two-dimensional data for manual key punching or for automatic comparator.

Col. 41 - Kind of run option for lower cell. This needs to be given only if the kind is different from upper cell.

Col. 49 - Beginning weight option:

Blank, 0: for conventional runs with more than one component or more than one cell, a special third cycle of quadratic least squares automatically occurs using the corrected times and adding the starting level at unit weight,

1-8: meniscus position at the timer zero is included as a point on the second cycle with weight 1-8 as indicated,

9: special cycle as for blank and 0 above, but for single component runs as well.

Cols. 50-59 - Timer correction in minutes. If left blank, no correction will be made.

Cols. 60-69 - Y-magnification factor. This includes the cell path length, the optical lever arm, magnification of the cylindrical lens, magnification of the comparator including dimensional changes, and specific refractive increment to give mg/ml units for concentrations.

C. Constants and options used on centrifuge "frame control card".

See card 3 of upper portion of Fig. 2.

Cols. 1-9 - Alphanumeric identification: normally, run-plate-frame.

Cols. 10-19 - Time in minutes.

Cols. 20-29 - Phaseplate angle θ in degrees.

Col. 31 - Baseline option:

Blank, 0: baseline reading either follows or precedes each solution pattern reading on two-dimensional data (typically a double sector cell experiment),

1: baseline readings do not correspond to pattern points (typically a single sector cell experiment). Up to 50 baseline points may be given. If there are none given, the baseline will be assumed to be zero, otherwise, the best fitting least squares interpolating polynomial will be computed.

Col. 33 - Baseline option for lower cell:

This needs to be given only if the lower pattern is read differently from the upper cell. Note: the baseline option must be given for each frame and, hence, baselines can be read for each point in one frame, and then only for a few in another frame, if desired.

Cols. 40-44 - Standard error of comparator ordinate readings (SE Y):

If blank or zero, $0.05/\tan \theta$ is assumed for purposes of estimating the standard error of the concentration calculation for double sector cell measurements. If the baseline option 1 is used, the residual standard error of the interpolating polynomial is used for SE Y.

D. Reading codes for comparator data.

In order to permit the operator of the comparator to read the plate in any sequence desired, a 3 digit code precedes each x and y

FIG. 3 READING CODES

coordinate as indicated on cards 4 and 5 of Fig. 2. A schematic representation of a schlieren pattern is given in Fig. 3. Here b stands for blank in the reading code and the dots represent points on the solution pattern, whereas the crosses are points on the solvent or baseline pattern.

1. One-dimensional data.

a. First digit.

Blank, 0 to 4: interpreted as blank (available in future for special data sequences),
5: inner meniscus (between air and solution),
6: outer meniscus (between solution and more dense immiscible fluid, or cell bottom),
7: inner reference edge,
8: outer reference edge,
9: center of rotor reference hole.

b. Second digit (ignored if first digit is 5-9).

Blank, zero: not used,
1: fastest peak,
2,3: intermediate peaks,
4: slowest peak,
5-8: special points recorded but not processed,
9: not used.

c. Third digit.

Blank, 0, 1: upper cell or only cell read,
2: lower cell,
3-4: special points neither recorded nor processed,
5-9: used in end codes.

2. Two-dimensional data.

a. First digit.

Blank, 0: x,y points are read in sequence at increasing radii,
1-4: available for special sequences of data,
5: upper meniscus
6: lower meniscus
7-9: not used, interpreted as blank.
(For single sector runs do not code baseline at meniscus as 5 or 6. A 5 on solution pattern must be first reading for that cell and 6 the last).

b. Second digit.
Blank, 0: baseline point,
1-4: x,y point belongs to the numbered peak,
5-8: not used, x,y point recorded, but not processed,
9: point is a minimum between peaks.

c. Third digit.
Blank, 0, 1: upper cell or only cell used,
2: lower cell,
3-4: special points neither recorded nor processed,
5-9: used in end codes.

d. The same code is used for the x and y coordinate readings, x must precede y.

3. End codes.

555: delete current frame including one-dimensional data,

666: delete preceding reading,

777: end of one-dimensional reading, two-dimensional data follow. If used in two-dimensional data, then delete any preceding x,y data given for that frame,

888: end of frame,

999: end of run.

E. Constants and options used on polynomial "options card".

See card 2 of lower portion of Fig. 2.

Cols. 2 and 4. MIN, MAX: Corresponding to the integer lowest and highest degree, respectively, of polynomial to be fit (may be 0-6). Program will not make fit if the number of data

points is less than 2 more than the degree requested. Use MIN = MAX for a single degree. Use MIN > MAX for degree starting at MAX and reducing until last coefficient is significant. Final degree will be overwritten as MIN.

Col. 6. Weight option:

- 0: all weights assumed unity,
- 1: weight taken as WINPUT,
- 2: weight taken as $1/\text{WINPUT}$,
- 3: weight taken as $(1/\text{WINPUT})^2$,

Col. 8. Increase in precision of computation option (MEAN):

- 0: means not taken out of sums of squares,
- 1: sums of squares corrected for mean (only necessary for high degrees).

Col. 10. Input option: Must be 1 to effect reading of data cards.

Col. 12. Function option:

- 0: normal,
- 1: fit $\ln y$ vs. x , for points with nonzero weight.

Col. 14. Scale option:

- 0: normal,
- 1: x data are multiplied by XSCALE
before fitting,
- 2: x data are multiplied by XSCALE
and y data are multiplied by
YSCALE (scaling done before
log function).

Cols. 15,16. Print option:

- negative: no printed output,
- 0: heading, coefficients and
their errors, residual standard
error, F-test value,
- 1: preceding plus input data and
residuals,
- 2: preceding plus variance-co-
variance matrix and reinversion
of matrix if highest term is
nonsignificant,
- 3: preceding plus detailed sums
of squares, reinversion of all
matrices, and implicit output
of MATINV subroutine.

Cols. 20-39.

Scale factor for x data (XSCALE,
E20.7).

Cols. 40-59. Scale factor for y data (YSCALE,
E20.7).

Cols. 60-69. Zero correction for x data (XZERO, F10.5).

F. Format for coordinates for polynomial curve fitting.

See card 3 of lower portion of Fig. 2.

Cols. 1-9: alphanumeric identification (may
be blank),

Cols. 10-29: XINPUT (E20.7),

Cols. 30-49: YINPUT (E20.7),

Cols. 50-69: WINPUT (E20.7),

Cols. 70,71,72: blank, 000: another data card
follows,

999: this is last data card.

G. Relaxation of key punching requirements and compromises.

1. Frames do not have to be in chronological order and more than one frame may have the same time (say, if an entire frame is re-read).

2. Replicates are permitted on one-dimensional readings; but not on two-dimensional readings.

3. Timer can be started at any time, a constant correction of all the values will be made by the program only if the timer zero is given on the constants card.

4. The comparator scales do not have to be set to read true distance on the magnified rotor.
5. Data can be in any order.
6. Blanks are interpreted as zeros.
7. Cell number does not have to be indicated anywhere in single cell runs, but lower cell must be indicated on both x and y readings.
8. Two-dimensional readings do not have to be made.
9. Up to 8 peaks may be read, but only the first 4 will be processed. The remaining 5 through 8 may be used for other points that the operator wishes to record while reading the plate, possibly for future processing.
10. Several choices of reference marks are possible. No coding is necessary to list which combination is desired. The ones not used are merely left blank. For example, if the center of the reference hole is used, code as a 9 and give no readings coded 7 or 8. If 7 and 8 are to be averaged, then both must be given. If either 7 or 8 is to be used separately, then the one not used must merely be omitted.
11. Special relaxation for double cell runs is possible for meniscus readings. If both menisci are identical, the reading need only be entered once (coded as 051 for the upper cell) and the program will assume that it also applies to the lower cell. Possible undesirable consequences of this compromise are:
 - a. If no peaks are read in the lower pattern, the common meniscus will not be included as the lower meniscus reading for that frame.

b. If no peaks are read in the upper pattern and the common meniscus is coded 052 instead of 051, it will not be included as a meniscus reading for the upper cell.

c. If the menisci are different and the upper one (code 051) is read in a given frame, the lower one must also be read (code 052) unless no peaks in the lower pattern are read.

12. It is not necessary to give the number of frames, the number of data points, the number of replicates, the number of cells, or the number of components. The program will determine these from the data that are given.

13. Two-dimensional x,y data must be in order from slowest to fastest component, but can be intermixed between the two cells. Points do not have to be equally spaced either on linear or cube of the radius scales.

14. The x,y data do not have to start at baseline. The program will assume the curve is zero at a distance preceding the first point equal to the first interval given. Similarly, the leading side of the peak is augmented with a final zero.

15. If the minimum (valley) is not coded (091), then the first reading of the next peak will be taken as the minimum.

16. Decimal override can be used on input punching.

17. Missing data. Any reading can be omitted in any frame except as follows:

a. The reference cannot be omitted.

b. The comparator must not be set such that a legitimate zero reading can occur.

FIG. 4

c. The meniscus cannot be omitted in all frames except for synthetic boundary cell runs.

18. The baseline reading may precede or follow each solution pattern point. It can have any code for double sector cell readings.

IV. Formula Summary.

A. Introduction.

The sedimentation coefficient ("s-rate") of a particular solute is the velocity that its molecules would have in a unit centrifugal field. It is determined from measurements of the position of a boundary between a solution containing the solute and its supernatant fluid at various times after the ultracentrifuge attains a constant angular velocity. In Fig. 4, the logarithm of the boundary position measured from the center of rotation is plotted (with its standard error) against the timer values $\underline{T}$ (shown with negligible error since the photographs are generally taken automatically with a precise interval timing mechanism). The boundary started at $\ln \underline{r}_a$ and moved to point A during the acceleration period. The zero time correction $\underline{T}_0$ is the timer value at which centrifugation would have started if the rotor could have been accelerated instantaneously to the final operating speed. Three s-rates are indicated: a) the initial, which is the slope of the curve extrapolated to zero time, b) the internal or tangent s-rate, which is the slope at the mean time of the data, and c) the linear s-rate, which is the slope of the least squares straight line through the data. The internal s-rate is the

recommended value to use since it has the smallest standard error.

The basic problem is to determine the s-rate of each component from the given data, and the concentration and pressure for which the s-rate is applicable, along with internal standard errors. The algorithms are developed from either substitution in or least squares treatment of the following formulas. A wavy line indicates the quantity computed, all other constants or variables are either input quantities or directly computed from such.

B. Centrifuge theory.

1. Schlieren pattern coordinates.

$$\tilde{x} = M_o M_e r_{ref} - (X_{ref} - X)$$

$$\tilde{r} = x / (M_o M_e)$$

$$\tilde{y} = Y_{soln} - Y_{solv}$$

$$\partial c / \partial r = y \tan \theta / (a \hat{b} M_c M_e R_1)$$

where $\underline{M_o}$ is the magnification of camera lens; $\underline{M_e}$, magnification of comparator; $\underline{M_c}$ magnification of cylinder lens; $\underline{a}$, optical path length of cell; $\underline{b}$, optical lever arm of schlieren camera; $\underline{\theta}$, phaseplate angle; $\underline{R_1}$, specific refractive increment; $(\underline{x}, \underline{y})$, absolute coordinates representing magnified rotor seen on plate-comparator system; (X, Y) arbitrary comparator coordinates; $\underline{r}$, radius in cm; $\underline{c}$, concentration at $\underline{r}$ in mg/ml; $\underline{c^0}$, initial

concentration; soln, solution; solv, solvent or baseline; and ref, fiducial or reference mark.

2. Background moving boundary s-rate relationships.

The instantaneous s-rate in Svedbergs of a moving boundary is

$$s = (10^{13}/\omega^2) d \ln \bar{r}/dt$$

and the average s-rate of the boundary is

$$s^* = (10^{13}/\omega^2) (\ln \bar{r} - \ln r_a)/t$$

where $\bar{r}$ is the boundary position at time t (in sec) and r_a its position at zero time, and ω is the angular velocity of the rotor $[2\pi(\text{rpm})/60]$.

In general, the instantaneous s-rate is not constant during a run. For sedimentation, radial dilution decreases the viscosity and the s-rate increases; with aggregating systems the dilution favors slower sedimenting species and the weight average s-rate decreases; with pressure dependent systems the s-rate decreases. A general series expansion can be written as

$$\ln \bar{r} = \ln r_a + s_0(\omega^2 t) + q s_0(\omega^2 t)^2 + \dots$$

Billick (1962a) has given the relationship between q and more fundamental parameters for the concentration-pressure dependent case

$$q = [a - b(2a+1)]/(1+a)$$

where $a = \frac{kc^0}{s_0^0}$ is the concentration dependence; $b = k'' \omega^2 r_a^2 \rho_a/2$, the pressure dependence; ρ_a , the density at one atmosphere, such that the instantaneous s-rate is related to that at atmospheric pressure and infinite dilution s_0^0 by

$$s = \frac{1-b[(r/r_a)^2-1]}{1+a(c/c^0)} s_0^0$$

3. Formulas used for s-rate.

The one-dimensional input data of the schlieren peak position is assumed to represent $\bar{r}$ and to have the parabolic relationship

$$\ln r_{\max} = \underline{b}_0 + \underline{b}_1 (\omega^2 t) + \underline{b}_2 (\omega^2 t)^2$$

where the coefficients $\underline{b}_0$, $\underline{b}_1$, and $\underline{b}_2$ are computed using an algorithm based on standard quadratic least squares curve fitting formulas. The initial s-rate is $\underline{b}_1$ and the internal s-rate is $\underline{b}_1 + 2\underline{b}_2 \omega^2 \bar{t}$, where $\bar{t}$ is the mean of the input time values. The concentration-pressure dependence coefficient $q = \underline{b}_2 / \underline{b}_1^2$.

4. Distribution function $\underline{g}^*(s^*)$.

Point-by-point conversion of a schlieren moving boundary pattern to a distribution with respect to s-rate with area $\underline{c}^0$ is

$$(\underline{c}^0 \underline{g}^*) = \frac{(\omega^2 r^3 t)}{r_a^2} \left(\frac{\partial c}{\partial r} \right)$$

$$\underline{g}^* = (10^{13} / \omega^2) (\ln r - \ln r_a) / t$$

5. Concentration.

$$c_p = c_a + \int_{r_a}^{r_p} (\partial c / \partial r) dr$$

$$c^0 = c_a + \int_{r_a}^{r_p} (r/r_a)^2 (\partial c / \partial r) dr = c_p (\bar{r}/r_a)^2$$

where $\underline{c}_a$ is the concentration at the starting level after the boundary has moved to $\bar{r}$ and $\underline{c}^0$ is the initial concentration before dilution to the

plateau concentration $\underline{c}_p$ ahead of the boundary.

These general relationships are used by first assuming $\underline{c}_a$ to be zero and second that the definite integrals of the form $\int_{x_1}^{x_n} y \, dx$ and

$\int_{x_1}^{x_n} x^2 y \, dx$ can be obtained adequately by summation using the trapezoidal rule. The n ordinates including the start at $\underline{x}_1$ and the end at $\underline{x}_n$ may be spaced at random, so each interval is considered separately, computing the mid point $\underline{x}'$, $\underline{y}'$ of the interval $\underline{\Delta x}$ as

$$\underline{\underline{x'}} = (\underline{x}_{i+1} + \underline{x}_i)/2$$

$$\underline{\underline{y'}} = (\underline{y}_{i+1} + \underline{y}_i)/2$$

$$\underline{\underline{\Delta x}} = \underline{x}_{i+1} - \underline{x}_i$$

and approximating the integrals as sums of the individual contributions

$$\int_{x_i}^{x_{i+1}} y \, dx = \underline{\underline{y'}} \underline{\Delta x}$$

and

$$\int_{x_i}^{x_{i+1}} x^2 y \, dx = \underline{\underline{x'^2}} \underline{\Delta x}$$

The "true" boundary position $\underline{\underline{r}}$, the square root of the second moment or radius of gyration of the schlieren peak, is computed from the ratio of the summations as

$$\underline{\underline{r}} = r_a [c^0/c_p]^{\frac{1}{2}}$$

C. Standard errors.

1. Standard least squares statistical relations are used, computing standard errors from the square root of the variance.

2. For functional relationships, the variance v_y and the covariance cov , are combined as (Davies, 1961)

$$y = f(x_1, x_2, \dots, x_n)$$

$$v_y = \left(\frac{\partial y}{\partial x_1}\right)^2 v_{x_1} + \left(\frac{\partial y}{\partial x_2}\right)^2 v_{x_2} + \dots + 2\left(\frac{\partial y}{\partial x_1}\right)\left(\frac{\partial y}{\partial x_2}\right) \text{cov}_{x_1, x_2} + \dots$$

3. For the summations, this formula gives, for example

$$v_A = \Sigma(\Delta x_i)^2 v_y$$

$$v_W = \Sigma[(x'_i)^4 (\Delta x_i)^2] v_y$$

where $\frac{v}{y}$ is the variance of the y measurement,

$$A = \Sigma(y'_i) \Delta x_i, \text{ and } W = \Sigma(x'_i)^2 \Delta x_i.$$

4. The Student's $t = y/\sigma_y$ is used as its equivalent

$F_{n,1} = t^2$ (the first column of the F-table) to test the significance of the last term in least square curve fitting (Snedecor, 1956). The 5% level is used throughout.

V. Description of Main Program.

The actual computations are done by eleven subroutines. These may be building blocks for much more sophisticated centrifuge programs. Here they are called by the main program which can cope only with blocks of data, possibly intermixed, of centrifuge runs for s-rate and concentration analysis and sets of data for polynomial least squares curve fitting.

The listing of the FORTRAN program has numerous "comments" cards to indicate the algorithms. Loops have been drawn to aid in following the logic.

VI. Description of Subroutines.

A. D1-CS2 SUBROUTINE MAIN2 (LRETRN).

1. Director program for s-rate and concentration calculations, repeated for each block of centrifuge data. Sequence of "comments" cards:

- a. Read run identity and run control card.
- b. Read data (CALL DATA1 or DATA3).
- c. Main loop for all cells (through g).
- d. Check that cell has data.
- e. Make input timer zero correction, convert and test for leak (CALL CKDATA).
- f. Add starting level if LKIND = 2.
- g. Compute s-rate for all components and save results (CALL SRATE2).

h. Compute concentration for each component in each frame
(CALL C/NC).

i. Add respective starting level at weighted zero time of
both cells if neither is a synthetic boundary cell run, recompute all
s-rates (CALL SRATE2).

2. Arguments.

a. Explicit.

LRETRN: Integer return variable for future use in
main program. Regardless of LRETRN on call, a new value is read from
run identity card: negative, blank or zero means all runs in data deck
are to be processed for s-rate and concentration; and positive means
return to main program.

b. Implicit.

Subroutine uses C/COMMON /CS1CM/, /CS2XY/, and /WORKCM/.

3. Notes.

All sense lights turned off. Sense light 4 used.

B. D2-CS2 SUBROUTINE DATA1.

1. Read routine for one-dimensional data transcribed from
comparator listing or test data. Called from D1-CS2 by option LINPUT =
blank, 0 or 1. Single cell, single reference, no replicates. Assign
zero weight if absolute value of entry $< 10^{-10}$.

2. Input format.

Cards 1 and 2 of upper portion of Fig. 2 are applicable.
Card 3 must have the following format for each frame.

a. LINPUT = 0 (see appendix, first input data block).

cols. 1-4	alphanumeric frame identification,
cols. 5-9	time (F5.1),
cols. 10-19	reference (F10.5),
cols. 20-29	peak position (F10.5), component 1,
cols. 30-39	peak position (F10.5), component 2,
cols. 40-49	peak position (F10.5), component 3,
cols. 50-59	peak position (F10.5), component 4,
cols. 60-69	meniscus position (F10.5),
cols. 70-79	blank, another frame card follows,
	999, last frame.

b. LINPUT = 1.

Data are in centimeters on rotor, magnification must be 1.0, neither comparator nor rotor references need be given. Same format as above except as follows.

cols. 5-9	not used,
cols. 10-19	time (F10.5).

2. Implicit arguments.

Subroutine uses ~~COMMON~~ /CS1CM/.

C. D3-CS2 SUBROUTINE DATA3.

1. Read routine for one- and two-dimensional data, especially from digitized comparator. Called from D1-CS2 by option LINPUT = 2 or 3. Sequence of "comments" cards:

- a. Heading for input data on print out.
- b. Initialization.
- c. Main loop over all frames (through s).
- d. Initialization and read frame control card.
- e. Read data.
 - 1) Alternate input for two digit code (LINPUT = 2).
 - 2) Regular input using 3 digit code.
- f. Edit each record and sort by cell.
- g. Count maximum number of replicates and flag cells with no x data. (Write sorted input one-dimensional data.)
- h. Average replicates.
- i. Select reference: center, average, outer, or inner, respectively.
- j. Assign meniscus for various cells. Convert to standard comparator reference.
- k. Count components. Convert to standard comparator reference.
- l. Frame deleted by input code on either x or x,y data, or no x data.
- m. Input of x,y coordinates.
- n. Edit each record and sort by cell, count cells. (Write sorted input two-dimensional data.)
- o. Flag cell if x,y data are given in any frame, flag frame.

p. Baseline sequence may be different for each frame and each cell.

q. Correct solution ordinates for baseline.

- 1) Collect baseline readings if not given for each point.
- 2) Put least squares polynomial through baseline points (CALL LSPOLY).
- 3) Compute baseline for solution pattern points and subtract (skip to r).
- 4) Subtract input baseline ordinate from input solution ordinate. Take absolute value to permit either solution or solvent reading to be first.

r. Supply extra zero point if minimum, meniscus, or bottom ordinate is not given (as first or last point). Zero point is not supplied between peaks.

s. Identify peaks in sequence of readings, convert to fixed reference and store values as x and y.

t. Write converted and sorted x,y data corrected for baseline.

2. Implicit arguments.

Subroutine uses ~~COMMON~~ /CS1CM/, /CS2XY/, and /~~WORK~~CM/.

3. Notes.

a. Up to 8 components in 2 cells can be read and will be listed as input data. Only 4 components in each will be processed. If a peak or cell is coded above 8 or 2, respectively, the point will be deleted.

b. The sequence of x,y coordinates is divided according to peaks by an index array which gives the stopping number in the sequence. This code is printed if the corrected comparator data are requested (print option = 1) and is labeled STOP/START. Component 1 includes the data included in the first 2 listed numbers, component 2, the 2nd and 3rd numbers, etc. These numbers refer to the listing of the x,y data, and can be used to check the program interpretation of the input identification of peaks. When the sequence starts with 2, asterisks will appear as the 1st point, as a zero value was not supplied by the program.

c. The polynomial fitting of baseline points (when not given for each solution point) starts at the fourth degree. The degree is reduced until the last term is significant at the 5% level. The residual standard error at the selected degree is overwritten on the standard error of ordinate measurement, if it was given as input. The details of this curve fitting are given with print option = 1.

D. D4-CS2 SUBROUTINE CKDATA.

1. Conversion of one-dimensional comparator data to rotor centimeters and cell leak check. Called from D1-CS2. Sequence of "comments" cards:

a. Write one-dimensional comparator data converted to standard comparator reference (average only, if replicates were given).

b. Conversion (to rotor centimeters and logarithm).

c. Linear least squares analysis of meniscus values (CALL CFLS2).

1) Significant leak (CALL FTEST). Determine its s-rate (CALL CFLS2).

2) No leak.

d. Use most radial peak in first frame as preliminary starting level in synthetic boundary cell runs (with zero standard error).

2. Implicit arguments.

Subroutine uses ~~COMMON~~ /CS1CM/ and /CS2XY/.

3. Notes.

a. Sense light 4 used, turned off before return.

b. Point 1d above only important if details of first cycle are requested by print option 2 or higher, or if only a single component is read.

E. D5-CS2 SUBROUTINE SRATE2.

1. Director program for s-rate of all components in each cell incorporating zero time correction and starting level. Called by D1-CS2 for each cell separately, and then again in double cell conventional runs with combined zero time correction. Sequence of "comments" cards:

a. Skip to second cycle if final call in double cell runs.

b. First cycle. Loop over all components, linear and quadratic least squares (CALL CFLS2), make F-test (CALL FTEST).

c. Determine common intersection of all components (CALL CFLS2).

- 1) Synthetic boundary cell run (CALL CFLS2).
- 2) Conventional run (CALL CFLS2).
- 3) Check that starting time and level are reasonable.

d. Log $\underline{r}$ vs. $\underline{t}$ plot with origin as ± 2 standard errors from weighted zero time and weighted starting level (initialization).

- 1) Point by point s-rate ($\underline{s}^*$) for data editing.
- 2) Write converted data and $\underline{s}^*$.
- 3) Make s-rate plot (CALL PLOT) such that slope will have dimensions of Svedbergs. Use reference line to mark timer zero.

e. Prepare for second cycle. Include starting level with specified weight. Reset weight if second cell calculated has only one component.

f. Second cycle, quadratic used for additional zero time even if log $\underline{r}$ vs. $\underline{t}$ is not curved. Loop over all components (CALL CFLS2), write results.

g. Reset for additional cycles as required by options. Additional cycle automatically done with unit weight for starting level if more than one component, or if a double cell run.

h. Restore time values for other pattern or for different zero time correction except in final calculation for double cell.

2. Implicit arguments.

Subroutine uses ~~COMMON~~ /CSLCM/ and /WRKCM/.

3. Notes.

a. Output of first cycle can only be obtained by print option = 2 or higher.

b. Sense lights 1 and 4 used.

c. Listing of $\ln r$ vs. $\omega^2 t$ can be obtained with plot option = 1, the last four values are the starting level ± 2 standard errors. Deletion of plot achieved with negative value for plot option.

d. On s^* listing, the starting level is the average of meniscus values for conventional runs, and the weighted starting intercept for synthetic boundary cell runs. The standard error of starting time will be asterisks (indeterminate) for synthetic boundary cell runs, since timer is assumed true.

F. D6-CS2 SUBROUTINE CFLS2 (LDEGRE, M, W, Y, XL, YO, SEYO, LPRINT).

1. Curve fitting least squares quadratic; $y = a + (b_1)(x_1) + (b_2)(x_2)$, $x_2 = (x_1)^2$; b_3 is tangent at mean: $b_3 = b_1 + 2(b_2)(\bar{x}_1)$;

$Y_0 \pm SE_{Y_0}$ is value at $x_1 = 0$. Weight is interpreted as number of replicate points, absolute value $< 10^{-10}$ causes omission of entire point, and reduction of the total number accordingly. Linear fit after quadratic if $L = 3$, $L = 2$ gives quadratic, $L = 1$ gives linear, and $L = 0$ gives weighted average of y only. $LPRINT = 1$ gives no printed output, $LPRINT = 2$ gives implicit output and $LPRINT = 3$ gives detailed output. Double precision on sums, differences of sums, parameters a , b_1 and b_2 , and SSE. Standard errors are single precision. Sequence of "comments" cards:

- a. Initialization.
 - b. Form sums and count points.
 - c. Compute means and correct sums for mean.
 - d. $L = 0$: constant least squares.
 - e. $L = 1$: linear least squares.
 - f. Reduce degree requested if too few points.
 - g. $L = 2$: quadratic least squares.
 - h. Determine $\underline{x}$ for given $\underline{y}$.
 - i. $L = 3$: linear least squares after quadratic.
2. Arguments.
- a. Explicit (floating point variables except where noted):
 - 1) LDEGRE 0: weighted average of $\underline{y}$ (constant least squares),
 1: linear least squares,
 2: quadratic least squares,
 3: linear and quadratic least squares.
 - 2) M Integer size of data array (cannot exceed 30).
 - 3) W (I) $\underline{w}$ array: weight of each $\underline{x}, \underline{y}$ point.
 If $\underline{w} < 10^{-10}$ weight considered zero and point is omitted.
 - 4) Y (I) $\underline{y}$ data array.
 - 5) XL (I) $\underline{x}$ data array.
 - 6) YO $\underline{y}_0$: value of $\underline{y}$ for which the value $\underline{x}_0$ from the fitted curve is desired.

- 7) SEYO standard error of given value of y_0 .
- 8) LPRINT negative, 0, 1: no printed output,
 2: print out of implicit arguments,
 3: print out of detailed sums of
 squares and sums corrected for
 mean in addition to implicit argu-
 ments.

b. Implicit arguments appear in ~~COMMON~~ /CS1CM/ (floating point except where noted):

- 1) A fitted constant (double precision).
- 2) SEA standard error of A.
- 3) B1 fitted first degree coefficient (double
 precision).
- 4) SEB1 standard error of B1.
- 5) B2 fitted second degree coefficient (double
 precision).
- 6) SEB2 standard error of B2.
- 7) YBAR $\bar{y}$: weighted average of input y data
 (double precision).
- 8) TBAR $\bar{x}_1$: weighted average of input x data
 (single precision).
- 9) SEYBAR standard error of $\bar{y}$.
- 10) WMIN minimum value of nonzero input weights.
- 11) WN the total weight referred to the point
 with the smallest nonzero weight,
 $(\Sigma W / WMIN)$.

- 12) N integer total of data points with non-zero weight ($N \leq M$). If $N = 0$, warning note is printed and return to calling program is made.
- 13) RSQ correlation coefficient squared (overwritten with linear value if $L = 3$).
- 14) SE residual standard error of the y data after least squares fitting.
- 15) F2 F-test value for quadratic term.
- 16) XO $\underline{x}_0$: value of x for given value y₀.
- 17) SEXO standard error of $\underline{x}_0$.
- 18) ~~CO~~PR $B_2/(B_1)^2$: special function of the two coefficients.
- 19) ~~SECO~~PR standard error of ~~CO~~PR.
- 20) B3 tangent to quadratic at $\bar{x}_1$.
- 21) SEB3 standard error of B_3 .
- 22) AP, SEAP, BP, SEBP, SEP, ~~XO~~P, ~~SEXO~~P
linear least square quantities corresponding to 1), 2), 3), 4), 14), 16), and 17), respectively.

c. Routine does not use ~~COMMON~~ /~~CCOXY~~/, /~~WORKCM~~/ at present.

3. Notes.

- a. The input weights are interpreted as relative, i.e., as

a number of replicates compared to the point with minimum weight.

Standard errors are computed from the number of entries, not the sum of the given weights.

b. If the standard error of the weighted mean of a set of means is desired and the given weights are reciprocals of variance, then it must be computed by the calling program from outputs WN and WMIN as

$$1/ \sqrt{(WN) (WMIN)}.$$

c. If there are too few points to fit a quadratic, the linear equation is computed and, similarly, the constant, if fewer than 2 points are given.

d. When the linear fit is requested ($L = 1$), the output two parameters appear both as A and B1, and as AP and BP.

4. Formulas.

a) Sums.

$$x_2 = x_1^2$$

$$S_{11} = \sum wx_1^2 - (\sum wx_1)^2 / \sum w$$

$$S_{12} = \sum wx_1 x_2 - (\sum wx_1) (\sum wx_2) / \sum w$$

$$S_{22} = \sum wx_2^2 - (\sum wx_2)^2 / \sum w$$

$$S_{1y} = \sum wx_1 y - (\sum wx_1) (\sum wy) / \sum w$$

$$S_{2y} = \sum wx_2 y - (\sum wx_2) (\sum wy) / \sum w$$

$$S_{yy} = \sum wy^2 - (\sum wy)^2 / \sum w$$

$$\bar{x}_1 = \sum wx_1 / \sum w$$

$$\bar{x}_2 = \sum wx_2 / \sum w$$

$$\bar{y} = \sum wy / \sum w$$

$$w_n = \sum w / w_{\min}$$

n = number of data points, not w_n

v is variance, cov is covariance

b. Constant.

$$\hat{y} = \bar{y}$$

$$v_{\bar{y}} = S_{yy} / [n(n-1) w_{\min}]$$

c. Linear.

$$\hat{y} = a + b_1 x_1$$

$$b_1 = S_{1y} / S_{11}$$

$$a = \bar{y} - b_1 \bar{x}_1$$

$$SSE = S_{yy} - b_1 S_{1y}$$

$$v_e = SSE / [(n-2) w_{\min}]$$

$$v_{\bar{y}} = v_e / \sum w$$

$$v_a = (1/\Sigma w + \bar{x}_1^2/S_{11}) v_e$$

$$v_{b_1} = v_e/S_{11}$$

$$r^2 = b_1 S_{1y}/S_{yy}$$

$$x_0 = (y_0 - a)/b_1$$

$$v_{x_0} = [v_{y_0} + v_a + 2x_0^2 v_{b_1} + 2x_0 \text{cov}(a, b_1)]/b_1^2$$

$$\text{cov}(a, b_1) = -\bar{x}_1 v_{b_1}$$

d. Quadratic.

$$\hat{y} = a + b_1 x_1 + b_2 x_2$$

$$D = S_{11} S_{22} - S_{12}^2$$

$$b_2 = (S_{11} S_{2y} - S_{12} S_{1y})/D$$

$$b_1 = (S_{22} S_{1y} - S_{12} S_{2y})/D$$

$$a = \bar{y} - b_1 \bar{x}_1 - b_2 \bar{x}_2$$

$$SSE = S_{yy} - b_1 S_{1y} - b_2 S_{2y}$$

$$v_e = SSE/[(n-3) w_{\min}]$$

$$v_{\bar{y}} = v_e/\Sigma w$$

$$v_a = [1/\Sigma w + (S_{22} \bar{x}_1^2 - 2S_{12} \bar{x}_1 \bar{x}_2 + S_{11} \bar{x}_2^2)/D] v_e$$

$$v_{b_1} = S_{22} v_e/D$$

$$v_{b_2} = S_{11} v_e / D$$

$$r^2 = (b_1 S_{1y} + b_2 S_{2y}) / S_{yy}$$

$$F_2 = b_2^2 / v_{b_2}$$

$$\text{cov}(b_1, b_2) = -S_{12} v_e / D$$

$$\sigma_{PR} = b_2 / b_1^2 = q$$

$$v_{\sigma_{PR}} = [v_{b_2} / b_1^2 + 4b_2^2 v_{b_1} / b_1^4 - 4b_2 \text{cov}(b_1, b_2) / b_1^3] / b_1^2$$

$$x_0 = \{-b_1 + [b_1^2 - 4b_2(a - y_0)]^{1/2}\} / (2b_2)$$

$$v_{x_0} = \text{assumed the same as for linear}$$

$$b_3 = b_1 + 2b_2 \bar{x}_1$$

$$v_{b_3} = v_{b_1} + 4\bar{x}_1^2 v_{b_2} + 4\bar{x}_1 \text{cov}(b_1, b_2)$$

e. Note.

The standard error of the zero time correction computed from the quadratic fit is approximate. When several components or cells are combined, the weighted mean of these individual zero time corrections depends on the standard errors. Hence, it is possible to get a slightly different result if a large constant change in all the timer values is made.

G. D7-CS2 SUBROUTINE PLOT (TITLE 1, TITLE 2, XX, YY, NDATA, NF, XLINE, YLINE, NX, NY, LPLT).

1. Line printer plot using alphabetical symbols to represent up to four sets of 100 points each and up to 20 reference x and 20 reference y lines.

2. The maximum and minimum values of each coordinate of the data are found. The data are transformed linearly such that the range is 0 to 99 for the x coordinate and 1 to 50 for the y coordinate. Each plot thus fills the page. The scale factors are given in the heading. Each point is used to locate a corresponding point in a Hollerith blank 50 x 100 array. The x reference lines are decimal points, and the y reference lines are negative signs. The symbols for the four sets of data are, respectively, asterisk *, letter ϕ , letter H, and letter X. If a location is already occupied by one of these four symbols, an equal sign is substituted. A listing of the input data before transformation is optional.

3. This program was modified from JØ*FSF PLOT 4 709/7090 FORTRAN II program by D.C. Martin, December 1961, Florida State University Computing Center and translated to FORTRAN IV eliminating the FAP subroutine originally required. Sequence of "comments" cards:

- a. Set up blank matrix.
- b. Locate maxima and minima.
- c. Find transform constants.

d. Add reference lines.

e. Transform points and insert in matrix with proper symbol.

f. List input data.

4. Arguments.

a. Explicit (floating point except where noted):

- 1) TITLE1, TITLE2 12 word (72H) arrays each for identification and appear at top of plot page, and top of listing of input data.
- 2) XX (I) x coordinate, dimensioned (100, 4).
- 3) YY (I) y coordinate, dimensioned (100, 4).
- 4) NDATA (I) integer number of points to be plotted in each set, dimensioned (4), may be zero in any set.
- 5) NF integer number of sets to be plotted, must not exceed 4.
- 6) XLINE (I) x reference lines, not necessarily equally spaced, dimensioned (20).
- 7) YLINE (I) y reference lines, not necessarily equally spaced, dimensioned (20).

- 8) NX integer number of x reference
lines, not to exceed 20.
- 9) NY integer number of y reference
lines, not to exceed 20.
- 10) LPL~~O~~T ~~n~~egative: return without
plotting,
0: make plot,
1: make plot and list input
data.

b. Implicit.

The subroutine uses ~~C~~OMM~~O~~N /~~W~~ORKCM/, REALCM (1000),
INTCM (1000). Equivalence statement can be deleted as desired.

H. D8-CS2 SUBROUTINE C~~O~~NC.

1. Subroutine for plateau and initial concentration, second
moment boundary position, and distribution function $g^*(s^*)$. Sequence
of "comments" cards:

- a. Check that x,y data have been measured.
- b. Factors and initialization.
- c. Main loop over all frames (through e).
- d. Loop over all components (through e).
- e. Loop over all points, sum for concentration, convert x
to s* and y to g*.
- f. Write output.
- g. Make $g^*(s^*)$ plot (CALL PL~~O~~T).

2. Implicit arguments.

Subroutine uses ~~COMMON~~ /CS1CM/, /CS2XY/, and /~~WORKCM~~/.

3. Notes.

a. Listing of $\underline{g}^*$ and $\underline{s}^*$ values can be obtained by option $LPL\cancel{O}T = 1$, deletion of plot by $LPL\cancel{O}T$ negative. Plot and listing are labeled as $\underline{g}^*$ but are actually ($\underline{c}^0 \underline{g}^*$) since $\underline{c}^0$ is not known when $\underline{g}^*$ is computed.

b. The plot incorporates a zero horizontal reference line ($\underline{g}^* = 0$), a zero vertical reference line ($\underline{s}^* = 0$), and a vertical reference line for each s-rate computed by the one-dimensional data analysis (using the internal s-rate value). All frames are superimposed. The equal sign is used for the common point between components (minimum) as well as multiple points. If more than four frames are involved, the same four plot symbols are reused, in order by frame, until a maximum of 100 points for each symbol is reached.

c. The $\underline{s}^*$ values are computed using the corrected times from the one-dimensional s-rate analysis for each cell. The combined zero time correction from both cells in double cell runs is not available at this point in the program. This can be achieved by resubmission of the data with the zero time entered as a timer correction and the kind option changed to 2, both on the run control card. A zero time error affects the $\underline{g}^*(\underline{s}^*)$ calculation but does not affect the concentration values.

d. The standard error of the ordinate measurement required to estimate the standard error of the summations is taken a) from the input, if given, for double sector cells, b) as $0.05/\tan \theta$, if not given, or c) as the residual standard error of the baseline polynomial curve fitting for single sector cells.

I. D9-CS2 SUBROUTINE FTEST (NDFL, NDFG, F, PRØB).

1. F-table for first column at 5 percent level. The number of degrees of freedom, if less than 10, is used to select tabular value. For 10 and above, $F=4.96$ is used.

2. Explicit arguments:

NDFL integer number of degrees of freedom of lesser sum of squares.

NDFG integer not used (if table is extended in the future, it will be the number of degrees of freedom of greater sum of squares).

F input floating point F value to be tested for significance.

PRØB output floating point probability with only 2 values available: 100, if F value is not significant and 4.999 if significant at 5 percent level.

3. Use subroutine with IF statement:

CALL FTEST (NDFL, NDFG, F, PRØB)

IF (PRØB - 5.0) α ; α , β

α significant at 5 percent level.

β not significant.

4. Notes: Called by D4CS2, D5CS2, D10CS2.

J. D10CS2 LSPOLY (TITLE, NCARDS, MIN, MAX, LWT, MEAN, INPUT, LFNCTN, LSCALE, LPRINT, XSCALE, YSCALE, XINPUT, YINPUT, WINPUT, XZERO).

1. Polynomial least squares curve fitting routine. Single precision for powers of x and sums of squares. Incorporate options to use lower polynomial degrees with the same sums of squares, compute residuals and make test of significance of added polynomial term.

Matrix inversion done by another subroutine.

2. Sequence of "comments" cards:

- a. Read, count and print input data.
- b. Use weights to count points and determine number of replicates. Transform input data as indicated by options.
- c. Convert weights to relative values, take logs if requested.
- d. Safeguard if too few data points.
- e. Set up powers of x and determine mean values and SYX .
- f. Set up XX and XY matrices (SXX , SXY , etc.).
- g. Take out mean if option $MEAN = 1$.
- h. Write heading.
- i. Write detail sums if option $LPRINT = 3$.
- j. (Main loop) least squares matrix inversion for all degrees from MIN to MAX (through p), ($CALL MATINV$).

k. Calculate residuals, variance-covariance matrix and residual standard error (SE).

l. Calculate standard error of coefficients and F-test value of last coefficient.

m. F-test for significance of last term (CALL FTEST).

n. Print coefficients, standard error, SE and F. Write significance note.

o. Print variance-covariance matrix if LPRINT = 2 or 3.

p. Reinvert matrix if added term not significant and if LPRINT = 2. Reinvert all matrices if LPRINT = 3 (for check on computation).

q. Set up conditions for reducing degree until significant last term (if this option chosen by setting MIN > MAX).

r. Write transformed data and residuals for all degrees of polynomial computed.

3. Arguments.

a. Explicit (floating point except where noted). Most of these correspond to the quantities supplied from cards described in III E and Fig. 2. Only the additional information needed is given here.

1) TITLE	12 word (72H) array for identification,
2) NCARDS	integer variable (may be overwritten by subroutine). If data are supplied by explicit

arguments (INPUT = 0), then NCARDS must be the number of data points and it will not be overwritten. If data are read from cards (INPUT = 1), then the program will count the cards and overwrite NCARDS. If return to calling program is requested after any number of blocks of data have been read from cards, NCARDS will be overwritten with the actual positive integer option IRETRN used to effect return.

3) MIN, MAX

integer lowest and highest degree, respectively, of polynomial to be fit (may be 0-6). MIN may be overwritten (see III E).

4) LWT

weight option (see III E). If LWT > 3, subroutine returns to calling program without computation.

5) MEAN

see III E.

6) INPUT

negative: return to calling program,

0: input data are explicit in arguments,
 1: input data are to be read from cards and overwrite corresponding explicit arguments.

7) LFNCTN	see III E, function,
8) LSCALE	see III E, scale option,
9) LPRINT	see III E, print option,
10) XSCALE, YSCALE	factors for transforming input data (selected by LSCALE option). XSCALE used especially to get slopes in Svedbergs,
11) X INPUT (I)	<u>x</u> data input (max 30),
12) Y INPUT (I)	<u>y</u> data input (max 30),
13) W INPUT (I)	weight data input (max 30) (interpreted by LWT option),
14) XZERO	constant to be subtracted from all <u>x</u> data.

b. Implicit.

Subroutine uses ~~COMMON~~ /WORKCM/ REALCM (1000), INTTCM (1000). Output appears in common by equivalence statements as follows:

1) B (K)	coefficients: REALCM (K + 300),
2) SEB (K)	standard error of B: REALCM (K + 310),

- 3) SE (J) residual standard error for
degree J-1: REALCM (J + 320),
- 4) F (J) F-test value for last coef-
ficient for degree J-1: REALCM
(J + 330),
- 5) XBAR (J) means of $\underline{x}$ to power J-1: REALCM
(J + 400),
- 6) YBAR mean of $\underline{y}$: REALCM (410),
- 7) VARCOV (K,L) variance-covariance matrix:
REALCM (M), where M = K+7 (L-1)+
500,
- 8) RESID (I,J) residual $\underline{y}_i - \hat{\underline{y}}_i$ for degree of
polynomial J-1: REALCM (M),
where M = I+30 (J-1)+700.
- 9) PROB probability corresponding to F-
test for significance of last
term of polynomial: REALCM (991),
- 10) WN weighted number, i.e., total sum
of relative weights used: REALCM
(992),
- 11) WMIN minimum nonzero weight, used to
compute relative weights: REALCM
(993),
- 12) SUMW sum of weights before converting
to relative values: REALCM (994).

4. Notes.

a. The following implicit arguments are overwritten for each degree of polynomial fit: B, SEB, VARCOV. They represent the final degree used, if more than one are requested.

b. The standard error of a weighted mean, when each $\underline{x}_i$ is itself a mean is $1/\sqrt{\sum W}$ where W is the reciprocal of the variance of each mean. It is necessary to use SUMW output [= (WN) (WMIN)] for this and not SE (1), which is calculated from the internal deviations of the data treated with relative weights.

c. Input format for data read from cards (INPUT = 1) is given in III A,E.

d. Values from this least squares inversion may be slightly different from those of D6-CS2 because of using double precision there for some quantities, and the SE when using the log option is not converted to the antilog here.

e. Return to calling program after any number of blocks of data can be achieved with positive integer in cols. 73, 74 or 75 of a dummy identification card (typically use: 111). The integer actually used is overwritten on NCARDS and is available to calling routine.

5. Formulas.

a. Polynomial of degree $\underline{n}$.

$$\hat{y} = b_1 + b_2 x + b_3 x^2 + \dots + b_{n+1} x^n$$

b. Generalized notation for the fitted value $\hat{y}$.

$$\begin{aligned}
\hat{y}_1 &= b_1 x_{1,1} + \dots + b_j x_{1,j} + \dots + b_{\text{last}} x_{1,\text{last}} \\
&\vdots \\
\hat{y}_i &= b_1 x_{i,1} + \dots + b_j x_{i,j} + \dots + b_{\text{last}} x_{i,\text{last}} \\
&\vdots \\
\hat{y}_{\text{ndata}} &= b_1 x_{\text{ndata},1} + \dots + b_j x_{\text{ndata},j} + \dots + \\
&\quad b_{\text{last}} x_{\text{ndata},\text{last}}
\end{aligned}$$

where (x_i, y_i) is a general inputdata point and

$x_{i,1} = 1, x_{i,2} = x_i, x_{i,3} = x_i^2$, etc., and last = degree

1.

The minimum nonzero weight $w_{\min}$ is found and used to convert all weights to relative values.

c. $X(I,J)$: powers of X matrix.

		column j					
		1	2	3	4	...	LAST
row i	1	1	↑	↑	↑		
	2	1	x	squares			.
	.		data				.
	.				cubes		.
	NDATA	1	↓	↓	↓		

$$x_{i,j} = (x_{1,2}) (x_{1,j-1})$$

$$\bar{x}_j = \sum_i w_i x_{i,j} / \sum w_i$$

d. $XX(JR\emptyset W, JC\emptyset L)$: square matrix consisting of sums of squares of powers of $\underline{x}$.

$XX(JR\emptyset W, JC\emptyset L)$ is $S_{JR\emptyset W, JC\emptyset L}$ but computed to take advantage of the special symmetry of this matrix. Not only is $S_{k,l} = S_{l,k}$, but $S_{k,l} = S_{k-1,l+1}$. The first relationship is evident from the definition of $S_{k,l}$. The second follows from the definition of the $\underline{x}_{i,k}$ as powers:

$$x_{i,k} = x_i^{k-1}. \text{ Thus, } (x_{i,k}) (x_{i,l}) = (x_i^{k-1}) (x_i^{l-1}) = (x_i^{k-2}) (x_i^l) = (x_{i,k-1}) (x_{i,l+1}).$$

It is only necessary to compute the first row and last column and then set $XX(JR\emptyset W, J\emptyset L) = XX(JR\emptyset W-1, J\emptyset L+1)$. Note that this special relationship is not valid if the sums are corrected for the mean. The mean can be taken out of all except the upper left hand corner according to $C_{k,\ell} \equiv S_{k,\ell} - (\sum w_i) \bar{x}_k \bar{y}_\ell$.

e. SYY , $\bar{y}$ and $XY(JR\emptyset W)$: vector of sums of cross terms of $\underline{x}$ and $\underline{y}$.

$$SYY = \sum w_i y_i^2$$

$$\bar{y} = \sum w_i y_i / \sum w_i$$

$$S_{k,y} \equiv \sum_1^{NDATA} w_i x_{ik} y_i$$

$$XY(JR\emptyset W) \text{ is } S_{JR\emptyset W,y}$$

The mean is taken out by

$$C_{k,y} = S_{k,y} - (\sum w_i) \bar{x}_k \bar{y}$$

f. The coefficients and inverse matrix are obtained by matrix algebra used in SUBROUTINE MATINV. It is not necessary to recompute the sums of squares for each degree of polynomial used. The XX matrix is set up for the highest degree $LAST = MAX + 1$, and each polynomial requested is computed by inverting the upper left hand submatrix of order $K\emptyset RDER = DEGREE + 1$. If the mean is taken out, the rank of the matrix is the same, but the first row and first column have all zeros except for the first

element. This effectively reduces the order by one, usually improves the scaling of the matrix, and gives greater precision in the inversion.

g. The variance of the y measurements unaccounted for by the least squares fitting, the residual random error contribution, is computed from the residuals $y_i - \hat{y}_i$ and the number of degrees of freedom NDF as

$$SEE = \sum w_i (y_i - \hat{y}_i)^2$$

$$NDF = NDATA - KORDER$$

$$VE = SSE/NDF$$

The matrix computed by multiplying each element of the inverse matrix by VE is called here the variance-covariance matrix. The residual standard error referred to the point with the fewest equivalent replicates is

$$SE = \sqrt{VE}.$$

h. The standard error of each coefficient is computed as the square root of the corresponding main diagonal member of the variance-covariance matrix. If the mean was taken out before matrix inversion, the first coefficient b_1 is actually $\bar{y}$ and must be converted back as

$$b_1 - (b_2 \bar{x}_2 + \dots + b_{KORDER} \bar{x}_{KORDER})$$

and the standard error computed from the variance-covariance matrix VARCOV as

$$SE_{b_1} = \left[\sum_{JROW}^{KORDER} \sum_{JCOL}^{KORDER} (VARCOV_{JROW, JCOL}) (\bar{x}_{JROW}) (\bar{x}_{JCOL}) \right]$$

i. The F-test value for the significance of the additional reduction in the sums of squares by adding one more term of the polynomial is equivalent to the square of the Student's t-test value of the last coefficient

$$F = (b_{KORDER} / SE_{b_{KORDER}})^2$$

with the number of degrees of freedom for that degree

$$NDF = NDATA - KORDER.$$

K. D11CS2 SUBROUTINE MATINV (XARRAY, A, N, YARRAY, B, M, DETERM, MAXDX, MAXDY, LINPUT, LPRINT).

1. Matrix inversion with accompanying solution of linear equations.

2. Program obtained from SHARE Distribution Number 664, written by B.S. Garbow, February 23, 1959, Argonne National Laboratory, ANF402. Single precision matrix inversion by pivotal method (Gauss-Jordan elimination). It was translated to FORTRAN IV using variable dimensions not to exceed a 10 x 10 square matrix for inversion, but there is no limit on the number of y array columns for specific linear equation solutions. Sequence of "comments" cards:

- a. Initialization.
- b. Search for pivot element.
- c. Interchange rows to put pivot element on diagonal.
- d. Divide pivot row by pivot element.
- e. Reduce non-pivot rows.

- f. Determine coefficients of solution to linear equations.
- g. Interchange columns.
- h. Write input matrix, inverted matrix, input constant array and least squares coefficients.

3. Explicit arguments (floating point except where noted):

- a. XARRAY (I,J) input square matrix, rank N,
- b. A (I,J) output inverted square matrix, rank N,
- c. N integer rank of matrix (must be >0,
but must not exceed MAXDX),
- d. YARRAY (I,K) input rectangular constants array,
row rank N, column rank M,
- e. B (I,K) output coefficients array, row rank
N, column rank M,
- f. M integer number of sets of constants
for sets of linear solutions to be
computed corresponding to the number
of column vectors in YARRAY (must not
exceed MAXDY). Negative or zero
gives inversion only.
- g. DETERM determinant of input square matrix,
- h. MAXDX integer maximum dimension of input
square matrix and first dimension of
constants matrix (must not exceed 10),
- i. MAXDY integer maximum second dimension of
constants array (no limit),

- j. LINPUT integer option not used at present,
 supply dummy argument,
- k. LPRINT negative, 0: no printed output,
 1: input matrix, inverted matrix,
 input constants array, solutions to
 linear equations printed.

4. Notes.

- a. No test for an ill-conditioned matrix is made, FORTRAN
IV monitor will supply overflow or under flow warning notes.
- b. For this program (CS2), MAXDX = 7, MAXDY = 1.

VII. Acknowledgments and Disclaimer.

The use of digital computers for ultracentrifuge data processing was started in the summer of 1956 when the author was a research collaborator with W.L. Hughes, Medical Department, Brookhaven National Laboratory. At that time, portion of a table of useful plate reading functions was computed on the UNIVAC. These tables have been completed by the author while at Rockefeller Institute and Plum Island Animal Disease Laboratory (Trautman, 1956, 1963). The limited memory and plug board arrangement of the computer at that time slowed development of direct data processing. A fresh look was made in the fall of 1962 when I.H. Billick gave the author and P.N. Reilly, Medical Department, an early version of his quadratic least squares one-dimensional data processing program for a

single component in a single cell written in FORTRAN II (Billick, 1962 b,c). This was slowly rewritten and extended slightly using the IBM 7090 then available at Brookhaven.

A major investigation of the applicability of digital computers was made in 1964 when the author was on sabbatical leave. The extension to four components and incorporation of a line-printer plot was done at Florida State University under E. Frieden of the Institute of Molecular Biophysics. The extension to double cells and applicability to a semiautomatic digitized comparator (Benson-Lehner OSCAR) was made at the University of Birmingham, England, under G.A. Gilbert and S.P. Spragg. The foundation of the statistical application was queried when it became apparent in processing a large number of hemoglobulin runs made there by E. Chiacone that the initial s-rate concept of Billick (1962a) from the first term of the least squares parabola had much too large a standard error to be useful with aqueous data that were essentially "straight".

Sponsored by E.A. Popenoe, Medical Department, the author continued as a research collaborator at Brookhaven in 1965 to incorporate the tangent to the parabola at the mean time for the internal s-rate, to extend the program for two-dimensional data with the second line-printer data editing plot, to incorporate the numerous cautionary notes and program options and to convert it entirely to FORTRAN IV. The data input routine was designed to accept the output from a digitized Gaertner comparator patterned after ones used in the Bubble Chamber Group, and recently described by Bartulovitch and Ward (1965).

This program shows, unmistakably, its evolutionary history containing still many awkward and vestigial steps. It is hoped that it can be simplified and rewritten later. It has been shown to be useful in its present condition and it has been checked on numerous hand calculated data and in many types of situations. However, any ultimate correctness cannot be claimed at this time.

A preliminary report on the internal s-rate and editing concepts of this program was made at the Biophysical Society National Meeting, February, 1966, Boston.

VIII. References

- Bartulovitch, J.J., and Ward, W.H. (1965). Recording, plate-measuring system for the ultracentrifuge. *Anal. Biochem.* 11, 42.
- Billick, I.H. (1962a). The variation of the sedimentation coefficient with pressure and concentration. *J. Phys. Chem.* 66, 565.
- Billick, I.H. (1962b). Fortran program for the calculation of sedimentation coefficients. Esso Research and Engineering Company, Analytical Research Division, Linden, N.J. ARD Memorandum No. 62-50, Nov. 1, 1962.
- Billick, I.H. (1962c). Velocity sedimentation studies on pressure and concentration dependent systems. *J. Phys. Chem.* 66, 1941.
- Davies, O.L. (1961). Statistical methods in research and production. Oliver and Boyd, Edinburgh.
- Lauffer, M.A. (1944). The influence of concentration upon the sedimentation rate of tobacco mosaic virus. *J. Am. Chem. Soc.* 66, 1195.
- Snedecor, G.W. (1956). Statistical Methods. Iowa State College Press, Ames, Iowa, Fifth edition, p. 419.
- Trautman, R. (1956). Operating and comparing procedures facilitating schlieren pattern analysis in analytical ultracentrifugation. *J. Phys. Chem.* 60, 1211.
- Trautman, R. (1963). Computational methods in ultracentrifugation. In "Ultracentrifugal Analysis in Theory and Experiment", J.W. Williams, ed., Academic Press.
- Wales, M. (1959). The effect of pressure on sedimentation rate. *J. Am. Chem. Soc.* 81, 4758.

\$JOB		TRAUTMAN	
\$EXECUTE	IBJOB		
\$IBJOB	MAP		
\$IBFTC CS2	LIST,M94		

C*****PROGRAM CS2 S-RATE AND CONCENTRATION IN MOVING BOUNDARY CENTRIFUGE	CS2	001
C	CS2	2
DIMENSION TITLE(12),XINPUT(30),WINPUT(30),YINPUT(30)	CS2	003
C	CS2	4
10 LRETRN = 1	CS2	005
CALL MAIN2 (LRETRN)	CS2	6
INPUT = 1	CS2	007
NCARDS = 1	CS2	8
MIN = 1	CS2	009
MAX = 1	CS2	10
LWT = 1	CS2	011
LFNCTN = 0	CS2	12
LSCALE = 0	CS2	013
LPRINT = 1	CS2	14
XSCALE = 1.0	CS2	015
YSCALE = 1.0	CS2	16
XZERO = 0.0	CS2	017
CALL LSPOLY (TITLE,NCARDS,MIN,MAX,LWT,MEAN,INPUT,LFNCTN,LSCALE,	CS2	18
11 LPRINT,XSCALE,YSCALE,XINPUT,YINPUT,WINPUT,XZERO)	CS2	019
GO TO 10	CS2	20
END	CS2	021

\$IBFTC D1-CS2 LIST,M94		
C*****DIRECTOR PROGRAM FOR S-RATE AND CONCENTRATION CALCULATIONS	D1	001
C	D1	2
SUBROUTINE MAIN2 (LRETRN)	D1	003
C	D1	4
COMMON /CS1CM/ A,B1,B2,YBAR,ALPHA(12),F2,FRAME(30),NCOMP,NFRAME,N,	D1	005
10MSQT(30),RBEGLN,RBEG,RMEN(30),RPK(30,4),RSQ,SEA,SEB1,SEB2,SE,	D1	6
2SETZOA,SEX0,SEYBAR,STAR(30,4),TIME(30),TZOA,WMIN,WN,X0,AP,BP,SEAP,	D1	007
3SEBP,SEP,TBAR,OMF,SERBLN,SPEED,REFR,FMOME,LKIND,LPRINT,LPLOT,	D1	8
4LINPUT,LBEGWT,NCELL,Z,XLINE(20),YLINE(20),NDATA(4),XX(100,4),	D1	009
5YY(100,4),COPR,SECOPR,SERBEG,XOP,SEXOP,B3,SEB3,STANRM(4,2),	D1	10
6SESTAN(4,2),DILN(4,2),METHOD,KIND(10),SEORD(10,2)	D1	011
DOUBLE PRECISION A,B1,B2,YBAR	D1	12
COMMON /CS2XY/ XDATA(10,50,2),START(10,9,2),RBAR(10,4),	D1	013
1STARRB(10,4),STARRM(10,4),CP(10,4),CU(10,4),TOPX(10,2),TOPY(10,2),	D1	14
2 BOTX(10,2),BOTY(10,2),XREF,	D1	015
3MENW(30,2),PKX(30,4,2),PKW(30,4,2),PKLN(30,4,2),NCOMPS(2),	D1	16
4FLAGCL(2),FY,	D1	017
5BMENX(30,2),BMENW(30,2),ANGLE(30)	D1	18
INTEGER START,FLAGCL,FLAGFR	D1	019
REAL MENX,MENW	D1	20
COMMON /WORKCM/REALCM(1000),INTCM(1000)	D1	021
C	D1	22
DIMENSION W(2),Y(2),SERB(2),TZERO(2),SET(2),BEGLN(2),SEBL(2),RB(2)	D1	023
C*****READ RUN IDENTITY CARD AND RUN CONTROL CARD	D1	24
5 READ (5,1005) ALPHA,LRETRN	D1	025
1005 FORMAT (12A6,I3)	D1	26
IF (LRETRN) 10,10,6	D1	027
6 RETURN	D1	28
10 READ (5,1010) SPEED,REFR,FMOME,METHOD,KIND(1),LPRINT,LPLOT,	D1	029
11 LINPUT,(KIND(I),I=2,6),TMRZRO,FY	D1	30
1010 FORMAT(F9.1,2F10.5,10I2,2F10.5)	D1	031
11 OMF = (((SPEED*0.10471976)**2)*60.0)*1.E-13	D1	32
12 CALL SLITE (0)	D1	033

XREF = REFR * FMOME	D1	34
Z = 1.0E20	D1	035
LBEGWT = KIND(6)	D1	36
C*****READ DATA	D1	037
30 IF (LINPUT - 2) 31,33,33	D1	38
31 CALL DATA1	D1	039
GO TO 34	D1	40
33 CALL DATA3	D1	041
C*****MAIN LOOP FOR ALL CELLS	D1	42
34 NSAVED = NCELL	D1	043
DO 87 NCELL = 1,NSAVED	D1	44
C*****CHECK THAT CELL HAS DATA	D1	045
35 IF (FLAGCL(NCELL)) 87,87,36	D1	46
36 NCOMP = NCOMPS(NCELL)	D1	047
IF (KIND(NCELL)) 41,41,42	D1	48
41 LKIND = KIND(1)	D1	049
GO TO 50	D1	50
42 LKIND = KIND(NCELL)	D1	051
C*****MAKE INPUT TIMER ZERO CORRECTION, CONVERT AND TEST FOR LEAK	D1	52
50 IF (ABS(TMRZRO) - 1.E-10) 54,54,51	D1	053
51 CALL SLITE (4)	D1	54
TZOA = TMRZRO	D1	055
IF (NCELL - 1) 54,52,54	D1	56
[52 DO 53 I = 1,NFRAME	D1	057
53 TIME(I) = TIME(I) - TMRZRO	D1	58
54 CALL CKDATA	D1	059
C*****ADD STARTING LEVEL IF LKIND = 2	D1	60
IF (LKIND - 2) 59,56,59	D1	061
56 NFRAME = NFRAME + 1	D1	62
OMSQT (NFRAME) = 0.0	D1	063
TIME(NFRAME) = 0.0	D1	64
DO 58 J= 1,NCOMP	D1	065
RPK(NFRAME,J) = RBEG	D1	66
PKLN(NFRAME,J,NCELL) = RBEGLN	D1	067
FRAME(NFRAME) = 0.0	D1	68
RMEN(NFRAME) = 0.0	D1	069
MENW(NFRAME,NCELL) = 0.0	D1	70
58 PKW(NFRAME,J,NCELL) = 1.0	D1	071
C*****COMPUTE S-RATE FOR ALL COMPONENTS AND SAVE RESULTS	D1	72
59 CALL SRATE2	D1	073
IF (LINPUT - 1) 999,999,70	D1	74
70 TZERO(NCELL) = TZOA	D1	075
SET(NCELL) = SETZOA	D1	76
BEGLN(NCELL) = RBEGLN	D1	077
SEBL(NCELL) = SERBLN	D1	78
RB(NCELL) = RBEG	D1	079
SERB(NCELL) = SERBEG	D1	80
IF (LKIND - 2) 80,75,80	D1	081
75 NFRAME = NFRAME - 1	D1	82
C*****COMPUTE CONCENTRATION FOR EACH COMPONENT IN EACH FRAME	D1	083
80 CALL CONC	D1	84
87 CONTINUE	D1	085
C*****ADD RESPECTIVE STARTING LEVEL AT WEIGHTED ZERO TIME OF BOTH CELLS	D1	86
C IF NEITHER IS A SYNTHETIC BOUNDARY CELL RUN, RECOMPUTE ALL S-RATES	D1	087
IF (NSAVED - 1) 999,999,201	D1	88
[201 DO 209 NCELL = 1,NSAVED	D1	089
IF (KIND(NCELL) - 2) 202,202,999	D1	90
202 W(NCELL) = (1.0/SET(NCELL))*2	D1	091
Y(NCELL) = TZERO(NCELL)	D1	92
[209 CONTINUE	D1	093
CALL CFLS2 (0,NSAVED,W,Y,TIME,0.0,0.0,LPRINT)	D1	94

TZOA = SNGL(YBAR)	D1	95
SETZOA=SQRT(1.0/(WN*WMIN))	D1	096
OMT0 = OMF*TZOA	D1	97
DO 221 IFRAME = 1,NFRAME	D1	098
221 OMSQT(IFRAME) = OMSQT(IFRAME) - OMT0	D1	99
LKIND = 0	D1	100
LBEGWT = 1	D1	101
CALL SLITE (4)	D1	102
DO 240 NCELL = 1,NSAVED	D1	103
RBEG = RB(NCELL)	D1	104
SERBEG = SERB(NCELL)	D1	105
RBEGLN = RBEGLN(NCELL)	D1	106
SERBLN = SEBL(NCELL)	D1	107
NCOMP = NCOMPS(NCELL)	D1	108
240 CALL SRATE2	D1	109
999 GO TO 5	D1	110
END	D1	111

\$IBFTC D2-CS2 LIST,M94

C*****READ ROUTINE FOR ONE-DIMENSIONAL DATA TRANSCRIBED FROM COMPARATOR	D2	1
C LINPUT=0,1. SINGLE CELL, SINGLE REFERENCE, NO REPLICATES	D2	002
C	D2	3
C SUBROUTINE DATA1	D2	004
C	D2	5
COMMON /CSICM/ A,B1,B2,YBAR,ALPHA(12),F2,FRAME(30),NCOMP,NFRAME,N,	D2	006
1OMSQT(30),RBEGLN,RBEG,RMEN(30),RPK(30,4),RSQ,SEA,SEB1,SEB2,SE,	D2	7
2SETZOA,SEX0,SEYBAR,STAR(30,4),TIME(30),TZOA,WMIN,WN,X0,AP,BP,SEAP,	D2	8
3SEBP,SEP,TBAR,OMF,SERBLN,SPEED,REFR,FMOME,LKIND,LPRINT,LPLOT,	D2	009
4LINPUT,LBEGWT,NCELL,Z,XLINE(20),YLINE(20),NDATA(4),XX(100,4),	D2	10
5YY(100,4),COPR,SECOPR,SERBEG,XOP,SEXOP,B3,SEB3,STANRM(4,2),	D2	011
6SESTAN(4,2),DILN(4,2),METHOD,KIND(10),SEORD(10,2)	D2	12
DOUBLE PRECISION A,B1,B2,YBAR	D2	013
COMMON /CS2XY/ XDATA(10,50,2),START(10,9,2),RBAR(10,4),	D2	14
1STARRB(10,4),STARRM(10,4),CP(10,4),CO(10,4),TOPX(10,2),TOPY(10,2),	D2	015
2 BOTX(10,2),BOTY(10,2),XREF, MENX(30,2),	D2	16
3MENW(30,2),PKX(30,4,2),PKW(30,4,2),PKLN(30,4,2),NCOMPS(2),	D2	017
4FLAGCL(2),FY, YDATA(10,50,2),NPOINT(10,4),FLAGFR(30,2),	D2	18
5BMENX(30,2),BMENW(30,2),ANGLE(30)	D2	019
INTEGER START,FLAGCL,FLAGFR	D2	20
REAL MENX,MENW	D2	021
COMMON /WORKCM/REALCM(1000),INTCM(1000)	D2	22
C	D2	023
NCOMP = 1	D2	24
NCELL = 1	D2	025
ISTOP = 0	D2	26
C*****READ DATA FRAME BY FRAME ASSIGNING ZERO WEIGHT IF ABSOLUTE VALUE	D2	027
C OF ENTRY LESS THAN E-10	D2	28
10 DO 29 I =1,30	D2	029
IF (LINPUT) 11,11,12	D2	30
11 READ (5,1011) FRAME(I),TIME(I),REFX,(PKX(I,J,NCELL),J=1,4),	D2	031
1MENX(I,NCELL),ISTOP	D2	32
1011 FORMAT(A4,F5.1,6F10.5,I3)	D2	033
GO TO 13	D2	34
C*****LINPUT = 1HAS TIME IN REF FIELD, DISTANCES IN ROTOR CM.	D2	035
12 READ (5,1011) FRAME(I),REFX,TIME(I),(PKX(I,J,NCELL),J=1,4),	D2	36
1MENX(I,NCELL),ISTOP	D2	037
BMENX(I,NCELL) = Z	D2	38
REFX = 0.0	D2	039
XREF = 0.0	D2	40
13 REFX = REFX - XREF	D2	041

IF (ABS(MENX(I,NCELL)) - 1.E-10) 14,14,15	D2	42
14 MENW(I,NCELL) = 0.0	D2	043
GO TO 16	D2	44
15 MENW(I,NCELL) = 1.0	D2	045
MENX(I,NCELL) = MENX(I,NCELL) - REF	D2	46
16 DO 22 J = 1,4	D2	047
IF (ABS(PKX(I,J,NCELL)) - 1.E-10) 18,18,20	D2	48
18 PKW(I,J,NCELL) = 0.0	D2	049
GO TO 22	D2	50
20 PKW(I,J,NCELL) = 1.0	D2	051
PKX(I,J,NCELL) = PKX(I,J,NCELL) - REF	D2	52
NCOMP= MAX0(NCOMP,J)	D2	053
22 CONTINUE	D2	54
IF (ISTOP) 29,29,30	D2	055
29 CONTINUE	D2	56
30 NFRAME = I	D2	057
NCOMPS(NCELL) = NCOMP	D2	58
FLAGCL(NCELL) = 1	D2	059
999 RETURN	D2	60
END	D2	061

\$IBFTC D3-C52. LIST,M94

C*****READ ROUTINE FOR ONE AND TWO DIMENSIONAL DATA	D3	001
C ESPECIALLY DESIGNED FOR DIGITIZED COMPARATOR. LINPUT=2,3	D3	2
C	D3	003
SUBROUTINE DATA3	D3	4
C	D3	005
COMMON /CS1CM/ A,B1,B2,YBAR,ALPHA(12),F2,FRAME(30),NCOMP,NFRAME,N,	D3	6
10MSQT(30),RBEGLN,RBEG,RMEN(30),RPK(30,4),RSQ,SEA,SEB1,SEB2,SE,	D3	007
2SETZOA,SEX0,SEYBAR,STAR(30,4),TIME(30),TZOAWMIN,WN,XO,AP,BP,SEAP,	D3	8
3SEBP,SEP,TBAR,OMF,SERBLN,SPEED,REFR,FMOME,LKIND,LPRINT,LPLLOT,	D3	009
4LINPUT,LBEGWT,NCELL,Z,XLINE(20),YLINE(20),NDATA(4),XX(100,4),	D3	10
5YY(100,4),COPR,SECOPR,SERBEG,XOP,SEXOP,B3,SEB3,STANRM(4,2),	D3	011
6SESTAN(4,2),DILN(4,2),METHOD,KIND(10),SEORD(10,2)	D3	12
DOUBLE PRECISION A,B1,B2,YBAR	D3	013
COMMON /CS2XY/ XDATA(10,50,2),START(10,9,2),RBAR(10,4),	D3	14
1STARRB(10,4),STARRM(10,4),CP(10,4),CO(10,4),TOPX(10,2),TOPY(10,2),	D3	015
2 ROTX(10,2),ROTY(10,2),XREF, MENX(30,2),	D3	16
3MENW(30,2),PKX(30,4,2),PKW(30,4,2),PKLN(30,4,2),NCOMPS(2),	D3	017
4FLAGCL(2),FY, YDATA(10,50,2),NPOINT(10,4),FLAGFR(30,2),	D3	18
5BMENX(30,2),BMENW(30,2),ANGLE(30)	D3	019
INTEGER START,FLAGCL,FLAGFR	D3	20
REAL MENX,MENW	D3	021
COMMON /WORKCM/REALCM(1000),INTCM(1000)	D3	22
C	D3	023
DIMENSION ID1(200,2),ID2(200,2),VALUE(200,2),KARD1(9),KARD2(9),	D3	24
1KARD3(9),CARD(9),KOUNT(13,2),XA(13,2),MAXREP(2),LBASLN(5),	D3	025
2WORK(5,13,2)	D3	26
DIMENSION W(30),X(30),Y(30),NFRXY(2)	D3	027
EQUIVALENCE (CARD(1),REALCM(601)),(XA(1,1),	D3	28
1REALCM(611)),(WORK(1,1,1),REALCM(701)),(ID1(1,1),INTCM(1)),	D3	029
2(ID2(1,1),INTCM(401)),(KARD1(1),INTCM(901)),(KARD2(1),INTCM(911)),	D3	30
3(KARD3(1),INTCM(921)),(KOUNT(1,1),INTCM(931)),(MAXREP(1),INTCM(961),	D3	031
4), (LBASLN(1),INTCM(971)),(NFRXY(1),INTCM(981)),(W(1),REALCM(901))	D3	32
5, (X(1),REALCM(931)),(Y(1),REALCM(961))	D3	033
C*****HEADING FOR INPUT DATA ON PRINTOUT	D3	34
IF (LPRINT) 11,10,10	D3	035
10 WRITE (6,1010) ALPHA	D3	36
1010 FORMAT(1H16X12A6,9X10HINPUT DATA//7H FRAME16X109HTIMER PEAK 1	D3	037
1PEAK 2 PEAK 3 PEAK 4 PEAK 5 PEAK 6 PEAK 7 PEAK 8 TOP MEN BOTD3	D3	38

2 MEN IN REF OUT REF CENTER/40X38HX,Y DATA WITH FIRST TWO DIGITS	OD3	39
3F CODE)	D3	040
C*****INITIALIZATION	D3	41
11 ISTOP = 0	D3	042
LSAVE = LPRINT	D3	43
NCELL = 1	D3	044
MXCELL = 2	D3	45
MXCOMP = 4	D3	046
MXX = 30	D3	47
MXXY = 10	D3	048
MXREPL = 5	D3	49
MXCARD = 30	D3	050
MXPTS = 200	D3	51
DO 12 LCELL = 1,MXCELL	D3	052
FLAGCL(LCELL) = 0	D3	53
NCOMPS(LCELL) = 0	D3	054
NFRXY(LCELL) = 0	D3	55
DO 12 IFRAME = 1,MXXY	D3	056
TOPX(IFRAME,LCELL) = Z	D3	57
TOPY(IFRAME,LCELL) = Z	D3	058
BOTX(IFRAME,LCELL) = Z	D3	59
BOTY(IFRAME,LCELL) = Z	D3	060
START(IFRAME,9,LCELL) = 0	D3	61
XDATA(IFRAME,1,LCELL) = Z	D3	062
YDATA(IFRAME,1,LCELL) = Z	D3	63
DO 12 JPEAK = 1,MXCOMP	D3	064
START(IFRAME,JPEAK,LCELL) = 0	D3	65
12 CONTINUE	D3	066
C*****MAIN LOOP OVER ALL FRAMES	D3	67
IFRAME = 0	D3	068
DO 300 III = 1,MXX	D3	69
IFRAME = IFRAME + 1	D3	070
C*****INITIALIZATION AND READ FRAME CONTROL CARD	D3	71
ICONT = 0	D3	072
IWARN = 0	D3	73
DO 14 LCELL = 1,MXCELL	D3	074
FLAGFR(IFRAME,LCELL) = 0	D3	75
MENX(IFRAME,LCELL) = Z	D3	076
MENW(IFRAME,LCELL) = 0.0	D3	77
BMENX(IFRAME,LCELL) = Z	D3	078
BMENW(IFRAME,LCELL) = 0.0	D3	79
DO 13 JPEAK = 1,MXCOMP	D3	080
PKW(IFRAME,JPEAK,LCELL) = 0.0	D3	81
PKX(IFRAME,JPEAK,LCELL) = Z	D3	082
13 CONTINUE	D3	83
DO 14 KODE = 1,13	D3	084
KOUNT(KODE,LCELL) = 0	D3	85
DO 14 KK = 1,5	D3	086
14 WORK(KK,KODE,LCELL) = Z	D3	87
15 READ (5,1015) RUN,FRAME(IFRAME),TIME(IFRAME),ANGLE(IFRAME),	D3	088
1(LBASLN(KD),KD=1,5),SEY	D3	89
1015 FORMAT(A5,A4,F10.5,F10.5,5I2,F5.3)	D3	090
C*****READ DATA	D3	91
KTOTAL = 0	D3	092
LCELL = 1	D3	93
KODE = 1	D3	094
IREPL = 0	D3	95
DO 35 KARD = 1,MXCARD	D3	096
C*****ALTERNATE INPUT FOR 2 DIGIT CODE (LINPUT = 2)	D3	97
IF (LINPUT = 2) 16,16,20	D3	098
16 READ (5,1016) (KARD2(KD),KARD3(KD),CARD(KD),KD=1,9)	D3	99

1016	FORMAT(9(2I1,F6.3))	D3	100
	DO 19 KD = 1,9	D3	101
	IF (KARD2(KD) - 5) 18,17,17	D3	102
17	KARD1(KD) = KARD2(KD)	D3	103
	KARD2(KD) = 0	D3	104
	GO TO 19	D3	105
18	KARD1(KD) = 0	D3	106
19	CONTINUE	D3	107
	GO TO 21	D3	108
	C*****REGULAR INPUT USING 3 DIGIT CODE	D3	109
20	READ (5,1020) (KARD1(KD),KARD2(KD),KARD3(KD),CARD(KD),KD=1,9)	D3	110
1020	FORMAT(9(3I1,F5.3))	D3	111
	C*****EDIT EACH RECORD AND SORT BY CELL	D3	112
21	DO 35 KD = 1,9	D3	113
	INDEX = KARD3(KD) + 1	D3	114
	GO TO (24,25,25,25,25,90,22,38,39,37),INDEX	D3	115
22	IF (KOUNT(KODE,LCELL)) 35,35,23	D3	116
23	KOUNT(KODE,LCELL) = KOUNT(KODE,LCELL) - 1	D3	117
	GO TO 35	D3	118
24	KARD3(KD) = 1	D3	119
25	IF (CARD(KD) - 1.E-20) 35,35,26	D3	120
26	IF (KARD1(KD) - 4) 29,29,27	D3	121
27	KODE = KARD1(KD) + 4	D3	122
	IF (KARD1(KD) - 6) 31,31,28	D3	123
28	KARD3(KD) = 1	D3	124
	GO TO 31	D3	125
29	IF (KARD2(KD) - 9) 30,35,35	D3	126
30	KODE = KARD2(KD)	D3	127
31	IF (KARD3(KD) - MXCELL) 32,32,35	D3	128
32	LCELL = KARD3(KD)	D3	129
	NCELL = MAX0 (NCELL,LCELL)	D3	130
	IF (KOUNT(KODE,LCELL) - MXREPL) 33,35,35	D3	131
33	KOUNT(KODE,LCELL) = KOUNT(KODE,LCELL) + 1	D3	132
	IREPL = KOUNT(KODE,LCELL)	D3	133
	WORK(IREPL,KODE,LCELL) = CARD(KD)	D3	134
35	CONTINUE	D3	135
	GO TO 39	D3	136
37	ISTOP = 1	D3	137
	GO TO 39	D3	138
38	ICONT = 1	D3	139
39	IF (IREPL) 999,90,50	D3	140
	C*****COUNT MAX NO. OF REPLICATES AND FLAG CELLS WITH X DATA	D3	141
50	DO 52 LCELL = 1,NCELL	D3	142
	MAXREP(LCELL) = 0	D3	143
	DO 52 KODE = 1,13	D3	144
	MAXREP(LCELL) = MAX0 (MAXREP(LCELL),KOUNT(KODE,LCELL))	D3	145
52	FLAGCL(LCELL) = MAX0 (FLAGCL(LCELL),MAXREP(LCELL))	D3	146
	C	D3	147
	IF (LPRINT) 55,53,53	D3	148
53	DO 54 LCELL = 1,NCELL	D3	149
	M = MAXREP(LCELL)	D3	150
54	WRITE (6,1054) RUN,FRAME(IFRAME),LCELL,TIME(IFRAME),((WORK(II,JJ,	D3	151
	1LCELL),JJ=1,13),II=1,M)	D3	152
1054	FORMAT(1H A5,A4,7H CELL13,14F8.3/(28X13F8.3))	D3	153
	C*****AVERAGE REPLICATES	D3	154
55	DO 59 LCELL = 1,NCELL	D3	155
	DO 59 KODE = 1,13	D3	156
	XA(KODE,LCELL) = 0.0	D3	157
	IF (KOUNT(KODE,LCELL)) 59,59,56	D3	158
56	M = KOUNT(KODE,LCELL)	D3	159
	DO 58 IREPL = 1,M	D3	160

58	XA(KODE,LCELL) = XA(KODE,LCELL) + WORK(IREPL,KODE,LCELL)	D3	161
	XA(KODE,LCELL) = XA(KODE,LCELL)/FLOAT(M)	D3	162
59	CONTINUE	D3	163
C*****	SELECT REFERENCE. CENTER,AVERAGE, OUTER, OR INNER, RESPECTIVELY	D3	164
	IF (KOUNT(13,1)) 68,68,66	D3	165
66	REFX = XA(13,1)	D3	166
	GO TO 75	D3	167
68	IF (KOUNT(11,1) * KOUNT(12,1)) 71,71,69	D3	168
69	REFX = (XA(11,1) + XA(12,1))/2.0	D3	169
	GO TO 75	D3	170
71	IF (KOUNT(12,1)) 74,74,72	D3	171
72	REFX = XA(12,1)	D3	172
	GO TO 75	D3	173
74	REFX = XA(11,1)	D3	174
75	IF (ABS(REFX) - 1.E-10) 90,90,76	D3	175
76	REFX = REFX - XREF	D3	176
C*****	ASSIGN MENISCUS FOR VARIOUS CELLS	D3	177
	DO 89 LCELL = 1,NCELL	D3	178
	IF (MAXREP(LCELL)) 89,89,78	D3	179
78	IF (KOUNT(10,LCELL)) 79,79,80	D3	180
79	BMENW(IFRAME,LCELL) = BMENW(IFRAME,1)	D3	181
	BMENX(IFRAME,LCELL) = BMENX(IFRAME,1)	D3	182
	GO TO 81	D3	183
80	BMENW(IFRAME,LCELL) = 1.0	D3	184
	BMENX(IFRAME,LCELL) = XA(10,LCELL) - REFX	D3	185
81	IF (KOUNT(9,LCELL)) 82,82,83	D3	186
82	MENW(IFRAME,LCELL) = MENW(IFRAME,1)	D3	187
	MENX(IFRAME,LCELL) = MENX(IFRAME,1)	D3	188
	GO TO 84	D3	189
83	MENW(IFRAME,LCELL) = 1.0	D3	190
	MENX(IFRAME,LCELL) = XA(9,LCELL) - REFX	D3	191
C*****	COUNT COMPONENTS	D3	192
84	DO 88 KODE = 1,8	D3	193
	IF (KOUNT(KODE,LCELL)) 88,88,85	D3	194
85	PKW(IFRAME,KODE,LCELL) = 1.0	D3	195
	PKX(IFRAME,KODE,LCELL) = XA(KODE,LCELL) - REFX	D3	196
	NCOMPS(LCELL) = MAX0(NCOMPS(LCELL),KODE)	D3	197
	IF (NCOMPS(LCELL) - MXCOMP) 88,88,86	D3	198
86	NCOMPS(LCELL) = MXCOMP	D3	199
88	CONTINUE	D3	200
89	CONTINUE	D3	201
	GO TO 91	D3	202
C*****	FRAME DELETED BY INPUT CODE ON EITHER X OR X,Y DATA OR NO X DATA	D3	203
90	WRITE (6,1090) RUN,FRAME(IFRAME)	D3	204
1090	FORMAT(18H **CAUTION** FRAME2XA5,A4,9H DELETED)	D3	205
	IFRAME = IFRAME - 1	D3	206
	IWARN = 1	D3	207
91	IF (ICONT) 999,290,92	D3	208
C*****	INPUT OF X,Y COORDINATES	D3	209
92	DO 93 LCELL = 1,MXCELL	D3	210
	VALUE(1,LCELL) = Z	D3	211
	VALUE(2,LCELL) = Z	D3	212
	ID1(3,LCELL) = 1000000	D3	213
	ID2(3,LCELL) = 1000000	D3	214
	VALUE(3,LCELL) = Z	D3	215
	KOUNT(1,LCELL) = 2	D3	216
93	KOUNT(2,LCELL) = 0	D3	217
	LCELL = 1	D3	218
	DO 110 KARD = 1,MXCARD	D3	219
	READ (5,1020) (KARD1(KD),KARD2(KD),KARD3(KD),CARD(KD),KD=1,9)	D3	220
C*****	EDIT EACH RECORD AND SORT BY CELL, COUNT CELLS	D3	221

DO 110 KD = 1,9	D3	222
INDEX = KARD3(KD) + 1	D3	223
GO TO (97,98,98,98,110,111,95,92,113,112),INDEX	D3	224
95 IF (KOUNT(1,LCELL))110,110,96	D3	225
96 KOUNT(1,LCELL) = KOUNT(1,LCELL) - 1	D3	226
GO TO 110	D3	227
97 KARD3(KD) = 1	D3	228
98 IF (CARD(KD) - 1.E-20) 110,110,99	D3	229
99 IF (KARD3(KD) - MXCELL) 100,100,110	D3	230
100 IF (KOUNT(1,LCELL) - MXPTS) 101,110,110	D3	231
101 LCELL = KARD3(KD)	D3	232
KOUNT(1,LCELL) = KOUNT(1,LCELL) + 1	D3	233
KTOTAL = KOUNT(1,LCELL)	D3	234
ID1(KTOTAL,LCELL) = KARD1(KD)	D3	235
IF (KARD2(KD)) 104,102,104	D3	236
102 IF (KARD1(KD) - 5) 103,104,104	D3	237
103 ID2(KTOTAL,LCELL) = 10	D3	238
GO TO 105	D3	239
104 ID2(KTOTAL,LCELL) = KARD2(KD)	D3	240
105 VALUE(KTOTAL,LCELL) = CARD(KD)	D3	241
NCELL = MAX0(NCELL,LCELL)	D3	242
110 CONTINUE	D3	243
GO TO 113	D3	244
111 ICONT = 0	D3	245
GO TO 90	D3	246
112 ISTOP = 1	D3	247
113 CONTINUE	D3	248
C	D3	249
115 IF (LPRINT) 120,116,116	D3	250
116 DO 117 LCELL = 1,NCELL	D3	251
KTOTAL = KOUNT(1,LCELL)	D3	252
117 WRITE (6,1117) LCELL,ANGLE(IFRAME),(ID1(KD,LCELL),ID2(KD,LCELL),	D3	253
1VALUE(KD,LCELL),KD=3,KTOTAL)	D3	254
1117 FORMAT(6H CELL13,F7.2,8H DEGREES4(I6,I2,F7.3,I3,I2,F7.3)/(24X4(I6D3	D3	255
1,I2,F7.3,I3,I2,F7.3)))	D3	256
C*****FLAG CELL IF X,Y DATA ARE GIVEN IN ANY FRAME, FLAG FRAME	D3	257
120 IF (IWARN) 121,121,290	D3	258
121 DO 127 LCELL = 1,NCELL	D3	259
KTOTAL = KOUNT(1,LCELL) - 2	D3	260
IF (KTOTAL) 125,125,122	D3	261
122 FLAGCL(LCELL)=MAX0(FLAGCL(LCELL),KTOTAL)	D3	262
IF (NFRXY(LCELL) - MXXY) 123,125,125	D3	263
123 NFRXY(LCELL) = NFRXY(LCELL) + 1	D3	264
FLAGFR(IFRAME,LCELL) = NFRXY(LCELL)	D3	265
C*****BASELINE SEQUENCE MAY BE DIFFERENT FOR EACH FRAME AND EACH CELL	D3	266
125 IF (LBASLN(LCELL)) 127,126,127	D3	267
126 LBASLN(LCELL) = LBASLN(1)	D3	268
127 CONTINUE	D3	269
C*****CORRECT SOLUTION ORDINATES FOR BASELINE	D3	270
DO 149 LCELL = 1,NCELL	D3	271
IF (FLAGFR(IFRAME,LCELL)) 149,149,130	D3	272
130 IF (LBASLN(LCELL)) 290,145,131	D3	273
C*****COLLECT BASELINE READINGS IF NOT GIVEN FOR EACH POINT	D3	274
131 KTOTAL = 2	D3	275
KPRIME = KOUNT(1,LCELL) - 1	D3	276
DO 134 KD = 3,KPRIME,2	D3	277
IF (ID2(KD,LCELL) - 10) 133,132,133	D3	278
132 KOUNT(2,LCELL) = KOUNT(2,LCELL) + 1	D3	279
INDEX = KOUNT(2,LCELL)	D3	280
XX(INDEX,LCELL) = VALUE(KD,LCELL)	D3	281
YY(INDEX,LCELL) = VALUE(KD+1,LCELL)	D3	282

GO TO 134	D3	283
133 KTOTAL = KTOTAL + 1	D3	284
ID1(KTOTAL,LCELL) = ID1(KD,LCELL)	D3	285
ID2(KTOTAL,LCELL) = ID2(KD,LCELL)	D3	286
VALUE(KTOTAL,LCELL) = VALUE(KD,LCELL)	D3	287
KTOTAL = KTOTAL + 1	D3	288
ID1(KTOTAL,LCELL) = ID1(KD+1,LCELL)	D3	289
ID2(KTOTAL,LCELL) = ID2(KD+1,LCELL)	D3	290
VALUE(KTOTAL,LCELL) = VALUE(KD+1,LCELL)	D3	291
134 CONTINUE	D3	292
KOUNT(1,LCELL) = KTOTAL	D3	293
C*****PUT LEAST SQUARES POLYNOMIAL THROUGH BASELINE POINTS	D3	294
IF (KOUNT(2,LCELL)) 135,135,136	D3	295
135 WRITE (6,1135)	D3	296
1135 FORMAT(34H **CAUTION**BASELINE ASSUMED = 0.0)	D3	297
XX(1,LCELL) = 0.0	D3	298
KOUNT(2,LCELL) = 1	D3	299
136 KOUNT(2,LCELL) = MIN0(KOUNT(2,LCELL),30)	D3	300
IF (KOUNT(2,LCELL) - 6) 138,139,139	D3	301
138 MAX = KOUNT(2,LCELL) - 2	D3	302
GO TO 140	D3	303
139 MAX = 4	D3	304
140 MIN = MAX + 1	D3	305
CALL LSPOLY (ALPHA,KOUNT(2,LCELL),MIN,MAX,0,1,0,0,0,LPRINT-1,1.0,	D3	306
11.0,XX(1,LCELL),YY(1,LCELL),W,0.0)	D3	307
C*****COMPUTE BASELINE FOR SOLUTION PATTERN POINTS AND SUBTRACT	D3	308
KTOTAL = KOUNT(1,LCELL)	D3	309
DO 143 INDEX = 4,KTOTAL,2	D3	310
BL = REALCM(301)	D3	311
DO 142 KDEGRE = 1,MIN	D3	312
142 BL=BL + REALCM(KDEGRE+301)*VALUE(INDEX-1,LCELL)**KDEGRE	D3	313
143 VALUE(INDEX,LCELL) = VALUE(INDEX,LCELL) - BL	D3	314
SEY = REALCM(MIN+321)	D3	315
KTOTAL = KOUNT(2,LCELL)	D3	316
144 WRITE (6,1144) LCELL,MIN,KTOTAL,SEY	D3	317
1144 FORMAT(16H **CAUTION**CELLI3,22H POLYNOMIAL OF DEGREEI3,12H PUT TD3	D3	318
1THROUGH I4,61H BASELINE POINTS GIVING STANDARD ERROR OF COMPARATOR OD3	D3	319
2RDINATEIPE11.3)	D3	320
GO TO 149	D3	321
C*****SUBTRACT INPUT BASELINE ORDINATE FROM INPUT SOLUTION ORDINATE	D3	322
145 KTOTAL = KOUNT(1,LCELL)	D3	323
DO 148 KD = 6,KTOTAL,4	D3	324
IF (ABS(VALUE(KD-3,LCELL) - VALUE(KD-1,LCELL)) - 1.E-2) 147,147,146D3	D3	325
146 WRITE(6,1146) LCELL	D3	326
1146 FORMAT(16H **CAUTION**CELLI3,35H BASELINE NOT GIVEN FOR EACH POIND3	D3	327
1T)	D3	328
FLAGFR (IFRAME,LCELL) = 0	D3	329
GO TO 149	D3	330
147 K = KD/2	D3	331
ID1(K,LCELL) = ID1(KD-3,LCELL)	D3	332
ID2(K,LCELL) = MIN0(ID2(KD-3,LCELL),ID2(KD-1,LCELL))	D3	333
VALUE(K,LCELL) = VALUE(KD-3,LCELL)	D3	334
ID1(K+1,LCELL) = ID1(K,LCELL)	D3	335
ID2(K+1,LCELL) = ID2(K,LCELL)	D3	336
VALUE(K+1,LCELL) = ABS(VALUE(KD,LCELL) - VALUE(KD-2,LCELL))	D3	337
148 CONTINUE	D3	338
KOUNT(1,LCELL) = K + 1	D3	339
149 CONTINUE	D3	340
C*****SUPPLY EXTRA ZERO POINT IF MIN, MEN, OR BOT ORD IS NOT GIVEN	D3	341
DO 190 LCELL = 1,NCELL	D3	342
IF (FLAGFR(IFRAME,LCELL)) 190,190,150	D3	343

150	JFRAME = NFRXY(LCELL)	D3	344
	SEORD(JFRAME,LCELL) = SEY	D3	345
	JPEAK = ID2(5,LCELL)	D3	346
	IF (ID1(3,LCELL) - 5) 152,151,152	D3	347
151	TOPX(JFRAME,LCELL) = VALUE(3,LCELL)	D3	348
	TOPY(JFRAME,LCELL) = VALUE(4,LCELL)	D3	349
	START(JFRAME,JPEAK+1,LCELL) = 2	D3	350
	ID2(1,LCELL) = JPEAK	D3	351
	ID2(3,LCELL) = JPEAK	D3	352
	GO TO 155	D3	353
152	IF (ID2(3,LCELL) - 9) 154,153,154	D3	354
153	ID2(3,LCELL) = JPEAK	D3	355
	ID2(1,LCELL) = JPEAK	D3	356
	START(JFRAME,JPEAK+1,LCELL) = 2	D3	357
	GO TO 155	D3	358
154	ID1(1,LCELL) = ID1(5,LCELL)	D3	359
	ID2(1,LCELL) = JPEAK	D3	360
	VALUE(1,LCELL) = VALUE(3,LCELL) - (VALUE(5,LCELL) - VALUE(3,LCELL))	D3	361
	ID1(2,LCELL) = ID1(1,LCELL)	D3	362
	ID2(2,LCELL) = JPEAK	D3	363
	VALUE(2,LCELL) = 0.0	D3	364
	START(JFRAME,JPEAK+1,LCELL) = 1	D3	365
155	KTOTAL = KOUNT(1,LCELL)	D3	366
	JPEAK = ID2(KTOTAL - 3,LCELL)	D3	367
	IF (ID1(KTOTAL-1,LCELL) - 6) 157,156,157	D3	368
156	BOTX(JFRAME,LCELL) = VALUE(KTOTAL - 1,LCELL)	D3	369
	BOTY(JFRAME,LCELL) = VALUE(KTOTAL,LCELL)	D3	370
	START(JFRAME,JPEAK ,LCELL) = KOUNT(1,LCELL)/2	D3	371
	ID2(KTOTAL-1,LCELL) = JPEAK	D3	372
	GO TO 160	D3	373
157	IF (ID2(KTOTAL-1,LCELL) - 9) 159,158,159	D3	374
158	ID2(KTOTAL-1,LCELL) = JPEAK	D3	375
	START(JFRAME,JPEAK,LCELL) = KOUNT(1,LCELL)/2	D3	376
	GO TO 160	D3	377
159	KPRIME = KOUNT(1,LCELL) + 1	D3	378
	KTOTAL = KPRIME + 1	D3	379
	ID1(KPRIME,LCELL) = ID1(KTOTAL-5,LCELL)	D3	380
	ID2(KPRIME,LCELL) = JPEAK	D3	381
	VALUE(KPRIME,LCELL) = VALUE(KPRIME-2,LCELL) + (VALUE(KPRIME-2,LCELL)	D3	382
	1 - VALUE(KPRIME-4,LCELL))	D3	383
	ID1(KTOTAL,LCELL) = ID1(KPRIME,LCELL)	D3	384
	ID2(KTOTAL,LCELL) = JPEAK	D3	385
	VALUE(KTOTAL,LCELL) = 0.0	D3	386
	START(JFRAME,JPEAK ,LCELL) = KTOTAL/2	D3	387
160	KOUNT(1,LCELL) = KTOIAL	D3	388
C****	IDENTIFY PEAKS IN SEQUENCE OF READINGS, CONVERT TO FIXED REFERENCE	D3	389
C	AND STORE VALUES AS X AND Y	D3	390
	JPEAK = ID2(1,LCELL)	D3	391
	DO 180 KD = 2,KTOTAL,2	D3	392
	JSEQ = KD/2	D3	393
	XDATA(JFRAME,JSEQ,LCELL) = VALUE(KD-1,LCELL) REFx	D3	394
	YDATA(JFRAME,JSEQ,LCELL) = VALUE(KD,LCELL)	D3	395
	IF (ID2(KD-1,LCELL) - 9) 161,166,161	D3	396
161	IF (JPEAK - ID2(KD-1,LCELL)) 167,162,165	D3	397
162	JPEAK = ID2(KD-1,LCELL)	D3	398
	GO TO 180	D3	399
165	JPEAK = ID2(KD-1,LCELL) + 1	D3	400
166	START(JFRAME,JPEAK,LCELL) = JSEQ	D3	401
	JPEAK = JPEAK - 1	D3	402
	GO TO 180	D3	403
167	JPRIME = ID2(1,LCELL) + 1	D3	404

JPEAK = ID2(KD-1,LCELL)	D3	405
START(JFRAME,JPEAK+1,LCELL) = START(JFRAME,JPRIME,LCELL)	D3	406
168. WRITE (6,1168) LCELL,JPEAK	D3	407
1168. FORMAT(16H **CAUTION**CELLI3,10H COMPONENTI3,71H NUMBERED WRONG, CD3	408	
10NC INCLUDES ALL SLOWER COMPONENTS READ IN THIS FRAME)	D3	409
IF (LPRINT) 180,175,180	D3	410
175 LPRINT = 1	D3	411
180 CONTINUE	D3	412
190 CONTINUE	D3	413
290 IF (ISTOP) 999,300,301	D3	414
300 CONTINUE	D3	415
301 NFRAME = IFRAME	D3	416
C	D3	417
IF (LPRINT) 999,999,305	D3	418
305 WRITE (6,1305)	D3	419
1305 FORMAT(66H X,Y DATA CORRECTED TO FIXED COMPARATOR REFERENCE AND FOD3	420	
1R BASELINE)	D3	421
DO 316 LCELL = 1,NCELL	D3	422
IF (FLAGCL(LCELL)) 316,316,306	D3	423
306 DO 315 IFRAME = 1,NFRAME	D3	424
IF (FLAGFR(IFRAME,LCELL)) 315,315,307	D3	425
307 JFRAME = FLAGFR(IFRAME,LCELL)	D3	426
NTOTAL = NCOMPS(LCELL) + 1	D3	427
KTOTAL = 0	D3	428
DO 309 JPEAK = 1,NTOTAL	D3	429
309 KTOTAL = MAX0(KTOTAL,START(JFRAME,JPEAK,LCELL))	D3	430
313 WRITE (6,1313) LCELL,RUN,FRAME(IFRAME),(START(JFRAME,JPEAK,LCELL),D3	431	
1JPEAK = 1,NTOTAL)	D3	432
1313 FORMAT(5H0CELLI3,5X2A5,12H STOP/START9(I6))	D3	433
314 WRITE (6,1314) (XDATA(JFRAME,JSEQ,LCELL),YDATA(JFRAME,JSEQ,LCELL),D3	434	
1JSEQ=1,KTOTAL)	D3	435
1314 FORMAT(4F8.3,1X4F8.3,2X4F8.3,1X4F8.3)	D3	436
315 CONTINUE	D3	437
316 CONTINUE	D3	438
999 LPRINT = LSAVE	D3	439
RETURN	D3	440
END	D3	441

\$IBFTC D4-CS2 LIST,M94

C*****CONVERT 1-DIMENSION COMPARATOR DATA TO ROTOR, CHECK FOR CELL LEAK	D4	1
C	D4	002
SUBROUTINE CKDATA	D4	3
C	D4	004
COMMON /CS1CM/ A,B1,B2,YBAR,ALPHA(12),F2,FRAME(30),NCOMP,NFRAME,N,D4	5	
10MSQT(30),RBEGLN,RBEG,RMEN(30),RPK(30,4),RSQ,SEA,SEB1,SEB2,SE,	D4	006
2SETZOA,SEX0,SEYBAR,STAR(30,4),TIME(30),TZOAWMIN,WN,X0,AP,BP,SEAP,D4	7	
3SEBP,SEP,TBAR,OMF,SERBLN,SPEED,REFR,FMOME,LKIND,LPRINT,LPLOT,	D4	008
4LINPUT,LBEGWT,NCELL,Z,XLINE(20),YLINE(20),NDATA(4),XX(100,4),	D4	9
5YY(100,4),COPR,SECOPR,SERBEG,X0P,SEX0P,B3,SEB3,STANRM(4,2),	D4	010
6SESTAN(4,2),DILN(4,2),METHOD,KIND(10),SEORD(10,2)	D4	11
DOUBLE PRECISION A,B1,B2,YBAR	D4	012
COMMON /CS2XY/ XDATA(10,50,2),START(10,9,2),RBAR(10,4),	D4	13
1STARRB(10,4),STARRM(10,4),CP(10,4),C0(10,4),TOPX(10,2),TOPY(10,2),D4	014	
2BOTX(10,2),BOTY(10,2),XREF,	D4	15
3MENW(30,2),PKX(30,4,2),PKW(30,4,2),PKLN(30,4,2),NCOMPS(2),	D4	016
4FLAGCL(2),FY,	D4	17
5BMENX(30,2),BMENW(30,2),ANGLE(30)	D4	018
INTEGER START,FLAGCL,FLAGFR	D4	19
REAL MENX,MENW	D4	020
COMMON /WORKCM/REALCM(1000),INTCM(1000)	D4	21

C	IF (FLAGCL(NCELL)) 999,999,1	D4	22
	1 IF (LPRINT+2) 10,10,2	D4	023
	2 WRITE (6,1002) ALPHA,NCELL	D4	24
	1002 FORMAT(1H112A6,10X4HCELLI3//)	D4	025
	CALL SLITET (4,INDEX)	D4	26
	GO TO (4,5),INDEX	D4	027
	4 WRITE (6,1004) TZO	D4	28
	1004 FORMAT(55H0**CAUTION**INPUT TIMER VALUES REDUCED BY INPUT ZERO OF	D4	029
	1F11.5,3X5H(MIN))	D4	30
	5 IF (LPRINT) 10,6,7	D4	031
	6 IF (LINPUT - 1) 7,7,10	D4	32
	7 WRITE (6,1007) XREF,SPEED,REFR,FMOME, NFRAME,LKIND, LPRINT,LPLOT,	D4	033
	1LINPUT,NCOMP,LBEGWT,NCELL	D4	34
	1007 FORMAT(51H0INPUT DATA CORRECTED TO FIXED COMPARATOR REFERENCEF11.6D4	D4	035
	1,6X52HFRAMES KIND PRINT PLOT INPUT COMPS BEGWT CELL/6H SPEED4	D4	36
	2DF8.1,13H RPM ROT REFF8.5,20H COMP-PLATE RAD MAGF9.5,8(5X12)/42HD4	D4	037
	3 I FRAME TIMER TOP MENISCUS BOTTOM5X5HPEAKS/12X5H(MIN)6X23D4	D4	38
	4H(C O M P A R A T O R))	D4	039
	DO 8 I = 1,NFRAME	D4	40
	[8 WRITE (6,1008) I,FRAME(I),TIME(I),MENX(I,NCELL),BMENX(I,NCELL),	D4	041
	1(PKX(I,J,NCELL),J=1,NCOMP)	D4	42
	1008 FORMAT(1X12,2XA4,F9.2,2X10F10.5)	D4	043
	C*****CONVERSION	D4	44
	10 RECIP = 1.0/FMOME	D4	045
	DO 29 I = 1,NFRAME	D4	46
	OMSQT(I) = TIME(I)*OMF	D4	047
	12 IF (MENW(I,NCELL) - 1.E-10) 13,13,15	D4	48
	13 RMEN(I) = 0.0	D4	049
	GO TO 16	D4	50
	15 RMEN(I) = RECIP * MENX(I,NCELL)	D4	051
	16 DO 29 J = 1,NCOMP	D4	52
	17 IF (PKW(I,J,NCELL) - 1.E-10) 18,18,20	D4	053
	18 RPK(I,J) = 0.0	D4	54
	PKLN(I,J,NCELL) = 0.0	D4	055
	GO TO 29	D4	56
	20 RPK(I,J) = RECIP * PKX(I,J,NCELL)	D4	057
	PKLN(I,J,NCELL) = ALOG(RPK(I,J))	D4	58
	29 CONTINUE	D4	059
	C*****LINEAR LEAST SQUARES ANALYSIS OF MENISCUS VALUES	D4	60
	CALL CFLS2 (1,NFRAME,MENW(1,NCELL),RMEN,TIME,0.0,0.0,LPRINT)	D4	061
	CALL FTEST (N-2,1,(B1/SEB1)**2,PROB)	D4	62
	IF (PROB - 5.0) 71,71,80	D4	063
	C*****SIGNIFICANT LEAK. DETERMINE ITS S-RATE	D4	64
	71 RMENA = SNGL(A)	D4	065
	SFERMA = SFA	D4	66
	DO 75 I = 1,NFRAME	D4	067
	IF (MENW(I,NCELL) - 1.E-10) 75,75,74	D4	68
	74 MENX(I,NCELL) = ALOG(RMEN(I))	D4	069
	75 CONTINUE	D4	70
	CALLCFLS2(1,NFRAME,MENW(1,NCELL),MENX(1,NCELL),OMSQT,0.,0.,LPRINT)	D4	071
	76 WRITE (6,1076) B1,SEB1	D4	72
	1076 FORMAT(33H **CAUTION**CELL LEAK WITH S-RATEF10.5,2X9HSTD ERRORF10.D4	D4	073
	15,2X6H(SVED))	D4	74
	GO TO 85	D4	075
	C*****NO LEAK	D4	76
	80 RMENA = SNGL(YBAR)	D4	077
	IF (RMENA - 1.E-10) 82,82,84	D4	78
	82 SERMA = Z	D4	079
	RBEGLN = Z	D4	80
	RMENA = 1.E-10	D4	081
		D4	82

LKIND = 3	D4	83
GO TO 87	D4	084
84 SERMA = SEYBAR	D4	85
85 RBEGLN= ALOG(RMENA)	D4	086
C*****USE MOST RADIAL PEAK FIRST FRAME AS PRELIM STARTING LEVEL IN SBC	D4	87
86 IF (LKIND - 2) 93,93,87	D4	088
87 RBEGLN = 0.0	D4	89
DO 90 J = 1,NCOMP	D4	090
TEST = PKLN(1,J,NCELL) * PKW(1,J,NCELL)	D4	91
90 RBEGLN = AMAX1(RBEGLN,TEST)	D4	092
SERBLN = 0.0	D4	93
GO TO 94	D4	094
93 SERBLN = SERMA/RMENA	D4	95
94 CALL SLITET (4,INDEX)	D4	096
999 RETURN	D4	97
END	D4	098

\$IBFTC D5-CS2 LIST,M94

C*****DIRECTOR PROGRAM FOR S-RATE OF ALL COMPONENTS IN EACH CELL	D5	001
C INCORPORATING ZERO TIME CORRECTION AND STARTING LEVEL	D5	2
C	D5	003
SUBROUTINE SRATE2	D5	4
C	D5	005
COMMON /CS1CM/ A,B1,B2,YBAR,ALPHA(12),F2,FRAME(30),NCOMP,NFRAME,N,	D5	6
10MSQT(30),RBEGLN,RBEG,RMEN(30),RPK(30,4),RSQ,SEA,SEB1,SEB2,SE,	D5	007
2SETZOA,SEX0,SEYBAR,STAR(30,4),TIME(30),TZOAWMIN,WN,X0,AP,BP,SEAP,	D5	8
3SEBP,SEP,TBAR,OMF,SERBLN,SPEED,REFR,FMOME,LKIND,LPRINT,LPLOT,	D5	009
4LINPUT,LBEGWT,NCELL,Z,XLINE(20),YLINE(20),NDATA(4),XX(100,4),	D5	10
5YY(100,4),COPR,SECOPR,SERBEG,XOP,SEXOP,B3,SEB3,STANRM(4,2),	D5	011
6SESTAN(4,2),DILN(4,2),METHOD,KIND(10),SEORD(10,2)	D5	12
DOUBLE PRECISION A,B1,B2,YBAR	D5	013
COMMON /CS2XY/ XDATA(10,50,2),START(10,9,2),RBAR(10,4),	D5	14
1STARRB(10,4),STARRM(10,4),CP(10,4),CO(10,4),TOPX(10,2),TOPY(10,2),	D5	015
2 BOTX(10,2),BOTY(10,2),XREF, MENX(30,2),	D5	16
3MENW(30,2),PKX(30,4,2),PKW(30,4,2),PKLN(30,4,2),NCOMPS(2),	D5	017
4FLAGCL(2),FY, YDATA(10,50,2),NPOINT(10,4),FLAGFR(30,2),	D5	18
5BMENX(30,2),BMENW(30,2),ANGLE(30)	D5	019
INTEGER START,FLAGCL,FLAGFR	D5	20
REAL MENX,MENW	D5	021
COMMON /WORKCM/REALCM(1000),INTCM(1000)	D5	22
C	D5	023
DIMENSION W(30),Y(30),RBLN(4), SRBLN(4),TZO(4),SETZO(4),TITLE1(12)	D5	24
EQUIVALENCE (W(1),REALCM(1)),(Y(1),REALCM(51)),(RBLN(1),REALCM(61))	D5	025
1),(SRBLN(1),REALCM(71)),(TZO(1),REALCM(81)),(SETZO(1),REALCM(91))	D5	26
C*****SKIP TO SECOND CYCLE IF FINAL CALL IN DOUBLE CELL RUNS	D5	027
5 CALL SLITET (4,INDEX)	D5	28
GO TO (6,10),INDEX	D5	029
6 CALL SLITE (4)	D5	30
GO TO 256	D5	031
C	D5	32
10 IF (LPRINT + 1) 130,120,120	D5	033
120 IF (LKIND - 2) 125,126,121	D5	34
121 WRITE (6,1121)	D5	035
1121 FORMAT(104H0**CAUTION**STARTING LEVEL DETERMINED AS AVERAGE OF INTD	D5	36
1ERCEPTS AT TIMER ZERO FOR SYNTHETIC BOUNDARY CELL)	D5	037
122 GO TO 130	D5	38
125 WRITE (6,1125)	D5	039
1125 FORMAT(62H0**CAUTION**ZERO TIME DETERMINED BY STARTING PEAKS AT MED	D5	40
1NISCUS)	D5	041
GO TO 130	D5	42

126 WRITE (6,1126)	D5	43
1126 FORMAT(69H0**CAUTION**MENISCUS USED AS A POINT, ZERO TIME CORRECTIO	D5	044
10N STILL MADE)	D5	45
C*****LOOP OVER ALL COMPONENTS, QUADRATIC LEAST SQUARES, MAKE F-TEST	D5	046
130 DO 139 J = 1,NCOMP	D5	47
CALL CFLS2 (3,NFRAME,PKW(1,J,NCELL),PKLN(1,J,NCELL),OMSQT,RBEGLN,	D5	048
1SERBLN,LPRINT)	D5	49
133 IF (N - 3) 500,134,135	D5	050
500 WRITE (6,2500) J	D5	51
2500 FORMAT(21H0**CAUTION**COMPONENTI2,23H HAS LESS THAN 3 POINTS)	D5	052
RBLN(J)=RBEGLN	D5	53
SRBLN(J) = Z	D5	054
GO TO 536	D5	55
134 WRITE (6,2134)J	D5	056
2134 FORMAT(21H0**CAUTION**COMPONENTI2,40H HAS JUST 3 POINTS, ONLY LINED	D5	57
1AR FIT MADE)	D5	058
GO TO 535	D5	59
135 CALL FTEST(N=3,1,F2,PROB)	D5	060
IF (PROB - 5.0) 530,530,520	D5	61
520 WRITE (6,2520)J	D5	062
2520 FORMAT(21H0**CAUTION**COMPONENTI2,59H HAS LESS THAN 5 PERCENT CHAND	D5	63
ICE OF A CURVED LN R VS. T PLOT)	D5	064
TZ0(J) = X0P/OMF	D5	65
SETZ0(J) = SEX0P/OMF	D5	066
RBLN(J) = AP	D5	67
SRBLN(J) = SEAP	D5	068
GO TO 139	D5	69
530 WRITE(6,2530)J	D5	070
2530 FORMAT(21H0**CAUTION**COMPONENTI2,60H HAS SIGNIFICANTLY CURVED LN	D5	71
1R VS. T PLOT AT 5 PERCENT LEVEL)	D5	072
535 SRBLN(J) = SEA	D5	73
RBLN(J) = SNGL(A)	D5	074
536 TZ0(J) = X0/OMF	D5	75
SETZ0(J) = SEX0/OMF	D5	076
139 CONTINUE	D5	77
C*****DETERMINE COMMON INTERSECTION OF ALL COMPONENTS	D5	078
140 IF (LKIND - 2) 171,171,141	D5	79
C*****SYNTHETIC BOUNDARY CELL RUN	D5	080
141 TZ0A = 0.0	D5	81
142 SETZ0A = Z	D5	082
143 IF (NCOMP - 1)999,152,155	D5	83
152 RBEGLN = RBLN(1)	D5	084
153 SERBLN = SRBLN(1)	D5	85
154 GO TO 184	D5	086
155 DO 160 J = 1,NCOMP	D5	87
156 IF (SRBLN(J) - 1.E-5)157,157,159	D5	088
157 W(J) = 1.E+5	D5	89
158 GO TO 160	D5	090
159 W(J) = (1.0/SRBLN(J))**2	D5	91
160 CONTINUE	D5	092
161 CALL CFLS2 (0,NCOMP,W,RBLN,TIME,0.0,0.0,LPRINT)	D5	93
162 RBEGLN = SNGL(YBAR)	D5	094
163 SERBLN = SQRT(1.0/(WN*WMIN))	D5	95
166 GO TO 184	D5	096
C*****CONVENTIONAL RUN	D5	97
171 IF (NCOMP - 1)999,172,175	D5	098
172 TZ0A = TZ0(1)	D5	99
173 SETZ0A = SETZ0(1)	D5	100
174 GO TO 184	D5	101
175 DO 180 J = 1,NCOMP	D5	102
176 IF (SETZ0(J) - 1.E-3) 177,177,179	D5	103

177 W(J) = 1.E+3	D5	104
178 GO TO 180	D5	105
179 W(J) = (1.0/SETZO(J))**2	D5	106
180 CONTINUE	D5	107
181 CALL CFLS2 (0,NCOMP,W,TZO,TIME,0.0,0.0,LPRINT)	D5	108
182 TZOA = SNGL(YBAR)	D5	109
183 SETZOA = SQRT(1.0/(WN*WMIN))	D5	110
C*****CHECK THAT STARTING TIME AND LEVEL ARE REASONABLE	D5	111
184 RBEG = EXP(RBEGLN)	D5	112
SERBEG = RBEG*SERBLN	D5	113
OMTO = TZOA*OMF	D5	114
SEOMTO = SETZOA*OMF	D5	115
SAVET = SEOMTO	D5	116
IF (SETZOA - 10.0) 190,190,185	D5	117
185 WRITE (6,1185)	D5	118
1185 FORMAT(69H0**CAUTION**STANDARD ERROR OF ZERO TIME TOO LARGE, SET =	D5	119
1 0.0 FOR PLOT)	D5	120
SEOMTO = 0.0	D5	121
190 SAVER = SERBLN	D5	122
IF (SERBLN - 0.2) 200,200,191	D5	123
191 WRITE (6,1191)	D5	124
1191 FORMAT(74H0**CAUTION**STANDARD ERROR OF STARTING LEVEL TOO LARGE,	D5	125
1SET = 0.0 FOR PLOT)	D5	126
SERBLN = 0.0	D5	127
C*****LOG R VS. T PLOT WITH ORIGIN AS +/- 2 STD ERROR FROM (TZOA,RBEGLN)	D5	128
200 XLINE(1) = 0.0	D5	129
202 DO 214 J = 1,NCOMP	D5	130
203 K = 0	D5	131
204 DO 211 I = 1,NFRAME	D5	132
C*****POINT-BY-POINT S-RATE (S*) FOR DATA EDITING	D5	133
IF (PKW(I,J,NCELL) - 1.E-10) 206,206,207	D5	134
206 STAR(I,J) = Z	D5	135
GO TO 211	D5	136
207 DUMMY = OMSQT(I) - OMTO	D5	137
IF (ABS(DUMMY) - 1.E-28) 208,208,209	D5	138
208 STAR(I,J) = Z	D5	139
GO TO 210	D5	140
209 STAR(I,J) = (PKLN(I,J,NCELL) - RBEGLN)/DUMMY	D5	141
210 K = K + 1	D5	142
YY(K,J) = PKLN(I,J,NCELL)	D5	143
XX(K,J) = OMSQT(I)	D5	144
211 CONTINUE	D5	145
YY(K+1,J) = RBEGLN + 2.0 * SERBLN	D5	146
YY(K+2,J) = RBEGLN - 2.0 * SERBLN	D5	147
YY(K+3,J) = YY(K+1,J)	D5	148
YY(K+4,J) = YY(K+2,J)	D5	149
IF (LKIND - 2) 213,213,212	D5	150
212 XX(K+1,J) = 0.0	D5	151
XX(K+2,J) = 0.0	D5	152
XX(K+3,J) = 0.0	D5	153
XX(K+4,J) = 0.0	D5	154
GO TO 214	D5	155
213 XX(K+1,J) = OMTO - 2.0*SEOMTO	D5	156
XX(K+2,J) = OMTO + 2.0*SEOMTO	D5	157
XX(K+3,J) = XX(K+2,J)	D5	158
XX(K+4,J) = XX(K+1,J)	D5	159
214 NDATA(J) = K + 4	D5	160
C	D5	161
IF (LPRINT) 235,231,231	D5	162
231 WRITE (6,1231)	D5	163
1231 FORMAT(// 6X8HI FRAME2X5HTIMER 4X8HMENISCUS4(6X4HPEAK6X6HS-RATE)	D5	164

1/16X5H(MIN)6X13H(CM ON ROTOR)9X6H(SVED))	D5	165
[232 DO 233 I = 1,NFRAME	D5	166
233 WRITE (6,1233)I,FRAME(I),TIME(I),RMEN(I),(RPK(I,J), STAR(I,J),J=1,D5	D5	167
INCOMP)	D5	168
1233 FORMAT(5X12,2XA4,F10.3,F10.5,(4(F12.5,F10.3)))	D5	169
234 WRITE (6,1234) RBEG,SERBEG,TZ0A,SETZ0A,OMF	D5	170
1234 FORMAT(9X14HSTARTING LEVELF10.5,16H STANDARD ERRORF10.5/6X9HZERO	D5	171
1TIMEF10.5,16H STANDARD ERRORF10.5,9X32HCONVERSION FACTOR TIMER TOD5	D5	172
2 OMSQT1PE14.5)	D5	173
235 IF (LPL0T) 248,236,236	D5	174
DATA TITLE1(1)/72HLN R VS. OMSQT (IN 1/SVED) COMPUTED START +/- 2D5	D5	175
1 SE, DOTS ARE TIMER ZERO/	D5	176
236 CALL PLOT (ALPHA,TITLE1,XX,YY,NDATA,NCOMP,XLINE,YLINE,1,0,LPL0T)	D5	177
C*****PREPARE FOR SECOND CYCLE. INCLUDE STARTING LEVEL WITH SPECIFIED WTD5	D5	178
C RESET BEGWT IF SECOND CELL CALCULATED HAS ONLY 1 COMPONENT	D5	179
248 SEOMT0 = SAVET	D5	180
SERBLN = SAVER	D5	181
[250 DO 251 I = 1,NFRAME	D5	182
251 OMSQT(I) = OMSQT(I) - OMT0	D5	183
LSAVE - LBEGWT	D5	184
IF (LBEGWT - 8) 252,252,255	D5	185
252 IF (LBEGWT) 254,253,256	D5	186
253 IF (NCOMP - 1) 256,256,254	D5	187
254 LBEGWT = 9	D5	188
255 BEGWT = 0.0	D5	189
GO TO 257	D5	190
256 BEGWT = FLOAT(LBEGWT)	D5	191
257 CALL SLITET(1,INDEX)	D5	192
GO TO (300,280),INDEX	D5	193
280 CALL SLITET(4,INDEX)	D5	194
GO TO (281,290),INDEX	D5	195
281 CALL SLITE (4)	D5	196
C	D5	197
IF (LPRINT + 1) 303,282,282	D5	198
282 WRITE (6,1282)ALPHA,NCELL,TZ0A,SETZ0A	D5	199
1282 FORMAT(84H1**CAUTION**SPECIAL CYCLE FOR BOTH CELLS ADDING STARTINGD5	D5	200
1 LEVEL AT WEIGHTED ZERO TIME/25X12A6,10X4HCELLI2/3XF10.5,2X5H(MIN)D5	D5	201
2F10.5,2X9HSTD ERROR)	D5	202
GO TO 302	D5	203
290 IF (LPRINT + 1) 303,291,291	D5	204
291 IF (LPL0T) 293,292,292	D5	205
292 WRITE (6,1292)	D5	206
1292 FORMAT(1H1)	D5	207
293 WRITE (6,1293)ALPHA,SPEED,REFR,FMOME,NFRAME,LKIND, LPRINT,LPL0T,	D5	208
1LINPUT,NCOMP,LBEGWT,NCELL,BEGWT	D5	209
1293 FORMAT(1H0 7X35HSECOND CYCLE 6X12A6//2X48HD5	D5	210
1PROGRAM CS2 SEDIMENTATION COEFFICIENTS18X52HFRAMES KINDD5	D5	211
2 PRINT PLOT INPUT COMPS BEGWT CELL/1X5HSPEED F8.1,1X3HRPM 2XD5	D5	212
37HROT REF F8.5,2X18HCOMP-PLATE RAD MAG F9.5,8(5X12)/2X6HWEIGHTF3.0D5	D5	213
4,39H USED FOR STARTING LEVEL FROM 1ST CYCLE)	D5	214
GO TO 302	D5	215
300 CALL SLITE (1)	D5	216
IF (LPRINT + 1) 303,301,301	D5	217
301 WRITE (6,1301)BEGWT,NCELL	D5	218
1301 FORMAT(33H0**CAUTION**SPECIAL CYCLE--WEIGHTF3.0,24H USED FOR STARTD5	D5	219
1ING LEVEL28X4HCELLI2)	D5	220
302 WRITE(6,1302)	D5	221
1302 FORMAT (132H0 COMPONENT TOTAL INTERNAL S-RATE CONC INITIAL S-RD5	D5	222
1ATE CONC-PRES ADDL-ZERO PARABOLIC COMPARATOR MEAN S-RATED5	D5	223
2(LINEAR LSQ)/12X120HPOINTS (SVED) FACTOR (SVED) D5	D5	224
3EPENDENCE TIME (MIN) TERM F ERROR (SE) TIME (SVED) ERD5	D5	225

4ROR (SE))	D5	226
C*****SECOND CYCLE, QUADRATIC USED FOR ADDL ZERO TIME EVEN IF NOT CURVED	D5	227
303 NFRAME = NFRAME + 1	D5	228
OMSQT(NFRAME) = 0.0	D5	229
DO 315 J = 1,NCOMP	D5	230
PKLN(NFRAME,J,NCELL) = RBEGLN	D5	231
PKW(NFRAME,J,NCELL) = BEGWT	D5	232
CALL CFLS2 (3,NFRAME,PKW(1,J,NCELL),PKLN(1,J,NCELL),OMSQT,RBEGLN,	D5	233
1SERBLN,LPRINT)	D5	234
TZ0(J) = X0/OMF	D5	235
SETZ0(J) = SEX0/OMF	D5	236
SE = RBEG*FMOME*SE	D5	237
SEP = RBEG*FMOME*SEP	D5	238
TBAR = TBAR/OMF	D5	239
IF (N) 306,306,307	D5	240
306 FACTOR = 1.0	D5	241
GO TO 308	D5	242
307 FACTOR = EXP(-2.0*(YBAR - RBEGLN))	D5	243
308 STANRM(J,NCELL) = B3	D5	244
SESTAN(J,NCELL) = SEB3	D5	245
DILN(J,NCELL) = FACTOR	D5	246
IF (N - 3) 309,309,310	D5	247
309 B1 = Z	D5	248
SEB1 = Z	D5	249
GO TO 313	D5	250
310 IF (B1 * B3) 311,313,313	D5	251
311 WRITE (6,1311) J	D5	252
1311 FORMAT(21H0**CAUTION**COMPONENT13,68H HAS ERROR IN DATA, OR DID NOT	D5	253
1T START AT SAME TIME OR PLACE AS OTHERS)	D5	254
313 IF (LPRINT + 1) 315,314,314	D5	255
314 WRITE (6,1314)J,WN,B3,FACTOR,B1,COPR,TZ0(J),F2,SE,BP,SEP,SEB3,SEB1	D5	256
1,SECOPR,SETZ0(J),TBAR,SEBP	D5	257
1314 FORMAT(5X12,5XF4.0,F14.4,F11.4,F13.4,F12.5,F11.4,F12.2,F11.5,7XF14	D5	258
1.4,F10.5/8X10HSTD ERRORSF12.4,10XF14.4,F12.5,F11.4,24X2F10.4//)	D5	259
315 CONTINUE	D5	260
C*****RESET FOR ADDITIONAL CYCLES AS REQUIRED BY OPTIONS	D5	261
C REUSE SENSE LIGHT 1 TO RESTORE LBEGWT FOR UPPER PATTERN	D5	262
C LBEGWT = 9 MEANS 2 CYCLES, 1ST WITH BEGWT = 0 AND 2ND = 1	D5	263
NFRAME = NFRAME - 1	D5	264
316 IF (LBEGWT - 8) 320,320,317	D5	265
317 CALL SLITE (1)	D5	266
LBEGWT = 1	D5	267
GO TO 256	D5	268
320 CALL SLITET(1,INDEX)	D5	269
GO TO (321,330),INDEX	D5	270
321 LBEGWT = LSAVE	D5	271
C*****RESTORE OMSQT FOR OTHER PATTERN OR FOR DIFFERENT ZERO TIME CORR-	D5	272
C ECTION EXCEPT IN FINAL CALC FOR DOUBLE CELL	D5	273
330 CALL SLITET(4,INDEX)	D5	274
GO TO (340,332),INDEX	D5	275
332 DO 333 I = 1,NFRAME	D5	276
333 OMSQT(I) = OMSQT(I) + OMT0	D5	277
334 GO TO 999	D5	278
340 CALL SLITE (4)	D5	279
CALL SLITE (1)	D5	280
999 RETURN	D5	281
END	D5	282

TIBFTC D6-CS2 LIST,M94

*****CURVE FITTING LEAST SQUARES QUADRATIC, LINEAR AND ZERO DEGREES D6 1

C	Y = A + (B1)(X1) + (B2)(X2)	X2 = (X1)**2	D6	2
C	B3 IS TANGENT AT MEAN	B3 = B1 + 2 * B2 * X1BAR	D6	003
C	YO PLUS OR MINUS SE YO IS VALUE AT X1 = 0.	WEIGHT IS INTERPRETED	D6	4
C	AS RELATIVE NUMBER.	ZERO VALUE OF W CAUSES OMISSION OF ENTIRE	D6	005
C	POINT AND REDUCTION IN NUMBER OF ENTRIES N.		D6	6
C	L = 2 IS QUADRATIC, 1 LINEAR, 0 WEIGHTED AVERAGE OF Y ONLY.		D6	007
C	LINEAR FIT AFTER QUADRATIC IF L=3		D6	8
C	LPRINT = 1 NONE, 2 IMPLICIT OUTPUT IS PRINTED, 3 CHECK POINTS.		D6	009
C	DOUBLE PRECISION ON SUMS, DIFFERENCES OF SUMS, PARAMETERS A, B1,		D6	10
C	B2, AND SSE. STANDARD ERRORS ARE SINGLE PRECISION.		D6	011
C			D6	12
C	SUBROUTINE CFLS2 (LDEGRE,M,W,Y,X1,YO,SEYO,LPRINT)		D6	013
C			D6	14
C	COMMON /CS1CM/ A,B1,B2,YBAR,ALPHA(12),F2,FRAME(30),NCOMP,NFRAME,N,		D6	015
C	10MSQT(30),RBEGLN,RBEG,RMEN(30),RPK(30,4),RSQ,SEA,SEB1,SEB2,SE,		D6	16
C	2SETZOA,SEX0,SEYBAR,STAR(30,4),TIME(30),TZOA,WMIN,WN,X0,AP,BP,SEAP,		D6	017
C	3SEBP,SEP,TBAR,OMF,SERBLN,SPEED,REFR,FMOME,LKIND,LPRINT,LPLOT,		D6	18
C	4LINPUT,LBEGWT,NCELL,Z,XLINE(20),YLINE(20),NDATA(4),XX(100,4),		D6	019
C	5YY(100,4),COPR,SECOPR,SERBEG,XOP,SEXOP,B3,SEB3,STANRM(4,2),		D6	20
C	6SESTAN(4,2),DILN(4,2),METHOD,KIND(10),SEORD(10,2)		D6	021
C	DOUBLE PRECISION A,B1,B2,YBAR		D6	22
C	COMMON /CS2XY/ XDATA(10,50,2),START(10,9,2),RBAR(10,4),		D6	023
C	1STARRB(10,4),STARRM(10,4),CP(10,4),CO(10,4),TOPX(10,2),TOPY(10,2),		D6	24
C	2 BOTX(10,2),BOTY(10,2),XREF,	MENX(30,2),	D6	025
C	3MENW(30,2),PKX(30,4,2),PKW(30,4,2),PKLN(30,4,2),NCOMPS(2),		D6	26
C	4FLAGCL(2),FY,	YDATA(10,50,2),NPOINT(10,4),FLAGFR(30,2),	D6	027
C	5BMENX(30,2),BMENW(30,2),ANGLE(30)		D6	28
C	INTEGER START,FLAGCL,FLAGFR		D6	029
C	REAL MENX,MENW		D6	30
C	COMMON /WORKCM/REALCM(1000),INTCM(1000)		D6	031
C			D6	32
C	DIMENSION W(30),X1(30),Y(30)		D6	033
C	DIMENSION YDP(30),SUMY(1),WDP(30),X1DP(30),SUMX1(1),X2DP(30),		D6	34
C	1 SUMX2(1),SUMW(1),SNUM(1),SSE(1),X1BAR(1),X2BAR(1),		D6	035
C	2 S2Y(1),SM11(1),S11(1),SM12(1),S12(1),SM22(1),S22(1),		D6	36
C	3 SMYY(1),SYY(1),SM1Y(1),S1Y(1),SM2Y(1),SDEN(1)		D6	037
C	DOUBLE PRECISION SUMY,WDP,X1DP,SUMX1,X2DP,SUMX2,SUMW,SNUM,SSE,		D6	38
C	1X1BAR,X2BAR,S2Y,SM11,S11,SM12,S12,SM22,S22,SMYY,SYY,SM1Y,S1Y,		D6	039
C	2SM2Y,SDEN		D6	40
C	C*****INITIALIZATION		D6	041
C	L = LDEGRE		D6	42
C	YBAR = 0.0D0		D6	043
C	SEYBAR = Z		D6	44
C	A = 0.0D0		D6	045
C	SEA = Z		D6	46
C	N1 = 0.0D0		D6	047
C	SEB1 = Z		D6	48
C	D2 = 0.0D0		D6	049
C	SEB2 = Z		D6	50
C	B3 = 0.0		D6	051
C	SEB3 = Z		D6	52
C	AP = 0.0		D6	053
C	SEAP = Z		D6	54
C	BP = 0.0		D6	055
C	SEBP = Z		D6	56
C	X0 = 0.0		D6	057
C	SEX0 = Z		D6	58
C	XOP = 0.0		D6	059
C	SEXOP = Z		D6	60
C	SE = Z		D6	061
C	SEP = Z		D6	62

RSQ = 0.0	D6	63
RSQP = 0.0	D6	064
SNUM = 0.0D0	D6	65
SDEN = 0.0D0	D6	066
COVAB1 = 0.0	D6	67
COVB12 = 0.0	D6	068
X1BAR = 0.0D0	D6	69
X2BAR = 0.0 D0	D6	070
F2 = 0.0	D6	71
COPR = 0.0	D6	072
SECOPR = Z	D6	73
IF (L-1) 9,6,2	D6	074
2 SUMX2(1)= 0.0D0	D6	75
3 SM22(1)= 0.0D0	D6	076
4 SM12(1)= 0.0D0	D6	77
5 SM2Y(1)= 0.0D0	D6	078
6 SUMX1(1)= 0.0D0	D6	79
7 SM11(1)= 0.0D0	D6	080
8 SM1Y(1)= 0.0D0	D6	81
9 SUMY(1)= 0.0D0	D6	082
10 SMYY(1)= 0.0D0	D6	83
11 SUMW(1)= 0.0D0	D6	084
12 N = 0	D6	85
WN = 0.0	D6	086
C	D6	87
14 IF (LPRINT - 2) 20,20,15	D6	088
15 WRITE (6,2015)	D6	89
2015 FORMAT (1H1 4X1HW 16X1HY 15X2HX1 15X2HX2 15X4HSM11 13X4HSM12 13X	D6	090
1 4HSM22/12X4HSUMW 13X4HSUMY 13X5HSUMX1 12X5HSUMX2 12X	D6	91
2 4HSMYY 13X4HSM1Y 13X4HSM2Y)	D6	092
C*****FORM SUMS AND COUNT POINTS	D6	93
20 DO 49 I = 1,M	D6	094
21 IF (ABS(W(I)) - 1.E-10) 49,49,22	D6	95
22 N = N + 1	D6	096
23 IF (L - 1) 27,24,24	D6	97
24 X1DP(I) = 0.0D0	D6	098
25 CALL STORE(X1DP,X1DP(I),30,X1(I))	D6	99
26 X2DP(I) = X1DP(I)**2	D6	100
27 WDP(N) = 0.0D0	D6	101
28 CALL STORE(WDP,WDP(N),30,W(I))	D6	102
29 YDP(I) = 0.0D0	D6	103
30 CALL STORE(YDP,YDP(I),30,Y(I))	D6	104
31 IF (L-1) 39,36,32	D6	105
32 SUMX2(1)= SUMX2(1)+ WDP(N)*X2DP(I)	D6	106
33 SM22(1)= SM22(1)+ WDP(N)*X2DP(I)**2	D6	107
34 SM12(1)= SM12(1)+ WDP(N)*X1DP(I)*X2DP(I)	D6	108
35 SM2Y(1)= SM2Y(1)+ WDP(N)*X2DP(I)*YDP(I)	D6	109
36 SUMX1(1)= SUMX1(1)+ WDP(N)*X1DP(I)	D6	110
37 SM11(1)= SM11(1)+ WDP(N)*X1DP(I)**2	D6	111
38 SM1Y(1)= SM1Y(1)+ WDP(N)*X1DP(I)*YDP(I)	D6	112
39 SUMY(1)= SUMY(1)+ WDP(N)*YDP(I)	D6	113
40 SMYY(1)= SMYY(1)+ WDP(N)*YDP(I)**2	D6	114
41 SUMW(1)= SUMW(1)+ WDP(N)	D6	115
C	D6	116
42 IF (LPRINT-2) 49,49,43	D6	117
43 IF (L - 1) 44,45,48	D6	118
44 X1(I) = 0.0	D6	119
CALL STORE(SUMX1,SUMX1,1,0.0)	D6	120
CALL STORE(SM11,SM11,1,0.0)	D6	121
CALL STORE(SM1Y,SM1Y,1,0.0)	D6	122
45 CALL STORE(X2DP,X2DP(I),30,0.0)	D6	123

CALL STORE(SUMX2,SUMX2,1,0.0)	D6	124
CALL STORE(SM22,SM22,1,0.0)	D6	125
CALL STORE(SM12,SM12,1,0.0)	D6	126
CALL STORE(SM2Y,SM2Y,1,0.0)	D6	127
48 WRITE (6,2048)W(I),Y(I),X1(I),X2DP(I),SM11,SM12,SM22, SUMW,SUMY,SUD6	D6	128
1MX1,SUMX2,SMYY,SM1Y,SM2Y	D6	129
2048 FORMAT (1H 1PE12.5,6E17.5/2X7E17.5)	D6	130
49 CONTINUE	D6	131
IF (N) 998,998,50	D6	132
C*****COMPUTE MEANS AND CORRECT SUMS FOR MEANS	D6	133
50 IF (L-1) 58,55,51	D6	134
51 S22(1)= SM22(1)- SUMX2(1)**2/SUMW(1)	D6	135
52 S12(1)= SM12(1)- SUMX1(1)*SUMX2(1)/SUMW(1)	D6	136
53 S2Y(1)= SM2Y(1)- SUMX2(1)*SUMY(1)/SUMW(1)	D6	137
54 X2BAR(1)= SUMX2(1)/ SUMW(1)	D6	138
55 S11(1)= SM11(1)- SUMX1(1)**2/SUMW(1)	D6	139
56 S1Y(1)= SM1Y(1)- SUMX1(1)*SUMY(1)/SUMW(1)	D6	140
57 X1BAR(1)= SUMX1(1)/ SUMW(1)	D6	141
YBAR = SNGL(X1BAR)	D6	142
58 SYY(1)= SMYY(1)- SUMY(1)**2/SUMW(1)	D6	143
59 YBAR = SUMY(1)/SUMW(1)	D6	144
61 WMIN = PART(WDP,WDP(1),30)	D6	145
62 DO 63 J = 1,N	D6	146
63 WMIN= AMIN1(WMIN,PART(WDP,WDP(J),30))	D6	147
64 WN = SNGL(SUMW)/WMIN	D6	148
70 IF (N - 1) 998,999,71	D6	149
71 IF (L - 1) 75,80,110	D6	150
C*****L = 0, CONSTANT LEAST SQUARES	D6	151
75 SEYBAR = SQRT(ABS(SNGL(SYY)/(WMIN*FLOAT(N*(N-1))))	D6	152
77 GO TO 150	D6	153
C*****L = 1, LINEAR LEAST SQUARES	D6	154
80 B1 = S1Y(1)/S11(1)	D6	155
91 CALL STORE(A,A,1,SNGL(YBAR)- SNGL(B1)*SNGL(X1BAR))	D6	156
AP = A	D6	157
BP = B1	D6	158
B3 = B1	D6	159
IF (N-2) 999,93,100	D6	160
93 SEYBAR = SQRT(ABS(SNGL(SYY)/FLOAT(N*(N-1))))	D6	161
96 GO TO 150	D6	162
100 SSE(1) = SYY(1) - B1 * S1Y(1)	D6	163
IF (ABS (SYY) - 1.E-20) 104,104,103	D6	164
103 RSQ = SNGL(B1)*SNGL(S1Y)/SNGL(SYY)	D6	165
104 VE = ABS(SNGL(SSE)/(WMIN*FLOAT(N-2)))	D6	166
105 SEB1 = SQRT(VE/SNGL(S11))	D6	167
106 SEYBAR = SQRT(VE/SNGL(SUMW))	D6	168
107 SEA = SQRT(VE * (1.0/SNGL(SUMW)+ (SNGL(X1BAR)**2)/SNGL(S11)))	D6	169
SE = SQRT(VE)	D6	170
SEAP = SEA	D6	171
SEBP = SEB1	D6	172
SEB3 = SEB1	D6	173
SEP = SE	D6	174
108 GO TO 140	D6	175
C*****REDUCE DEGREE REQUESTED IF TOO FEW POINTS	D6	176
110 IF (N - 3) 111,111,120	D6	177
111 L = 1	D6	178
114 GO TO 80	D6	179
C*****L = 2, QUADRATIC LEAST SQUARES	D6	180
120 SDEN(1)= S11(1)*S22(1)- S12(1)**2	D6	181
121 SNUM(1)= S22(1)*(X1BAR(1)**2) - 2.0D0*(S12(1)*(X1BAR(1)*X2BAR(1)))	D6	182
1 + S11(1)*(X2BAR(1)**2)	D6	183
122 B2 = (S11(1)*S2Y(1)- S12(1)*S1Y(1))/SDEN(1)	D6	184

123	B1 = (S22(1)*S1Y(1)- S12(1)*S2Y(1))/SDEN(1)	D6	185
124	CALL STORE(A,A,1,SNGL(YBAR)- SNGL(B1)*SNGL(X1BAR)- SNGL(B2)*SNGL(X2BAR))	D6	186
	SSE(1) = SY(1) - B1 * S1Y(1) - B2 * S2Y(1)	D6	187
	IF (ABS (SY) - 1.E-20) 127,127,126	D6	188
126	RSQ = (SNGL(B1)*SNGL(S1Y)+ SNGL(B2)*SNGL(S2Y))/SNGL(SY)	D6	189
127	VE = ABS(SNGL(SSE)/(WMIN*FLOAT(N-3)))	D6	190
128	SEB2 = SQRT(VE*SNGL(S11)/SNGL(SDEN))	D6	191
129	SEB1 = SQRT(VE*SNGL(S22)/SNGL(SDEN))	D6	192
130	SEYBAR = SQRT(VE/SNGL(SUMW))	D6	193
131	SEA = SQRT(VE*(1.0/SNGL(SUMW)+ SNGL(SNUM)/SNGL(SDEN)))	D6	194
132	F2 = (SNGL(B2)/SEB2)**2	D6	195
133	COVB12 = - VE*SNGL(S12)/SNGL(SDEN)	D6	196
134	COPR = SNGL(B2)/(SNGL(B1)**2)	D6	197
135	SECOPR=(SQRT((SEB2/SNGL(B1))**2+4.0*((COPR*SEB1)**2-COPR*COVB12/SNGL(B1))))/ABS(SNGL(B1))	D6	198
	B3 = B1 + 2.0*B2*X1BAR	D6	199
136	SEB3=SQRT(SEB1**2+(2.0*X1BAR*SEB2)**2+4.0*X1BAR*COVB12)	D6	200
	SE = SQRT(VE)	D6	201
C*****	DETERMINE X FOR GIVEN Y	D6	202
140	IF (ABS(Y0) - 1.E-10) 150,150,141	D6	203
141	IF (L - 1) 150,142,143	D6	204
142	X0 = (Y0 - SNGL(A))/SNGL(B1)	D6	205
	COVB12 = 0.0	D6	206
	GO TO 146	D6	207
143	X0 = SNGL(B1)**2-4.0*SNGL(B2)*(SNGL(A)-Y0)	D6	208
	IF (X0) 144,145,145	D6	209
144	WRITE (6,2144)	D6	210
2144	FORMAT(65H0**CAUTION**TOO LARGE ERROR IN DATA, ZERO TIME CANNOT BE D	D6	211
	1 COMPUTED)	D6	212
	X0 = 0.0	D6	213
	GO TO 148	D6	214
145	X0 = (SNGL(B1) - SQRT(X0))/(-2.*SNGL(B2))	D6	215
146	COVAB1 = -SNGL(X1BAR)*(SEB1**2) - SNGL(X2BAR)*COVB12	D6	216
	SEX0 = SEY0**2+SEA**2+(X0*SEB1)**2+2.0*X0*COVAB1	D6	217
	IF (SEX0) 300,147,147	D6	218
300	WRITE (6,2300)	D6	219
2300	FORMAT(71H0**CAUTION**TOO LARGE ERROR IN DATA, ZERO TIME ERROR CAND	D6	220
	1 NOT BE COMPUTED)	D6	221
	SEX0 = Z	D6	222
	GO TO 148	D6	223
147	SEX0 = (SQRT (SEX0))/ABS(SNGL(B1))	D6	224
	GO TO 150	D6	225
148	SEX0 = Z	D6	226
C		D6	227
150	IF (LPRINT - 2) 160,152,151	D6	228
151	WRITE (6,2151)SNUM(1),SDEN(1),S11(1),SY(1),S12(1), S1Y(1),S22(1),D6	D6	229
	1S2Y(1),SSE(1)	D6	230
2151	FORMAT (1H0 6X4HSNUM 9X4HSDEN 10X3HS11 10X3HSY 10X3HS12 10X3HS1Y D6	D6	231
	110X3HS22 10X3HS2Y 10X3HSSE/3X1P9E13.5)	D6	232
152	WRITE (6,2152)L,M,YBAR,Y0,X1BAR,X0,A,B1,B2,N,SEYBAR, SEY0,X2BAR,SED6	D6	233
	1X0,SEA,SEB1,SEB2,WN,WMIN,COVAB1,COVB12,RSQ,SE,F2,B3,SEB3	D6	234
2152	FORMAT (1H0 4X5HL M 11X5HY BAR 11X2HY0 12X6HX1 BAR 10X2HX0 13X D6	D6	235
	1 1HA 14X2HB1 13X2HB2/5X11,2X12,5X1P7E15.5/7X1HN 12X D6	D6	236
	2 8HSE Y BAR 8X5HSE Y0 10X6HX2 BAR 8X5HSE X0 10X4HSE A 11X D6	D6	237
	35HSE B1 11X5HSE B2/6X12,7X7E15.5/6X2HWN 12X5HW MIN 11X9HCOV(A,B1) D6	D6	238
	46X10HCOV(B1,B2) 6X3HRSQ 11X2HSE 10X18HF (PARABOLIC TERM)/1XE14.5, D6	D6	239
	53E15.5,0PF15.9,1P2E15.5/30X2HB3E15.5,6H SEB3E15.5)	D6	240
C*****	L = 3, LINEAR LEAST SQUARES AFTER QUADRATIC	D6	241
160	IF (L - 3) 999,161,999	D6	242
161	BP = SNGL(S1Y)/SNGL(S11)	D6	243

162	AP = SNGL(YBAR)- BP*SNGL(X1BAR)	D6	24
	SSE(1)= SYY(1)- (S1Y(1)**2)/S11(1)	D6	24
	IF (ABS (SYY) - 1.E-20) 165,165,164	D6	248
164	RSQ = (SNGL(S1Y)**2)/(SNGL(S11)*SNGL(SYY))	D6	249
165	VE = ABS(SNGL(SSE)/(WMIN*FLOAT(N-2)))	D6	250
166	SEBP = SQRT(VE/SNGL(S11))	D6	251
167	SEAP = SQRT(VE*(1.0/SNGL(SUMW)+ (SNGL(X1BAR)**2)/SNGL(S11)))	D6	252
168	COVAB1 = -SNGL(X1BAR)* (SEBP**2)	D6	253
169	SEP = SQRT(VE)	D6	254
172	IF (ABS(Y0)-1.E-10) 179,179,176	D6	255
176	XOP = (Y0-AP)/BP	D6	256
177	SEXOP = (SQRT(SEY0**2+SEAP**2+(XOP*SEBP)**2)+2.0*X0*COVAB1)/BP	D6	257
C		D6	258
179	IF (LPRINT - 2) 999,180,180	D6	259
180	WRITE (6,2180)RSQ ,SEP,AP,SEAP,BP,SEBP,COVAB1,XOP,SEXOP	D6	260
2180	FORMAT(42H LINEAR LEAST SQUARES FITTING OF SAME DATA/8X3HRSQ 11X2HD6	D6	261
	1SE 12X1HA 12X4HSE A 12X1HB 11X4HSE B 7X8HCOV(A,B) 12X2HX012X5HSE XD6	D6	262
	20/F15.9,1P8E14.5//)	D6	263
	GO TO 999	D6	264
998	WRITE (6,2998)	D6	265
2998	FORMAT(47H **CAUTION**ALL WEIGHTS ARE ZERO, CFLS NOT DONE)	D6	266
	WN = 1.E-10	D6	267
	WMIN = 1.E-10	D6	268
999	RETURN	D6	269
	END	D6	270
\$IBFTC D7-CS2 LIST,M94			
C*****PLOTING SUBROUTINE			
C		D7	1
	SUBROUTINE PLOT(TITLE1,TITLE2,XX,YY,NDATA,NF,XLINE,YLINE,NX,NY,	D7	002
	1LPLOT)	D7	3
C		D7	004
	DIMENSION PAGE(50,17),SYMBOL(4),AMASK(6),XLINE(20),YLINE(20),	D7	5
	1NDATA(4),XX(100,4),YY(100,4)	D7	006
	DIMENSION TITLE1(12),TITLE2(12)	D7	7
	COMMON /WORKCM/REALCM(1000),INTCM(1000)	D7	008
	EQUIVALENCE (PAGE(1,1),REALCM(1))	D7	9
	DATA AMASK(1)/07700000000000/	D7	010
	DATA AMASK(2)/077000000000/	D7	11
	DATA AMASK(3)/0770000000/	D7	012
	DATA AMASK(4)/0770000/	D7	13
	DATA AMASK(5)/07700/	D7	014
	DATA AMASK(6)/077/	D7	15
	DATA SYMBOL(1)/0545454545454/	D7	016
	DATA SYMBOL(2)/0464646464646/	D7	17
	DATA SYMBOL(3)/0303030303030/	D7	018
	DATA SYMBOL(4)/0676767676767/	D7	19
	DATA BLANK/0606060606060/	D7	020
	DATA DASH/0404040404040/	D7	21
	DATA UPLINE/0333333333333/	D7	022
	DATA EQUAL/0131313131313/	D7	23
	IF (LPLOT) 999,10,10	D7	024
C*****SET UP BLANK MATRIX		D7	25
10	DO 12 I=1,50	D7	026
11	DO 12 J=1,17	D7	27
12	PAGE(I,J)=BLANK	D7	028
C*****LOCATE MAXIMA AND MINIMA		D7	29
20	XMAX=XX(1,1)	D7	030
21	XMIN=XMAX	D7	31
22	YMAX=YY(1,1)	D7	032
		D7	3

23	YMIN=YMAX	D7	34
24	DO 30 K=1,NF	D7	035
25	NDF=NDATA(K)	D7	36
	IF (NDF) 30,30,26	D7	037
26	DO 29 J=1,NDF	D7	38
27	XMAX=AMAX1(XMAX,XX(J,K))	D7	039
28	XMIN=AMIN1(XMIN,XX(J,K))	D7	40
	YMAX=AMAX1(YMAX,YY(J,K))	D7	041
29	YMIN=AMIN1(YMIN,YY(J,K))	D7	42
30	CONTINUE	D7	043
31	IF(NX)35,35,32	D7	44
32	DO 34 J=1,NX	D7	045
33	XMAX=AMAX1(XMAX,XLINE(J))	D7	46
34	XMIN=AMIN1(XMIN,XLINE(J))	D7	047
35	IF(NY)39,39,36	D7	48
36	DO 38 J=1,NY	D7	049
37	YMAX=AMAX1(YMAX,YLINE(J))	D7	50
38	YMIN=AMIN1(YMIN,YLINE(J))	D7	051
C*****	FIND TRANSFORM CONSTANTS	D7	52
39	XSC= 99.0/(XMAX-XMIN)	D7	053
	YSC= 49.0/(YMAX-YMIN)	D7	54
C*****	ADD REFERENCE LINES	D7	055
40	IF(NX)50,50,41	D7	56
41	DO 47 J=1,NX	D7	057
42	JX=((XLINE(J)-XMIN)*XSC+0.5)	D7	58
43	JWORD=(JX/6)+1	D7	059
44	JPOS=MOD(JX,6)+1	D7	60
45	DO 46 K=1,50	D7	061
46	PAGE(K,JWORD)=OR(AND(PAGE(K,JWORD),COMPL(AMASK(JPOS))),AND(AMASK(JD7	D7	62
	1POS),UPLINE))	D7	063
47	CONTINUE	D7	64
50	IF(NY)60,60,51	D7	065
51	DO 55 J=1,NY	D7	66
52	JY=((YLINE(J)-YMIN)*YSC+1.5)	D7	067
53	DO 54 K=1,17	D7	68
54	PAGE(JY,K)=DASH	D7	069
55	CONTINUE	D7	70
C*****	TRANSFORM POINTS AND INSERT IN MATRIX WITH PROPER SYMBOL	D7	071
60	DO 90 K=1,NF	D7	72
61	NDF=NDATA(K)	D7	073
	IF (NDF) 90,90,62	D7	74
62	DO 89 J=1,NDF	D7	075
75	JY=((YY(J,K)-YMIN)*YSC+1.5)	D7	76
76	JX=((XX(J,K)-XMIN)*XSC+0.5)	D7	077
77	JWORD=(JX/6)+1	D7	78
78	JPOS=MOD(JX,6)+1	D7	079
79	TEST=AND(PAGE(JY,JWORD),AMASK(JPOS))	D7	80
	TUP=AND(UPLINE,AMASK(JPOS))	D7	081
	TDASH=AND(DASH,AMASK(JPOS))	D7	82
	TBLANK=AND(BLANK,AMASK(JPOS))	D7	083
82	IF(TEST.EQ.TBLANK)GOTO85	D7	84
83	IF(TEST.EQ.TDASH)GOTO85	D7	085
84	IF(TEST.EQ.TUP)GOTO85	D7	86
	SYM=EQUAL	D7	087
	GOTO88	D7	88
85	SYM=SYMBOL(K)	D7	089
88	PAGE(JY,JWORD)=OR(AND(PAGE(JY,JWORD),COMPL(AMASK(JPOS))),AND(SYM,AD7	D7	90
	1MASK(JPOS)))	D7	091
89	CONTINUE	D7	92
90	CONTINUE	D7	093
		D7	94

XUNIT=1.0/XSC	D7	9
YUNIT=1.0/YSC	D7	09
WRITE (6,100) TITLE1,TITLE2,XUNIT,YUNIT	D7	97
100 FORMAT(1H120X12A6/1H 12A6, 8X12HX SCALE UNIT 1PE11.3,3X12HY SCALE	D7	098
1UNIT E11.3/5X19H= IS MULTIPLE POINT)	D7	99
108 WRITE (6,109)	D7	100
109 FORMAT(16X20(5H+I+++),4H+I++)	D7	101
110 FORMAT(16X2H+ 16A6,A4,2H +)	D7	102
111 DO 113 J=1,50	D7	103
112 JC=51-J	D7	104
113 WRITE (6,110) (PAGE(JC,K),K=1,17)	D7	105
115 WRITE (6,109)	D7	106
C*****LIST INPUT DATA	D7	107
120 IF (LPL0T - 1) 999,121,121	D7	108
121 WRITE (6,122) TITLE1,TITLE2	D7	109
122 FORMAT(1H1 10X12A6/10X12A6,20X13H(X,Y) PLOTTED)	D7	110
DO 126 J = 1,NF	D7	111
WRITE (6,123) SYMBOL(J)	D7	112
123 FORMAT(1H 30X6HSYMBOL3XA6)	D7	113
K = NDATA(J)	D7	114
IF (K) 126,126,124	D7	115
124 WRITE (6,125) (XX(I,J),YY(I,J),I=1,K)	D7	116
125 FORMAT(5(1PE13.5,1H,E12.5))	D7	117
126 CONTINUE	D7	118
999 RETURN	D7	119
END	D7	120

\$IBFTC D8-CS2 LIST,M94

C*****SUBROUTINE FOR PLATEAU AND INITIAL CONCENTRATION, SECOND MOMENT	D8	001
C BOUNDARY POSITION, AND G*(S*)	D8	2
C	D8	003
C SUBROUTINE CONC	D8	4
C	D8	005
COMMON /CS1CM/ A,B1,B2,YBAR,ALPHA(12),F2,FRAME(30),NCOMP,NFRAME,N,	D8	6
10MSQT(30),RBEGLN,RBEG,RMEN(30),RPK(30,4),RSQ,SEA,SEB1,SEB2,SE,	D8	007
2SETZOA,SEXO,SEYBAR,STAR(30,4),TIME(30),TZOAWMIN,WN,XO,AP,BP,SEAP,	D8	8
3SEBP,SEP,TBAR,OMF,SERBLN,SPEED,REFR,FMOME,LKIND,LPRINT,LPL0T,	D8	009
4LINP0T,LBEGWT,NCELL,2,XLINE(20),YLINE(20),NDATA(4),XX(100,4),	D8	10
5YY(100,4),COPR,SECOPR,SERBEG,XOP,SEXOP,B3,SEB3,STANRM(4,2),	D8	011
6SESTAN(4,2),DILN(4,2),METHOD,KIND(10),SEORD(10,2)	D8	12
DOUBLE PRECISION A,B1,B2,YBAR	D8	013
COMMON /CS2XY/ XDATA(10,50,2),START(10,9,2),RBAR(10,4),	D8	14
1STARRB(10,4),STARRM(10,4),CP(10,4),CO(10,4),TOPX(10,2),TOPY(10,2),	D8	015
2 BOTX(10,2),BOTY(10,2),XREF, MENX(30,2),	D8	16
3MENW(30,2),PKX(30,4,2),PKW(30,4,2),NCOMPS(2),	D8	017
4FLAGCL(2),FY, YDATA(10,50,2),NPOINT(10,4),FLAGFR(30,2),	D8	18
5BMENX(30,2),BMENW(30,2),ANGLE(30)	D8	019
INTEGER START,FLAGCL,FLAGFR	D8	20
REAL MENX,MENW	D8	021
COMMON /WORKCM/REALCM(1000),INTCM(1000)	D8	22
C	D8	023
DIMENSION TITLE2(12),SECP(10,4),SECO(10,4)	D8	24
C*****CHECK THAT X,Y DATA HAVE BEEN MEASURED	D8	025
DO 20 IFRAME = 1,NFRAME	D8	26
IF (FLAGFR(IFRAME,NCELL)) 20,20,30	D8	027
20 CONTINUE	D8	28
GO TO 990	D8	029
C*****FACTORS AND INITIALIZATION	D8	30
30 FACT1 = 0.5 * FY/FMOME	D8	031
FACT2 = 0.25/(RBEG*FMOME)**2	D8	32

XBEGLN = RBEGLN + ALOG(FMOME)	D8	33
JPLOT = 0	D8	034
KPLOT = 0	D8	35
LSAVE = LPLOT	D8	036
DO 32 IFRAME = 1,NFRAME	D8	37
JFRAME = FLAGFR(IFRAME,NCELL)	D8	038
DO 32 J = 1,NCOMP	D8	39
32 NPOINT(JFRAME,J) = 0	D8	040
DO 33 J = 1,4	D8	41
33 NDATA(J) = 0	D8	042
C*****MAIN LOOP OVER ALL FRAMES	D8	43
DO 200 IFRAME = 1,NFRAME	D8	044
IF (FLAGFR(IFRAME,NCELL)) 200,200,40	D8	45
40 JFRAME = FLAGFR(IFRAME,NCELL)	D8	046
ANG = 0.0174533 * ANGLE(IFRAME)	D8	47
TANANG = SIN(ANG)/COS(ANG)	D8	048
FACTCP = FACT1 * TANANG	D8	49
FACTCO = FACT2 * FACTCP	D8	050
IF (FACTCO) 42,42,44	D8	51
42 WRITE (6,1042) FRAME(IFRAME)	D8	052
1042 FORMAT(18H0**CAUTION**FRAME A4,21H HAS ZERO CONC FACTOR)	D8	53
GO TO 200	D8	054
44 FACTG = OMSQT(IFRAME) - TZOA * OMF	D8	55
IF (ABS(FACTG) - 1.E-20) 45,45,46	D8	056
45 WRITE (6,1045) FRAME(IFRAME)	D8	57
1045 FORMAT(18H0**CAUTION**FRAME A4,39H HAS ZERO TIME, S* CANNOT BE CALD	D8	058
1CULATED)	D8	59
LPLOT = -1	D8	060
46 FACTS = 1.0/FACTG	D8	61
FACTG = 8. * FACTG * FACTCO	D8	062
IF (ABS(SEORD(JFRAME,NCELL)) - 1.E-10) 48,48,49	D8	63
48 SEORD(JFRAME,NCELL) = 0.05/TANANG	D8	064
49 SEY = SEORD(JFRAME,NCELL)	D8	65
JPLOT = MOD (JPLOT,4) + 1	D8	066
C*****LOOP OVER ALL COMPONENTS	D8	67
DO 100 J = 1,NCOMP	D8	068
JPEAK = NCOMP - J + 1	D8	69
CP (JFRAME,JPEAK) = 0.0	D8	070
CO (JFRAME,JPEAK) = 0.0	D8	71
SECP(JFRAME,JPEAK) = 0.0	D8	072
SECO(JFRAME,JPEAK) = 0.0	D8	73
INDEX1 = START(JFRAME,JPEAK+1,NCELL)	D8	074
INDEX2 = START(JFRAME,JPEAK,NCELL) - 1	D8	75
IF (INDEX2 - INDEX1 - 2) 100,50,50	D8	076
C*****LOOP OVER ALL POINTS, SUM FOR CONC, CONVERT X TO S* AND Y TO G*	D8	77
50 SIGNDX = XDATA(JFRAME,INDEX2,NCELL) - XDATA(JFRAME,INDEX1,NCELL)	D8	078
DO 90 KPOINT = INDEX1,INDEX2	D8	79
NPOINT(JFRAME,JPEAK) = NPOINT(JFRAME,JPEAK) + 1	D8	080
DELTAX = XDATA(JFRAME,KPOINT+1,NCELL)-XDATA(JFRAME,KPOINT,NCELL)	D8	81
IF (SIGNDX * DELTAX + 1.E-20) 54,54,56	D8	082
54 WRITE (6,1054) FRAME(IFRAME),JPEAK,KPOINT	D8	83
1054 FORMAT(18H0**CAUTION**FRAME A4,5H PEAKI3,6H POINTI3,16H IS OUT OF	D8	084
1ORDER)	D8	85
56 FACTOR = DELTAX**2	D8	086
SECP(JFRAME,JPEAK) = SECP(JFRAME,JPEAK) + FACTOR	D8	87
XMEAN = XDATA(JFRAME,KPOINT+1,NCELL) + XDATA(JFRAME,KPOINT,NCELL)	D8	088
YMEAN = YDATA(JFRAME,KPOINT+1,NCELL) + YDATA(JFRAME,KPOINT,NCELL)	D8	89
XMSQ = XMEAN**2	D8	090
FACTOR = FACTOR*(XMSQ**2)	D8	91
SECO(JFRAME,JPEAK) = SECO(JFRAME,JPEAK) + FACTOR	D8	092
FACTOR = YMEAN * DELTAX	D8	93

CP(JFRAME,JPEAK) = CP(JFRAME,JPEAK) + FACTOR	D8	9
CO(JFRAME,JPEAK) = CO(JFRAME,JPEAK) + FACTOR * XMSQ	D8	99
IF (LPLOT) 90,60,60	D8	96
60 IF (NDATA(JPLOT) - 99) 80,70,70	D8	097
70 JPLOT = MOD (JPLOT,4) + 1	D8	98
80 NDATA(JPLOT) = NDATA(JPLOT) + 1	D8	099
KPLOT = MAX0(KPLOT,JPLOT)	D8	100
IPLOT = NDATA(JPLOT)	D8	101
XX(IPLOT,JPLOT) = FACTS*(ALOG(XDATA(JFRAME,KPOINT,NCELL))-XBEGLN)	D8	102
YY(IPLOT,JPLOT) = FACTG*((XDATA(JFRAME,KPOINT,NCELL))**3)*YDATA(JFRAME,KPOINT,NCELL)	D8	103
1ME,KPOINT,NCELL)	D8	104
90 CONTINUE	D8	105
CP(JFRAME,JPEAK) = FACTCP * CP(JFRAME,JPEAK)	D8	106
CO(JFRAME,JPEAK) = FACTCO * CO(JFRAME,JPEAK)	D8	107
SECP(JFRAME,JPEAK) = SEY * FACTCP * SQRT(SECP(JFRAME,JPEAK))	D8	108
SECO(JFRAME,JPEAK) = SEY * FACTCO * SQRT(SECO(JFRAME,JPEAK))	D8	109
RBAR(JFRAME,JPEAK) = RBEG*SQRT(CO(JFRAME,JPEAK)/CP(JFRAME,JPEAK))	D8	110
STARRB(JFRAME,JPEAK) = FACTS*(ALOG(RBAR(JFRAME,JPEAK))-RBEGLN)	D8	111
IF (PKW(JFRAME,JPEAK,NCELL) - 1.E-10) 95,95,96	D8	112
95 STARRM(JFRAME,JPEAK) = 2	D8	113
GO TO 97	D8	114
96 STARRM(JFRAME,JPEAK) = FACTS * (PKLN(JFRAME,JPEAK,NCELL)-RBEGLN)	D8	115
97 IF (LPLOT) 100,98,98	D8	116
98 NDATA(JPLOT) = NDATA(JPLOT) + 1	D8	117
IPLOT = NDATA(JPLOT)	D8	118
KPOINT = INDEX2 + 1	D8	119
XX(IPLOT,JPLOT) = FACTS*(ALOG(XDATA(JFRAME,KPOINT,NCELL))-XBEGLN)	D8	120
YY(IPLOT,JPLOT) = FACTG*((XDATA(JFRAME,KPOINT,NCELL))**3)*YDATA(JFRAME,KPOINT,NCELL)	D8	121
1ME,KPOINT,NCELL)	D8	122
100 CONTINUE	D8	123
LPLOT = LSAVE	D8	124
200 CONTINUE	D8	125
C	D8	126
IF (LPRINT) 411,401,401	D8	127
401 WRITE (6,1401) ALPHA,NCELL,FY	D8	128
1401 FORMAT(1H012A6,5X30H CONCENTRATION ANALYSIS CELL13,13H CONC FACD8	D8	129
1TORF8.5/131HOFAME TIMER PEAK INITIAL MG/ML PLATEAU CONC RBAR	D8	130
2 S* MAX S* RBAR INTERVALS ANGLE SE CO SE CP	D8	131
3SE ORDINATE)	D8	132
DO 409 IFRAME = 1,NFRAME	D8	133
JFRAME = FLAGFR(IFRAME,NCELL)	D8	134
DO 409 JPEAK = 1,NCOMP	D8	135
IF (NPOINT(JFRAME,JPEAK)) 409,409,403	D8	136
403 WRITE (6,1403) FRAME(IFRAME),TIME(IFRAME),JPEAK,CO(JFRAME,JPEAK),	D8	137
1 CP(JFRAME,JPEAK),RBAR(JFRAME,JPEAK),STARRM(JFRAME,JPEAK),	D8	138
2STARRB(JFRAME,JPEAK),NPOINT(JFRAME,JPEAK),ANGLE(IFRAME),	D8	139
3SECO(JFRAME,JPEAK),SECP(JFRAME,JPEAK),SEORD(JFRAME,NCELL)	D8	140
1403 FORMAT(1H A5,F8.3,I3,2X5(1PE12.4),I4,4E12.4)	D8	141
409 CONTINUE	D8	142
C	D8	143
411 IF (LPLOT) 999,415,415	D8	144
DATA TITLE2(1)/72HSCHLIEREN DATA PLOTTED AS G*, VS. S*. ALL FRAMES	D8	145
1 ARE SUPERIMPOSED. /	D8	146
415 XLINE(1) = 0.0	D8	147
YLINE(1) = 0.0	D8	148
DO 416 JPEAK = 1,NCOMP	D8	149
416 XLINE(JPEAK+1) = STARRM(JPEAK,NCELL)	D8	150
CALL PLOT (ALPHA,TITLE2,XX,YY,NDATA,KPLOT,XLINE,YLINE,NCOMP+1,1,	D8	151
1LPLOT)	D8	152
GO TO 999	D8	153
990 WRITE (6,1990)	D8	15


```

1990 FORMAT(40H **CAUTION**CONCENTRATION NOT CALCULATED)
999 RETURN
END

```

```

D8 155
D8 156
D8 157

```

```

$IBFTC D9-CS2 LIST,M94
C*****F TABLE FOR FIRST COLUMN AT 5 PERCENT LEVEL

```

```

C
SUBROUTINE FTEST (NDFL,NDFG,F,PROB)
C
NDF = NDFL
PROB=100.0
IF(NDF)999,999,11
11 IF(F)999,13,13
13 IF(NDF-10)16,14,15
14 IF(F-4.96)999,100,100
15 IF(F-3.84)999,100,100
16 GO TO (21,22,23,24,25,26,27,28,29),NDF
21 IF(F-161.0)999,100,100
22 IF(F-18.51)999,100,100
23 IF(F-10.13)999,100,100
24 IF(F- 7.71)999,100,100
25 IF(F- 6.61)999,100,100
26 IF(F- 5.99)999,100,100
27 IF(F- 5.59)999,100,100
28 IF(F- 5.32)999,100,100
29 IF(F- 5.12)999,100,100
100 PROB=4.9999
999 RETURN
END

```

```

D9 1
D9 002
D9 3
D9 004
D9 5
D9 006
D9 7
D9 008
D9 9
D9 010
D9 11
D9 012
D9 13
D9 014
D9 15
D9 016
D9 17
D9 018
D9 19
D9 020
D9 21
D9 022
D9 23
D9 024

```

```

$IBFTC D10CS2 LIST,M94

```

```

C*****POLYNOMIAL LEAST SQUARES CURVE FITTING ROUTINE (SINGLE PRECISION)

```

```

C
SUBROUTINE LSPOLY (TITLE,NCARDS,MIN,MAX,LWT,MEAN,INPUT,LFNCTN,
1LSCALE,LPRINT,XSCALE,YSCALE,XINPUT,YINPUT,WINPUT,XZERO)
C
COMMON /WORKCM/REALCM(1000),INTCM(1000)
DIMENSION TITLE(12), X(30,7),Y(30),W(30),XBAR(7),XX(7,7),
1XY(7),B(7),SEB(7),SE(7),F(7),VARCOV(7,7),RESID(30,7),WINPUT(30),
2XXINV(7,7),EN(30),TRY(30),XINPUT(30),YINPUT(30)
EQUIVALENCE (X(1,1),REALCM(1)),(Y(1),REALCM(201)),(W(1),REALCM(231D10
1)), (B(1),REALCM(301)),(SEB(1),REALCM(311))D10
2,(SE(1),REALCM(321)),(F(1),REALCM(331)),(EN(1),REALCM(341)),(TRY(1D10
3),REALCM(371)),(XBAR(1),REALCM(401)),(XX(1),REALCM(411)),
4(XY(1),REALCM(461)),(VARCOV(1,1),REALCM(501)),(XXINV(1,1),REALCM
5(601)),(RESID(1,1),REALCM(701)), (YBAR,REALCM(410)),
6(PROB,REALCM(991)),(WN,REALCM(992)),(WMIN,REALCM(993)),
7(SUMW,REALCM(994))
C*****READ, COUNT AND PRINT INPUT DATA
IF (INPUT) 990,15,5
5 READ (5,1005) TITLE,LRETRN
1005 FORMAT(12A6,I3)
IF (LRETRN) 10,10,6
6 NCARDS = LRETRN
RETURN
10 READ (5,1010) MIN,MAX,LWT,MEAN,INPUT,LFNCTN,LSCALE,LPRINT,
1XSCALE,YSCALE,XZERO
1010 FORMAT(8I2,3X2E20.7,F10.5)
11 DO 13 I = 1,30

```

```

D10 001
D10 2
D10 003
D10 4
D10 005
D10 6
D10 007
D10 8
D10 009
D10 10
D10 011
D10 12
D10 013
D10 14
D10 015
D10 16
D10 017
D10 18
D10 019
D10 20
D10 021
D10 22
D10 023
D10 24
D10 025
D10 26
D10 027
D10 28

```

12 READ (5,1012)EN(I),TRY(I),XINPUT(I),YINPUT(I),WINPUT(I),LSTOP	D10	29
1012 FORMAT(A6,A3,3(E20.7),I3)	D10	030
IF (LSTOP) 13,13,14	D10	31
13 CONTINUE	D10	032
14 NCARDS = I	D10	33
C*****USE WEIGHTS TO COUNT POINTS AND DETERMINE NUMBER OF REPLICATES	D10	034
C TRANSFORM DATA AS INDICATED BY OPTIONS	D10	35
15 IF (NCARDS) 990,990,16	D10	036
16 IF (LWT-3) 162,162,990	D10	37
162 IF (LSCALE-1) 163,164,165	D10	038
163 XSC = 1.0	D10	39
YSC = 1.0	D10	040
GO TO 169	D10	41
164 YSC = 1.0	D10	042
GO TO 166	D10	43
165 YSC = YSCALE	D10	044
166 XSC = XSCALE	D10	45
169 NDATA=0	D10	046
SUMW=0.0	D10	47
WMIN=1.E30	D10	048
DO26 I=1,NCARDS	D10	49
IF(LWT)990,17,18	D10	050
17 W(I)=1.0	D10	51
GOTO25	D10	052
18 IF(WINPUT(I)-1.E-15)19,19,20	D10	53
19 W(I)=0.0	D10	054
X(I,2) = 0.0	D10	55
Y(I) = 0.0	D10	056
GO TO 26	D10	57
20 GOTO(21,22,23),LWT	D10	058
21 W(I)=WINPUT(I)	D10	59
GOTO25	D10	060
22 W(I)=1.0/WINPUT(I)	D10	61
GOTO25	D10	062
23 W(I)=1.0/WINPUT(I)**2	D10	63
25 WMIN=AMIN1(WMIN,W(I))	D10	064
SUMW=SUMW+W(I)	D10	65
NDATA=NDATA+1	D10	066
X(I,2) = (XINPUT(I) - XZERO) * XSC	D10	67
Y(I) = YINPUT(I) * YSC	D10	068
26 CONTINUE	D10	69
28 WN = SUMW/WMIN	D10	070
C*****CONVERT WEIGHTS TO RELATIVE VALUES, TAKE LOGS IF REQUESTED	D10	71
DO 31 I = 1,NCARDS	D10	072
IF (W(I) - 1.E-15) 31,31,29	D10	73
29 W(I)=W(I)/WMIN	D10	074
IF (LFNCTN) 31,31,30	D10	75
30 Y(I) = ALOG(Y(I))	D10	076
31 CONTINUE	D10	77
C*****SAFEGUARD IF TOO FEW DATA POINTS	D10	078
IF (NDATA - MIN - 1) 990,310,311	D10	79
310 LEAST = NDATA - 1	D10	080
GO TO 312	D10	81
311 LEAST = MIN + 1	D10	082
312 IF (NDATA - MAX - 1) 32,32,33	D10	83
32 LAST = NDATA - 1	D10	084
GO TO 34	D10	85
33 LAST = MAX + 1	D10	086
34 IF (MAX - MIN) 313 ,314,314	D10	87
313 LEAST = LAST	D10	088
LSAVE = LAST	D10	89

*****SET UP POWERS OF X AND DETERMINE MEAN VALUES, AND SYY	D10	90
314 LMAX = LAST - 1	D10	091
XBAR(1) = 1.0	D10	92
DO 35 I = 1,NCARDS	D10	093
[35 X(I,1) = 1.0	D10	94
IF (LAST - 2) 317,316,315	D10	095
[315 DO 36 J = 3, LAST	D10	96
DO 36 I = 1,NCARDS	D10	097
[36 X(I,J) = X(I,2)*X(I,J-1)	D10	98
[316 DO 39 J = 2, LAST	D10	099
XBAR(J) = 0.0	D10	100
DO 38 I = 1,NCARDS	D10	101
[38 XBAR(J) = XBAR(J) + X(I,J)*W(I)	D10	102
39 XBAR(J) = XBAR(J)/WN	D10	103
317 YBAR = 0.0	D10	104
SYY=0.0	D10	105
DO 41 I = 1,NCARDS	D10	106
YBAR = YBAR + W(I)*Y(I)	D10	107
[41 SYY=SYY+W(I)*(Y(I)**2)	D10	108
YBAR = YBAR/WN	D10	109
C*****SET UP XX AND XY MATRICES (SXX,SXY ETC.)	D10	110
DO 42 JCOL=1,LMAX	D10	111
XX(1,JCOL)=0.0	D10	112
DO 42 I=1,NCARDS	D10	113
[42 XX(1,JCOL)=XX(1,JCOL)+W(I)*X(I,1)*X(I,JCOL)	D10	114
DO 43 JROW=1, LAST	D10	115
XX(JROW, LAST)=0.0	D10	116
XY(JROW)=0.0	D10	117
DO 43 I=1,NCARDS	D10	118
XX(JROW, LAST)=XX(JROW, LAST)+W(I)*X(I,JROW)*X(I, LAST)	D10	119
[43 XY(JROW)=XY(JROW)+W(I)*X(I,JROW)*Y(I)	D10	120
DO 44 JROW=2, LAST	D10	121
DO 44 JCOL=1,LMAX	D10	122
[44 XX(JROW,JCOL)=XX(JROW-1,JCOL+1)	D10	123
C*****TAKE OUT MEAN IF OPTION MEAN=1	D10	124
IF(MEAN)50,50,45	D10	125
[45 DO 46 JROW=2, LAST	D10	126
DO 46 JCOL=2, LAST	D10	127
46 XX(JROW,JCOL)=XX(JROW,JCOL)-WN*XBAR(JROW)*XBAR(JCOL)	D10	128
DO 47 JROW=2, LAST	D10	129
[47 XY(JROW)=XY(JROW)-WN*XBAR(JROW)*YBAR	D10	130
DO 48 J=2, LAST	D10	131
XX(1,J)=0.0	D10	132
[48 XX(J,1)=0.0	D10	133
C	D10	134
50 IF(LPRINT)60,51,51	D10	135
51 IF (INPUT) 53,53,52	D10	136
52 WRITE (6,1052)	D10	137
1052 FORMAT(1H1)	D10	138
53 WRITE (6,1053) TITLE,XZERO,XSC,YSC,MIN,MAX,LWT,MEAN,INPUT,LFNCTN,	D10	139
1LSCALE,LPRINT	D10	140
1053 FORMAT(1H012A6,2X57HPOLYNOMIAL LOW HIGH WEIGHT MEAN INPUT FNCTN	D10	141
1SCALE PRINT/6H XZEROF10.5,23H X AND Y SCALE FACTORS1P2E14.5,9X	D10	142
26HDEGREE8I6)	D10	143
IF(LPRINT-2)60,60,54	D10	144
54 WRITE (6,1054)	D10	145
1054 FORMAT(101H0SUMS OF PRODUCTS OF POWERS OF X FIRST WITH Y AND THEN	D10	146
1WITH POWERS OF X (XY MATRIX, THEN XX MATRIX))	D10	147
DO55 I=1, LAST	D10	148
[55 WRITE (6,1055)XY(I),(XX(I,J),J=1, LAST)	D10	149
1055 FORMAT(1PE14.5,8X7E14.5)	D10	150

57 WRITE (6,1057)(J,J=1, LAST)	D10	15
1057 FORMAT(11H WTD NUMBER7X3HSYY9X4HYBAR7X6HXBAR--12,6(12X11))	D10	15
58 WRITE (6,1058)WN,SY,YBAR,(XBAR(J),J=1, LAST)	D10	153
1058 FORMAT(1P10E13.5)	D10	154
C*****LEAST SQUARES MATRIX INVERSION FOR ALL DEGREES FROM MIN TO MAX	D10	155
C KORDER IS ORDER OF SQUARE MATRIX = DEGREE OF POLYNOMIAL + 1	D10	156
60 DO 89 KORDER = LEAST, LAST	D10	157
CALL MATINV (XX,XXINV,KORDER,XY,B,1, DETERM,7,7,0, LPRINT-2)	D10	158
IF (MEAN) 65,65,63	D10	159
[63 DO 64 J = 2, KORDER	D10	160
64 B(1) = B(1) - B(J) * XBAR(J)	D10	161
C*****CALC RESIDUAL VARIANCE, VAR-COV MATRIX, AND RESIDUAL STD ERROR SE	D10	162
65 SSE = 0.0	D10	163
DO 69 I = 1, NCARDS	D10	164
IF(W(I)-1.E-15)66,66,67	D10	165
66 RESID(I, KORDER) = 0.0	D10	166
GO TO 69	D10	167
67 RESID(I, KORDER) = Y(I)	D10	168
DO 68 J = 1, KORDER	D10	169
[68 RESID(I, KORDER) = RESID(I, KORDER) - B(J)*X(I, J)	D10	170
SSE=SSE+(RESID(I, KORDER)**2)*W(I)	D10	171
69 CONTINUE	D10	172
NDF=NDATA-KORDER	D10	173
VE=SSE/FLOAT(NDF)	D10	174
DO 70 J = 1, KORDER	D10	175
DO 70 L = 1, KORDER	D10	176
[70 VARCOV(J, L) = VE * XXINV(J, L)	D10	177
SE(KORDER) = SQRT(ABS(VE))	D10	178
C*****CALCULATE STD ERROR OF COEFFICIENTS AND F-TEST VALUE OF LAST COEF.	D10	179
DO 71 J = 1, KORDER	D10	180
[71 SEB(J) = SQRT(ABS(VARCOV(J, J)))	D10	181
IF (MEAN) 74,74,72	D10	182
72 SEB(1) = 0.0	D10	183
DO 73 JROW = 1, KORDER	D10	184
DO 73 JCOL = 1, KORDER	D10	185
[73 SEB(1) = SEB(1) + VARCOV(JROW, JCOL)*XBAR(JROW)*XBAR(JCOL)	D10	186
SEB(1) = SQRT(ABS(SEB(1)))	D10	187
74 F(KORDER) = (B(KORDER)/SEB(KORDER))**2	D10	188
C*****F TEST FOR SIGNIFICANCE OF LAST TERM	D10	189
CALL FTEST (NDF,1,F(KORDER),PROB)	D10	190
IF (PROB - 5.0) 742,742,741	D10	191
741 NOTSIG = 1	D10	192
GO TO 743	D10	193
742 NOTSIG = 0	D10	194
C*****PRINT COEF STD ERROR, SE AND F	D10	195
743 IF(LPRINT)89,75,75	D10	196
75 KDEGRE=KORDER-1	D10	197
76 WRITE (6,1076)KDEGRE,SE(KORDER),F(KORDER)	D10	198
1076 FORMAT(7H0DEGREE13,10X2HSE1PE14.5,10X1HFE12.3)	D10	199
IF (NOTSIG) 78,78,77	D10	200
77 WRITE (6,1077)	D10	201
1077 FORMAT(11H+90X3HNOT)	D10	202
78 WRITE (6,1078)(B(J),J=1,KORDER)	D10	203
1078 FORMAT(1H+95X30HSIGNIFICANT AT 5 PERCENT LEVEL/17X8HCONSTANT4X15HSD10	D10	204
1UCESIVE TERMS/12H COEFFICIENT3X1P7E13.5).	D10	205
79 WRITE (6,1079)(SEB(J),J=1,KORDER)	D10	206
1079 FORMAT(15H STANDARD ERROR1P7E13.5)	D10	207
C*****PRINT VARIANCE-COVARIANCE MATRIX IF LPRINT = 2 OR 3	D10	208
IF(LPRINT-2)89,80,80	D10	209
80 WRITE (6,1080)	D10	210
1080 FORMAT(4H.ROW34X28HVARIANCE - COVARIANCE MATRIX)	D10	211

[DO82 J=1,KORDER	D10	212
82 WRITE (6,1082)J,(VARCOV(J,L),L=1,KORDER)	D10	213
1082 FORMAT(13,2X1P7E13.5)	D10	214
C*****REINVERT MATRIX IF ADDED TERM NOT SIGNIFICANT AND IF LPRINT = 2	D10	215
IF (LPRINT - 2) 89,84,85	D10	216
84 IF(NOTSIG)89,89,85	D10	217
85 CALL MATINV (XXINV,VARCOV,KORDER,XY,B,0,DETERM,7,7,0,LPRINT-2)	D10	218
86 WRITE (6,1086)	D10	219
1086 FORMAT(1H020X47HORIGIAL XX MATRIX WITH REINVERTED MATRIX BELOW)	D10	220
DO 88 I = 1,KORDER	D10	221
[87 WRITE (6,1087)(XX(I,J),J=1,KORDER)	D10	222
1087 FORMAT(1H01P7E14.5)	D10	223
88 WRITE (6,1088)(VARCOV(I,J),J=1,KORDER)	D10	224
1088 FORMAT(1H 1P7E14.5)	D10	225
89 CONTINUE	D10	226
C*****SET UP CONDITIONS FOR REDUCING DEGREE UNTIL SIGNIFICANT LAST TERM	D10	227
IF (MAX - MIN) 120,150,150	D10	228
120 IF (NOTSIG) 149,149,121	D10	229
121 IF (LEAST - 1) 149,149,122	D10	230
122 LEAST = LEAST - 1	D10	231
LAST = LEAST	D10	232
GO TO 60	D10	233
149 MIN = LAST - 1	D10	234
LAST = LSAVE	D10	235
C	D10	236
150 IF (LPRINT - 1) 995,92,91	D10	237
91 WRITE (6,1091)	D10	238
1091 FORMAT(1H1)	D10	239
92 I = LEAST - 1	D10	240
L = LAST - 1	D10	241
93 WRITE (6,1093) TITLE,(J,J=I,L)	D10	242
1093 FORMAT(1H012A6,5X20HRESIDUALS (Y - YHAT)/9X6HREPLI-19X4HDATA30X20HD	D10	243
1DEGREE OF POLYNOMIAL/9X5HCATES7X1HX14X1HY14X1HW6X7(9XI1))	D10	244
[95 DO96 I=1,NCARDS	D10	245
96 WRITE (6,1096) EN(I),TRY(I),W(I),XINPUT(I),YINPUT(I),WINPUT(I),	D10	246
1(RESID(I,J),J=LEAST,LAST)	D10	247
1096 FORMAT(1H A6,A3,F5.1,1P3E15.7,2X7E10.2)	D10	248
97 WRITE (6,1097)(SE(J),J=LEAST,LAST)	D10	249
1097 FORMAT(1H0 47H SE (REFERRED TO POINT WITH FEWEST REPLICATES)14X	D10	250
11P7E10.2)	D10	251
98 WRITE (6,1098)(F(J),J=LEAST,LAST)	D10	252
1098 FORMAT(1H0 44H F-TEST (FOR LAST COEF. D.F.=NDATA-DEGREE-1)17X	D10	253
11P7E10.2)	D10	254
GO TO 995	D10	255
990 WRITE (6,1990)	D10	256
1990 FORMAT(45H **CAUTION**LEAST SQUARES POLYNOMIAL NOT DONE)	D10	257
995 IF (INPUT) 999,999,5	D10	258
999 RETURN	D10	259
END	D10	260

\$IBFTC D11CS2 LIST,M94

C***** MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS	D11	1
C SHARE DISTRIBUTION NO. 664 (SINGLE PRECISION)	D11	002
C	D11	3
SUBROUTINE MATINV (XARRAY,A,N,YARRAY,B,M,DETERM,MAXDX,MAXDY,LINPUTD	D11	004
1,LPRINT)	D11	5
C	D11	006
DIMENSION IPIVOT(10),XARRAY(MAXDX,MAXDX),A(MAXDX,MAXDX),YARRAY(MAXD	D11	7
1DX,MAXDY),B(MAXDX,MAXDY),INDEX(10,2),PIVOT(10)	D11	008
EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX, T, SWAP)	D11	9

C*****INITIALIZATION	D11	11
DO 5 I = 1,N	D11	011
DO 4 J = 1,N	D11	12
4 A(I,J) = XARRAY(I,J)	D11	013
DO 5 K = 1,M	D11	14
5 B(I,K) = YARRAY(I,K)	D11	015
10 DETERM=1.0	D11	16
15 DO 20 J=1,N	D11	017
20 IPIVOT(J)=0	D11	18
30 DO 550 I=1,N	D11	019
C*****SEARCH FOR PIVOT ELEMENT	D11	20
40 AMAX=0.0	D11	021
45 DO 105 J=1,N	D11	22
50 IF (IPIVOT(J)-1) 60, 105, 60	D11	023
60 DO 100 K=1,N	D11	24
70 IF (IPIVOT(K)-1) 80, 100, 740	D11	025
80 IF (ABS(AMAX)-ABS(A(J,K))) 85, 100, 100	D11	26
85 IROW=J	D11	027
90 ICOLUM=K	D11	28
95 AMAX=A(J,K)	D11	029
100 CONTINUE	D11	30
105 CONTINUE	D11	031
110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1	D11	32
C*****INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL	D11	033
130 IF (IROW-ICOLUM) 140, 260, 140	D11	34
140 DETERM=-DETERM	D11	035
150 DO 200 L=1,N	D11	36
160 SWAP=A(IROW,L)	D11	037
170 A(IROW,L)=A(ICOLUM,L)	D11	38
200 A(ICOLUM,L)=SWAP	D11	039
205 IF(M) 260, 260, 210	D11	40
210 DO 250 L=1, M	D11	041
220 SWAP=B(IROW,L)	D11	42
230 B(IROW,L)=B(ICOLUM,L)	D11	043
250 B(ICOLUM,L)=SWAP	D11	44
260 INDEX(I,1)=IROW	D11	045
270 INDEX(I,2)=ICOLUM	D11	46
310 PIVOT(I)=A(ICOLUM,ICOLUM)	D11	047
320 DETERM=DETERM*PIVOT(I)	D11	48
C*****DIVIDE PIVOT ROW BY PIVOT ELEMENT	D11	049
330 A(ICOLUM,ICOLUM)=1.0	D11	50
340 DO 350 L=1,N	D11	051
350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT(I)	D11	52
C*****DETERMINE COEFFICIENTS OF SOLUTION TO LINEAR EQUATIONS	D11	053
355 IF(M) 380, 380, 360	D11	54
360 DO 370 L=1,M	D11	055
370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT(I)	D11	56
C*****REDUCE NON PIVOT ROWS	D11	057
380 DO 550 L1=1,N	D11	58
390 IF(L1-ICOLUM) 400, 550, 400	D11	059
400 T=A(L1,ICOLUM)	D11	60
420 A(L1,ICOLUM)=0.0	D11	061
430 DO 450 L=1,N	D11	62
450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T	D11	063
455 IF(M) 550, 550, 460	D11	64
460 DO 500 L=1,M	D11	065
500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T	D11	66
550 CONTINUE	D11	067
C*****INTERCHANGE COLUMNS	D11	68
600 DO 710 I=1,N	D11	069
610 L=N+1-I	D11	71

620 IF (INDEX(L,1)-INDEX(L,2)) 630, 710, 630	D11 71
630 JROW=INDEX(L,1)	D11 072
640 JCOLUMN=INDEX(L,2)	D11 73
650 DO 705 K=1,N	D11 074
660 SWAP=A(K,JROW)	D11 75
670 A(K,JROW)=A(K,JCOLUMN)	D11 076
700 A(K,JCOLUMN)=SWAP	D11 77
705 CONTINUE	D11 078
710 CONTINUE	D11 79
C	D11 080
715 IF (LPRINT) 740,740,720	D11 81
720 WRITE (6,1720)	D11 082
1720 FORMAT(1H110X35HSHARE 664 MATRIX INVERSION ROUTINE10X19HINPUT SQU	D11 83
1ARE MATRIX)	D11 084
DO 722 I = 1,N	D11 85
722 WRITE (6,1722) (XARRAY(I,J),J=1,N)	D11 086
1722 FORMAT(1P10E13.5)	D11 87
WRITE (6,1724)	D11 088
1724 FORMAT(1H010X22HINVERTED SQUARE MATRIX)	D11 89
DO 726 I = 1,N	D11 090
726 WRITE (6,1722) (A(I,J),J=1,N)	D11 91
IF (M) 740,740,730	D11 092
730 WRITE (6,1730)	D11 93
1730 FORMAT(1H010X75HINPUT CONSTANT ARRAY AND CORRESPONDING LEAST SQUARE	D11 094
1ES COEFS COLUMN BY COLUMN)	D11 95
DO 735 I = 1,N	D11 096
735 WRITE (6,1722) (YARRAY(I,J),B(I,J),J=1,M)	D11 97
740 RETURN	D11 098
END	D11 99

THE FOLLOWING CARDS SHOULD BE SUBSTITUTED FOR THE CORRESPONDING NUMBER (WITHOUT THE LETTER) IN THE PRECEEDING LISTING. THESE ARE NECESSARY TO MAKE THE BASELINE CORRECTION IF IT IS NOT SIGNIFICANTLY CURVED.

C	D3 61A
DO 12 JPEAK = 1,9	D3 064A
IF (KOUNT(2,LCELL)-1) 135,136,137	D3 295A
KOUNT(2,LCELL) = 1	D3 299A
136 MIN = 0	D3 299B
REALCM(301) = XX(1,LCELL)	D3 299C
REALCM(321) = SEY	D3 299D
GO TO 141	D3 299E
137 KOUNT(2,LCELL) = MIN0(KOUNT(2,LCELL),30)	D3 300A
141 KTOTAL = KOUNT(1,LCELL)	D3 309A
BL = REALCM(301)	D3 311A
IF (MIN) 143,143,1410	D3 311B
1410 DO 142 KDEGRE = 1,MIN	D3 312A
IF (LAST - 2) 316,316,315	D10 095A
IF (MEAN) 65,65,62	D10 159A
62 IF (KORDER - 1) 65,65,63	D10 159B

TEST DATA RT 15 RECTANGULAR, CONC-PRES, CONCENTRATION, AND LINEAR COMPS

11100.0	7.3	1.0						
A-6	10. 7.3	6.034	5.95125					
1-2	20. 7.3	6.234	6.06932	5.972			5.834	
1-4	30. 7.3	6.434	6.18789	6.043			5.834	
1-6	40. 7.3	6.634	6.30693	6.115			5.834	
B2	50. 7.3	6.834	6.42588	6.188			5.834	
B4	60. 7.3	7.034	6.54449	6.264	6.166			
B6	70. 7.3		6.66252	6.341	6.223		5.834	
3-2	80. 7.3		6.77925	6.419	6.281		5.834	
3-4	90. 7.3		6.89499	6.501	6.339		5.834	
3-6	100. 7.3		7.00882	6.584	6.397		5.834	
4B	110. 7.3			6.667	6.457		5.834	
4D	120. 7.3			6.750	6.516		5.834	
4F	130. 7.3			6.836	6.577		5.834	
5-2	140. 7.3			6.924	6.637		5.834	999

TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT

25979.6	7.40	20.44		3				.8352
RT18-1-2	2.	45.						
7	5285 8	4949 5	2290	1	2441	888		
RT18-1-3	4.	30.						
7	5285 8	4951 5	2288	1	2598	888		
RT18-1-4	6.	30.						
7	5286 8	4950 5	2289	1	2760	777		
1	2648	1 1525	0 2648	0 1522	1 2665	1 1556	0 2665	0 1511
1	2682	1 1592	0 2682	0 1505	1 2699	1 1795	0 2699	0 1499
1	2716	1 1983	0 2716	0 1495	1 2733	1 2464	0 2733	0 1479
1	2750	1 2693	0 2750	0 1474	1 2767	1 2734	0 2767	0 1475
1	2783	1 2553	0 2783	0 1487	1 2800	1 1933	0 2800	0 1476
1	2817	1 1798	0 2817	0 1482	1 2833	1 1612	0 2833	0 1488
1	2850	1 1559	0 2850	0 1495	1 2866	1 1534	0 2866	0 1495
1	2883	1 1516	0 2883	0 1494	1 2899	1 1505	0 2899	0 1502 888
RT18-1-5	8.	15.						
7	5284 8	4951 5	2290	1	2936	888		
RT18-1-6	10.	15.						
7	5285 8	4951 5	2288	1	3090	888		
RT18-2-1	12.	15.						
7	5286 8	4950 5	2289	1	3256	777		
1	3109	1 1448	0 3109	0 1443	1 3141	1 1531	0 3141	0 1466
1	3172	1 1767	0 3172	0 1463	1 3204	1 2247	0 3204	0 1447
1	3235	1 3112	0 3235	0 1440	1 3266	1 3199	0 3266	0 1438
1	3297	1 2820	0 3297	0 1430	1 3328	1 1931	0 3328	0 1440
1	3359	1 1595	0 3359	0 1439	1 3389	1 1500	0 3389	0 1438
1	3420	1 1457	0 3420	0 1439	1 3450	1 1443	0 3450	0 1440 888
RT18-2-2	14.							
7	5286 8	4949 5	2289	1	3443	888		
RT18-2-3	16.							
7	5284 8	4951 5	2288	1	3604	999		

TEST DATA RT 20 SINGLE SECTOR CELL

59780.	7.3	19.55		1	3			1.91
RT20-1-1	16.	60.						
8	427155	15415	1	2353	1888			
RT20-1-2	32.	60.						
8	427155	15439	2	20762	1 32300888			
RT20-1-3	48.	60.						
8	427155	15437	3	21236	2 23784			
8	427155	15444	3	21247	2 23788888			
RT20-1-4	64.	60.		1				
8	427155	15462	3	23186	2 26862777			
0	15462	0 18708	0	19500	0 18812			
0	26000	0 18234	0	30000	0 18294	0 35000	0 18454	0 38000 0 18838

3	18547	3	18768	3	20000	3	19329	3	21000	3	20529	3	22000	3	22684
3	22600	3	23940	3	23700	3	23917	3	24000	3	23511	3	24200	3	23188
3	24400	3	22831	9	24720	9	22664	2	25200	2	23142	2	25700	2	26082
2	26000	2	30040	2	26500	2	35571	2	27100	2	36048	2	27600	2	31717
2	28000	2	27552	2	28500	2	23320	2	29200	2	20304	9	32000	9	19063888

RT20-1-5 80. 60.
8 427155 15454 3 25195 2 30019888
RT20-1-6 96. 60.
8 427155 15410 3 27334 2 33243999

TRANSFER CARD

COMPONENT 2 TEST DATA RT 15 (CONCENTRATION-PRESSURE DEPENDENCE).

1 4 0 1 1 1 1	8.10689E-06
ASSUMED 0.0	5.834
A-6 10.	5.95125
1-2 20.	6.06932
1-4 30.	6.18789
1-6 40.	6.30693
B2 50.	6.42588
B4 60.	6.54449
B6 70.	6.66252
3-2 80.	6.77925
3-4 90.	6.89499
3-6 100.	7.00882

999

COMPONENT 3 TEST DATA RT 15 (CONCENTRATION DEPENDENCE)

1 4 0 1 1 1 1	8.10689E-06	-0.04819
ZERO TIME-0.04819	5.834	
1-2 20.	5.972	
1-4 30.	6.043	
1-6 40.	6.115	
B2 50.	6.188	
B4 60.	6.264	
B6 70.	6.341	
3-2 80.	6.419	
3-4 90.	6.501	
3-6 100.	6.584	
4B 110.	6.667	
4D 120.	6.750	
4F 130.	6.836	
5-2 140.	6.924	

999

TEST DATA RT 15 RECTANGULAR, CONC-PRES, CONCENTRATION, AND LINEAR COMPS

CELL 1

INPUT DATA CORRECTED TO FIXED COMPARATOR REFERENCE: 7.300000										FRAMES	KIND	PRINT	PLT	INPUT	COMPS	BEGWT	CELL
SPEED 11100.0 RPM RST REF 7.30000 COMP-PLATE RAD MAG 1.00000										14	-0	-0	-0	-0	4	-C	1
I	FRAME	TIMER	TOP MENISCUS BOTTOM		PEAKS												
		(MIN)	(C O M P A R A T O R)														
1	A-6	10.00	-0.00000	-0.00000	6.03400	5.95125	-0.00000	-0.00000									
2	1-2	20.00	5.83400	-0.00000	6.23400	6.06932	5.97200	-0.00000									
3	1-4	30.00	5.83400	-0.00000	6.43400	6.18789	6.04300	-0.00000									
4	1-6	40.00	5.83400	-0.00000	6.63400	6.30693	6.11500	-0.00000									
5	B2	50.00	5.83400	-0.00000	6.83400	6.42588	6.18800	-0.00000									
6	B4	60.00	-0.00000	-0.00000	7.03400	6.54449	6.26400	6.16600									
7	B6	70.00	5.83400	-0.00000	-0.00000	6.66252	6.34100	6.22300									
8	3-2	80.00	5.83400	-0.00000	-0.00000	6.77925	6.41900	6.28100									
9	3-4	90.00	5.83400	-0.00000	-0.00000	6.89499	6.50100	6.33900									
10	3-6	100.00	5.83400	-0.00000	-0.00000	7.00882	6.58400	6.39700									
11	4B	110.00	5.83400	-0.00000	-0.00000	-0.00000	6.66700	6.45700									
12	4D	120.00	5.83400	-0.00000	-0.00000	-0.00000	6.75000	6.51600									
13	4F	130.00	5.83400	-0.00000	-0.00000	-0.00000	6.83600	6.57700									
14	5-2	140.00	5.83400	-0.00000	-0.00000	-0.00000	6.92400	6.63700									

CAUTIONZERO TIME DETERMINED BY STARTING PEAKS AT MENISCUS

CAUTIONCOMPONENT 1 HAS SIGNIFICANTLY CURVED LN R VS. T PLOT AT 5 PERCENT LEVEL

CAUTIONCOMPONENT 2 HAS SIGNIFICANTLY CURVED LN R VS. T PLOT AT 5 PERCENT LEVEL

CAUTIONCOMPONENT 3 HAS SIGNIFICANTLY CURVED LN R VS. T PLOT AT 5 PERCENT LEVEL

CAUTIONCOMPONENT 4 HAS LESS THAN 5 PERCENT CHANCE OF A CURVED LN R VS. T PLOT

I	FRAME	TIMER	MENISCUS	PEAK	S-RATE	PEAK	S-RATE	PEAK	S-RATE	PEAK	S-RATE
		(MIN)	(CM ON ROTOR)		(SVED)						
1	A-6	10.000	0.00000	6.03400	413.791	5.95125	244.273	0.00000*****	0.00000*****		
2	1-2	20.000	5.83400	6.23400	408.023	6.06932	243.303	5.97200	143.846	0.00000*****	
3	1-4	30.000	5.83400	6.43400	401.866	6.18789	241.757	6.04300	144.491	0.00000*****	
4	1-6	40.000	5.83400	6.63400	395.806	6.30693	240.081	6.11500	144.893	0.00000*****	
5	B2	50.000	5.83400	6.83400	389.927	6.42588	238.162	6.18800	145.191	0.00000*****	
6	B4	60.000	0.00000	7.03400	384.246	6.54449	236.071	6.26400	146.088	6.16600	113.696
7	B6	70.000	5.83400	0.00000*****		6.66252	233.346	6.34100	146.747	6.22300	113.668
8	3-2	80.000	5.83400	0.00000*****		6.77925	231.398	6.41900	147.254	6.28100	113.764
9	3-4	90.000	5.83400	0.00000*****		6.89499	228.390	6.50100	148.290	6.33900	113.722
10	3-6	100.000	5.83400	0.00000*****		7.00882	226.200	6.58400	149.109	6.39700	113.585
11	4B	110.000	5.83400	0.00000*****		0.00000*****		6.66700	149.602	6.45700	113.728
12	4D	120.000	5.83400	0.00000*****		0.00000*****		6.75000	149.853	6.51600	113.600
13	4F	130.000	5.83400	0.00000*****		0.00000*****		6.83600	150.338	6.57700	113.703
14	5-2	140.000	5.83400	0.00000*****		0.00000*****		6.92400	150.870	6.63700	113.583
STARTING LEVEL			5.83400	STANDARD ERROR	0.00000						
ZERO TIME			-0.04819	STANDARD ERROR	0.02150	CONVERSION FACTOR TIMER TO SMSQT		8.10689E-C6			

TEST DATA RT 15 RECTANGULAR, CONC-PRES, CONCENTRATION, AND LINEAR COMPS
 LN R VS. ØMSQT (IA 1/SVED) COMPUTED START +/- 2 SE, ØØTS ARE TIMER ZERO X SCALE UNIT 1.147E-05 Y SCALE UNIT 3.817E-03
 = IS MULTIPLE POINT

SECOND CYCLE

TEST DATA RT 15 RECTANGULAR, CONC-PRES, CONCENTRATION, AND LINEAR COMPS

PROGRAM CS2 SEDIMENTATION COEFFICIENTS
 SPEED 11100.0 RPM ROT REF 7.30000 COMP-PLATE RAD MAG 1.00000
 WEIGHT 0. USED FOR STARTING LEVEL FROM 1ST CYCLE

FRAMES KIND PRINT PLOT INPUT COMPS BEGWT CELL
 14 -0 -0 -0 -0 4 9 1

COMPONENT	TOTAL POINTS	INTERNAL S-RATE (SVED)	CONC FACTOR	INITIAL S-RATE (SVED)	CONC-PRES DEPENDENCE	ADDL-ZERO TIME (MIN)	PARABOLIC TERM F	COMPARATOR ERROR (SE)	MEAN TIME	S-RATE (LINEAR LSQ) (SVED)	ERROR (SE)
1	6.	378.1665	0.7994	418.3012	-0.40769	-0.0281	4135.22	0.00026	35.0482	378.1665	0.00838
	STD ERRORS	0.1317		0.5455	0.00512	0.0236				4.2351	
2	10.	224.5863	0.8120	252.3762	-0.48884	0.2953	1450.33	0.00072	55.0482	224.5863	0.00972
	STD ERRORS	0.1677		0.7487	0.01003	0.0703				2.2631	
3	13.	152.3200	0.8247	143.5125	0.32529	0.2298	114.52	0.00108	80.0482	152.3200	0.00362
	STD ERRORS	0.1686		0.3310	0.03409	0.2041				0.5671	
4	9.	113.5506	0.8316	114.1529	-0.02849	0.1465	0.53	0.00034	100.0482	113.5506	0.00033
	STD ERRORS	0.0935		0.8312	0.03866	0.3472				0.0903	

CAUTIONSPECIAL CYCLE--WEIGHT 1. USED FOR STARTING LEVEL

CELL 1

COMPONENT	TOTAL POINTS	INTERNAL S-RATE (SVED)	CONC FACTOR	INITIAL S-RATE (SVED)	CONC-PRES DEPENDENCE	ADDL-ZERO TIME (MIN)	PARABOLIC TERM F	COMPARATOR ERROR (SE)	MEAN TIME	S-RATE (LINEAR LSQ) (SVED)	ERROR (SE)
1	7.	384.0976	0.8254	419.3487	-0.41155	-0.0067	9362.74	0.00026	30.0413	384.1128	0.01140
	STD ERRORS	0.1051		0.3790	0.00354	0.0116				4.5511	
2	11.	226.7741	0.8275	250.7337	-0.46970	0.1244	993.13	0.00105	50.0438	226.7788	0.01111
	STD ERRORS	0.2118		0.7872	0.01205	0.0672				2.2389	
3	14.	151.6087	0.8361	143.0656	0.34634	0.0860	244.69	0.00107	74.3305	151.3802	0.00492
	STD ERRORS	0.1456		0.5509	0.02472	0.1244				0.6689	
4	10.	113.5693	0.8471	113.8180	-0.01315	0.0048	1.42	0.00032	90.0434	113.6191	0.00033
	STD ERRORS	0.0695		0.1758	0.01099	0.0588				0.0570	

TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT

INPUT DATA

FRAME		TIMER	PEAK 1	PEAK 2	PEAK 3	PEAK 4	PEAK 5	PEAK 6	PEAK 7	PEAK 8	TOP MEN	BOT MEN	IN REF	OUT REF	CENTER
X,Y DATA WITH FIRST TWO DIGITS OF CODE															
RT18-1-2	CELL 1	2.000	24.410*****								22.900*****		52.850	49.490*****	
RT18-1-3	CELL 1	4.000	25.980*****								22.880*****		52.850	49.510*****	
RT18-1-4	CELL 1	6.000	27.600*****								22.890*****		52.860	49.500*****	
CELL 1 30.00 DEGREES			-0 1 26.480	-0 1 15.250	-010 26.480	-010 15.220	-0 1 26.650	-0 1 15.560	-010 26.650	-010 15.110					
			-0 1 26.820	-0 1 15.920	-010 26.820	-010 15.050	-0 1 26.990	-0 1 17.950	-010 26.990	-010 14.990					
			-0 1 27.150	-0 1 19.830	-010 27.160	-010 14.950	-0 1 27.330	-0 1 24.640	-010 27.330	-010 14.790					
			-0 1 27.530	-0 1 26.930	-010 27.500	-010 14.740	-0 1 27.670	-0 1 27.340	-010 27.670	-010 14.750					
			-0 1 27.830	-0 1 25.530	-010 27.830	-010 14.870	-0 1 28.000	-0 1 19.330	-010 28.000	-010 14.760					
			-0 1 28.170	-0 1 17.980	-010 28.170	-010 14.820	-0 1 28.330	-0 1 16.120	-010 28.330	-010 14.880					
			-0 1 28.530	-0 1 15.590	-010 28.500	-010 14.950	-0 1 28.660	-0 1 15.340	-010 28.660	-010 14.950					
			-0 1 28.830	-0 1 15.160	-010 28.830	-010 14.940	-0 1 28.990	-0 1 15.050	-010 28.990	-010 15.020					
RT18-1-5	CELL 1	8.000	29.360*****								22.900*****		52.840	49.510*****	
RT18-1-6	CELL 1	10.000	30.900*****								22.880*****		52.850	49.510*****	
RT18-2-1	CELL 1	12.000	32.560*****								22.890*****		52.860	49.500*****	
CELL 1 15.00 DEGREES			-0 1 31.090	-0 1 14.480	-010 31.090	-010 14.450	-0 1 31.410	-0 1 15.510	-010 31.410	-010 14.660					
			-0 1 31.720	-0 1 17.670	-010 31.720	-010 14.630	-0 1 32.040	-0 1 22.470	-010 32.040	-010 14.470					
			-0 1 32.350	-0 1 31.120	-010 32.350	-010 14.400	-0 1 32.660	-0 1 31.990	-010 32.660	-010 14.380					
			-0 1 32.970	-0 1 28.200	-010 32.970	-010 14.300	-0 1 33.280	-0 1 19.310	-010 33.280	-010 14.400					
			-0 1 33.590	-0 1 15.950	-010 33.590	-010 14.390	-0 1 33.890	-0 1 15.000	-010 33.890	-010 14.380					
			-0 1 34.200	-0 1 14.570	-010 34.200	-010 14.390	-0 1 34.500	-0 1 14.430	-010 34.500	-010 14.400					
RT18-2-2	CELL 1	14.000	34.430*****								22.890*****		52.860	49.490*****	
RT18-2-3	CELL 1	16.000	36.040*****								22.880*****		52.840	49.510*****	

TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT CELL 1

CAUTIONZERO TIME DETERMINED BY STARTING PEAKS AT MENISCUS

CAUTIONCOMPONENT 1 HAS LESS THAN 5 PERCENT CHANCE OF A CURVED LN R VS. T PLOT

I	FRAME	TIMER (MIN)	MENISCUS (CM ON FOTHR)	PEAK (SVED)	S-RATE	PEAK	S-RATE	PEAK	S-RATE	PEAK	S-RATE
1	1-2	2.000	6.01693	6.09080	145.936						
2	1-3	4.000	6.01546	6.16712	143.000						
3	1-4	6.000	6.01595	6.24638	143.261						
4	1-5	8.000	6.01668	6.33273	146.124						
5	1-6	10.000	6.01546	6.40783	143.420						
6	2-1	12.000	6.01595	6.48904	143.148						
7	2-2	14.000	6.01619	6.58077	145.291						
8	2-3	16.000	6.01570	6.65954	143.866						
STARTING LEVEL			6.01604	STANDARD ERROR	0.00019						
ZERO TIME			0.09433	STANDARD ERROR	0.06140	CONVERSION FACTOR TIMER TO SMSOT			4.44093E-05		

TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT
 LN R VS. QMSOT (IN 1/SVED) COMPUTED START +/- 2 SE, DOTS ARE TIMER ZERO X SCALE UNIT 7.190E-06 Y SCALE UNIT 2.075E-03
 = IS MULTIPLE POINT

SECOND CYCLE

TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT

PROGRAM CS2 SEDIMENTATION COEFFICIENTS
 SPEED 25979.6 RPM ROT REF 7.40000 COMP-PLATE RAD MAG 20.44000
 WEIGHT-0. USED FOR STARTING LEVEL FROM 1ST CYCLE

FRAMES KIND PRINT PLOT INPUT COMPS BEGWT CELL
 8 -0 -0 -0 3 1 -0 1

COMPONENT	TOTAL POINTS	INTERNAL S-RATE (SVED)	CONC FACTOR	INITIAL S-RATE (SVED)	CONC-PRES DEPENDENCE	ADDL-ZERO TIME (MIN)	PARABOLIC TERM F	COMPARATOR ERROR (SE)	MEAN TIME	S-RATE (LINEAR LSQ) (SVED)	ERROR (SE)
1	8.	144.1704	0.8922	143.8198	0.02143	-0.0080	0.01	0.06769	8.9057	144.1704	0.06183
	STD ERRORS	0.9563		4.3642	0.26153	0.1179				0.8735	

TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT

CONCENTRATION ANALYSIS CELL 1 CONC. FACTOR 0.83520

FRAME	TIMER	PEAK	INITIAL MG/ML	PLATEAU CONC	RBAR	S* MAX	S* RBAR	INTERVALS	ANGLE	SE CO	SE CP	SE ORDINATE
1-4	6.000	1	2.7618E-01	2.5618E-01	6.2464E 00	1.4326E 02	1.4326E 02	17	3.0000E 01	7.6030E-04	7.0389E-04	8.6602E-02
2-1	12.000	1	2.6709E-01	2.2945E-01	6.4908E 00	1.4315E 02	1.4365E 02	13	1.5000E 01	1.3331E-03	1.1421E-03	1.8660E-01

TEST DATA RT 18 S-RATE AND CONCENTRATION OF SINGLE COMPONENT
 SCHLIEREN DATA PLOTTED AS G* VS. S*. ALL FRAMES ARE SUPERIMPOSED.
 = IS MULTIPLE POINT

X SCALE UNIT 1.912E 00 Y SCALE UNIT 3.218E-04

TEST DATA RT 20 SINGLE SECTOR CELL

INPUT DATA

FRAME	TIMER	PEAK 1	PEAK 2	PEAK 3	PEAK 4	PEAK 5	PEAK 6	PEAK 7	PEAK 8	TOP MEN	BOT MEN	IN REF	OUT REF	CENTER
X,Y DATA WITH FIRST TWO DIGITS OF COD														
RT20-1-1	CELL 1	16.300	23.531	*****	*****	*****	*****	*****	*****	15.415	*****	*****	42.715	*****
RT20-1-2	CELL 1	32.300	32.300	20.762	*****	*****	*****	*****	*****	15.439	*****	*****	42.715	*****
RT20-1-3	CELL 1	48.000	*****	23.784	21.236	*****	*****	*****	*****	15.437	*****	*****	42.715	*****
			*****	23.788	21.247	*****	*****	*****	*****	15.444	*****	*****	42.715	*****
RT20-1-4	CELL 1	64.000	*****	26.862	23.186	*****	*****	*****	*****	15.462	*****	*****	42.715	*****
CELL 1	60.00 DEGREES	-010	15.462	-010	18.708	-010	19.500	-010	18.81	-010	26.000	-010	18.234	-010 30.000 -010 18.294
		-010	35.000	-010	18.454	-010	38.000	-010	18.83	-0 3	18.547	-0 3	18.768	-0 3 20.000 -0 3 19.329
		-0 3	21.000	-0 3	20.529	-0 3	22.000	-0 3	22.68	-0 3	22.600	-0 3	23.940	-0 3 23.700 -0 3 23.917
		-0 3	24.000	-0 3	23.511	-0 3	24.200	-0 3	23.18	-0 3	24.400	-0 3	22.831	-0 9 24.720 -0 9 22.664
		-0 2	25.200	-0 2	23.442	-0 2	25.700	-0 2	26.08	-0 2	26.000	-0 2	30.040	-0 2 26.500 -0 2 35.571
		-0 2	27.100	-0 2	36.048	-0 2	27.600	-0 2	31.71	-0 2	28.000	-0 2	27.552	-0 2 28.500 -0 2 23.320
		-0 2	29.200	-0 2	20.304	-0 9	32.000	-0 9	19.06					

TEST DATA RT 20 SINGLE SECTOR CELL

XZER0 0.00000 X AND Y SCALE FACTORS 1.00000E 00 1.00000E 00 P0 YNOMIAL LOW HIGH WEIGHT MEAN INPUT FNCTN SCALE PRINT

DEGREE 4 SE 1.27595E-01 F 1.255E 00 NOT SIGNIFICANT AT 5 PERCENT LEVEL

CONSTANT SUCCESSIVE TERMS
COEFFICIENT -2.04435E-01 3.06325E 00 -1.74990E-01 4.16486E-03 -3.51204E 05
STANDARD ERROR 1.32799E 01 2.18429E 00 1.30243E-01 3.34673E-03 3.13522E 05

DEGREE 3 SE 1.31410E-01 F 4.669E 00 NOT SIGNIFICANT AT 5 PERCENT LEVEL

CONSTANT SUCCESSIVE TERMS
COEFFICIENT 1.42299E 01 4.56494E-01 -3.00964E-02 4.21801E-04
STANDARD ERROR 3.31420E 00 4.06499E-01 1.57675E-02 1.95213E-04

DEGREE 2 SE 1.95878E-01 F 5.912E 00 NOT SIGNIFICANT AT 5 PERCENT LEVEL

CONSTANT SUCCESSIVE TERMS
COEFFICIENT 2.12182E 01 -2.12914E-01 3.89374E-03
STANDARD ERROR 1.07862E 00 8.61624E-02 1.60140E-03

DEGREE 1 SE 2.92380E-01 F 1.047E-01 NOT SIGNIFICANT AT 5 PERCENT LEVEL

CONSTANT SUCCESSIVE TERMS
COEFFICIENT 1.86886E 01 -4.82894E-03
STANDARD ERROR 4.24980E-01 1.49256E-02

DEGREE 0 SE 2.64913E-01 F 2.944E 04 SIGNIFICANT AT 5 PERCENT LEVEL

CONSTANT SUCCESSIVE TERMS
COEFFICIENT 1.85567E 01
STANDARD ERROR 1.08150E-01

CAUTIONCELL 1 P0 YNOMIAL OF DEGREE 0 PUT THROUGH 6 BASELINE POINTS GIVING STANDARD ERROR OF COMPARATOR ORDINATE 2.649E-01

RT20-1-5 CELL 1 80.000 ***** 30.019 25.195 ***** 15.454 ***** 42.715 *****

RT20-1-6 CELL 1 85.000 ***** 33.243 27.334 ***** 15.410 ***** 42.715 *****

X,Y DATA CORRECTED TO FIXED COMPARATOR REFERENCE AND FOR BASELINE

CELL 1	RT20-1-4	STOP/START	0	21	11	1									
117.094	0.000	118.547	0.211	120.000	0.772	121.000	1.972	122.000	4.127	122.500	5.383	123.700	5.360	124.000	4.954
124.700	4.631	124.400	4.274	124.720	4.107	125.200	4.585	125.700	7.525	126.000	11.483	126.500	17.014	127.100	17.461
1	00	13.160	128.000	8.495	128.500	4.763	129.200	1.747	132.000	0.506					

TEST DATA RT 20 SINGLE SECTOR CELL

CELL 1

INPUT DATA CORRECTED TO FIXED COMPARATOR REFERENCE 142.714998
 SPEED 59730.0 RPM ROT REF 7.30000 COMP-PLATE RAD MAG 19.55000

FRAMES K NO PRNT PLOT INPUT COMPS BEGWT CELL
 6 - 7 -0 3 3 -0 1

I	FRAME	TIMER (MIN)	TOP MENISCUS (C O M P A R A T O R)	BOTTOM (C O M P A R A T O R)	PEAKS
1	1-1	16.00	115.41500*****	123.53100*****	
2	1-2	32.00	115.43900*****	132.30000 120.74200*****	
3	1-3	48.00	115.44050*****	123.78600 121.24150	
4	1-4	64.00	115.46200*****	126.86200 123.18600	
5	1-5	80.00	115.45400*****	130.01900 125.19500	
6	1-6	96.00	115.41000*****	133.24300 127.33400	

CAUTIONZERO TIME DETERMINED BY STARTING PEAKS AT MENISCUS

CAUTIONCOMPONENT 1 HAS LESS THAN 3 POINTS

CAUTIONCOMPONENT 2 HAS LESS THAN 5 PERCENT CHANCE OF A CURVED LN R VS. T PLOT

CAUTIONCOMPONENT 3 HAS LESS THAN 5 PERCENT CHANCE OF A CURVED LN R VS. T PLOT

UNDERFLOW AT 31043 IN AC AND MQ.

I	FRAME	TIMER (MIN)	MENISCUS (CM ON ROTOR)	PEAK (SVED)	S-RATE	PEAK	S-RATE	PEAK	S-RATE	PEAK	S-RATE
1	1-1	16.000	5.90358	6.31872	21.456	0.00000*****	0.00000*****	0.00000*****	0.00000*****		
2	1-2	32.000	5.90481	6.76726	19.702	6.17708	6.516	0.00000*****	0.00000*****		
3	1-3	48.000	5.90488	0.00000*****		6.33176	6.537	6.20161	4.593		
4	1-4	64.000	5.90598	0.00000*****		6.48910	6.533	6.30107	4.498		
5	1-5	80.000	5.90558	0.00000*****		6.65059	6.534	6.40384	4.457		
6	1-6	96.000	5.90332	0.00000*****		6.81550	6.530	6.51325	4.465		
STARTING LEVEL			5.90469	STANDARD ERROR	0.00048						
ZERO TIME			2.56709	STANDARD ERROR	0.08344	CONVERSION FACTOR TIMER TO OMSOT 2.35137E-04					

TEST DATA HT 20 SINGLE SECTOR CELL
 LN R VS. Φ MSQT (IN 1/SVED) COMPUTED START +/- 2 SE. DOTS ARE TIMER ZERO
 = IS MULTIPLE POINT

X SCALE UNIT 2.280E-04 Y SCALE UNIT 2.931E-03

SECOND CYCLE

TEST DATA RT 20 SINGLE SECTOR CELL

PROGRAM CS2 SEDIMENTATION COEFFICIENTS
 SPEED 59780.0 RPM ROT REF 7.30000 COMP-PLATE RAD MAG 19.55000
 WEIGHT 0. USED FOR STARTING LEVEL FROM 1ST CYCLE

FRAMES K NO PRINT PLOT INPUT COMPS BEGWT CELL
 6 - -0 3 3 9 1

COMPONENT	TOTAL POINTS	INTERNAL S-RATE (SVED)	CONC FACTOR	INITIAL S-RATE (SVED)	CONC-PRES DEPENDENCE	ADDL-ZER TIME (MI)	PARABOLIC TERM F	COMPARATOR ERROR (SE)	MEAN TIME	S-RATE (LINEAR LSQ) (SVED)	ERROR (SE)
1	2	18.2287	0.8154	*****	0.00000	0.0000	0.00	*****	21.4329	*****	*****
STD ERRORS*****											
2	5	6.5343	0.8280	6.5988	-0.05125	0.2885	10.37	0.00424	61.4329	6.5343	0.00860
STD ERRORS		0.0031		0.0203	0.01561	0.1001				0.0063	
3	4	4.3396	0.8636	3.7456	1.29683	-8.0177	21.41	0.01285	69.4329	4.3396	0.04301
STD ERRORS		0.0132		0.1291	0.36928	1.4170				0.0443	

CAUTIONSPECIAL CYCLE--WEIGHT 1. USED FOR STARTING LEVEL

CELL 1

COMPONENT	TOTAL POINTS	INTERNAL S-RATE (SVED)	CONC FACTOR	INITIAL S-RATE (SVED)	CONC-PRES DEPENDENCE	ADDL-ZER TIME (MI)	PARABOLIC TERM F	COMPARATOR ERROR (SE)	MEAN TIME	S-RATE (LINEAR LSQ) (SVED)	ERROR (SE)
1	3	19.6551	0.8728	*****	0.00000	-0.4334	0.00	0.52158	14.2886	19.6551	0.52158
STD ERRORS		0.9221	*****			0.8922				0.9221	
2	6	6.5321	0.8545	6.5373	-0.00502	0.0207	0.12	0.00862	51.1941	6.5326	0.00762
STD ERRORS		0.0044		0.0141	0.01426	0.0707				0.0037	
3	5	4.4128	0.8893	4.6273	-0.38337	-0.0781	2.92	0.06361	55.5463	4.4532	0.08144
STD ERRORS		0.0403		0.1070	0.20763	0.5100				0.0419	

TEST DATA RT 20 SINGLE SECTOR CELL

CONCENTRATION ANALYSIS CELL 1 CONC FACTOR 1.91000

FRAME	TIMER	PEAK	INITIAL MG/ML	PLATEAU CONC	RBAR	S* MAX	S* RBAR	INTERVALS	ANGLE	SE CO	SE CP	SE ORDINATE
1-4	64.000	2	9.5272E 00	7.8532E 00	5.5036E 00	6.5335E 00	6.6883E	0 10	6.0000E 01	9.0411E-02	7.1481E-02	2.6491E-01
1-4	64.000	3	3.5887E 00	3.1796E 00	5.2730E 00	4.4979E 00	4.1890E	0 10	6.0000E 01	6.9077E-02	6.3653E-02	2.6491E-01

TES DATA RT 20 SINGLE SECTOR CELL

SCHLIEREN DATA PLOTTED AS G* VS. S*. ALL FRAMES ARE SUPERIMPOSED.
= IS MULTIPLE POINT

X SCALE UNIT 1.985E-01 Y SCALE UNIT 1.344E-01

UNDERFLOW AT 43054 IN M3

RFLOW AT 43055 IN M3

COMPONENT 2 TEST DATA RT 15 (CONCENTRATION-PRESSURE DEPENDENCE)
 XZERO -0.00000 X AND Y SCALE FACTORS 8.10689E-06 1.00000E 00

POLYNOMIAL LOW HIGH WEIGHT MEAN INPUT FNCTN SCALE PRINT
 DEGREE 1 4 0 1 1 1 1 1

DEGREE 1 SE 1.91792E-03 F 1.011E 04
 CONSTANT SUCCESSIVE TERMS
 COEFFICIENT 1.76643E 00 2.26828E 02
 STANDARD ERROR 1.08185E-03 2.25569E 00

SIGNIFICANT AT 5 PERCENT LEVEL

DEGREE 2 SE 1.63506E-04 F 1.231E 03
 CONSTANT SUCCESSIVE TERMS
 COEFFICIENT 1.76349E 00 2.50982E 02 -2.97950E 04
 STANDARD ERROR 1.24567E-04 7.14898E-01 8.49338E 02

SIGNIFICANT AT 5 PERCENT LEVEL

UNDRFLOW AT 43750 IN AC AND MQ.

DEGREE 3 SE 1.08588E-05 F 1.813E 03
 CONSTANT SUCCESSIVE TERMS
 COEFFICIENT 1.76370E 00 2.46832E 02 -1.63705E 04 -1.10396E 07
 STANDARD ERROR 9.65282E-06 1.08427E-01 3.20329E 02 2.59305E 05

SIGNIFICANT AT 5 PERCENT LEVEL

UNDRFLOW AT 43750 IN AC AND MQ.

DEGREE 4 SE -1.12991E-05 F 2.394E 00
 CONSTANT SUCCESSIVE TERMS
 COEFFICIENT 1.76371E 00 2.46566E 02 -1.47319E 04 -1.42736E 07 1.99462E 09
 STANDARD ERROR 1.08146E-05 2.05454E-01 1.11021E 03 2.10740E 06 1.28906E 09

NOT SIGNIFICANT AT 5 PERCENT LEVEL

COMPONENT 2 TEST DATA RT 15 (CONCENTRATION-PRESSURE DEPENDENCE)

RESIDUALS (Y - YHAT)

	REPLI- CATES	X	DATA			DEGREE OF POLYNOMIAL			
			Y	W	1	2	3	4	
ASSUMED	1.0	0.000000E-39	5.834000E 00	-0.000000E-39	-2.72E-03	2.13E-04	9.83E-07	-5.22E-06	
A-6	1.0	1.000000E 01	5.951250E 00	-0.000000E-39	-1.21E-03	-3.99E-05	2.46E-06	8.67E-06	
1-2	1.0	2.000000E 01	6.067320E 00	-0.000000E-39	4.18E-05	-1.54E-04	1.28E-06	7.49E-06	
1-4	1.0	3.000000E 01	6.187890E 00	-0.000000E-39	1.00E-03	-1.74E-04	-1.19E-05	-1.08E-05	
1-6	1.0	4.000000E 01	6.305930E 00	-0.000000E-39	1.67E-03	-9.54E-05	3.37E-06	-7.62E-07	
B2	1.0	5.000000E 01	6.425880E 00	-0.000000E-39	1.96E-03	4.62E-06	4.62E-06	-1.58E-06	
B4	1.0	6.000000E 01	6.544490E 00	-0.000000E-39	1.86E-03	1.02E-04	2.83E-06	-1.31E-06	
B6	1.0	7.000000E 01	6.662520E 00	-0.000000E-39	1.35E-03	1.75E-04	1.24E-05	1.34E-05	
3-2	1.0	8.000000E 01	6.779250E 00	-0.000000E-39	3.30E-04	1.34E-04	-2.15E-05	-1.52E-05	
3-4	1.0	9.000000E 01	6.894990E 00	-0.000000E-39	-1.13E-03	4.45E-05	2.11E-06	8.31E-06	
3-6	1.0	1.000000E 02	7.008820E 00	-0.000000E-39	-3.14E-03	-2.08E-04	4.17E-06	-2.03E-06	

SE (REFERRED TO POINT WITH FEWEST REPLICATES)

1.92E-03 1.64E-04 1.09E-05 1.13E-05

F-TEST (FOR LAST COEF. D.F.=NDATA-DEGREE-1)

1.01E 04 1.23E 03 1.81E 03 2.39E 00

COMPONENT 3 TEST DATA RT 15 (CONCENTRATION DEPENDENCE)
 XZERØ -0.04819 X AND Y SCALE FACTØRS 8.10689E-06 1.00000E 00

POLYNOMIAL LOW HIGH WEIGHT MEAN INPUT FNCTN SCALE PRINT
 DEGREE 1 4 0 1 1 1 1 1

DEGREE 1 SE 8.42655E-04 F 5.122E 04
 CONSTANT SUCESSIVE TERMS
 COEFFICIENT 1.76197E 00 1.51381E 02
 STANDARD ERROR 4.61701E-04 6.68862E-01

SIGNIFICANT AT 5 PERCENT LEVEL

DEGREE 2 SE 1.82553E-04 F 2.446E 02
 CONSTANT SUCESSIVE TERMS
 COEFFICIENT 1.76360E 00 1.43068E 02 7.08734E 03
 STANDARD ERROR 1.44562E-04 5.50941E-01 4.53175E 02

SIGNIFICANT AT 5 PERCENT LEVEL

DEGREE 3 SE 1.44163E-04 F 7.607E 00
 CONSTANT SUCESSIVE TERMS
 COEFFICIENT 1.76380E 00 1.40599E 02 1.24293E 04 -3.12371E 06
 STANDARD ERROR 1.34116E-04 9.62771E-01 1.96973E 03 1.13253E 06

SIGNIFICANT AT 5 PERCENT LEVEL

DEGREE 4 SE 1.26790E-04 F 3.891E 00
 CONSTANT SUCESSIVE TERMS
 COEFFICIENT 1.76372E 00 1.43181E 02 1.53676E 03 1.22151E 07 -6.76925E 09
 STANDARD ERROR 1.24434E-04 1.51646E 00 5.78734E 03 7.83927E 06 3.43104E 09

NOT SIGNIFICANT AT 5 PERCENT LEVEL

COMPONENT 3 TEST DATA RT 15 (CONCENTRATION DEPENDENCE)

RESIDUALS (Y - YHAT)

REPLI- CATES	X	Y	W	DEGREE OF POLYNOMIAL				
				1	2	3	4	
ZERØ TIME	1.0	-4.8190000E-02	5.8340000E 00	-0.0000000E-39	1.73E-03	1.00E-04	-9.37E-05	-1.55E-05
1-2	1.0	2.0000000E 01	5.9720000E 00	-0.0000000E-39	5.08E-04	3.96E-05	1.03E-04	4.26E-06
1-4	1.0	3.0000000E 01	6.0430000E 00	-0.0000000E-39	5.45E-05	2.66E-05	1.38E-04	5.99E-05
1-6	1.0	4.0000000E 01	6.1150000E 00	-0.0000000E-39	-3.74E-04	-5.40E-05	6.47E-05	3.57E-05
B2	1.0	5.0000000E 01	6.1880000E 00	-0.0000000E-39	-7.79E-04	-2.05E-04	-1.09E-04	-8.53E-05
B4	1.0	6.0000000E 01	6.2640000E 00	-0.0000000E-39	-8.44E-04	-1.09E-04	-5.56E-05	6.46E-06
B6	1.0	7.0000000E 01	6.3410000E 00	-0.0000000E-39	-8.99E-04	-9.58E-05	-9.55E-05	-1.89E-05
3-2	1.0	8.0000000E 01	6.4190000E 00	-0.0000000E-39	-9.45E-04	-1.67E-04	-2.20E-04	-1.57E-04
3-4	1.0	9.0000000E 01	6.5010000E 00	-0.0000000E-39	-5.24E-04	1.36E-04	3.90E-05	6.54E-05
3-6	1.0	1.0000000E 02	6.5840000E 00	-0.0000000E-39	-1.09E-04	3.38E-04	2.18E-04	1.94E-04
4B	1.0	1.1000000E 02	6.6670000E 00	-0.0000000E-39	1.46E-04	2.89E-04	1.74E-04	1.04E-04
4D	1.0	1.2000000E 02	6.7500000E 00	-0.0000000E-39	2.46E-04	-8.68E-05	-7.31E-05	-1.65E-04
4F	1.0	1.3000000E 02	6.8360000E 00	-0.0000000E-39	6.34E-04	-1.12E-04	-8.60E-05	-1.29E-04
5-2	1.0	1.4000000E 02	6.9240000E 00	-0.0000000E-39	1.15E-03	-1.77E-04	3.17E-06	1.03E-04

SE (REFERRED TO POINT WITH FEWEST REPLICATES)

8.43E-04 1.83E-04 1.44E-04 1.27E-04

F-TEST (FOR LAST COEF. D.F. = NDATA - DEGREE - 1)

5.12E 04 2.45E 02 7.61E 00 3.89E 00