

This article was downloaded by:

On: 25 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



## Journal of Macromolecular Science, Part A

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713597274>

### A Fortran II Computer Program for Calculation of Concentration-Dependent Sedimentation Coefficients

J. Ehrlich<sup>a</sup>; P. Weiner<sup>a</sup>; S. S. Stivala<sup>a</sup>

<sup>a</sup> DEPARTMENT OF CHEMISTRY AND CHEMICAL ENGINEERING, STEVENS INSTITUTE OF TECHNOLOGY, HOBOKEN, NEW JERSEY

**To cite this Article** Ehrlich, J. , Weiner, P. and Stivala, S. S.(1967) 'A Fortran II Computer Program for Calculation of Concentration-Dependent Sedimentation Coefficients', *Journal of Macromolecular Science, Part A*, 1: 6, 1127 — 1141

**To link to this Article:** DOI: 10.1080/10601326708053762

**URL:** <http://dx.doi.org/10.1080/10601326708053762>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

## A Fortran II Computer Program for Calculation of Concentration-Dependent Sedimentation Coefficients\*

J. EHRLICH, P. WEINER, and S. S. STIVALA

DEPARTMENT OF CHEMISTRY AND CHEMICAL ENGINEERING  
STEVENS INSTITUTE OF TECHNOLOGY  
HOBOKEN, NEW JERSEY

### Summary

A computer program for calculation of concentration-dependent sedimentation coefficients is presented. Provision is made for rejection of outlying experimental points. The method yields extremely rapid and precise results from original data without any intermediate steps.

Use of a computer program for calculation of concentration-dependent sedimentation constants assures a more rapid, precise, and sophisticated method. Excellent treatments of Fortran programming are given by Organick (1), Germain (2), and Stein and Munro (3). A general review of computation methods of ultracentrifugation was presented by Trautman (4) and processing of analytical ultracentrifugal data was given by Chun and Gehrke (5). In this discussion will be presented a detailed treatment of a complete Fortran program that can be utilized to get these sedimentation constants direct from the initial data without any intervening steps such as graph plotting or calculations. Rejection of outlying results is also a built-in feature. If desired, modification of the program will also allow for second moment calculations.

The sedimentation constant (or coefficient) is defined by the following differential equation:

$$S = \frac{1}{\omega^2 r} \frac{dr}{dt} = \frac{1}{\omega^2} \frac{d \ln r}{dt}$$

\* This work was supported in part by U.S. Public Health Service Grant HE-05943 and Public Health Service Fellowship 5-F2-HE-29,038-02.

```

DIMENSION X(6),AVERL(6,6),T(6),SLOPE(6),CONC(6)
DIMENSION SD(6),REBA(6),K(6),SLAPE(6),CA(6)
DIMENSION A(6),C(6),CALCY(6,6),DIF(6,6)
DIMENSION VEBA(6),DIFF(6),DIFS(6,6)
DIMENSION NSAVE(6),MAO(6)
DIMENSION COLCY(6,6),DAF(6,6),DAFS(6,6)
DIMENSION SO(6),CULCY(6),DOF(6),DOFS(6)
13 READ 1,(A(I),I=1,6)
PUNCH 1,(A(I),I=1,6)
READ 2,NCONC
DO 600 M=1,NCONC
READ 2,NT
NSAVE(M)=NT
MA=NSAVE(M)
DO 400 J=1,MA
READ 2,NX
READ 3,(X(I),I=1,NX)
AVER=0.
DO 300 I=1,NX
300 AVER=AVER+X(I)
EX=NX
400 AVERL(M,J)=LOG((AVER*0.48449/EX)+5.72)/2.3026
READ 3,(T(I),I=1,NT)
SUMX=0.
SUMY=0.
SUMXY=0.
SUMXX=0.
DO 500 L=1,MA
SUMX=SUMX+T(L)
SUMY=SUMY+AVERL(M,L)
SUMXX=SUMXX+T(L)**2
500 SUMXY=SUMXY+AVERL(M,L)*T(L)
G=MA
DENOM=SUMX**2-G*SUMXX
SLOPE(M)=(SUMX*SUMY-G*SUMXY)/DENOM
C(M)=(SUMX*SUMXY-SUMY*SUMXX)/DENOM
DO 501 IM=1,MA
CALCY(M,IM)=SLOPE(M)*T(IM)+C(M)
DIF(M,IM)=ABS(CALCY(M,IM)-AVERL(M,IM))
501 DIFS(M,IM)=DIF(M,IM)**2
SDS=0.
DO 502 IN=1,MA
502 SDS=SDS+DIFS(M,IN)
R=MA
SD(M)=(SDS/(R-1.))**.5
DIFF(M)=DIF(M,1)
K(M)=1
DO 503 IP=2,MA
REBA(M)=DIFF(M)-DIF(M,IP)
IF (REBA(M))504,504,503
504 DIFF(M)=DIF(M,IP)
K(M)=IP
503 CONTINUE
VEBA(M)=DIFF(M)-1.5*SD(M)
IF (VEBA(M))505,505,506
505 MOO=1
MAU(M)=1
GO TO 510
506 MB=K(M)

```

FIG. 1.

```

PUNCH 4,M,T(MB),AVERL(M,MB)
SAMX=0.
SAMY=0.
SAMXX=0.
SAMXY=0.
DO 509 IQ=1,MA
IF (K(M)-IQ)508,509,508
508 SAMX=SAMX+T(IQ)
SAMY=SAMY+AVERL(M,IQ)
SAMXX=SAMXX+T(IQ)**2
SAMXY=SAMXY+T(IQ)*AVERL(M,IQ)
509 CONTINUE
F=MA-1
DENAM=SAMX**2-F*SAMXX
SLAPE(M)=(SAMX*SAMY-F*SAMXY)/DENAM
CA(M)=(SAMX*SAMXY-SAMY*SAMXX)/DENAM
DO 700 JA=1,MA
COLCY(M,JA)=SLAPE(M)*T(JA)+CA(M)
DAF(M,JA)=ABS(COLCY(M,JA)-AVERL(M,JA))
700 DAFS(M,JA)=DAF(M,JA)**2
SOS=0.
DO 702 JB=1,MA
IF (K(M)-JB)701,702,701
701 SOS=SOS+DAFS(M,JB)
702 CONTINUE
RA=MA-2
SO(M)=(SOS/RA)**.5
MOD=2
MAO(M)=2
PUNCH 5,SLAPE(M),CA(M)
510 PUNCH 6,M,SLOPE(M),C(M)
IF (MOO-2)512,511,511
511 SLOPE(M)=SLAPE(M)
C(M)=CA(M)
512 CONTINUE
600 SLOPE(M)=1./(SLOPE(M)*9.7943E-10)
DO 601 J=1,NCONC
PUNCH 7,J,SD(J)
IF (MAO(J)-2)703,704,703
704 PUNCH 18,J,SD(J)
703 PUNCH 8
MC=NSAVE(J)
DO 601 I=1,MC
PUNCH 11,T(I),AVERL(J,I),CALCY(J,I),DIF(J,I)
601 CONTINUE
READ 3,(CONC(I),I=1,NCONC)
SMX=0.
SMY=0.
SMXY=0.
SMXX=0.
DO 610 LB=1,NCONC
SMX=SMX+CONC(LB)
SMY=SMY+SLOPE(LB)
SMXX=SMXX+CONC(LB)**2
610 SMXY=SMXY+CONC(LB)*SLOPE(LB)
H=NCONC
DENM=SMX**2-H*SMXX
SLOPF=(SMX*SMY-H*SMXY)/DENM
CU=(SMX*SMXY-SMY*SMXX)/DENM

```

FIG. 1. (continued).

```

DO 611 LC=1,NCONC
CALCY(LC,LC)=SLOPF*CONC(LC)+CO
DIF(LC,LC)=ABS(CALCY(LC,LC)-SLOPE(LC))
611 DIFS(LC,LC)=DIF(LC,LC)**2
SOD=0.
DO 612 LD=1,NCONC
612 SOD=SOD+DIFS(LD,LD)
R=NCONC
SD(1)=(SOD/(R-1.))**.5
DIFF(1)=DIF(1,1)
KA=1
DO 614 LE=2,NCONC
REBA(LE)=DIFF(1)-DIF(LE,LE)
IF(REBA(LE))613,613,614
613 DIFF(1)=DIF(LE,LE)
KA=LE
614 CONTINUE
VEBA(1)=DIFF(1)-1.3*SD(1)
IF(VEBA(1))615,615,616
615 MOO=1
MAD=1
GO TO 620
616 PUNCH 9,CONC(KA),SLOPE(KA)
SIMX=0.
SIMY=0.
SIMXX=0.
SIMXY=0.
DO 618 LG=1,NCONC
IF(KA=LG)617,618,617
617 SIMX=SIMX+CONC(LG)
SIMY=SIMY+SLOPE(LG)
SIMXY=SIMXY+CONC(LG)*SLOPE(LG)
SIMXX=SIMXX+CONC(LG)**2
618 CONTINUE
Z=NCONC-1
DENIM=SIMX**2-Z*SIMXX
BOOB=(SIMX*SIMXY-SIMY*SIMXX)/DENIM
E=1./BOOB
SLOM=(SIMX*SIMY-Z*SIMXY)/DENIM
DO 750 JC=1,NCONC
CULCY(JC)=SLOM*CONC(JC)+BOOB
DOF(JC)=ABS(CULCY(JC)-SLOPE(JC))
750 UOFS(JC)=DOF(JC)**2
SAS=0.
DO 762 JD=1,NCONC
IF(KA=JD)761,762,761
761 SAS=SAS+DOFS(JD)
762 CONTINUE
RO=NCONC-2
SA=(SAS/RO)**.5
MAD=2
MOO=2
620 U=1./CO
PUNCH 12
DO 630 LZ=1,NCONC
630 PUNCH 15,CONC(LZ),SLOPE(LZ),CALCY(LZ,LZ),DIF(LZ,LZ)
PUNCH 14,SD(1)
IF(MAD=2)770,771,770
771 PUNCH 19,SA

```

FIG. 1. (continued).

```

770 CONTINUE
    PUNCH 10,D
    IF(MOO-2)801,800,801
800 PUNCH 16,E
801 CONTINUE
    PUNCH 17
    1  FORMAT(10A4)
    2  FORMAT(11I5)
    3  FORMAT(7F10,2)
    4  FORMAT(5HCONC.,12,10HREJ. PT T=,F10,6,2X,6H AVERL=,F10,6)
    5  FORMAT(16HCORRECTED SLOPE=,E20,6,5X,10HINTERCEPT=,E20,6)
    6  FORMAT(8HIN CONC.,12,6HSLOPE=,E20,6,5X,10HINTERCEPT=,E20,6)
    7  FORMAT(/8HIN CONC.,12,16HTHE STAND. DEV.=,F10,6)
    8  FORMAT(12H      T      ,12H      AVERL ,12H      CALCY ,
        112H      DIF      )
    9  FORMAT(/8HIN CONC.,E15,6,2X,14HREJ. 1/S APP.=,E15,6)
   10  FORMAT(/27HTHE SEDIMENTATION CONSTANT=,E20,6)
   11  FORMAT(4F12,6)
   12  FORMAT(/15H      CONC      ,13H      1/S APP ,
        114H      CALC 1/S APP,5X 4H DIF)
   14  FORMAT(28HTHE STAND. DEV. OF 1/S APP.=,E12,6)
   15  FORMAT(4E14,6)
   16  FORMAT(22HCORRECTED SED. CONST.=,E12,6)
   17  FORMAT(9HABCDEFGHI)
   18  FORMAT(8HIN CONC.,12,18H CORR. STAND. DEV.=,F10,6)
   19  FORMAT(30HSTAND. DEV. OF CORR. 1/S APP.=,E20,6)
   20  FORMAT(F5,2)
      GO TO 13
      END

```

FIG. 1. Program.

*Program notes*

1. It is possible for an investigator if he so desires to raise or lower the standard deviation factor in statements 503 + 001, and 614 + 001.
2. In statement 400, the magnification factor, 0.48449, can be changed to fit the ultracentrifuge in use.
3. In statement 600, the factor  $9.7943 \times 10^{-10}$  can be altered if the speed of the rotor is changed.

*Definition of input symbols*

NCONC = number of concentrations

T = the time at a particular interval

NT = number of times

x = value of micrometer reading from reference line to the maximum ordinate

NX = number of x values

*Summary of arrangement of input data cards*

1. Title of experiment (columns 1-24)
2. Number of concentrations (fifth column)
3. Number of times for first concentration (fifth column)
4. Number of x values at first time and first concentration (fifth column)
5. x values at first time and first concentration

*Continued at bottom of p. 1133*

SAMPLE A10					
6					
5					
3	1.9452	1.9429	1.9428		
4	1.9910	1.9915	1.9915	1.9920	
3	2.0330	2.0337	2.0340		
3	2.0819	2.0827	2.0827		
4	2.1268	2.1315	2.1324	2.1319	
0.		8.	16.	24.	32.
5					
4	1.9413	1.9353	1.9378	1.9355	
4	1.9900	1.9872	1.9866	1.9851	
3	2.0355	2.0349	2.0333		
2	2.0866	2.0864			
2	2.1383	2.1382			
0.		8.	16.	24.	32.
5					
2	1.9391	1.9390			
2	1.9806	1.9804			
5	2.0272	2.0284	2.0250	2.0272	2.0276
4	2.0796	2.0775	2.0762	2.0760	
3	2.1318	2.1296	2.1317		
0.		8.	16.	24.	32.
5					
3	1.9371	1.9390	1.9380		
4	1.9950	1.9920	1.9925	1.9953	
2	2.0525	2.0527			
3	2.1038	2.1028	2.1040		
2	2.1570	2.1573			
0.		8.	16.	24.	32.
5					
4	1.9262	1.9270	1.9293	1.9300	
3	1.9813	1.9810	1.9823		
4	2.0389	2.0373	2.0360	2.0377	
3					

FIG. 2.

2.0987	2.0977	2.0972		
3				
2.1520	2.1500	2.1535		
0.	8.	16.	24.	32.
5				
3				
1.9895	1.9915	1.9915		
3				
2.0520	2.0530	2.0528		
2				
2.1080	2.1080			
3				
2.1653	2.1637	2.1633		
3				
2.2299	2.2324	2.2312		
0.	8.	16.	24.	32.
1.000000	.750000	.666667	.500000	.333333
				.25000000

FIG. 2. Example of input data.

where  $r$  = distance of boundary from center of rotation,  $\omega$  = angular velocity in radians per second, and  $t$  = time in seconds.

Therefore, if  $\ln r$  is plotted versus time, the slope divided by  $\omega^2$  gives the sedimentation constant directly. Also, if desired, this can be corrected to the standard state by multiplying by a correction factor (6).

If the polymer is pure and has a narrow molecular weight dis-

---

col. 1            10 11            20 21            30 31            40 41            50

Number of  $x$  values at second time and first concentration

---

col. 1            10 11            20 21            30 31            40 41            50

Do same for all  $x$  values of first concentration

6. Time values at first concentration

---

col. 1            10 11            20 21            30 31            40 41            50

Repeat cards 3-6 for all concentrations

7. Concentration values

---

col. 1            10 11            20 21            30 31            40 41            50 51            60

Notes

1. If a particular time is omitted, this fact must be accounted for in card 3 and its value omitted in the proper order in card 6.
2. If a particular concentration is omitted, this fact must be accounted for in card 2 and its value omitted in the proper order in card.
3. Cards must be checked and rechecked for proper content and order.



SAMPLF A10			
CONC. 1REJ. PT T=	16.000000	AVERL=	.826409
CORRECTED SLOPE=	18.248828E-05	INTERCEPT=	82.358957E-02
IN CONC. 1SLOPE=	18.249062E-05	INTERCEPT=	82.356950E-02
CONC. 2REJ. PT T=	16.000000	AVERL=	.826440
CORRECTED SLOPE=	19.638281E-05	INTERCEPT=	82.337917E-02
IN CONC. 2SLOPE=	19.638437E-05	INTERCEPT=	82.336303E-02
IN CONC. 3SLOPE=	18.898125E-05	INTERCEPT=	82.330578E-02
CONC. 4REJ. PT T=	16.000000	AVERL=	.827005
CORRECTED SLOPE=	21.476171E-05	INTERCEPT=	82.342031E-02
IN CONC. 4SLOPE=	21.476562E-05	INTERCEPT=	82.345015E-02
IN CONC. 5SLOPE=	22.103750E-05	INTERCEPT=	82.304725E-02
IN CONC. 6SLOPE=	23.100000E-05	INTERCEPT=	82.507646E-02
IN CONC. 1THE STAND. DEV.=	.000049		
IN CONC. 1CORR. STAND. DEV.=	.000025		
T	AVERL	CALCY	DIF
0.000000	.823577	.823569	.000008
8.000000	.825075	.825029	.000045
16.000000	.826409	.826489	.000080
24.000000	.827939	.827949	.000009
32.000000	.829444	.829409	.000035
IN CONC. 2THE STAND. DEV.=	.000039		
IN CONC. 2CORR. STAND. DEV.=	.000018		
T	AVERL	CALCY	DIF
0.000000	.823383	.823363	.000020
8.000000	.824953	.824934	.000019
16.000000	.826440	.826505	.000064
24.000000	.828067	.828076	.000009
32.000000	.829681	.829647	.000034
IN CONC. 3THE STAND. DEV.=	.000110		
T	AVERL	CALCY	DIF
0.000000	.823433	.823305	.000127
8.000000	.824740	.824817	.000076
16.000000	.826205	.826329	.000123
24.000000	.827811	.827841	.000029
32.000000	.829456	.829353	.000103
IN CONC. 4THE STAND. DEV.=	.000070		
IN CONC. 4CORR. STAND. DEV.=	.000024		
T	AVERL	CALCY	DIF
0.000000	.823400	.823450	.000049
8.000000	.825156	.825168	.000011
16.000000	.827005	.826886	.000119
24.000000	.828599	.828604	.000005
32.000000	.830269	.830322	.000052
IN CONC. 5THE STAND. DEV.=	.000053		
T	AVERL	CALCY	DIF
0.000000	.823087	.823047	.000040
8.000000	.824773	.824815	.000042
16.000000	.826531	.826583	.000052
24.000000	.828422	.828352	.000070
32.000000	.830104	.830120	.000015
IN CONC. 6THE STAND. DEV.=	.000094		

FIG. 3.

T	AVERL	CALCY	DIF
0.000000	.825066	.825076	.000010
8.000000	.827005	.826924	.000081
16.000000	.828738	.828772	.000033
24.000000	.830486	.830620	.000134
32.000000	.832565	.832468	.000097

IN CONC. 66.666700E-02 REJ. 1/S APP.= 54.026631F+11

CONC	1/S APP	CALC 1/S APP	DIF
10.000000E-01	55.948910E+11	56.665074E+11	71.616400E+09
75.000000E-02	51.990397E+11	52.655798E+11	66.540100E+09
66.666700E-02	54.026631F+11	51.319378E+11	27.072530E+10
50.000000E-02	47.541157E+11	48.646523E+11	11.053660E+10
33.333300E-02	46.191349E+11	45.973667E+11	21.768200E+09
25.000000E-02	44.199221E+11	44.637247E+11	43.802600E+09

THE STAND. DEV. OF 1/S APP.= .139613E+12  
 STAND. DEV. OF CORR. 1/S APP.= .43539656E+11

THE SEDIMENTATION CONSTANT= 24.613583E-14  
 CORRECTED SED. CONST.= .246976F-12

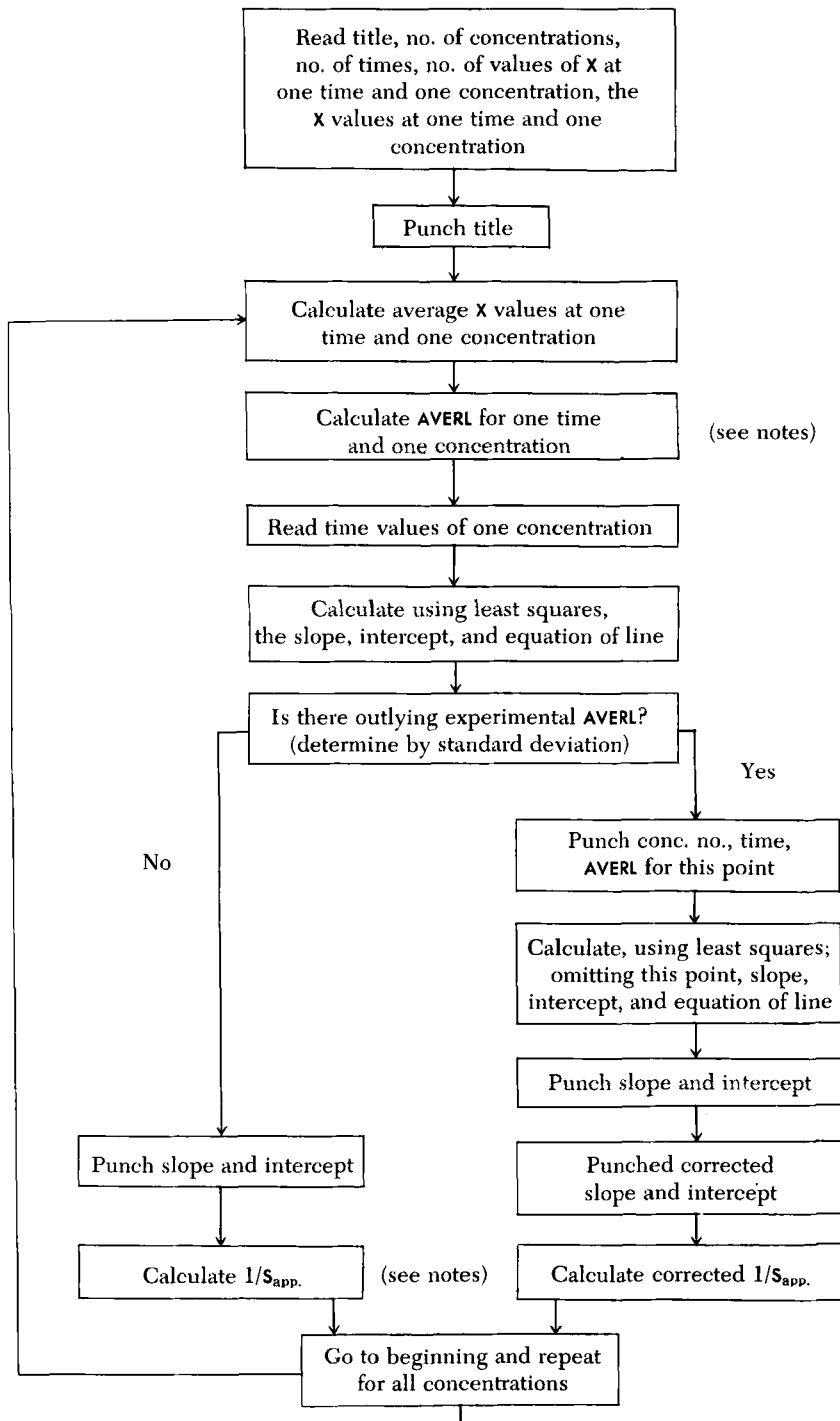
FIG. 3. Example of calculation.

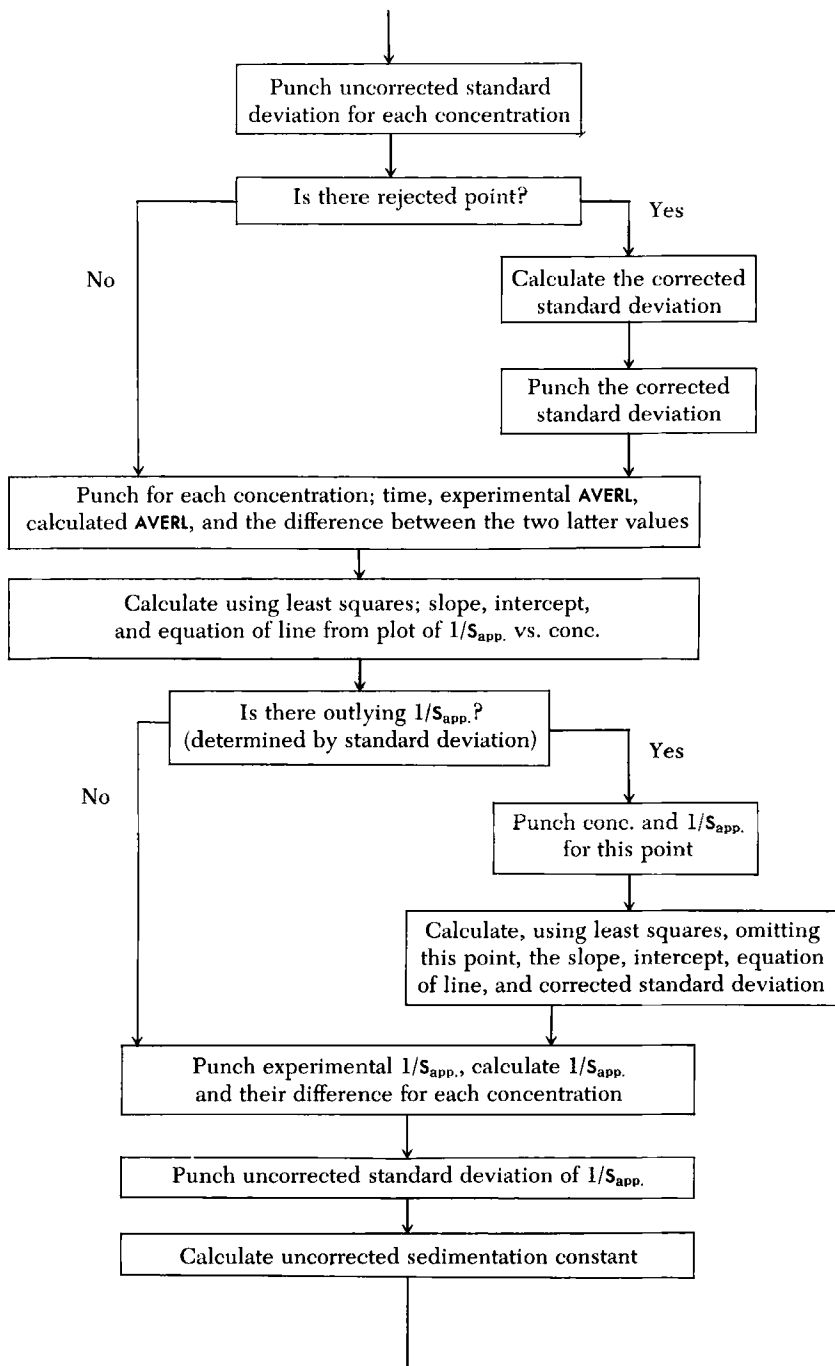
Notes for calculation

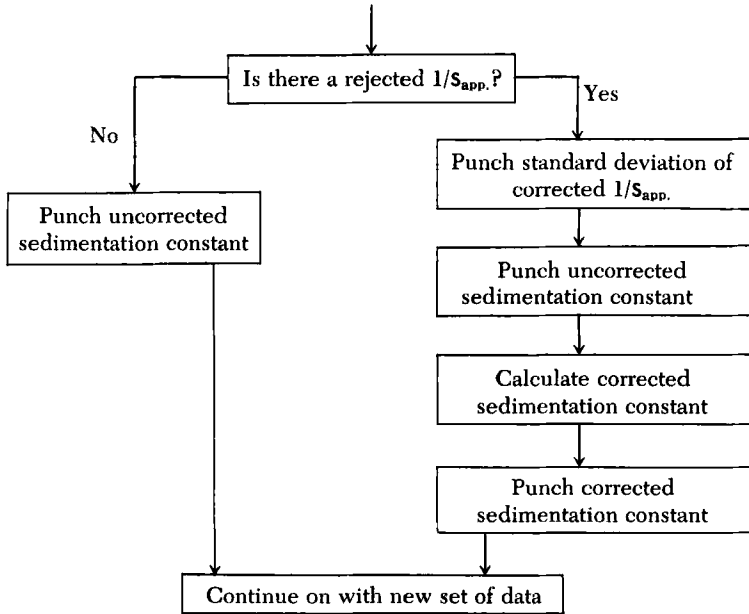
1. Abbreviations:
  - a. REJ. PT = rejected point
  - b. CORR. STAND. DEV. = standard deviation of new line after rejection of outlying point
  - c. REJ. 1/S APP. = rejected  $1/s_{\text{APPARENT}}$
  - d. STAND. DEV. OF CORR. 1/S APP. = standard deviation of new line after rejection of outlying  $1/s_{\text{APPARENT}}$
  - e. CORRECTED SED. CONST. = corrected sedimentation constant after rejection of outlying  $1/s_{\text{APPARENT}}$
  - f. CALCY = calculated AVERL
2. Since the intermediary as well as final results are printed out, it is possible for the investigator to spot check calculations if he so desires by plotting his own curves and reject his own outlying points and compare.
3. By comparing the corrected and uncorrected standard deviations one can see whether there is justification in rejecting an outlying point.
4. In difference column, computer truncates in print-out last digit rather than rounding it off.
5. The sedimentation constant reported should be rounded off to three significant figures.

tribution, the schlieren pattern obtained will be closely symmetrical and it will be possible to determine the maximum ordinate by bisecting the schlieren fringes without resorting to second moment calculations.

## FLOW CHART







#### Notes for Flow Chart

1.  $x$  = micrometer reading on comparator of distance from outer edge of inner reference hole to boundary
2.  $AVERL$  = natural logarithm/2.303 (average of  $x$  value at a particular time and conc.  $\times$  magnification factor<sup>\*</sup> + distance from outer edge of inner reference hole to center of rotation<sup>†</sup>)

$$3. \frac{1}{s_{app.}} = \frac{60(\omega^2)}{2.303(d \ln x/dx)}$$

$$= \frac{(2\pi \times \text{speed of rotor in rpm} \dagger / 60)^2}{\text{slope} \times 2.303/60} = \frac{1}{\text{slope} (9.7943 \times 10^{-10})}$$

## EXPERIMENTAL

### Materials

Commercial heparin sodium, derived from beef lungs, was obtained from Organon, Inc. Heparin is a charged polysaccharide. For use, 2% solutions of heparin in 0.5 M NaCl solution were dialyzed for 48 hr with constant magnetic stirring and under refrigeration against 0.5 M NaCl solution.

\* Magnification factor of our ultracentrifuge is 0.48449.

† This distance is 5.72 cm, taking into consideration the stretching of the rotor.

‡ Speed used is 59,780 rpm.

## Methods

All sedimentation velocity runs were made using the Beckman-Spinco Model E analytical ultracentrifuge. The An-D rotor was used with the R.T.I.C. system set at 20°C with a speed of 59,780 rpm. Single-sector capillary-type synthetic boundary cells with Epon centerpieces were filled with 0.25 ml of solute and about 0.2 ml of solvent in the reservoir. Precision volume measurements were made with Hamilton microliter syringes equipped with Chaney adaptors. The dialysate was used as solvent for all dilutions. Photographs were taken at 8-min intervals on Kodak II-G spectroscopic plates. Cells were checked for leakage in each run.

Computer used was the IBM 1620-(1) with 40K memory, equipped with Fortran or Kingston Fortran compiler. Calculations were checked by plotting and calculator.

## DISCUSSION OF PROGRAM

Two to five readings are made on a photographic plate from the reference line obtained from the inner reference hole of the counterbalance to a line bisecting the schlieren fringes. An average of these readings is calculated, multiplied by the magnification factor of the ultracentrifuge, and added to the distance of reference line from the center of rotation. This is done at each particular time interval. The logarithms of these values are plotted versus the particular times, from which the slopes, intercepts, and equation of the lines are obtained. If there is an outlying point in any concentration, it is rejected by using a modification of the 2.5-D rule (7). Because of the precision of the ultracentrifuge it was found experimentally that a point should be rejected if the absolute difference between its calculated and actual value is greater than 1.5 times the standard deviations of the line. If a point has been rejected, the line is replotted omitting this point and a new slope, intercept, and standard deviation obtained. The above procedure is repeated for all the concentrations and the apparent sedimentation constants are calculated from the slopes. Then the reciprocals of the apparent sedimentation constants are plotted versus concentrations. Again an outlying point will be rejected, but this time if the absolute difference between the calculated and actual value is greater than 1.3 times the standard deviation of the line. This result was arrived at by repeated runs. If a point is rejected, the line is

replotted omitting this point and a new slope, intercept, and standard deviation obtained. Through extrapolation to zero concentration, the sedimentation constant is found both for the case where a point is rejected and where none is rejected. At least five concentrations should be used for this determination. (See Figs. 1 to 3.)

## CONCLUSIONS

Concentration-dependent sedimentation constants can be calculated on a computer. A program in Fortran which can be compiled either in Fortran or Kingston Fortran was presented. Results are obtained quickly and efficiently from initial data without intermediate plotting and calculation. Also a built-in mechanism is supplied for eliminating outlying data. The program can be easily modified to allow for second moment calculations and for use with the IBM 360 computer.

## Acknowledgments

The authors acknowledge with pleasure the criticisms and suggestions of Mr. George Denzer. We wish to express our appreciation to the Stevens Institute of Technology computer center for permitting us to use their facilities and for their helpful assistance. The authors are grateful to Organon, Inc., for supplying the generous sample of heparin sodium.

## REFERENCES

1. E. J. Organick, *A Fortran Primer*, Addison-Wesley, Reading, Mass., 1966.
2. C. B. Germain, *Programming the IBM 1620*, Prentice-Hall, Englewood Cliffs, N.J., 1965.
3. M. L. Stein and W. D. Munro, *A Fortran Introduction to Programming and Computers*, Academic Press, New York, 1966.
4. R. Trautman, in *Ultracentrifugal Analysis in Theory and Experiment* (J. W. Williams, ed.), Academic Press, New York, 1963, p. 203.
5. P. Chun and C. W. Gehrke, *Anal. Biochem.*, **17**, 214 (1966).
6. H. K. Schachman, in *Methods in Enzymology*, Vol. IV (S. P. Colowick and N. O. Kaplan, eds.) Academic Press, New York, 1957, p. 32.
7. D. A. Skoog and D. M. West, in *Fundamentals of Analytical Chemistry*, Holt, New York, 1963, p. 58.

### Zusammenfassung

Eine Rechenprogram zur Berechnung von konzentrationsabhängigen Sedimentationskoeffizienten wird angegeben. Ausserhalb liegende experimentelle Daten werden hierbei eliminiert. Die Methode ergibt rasche und genaue Ergebnisse direkt aus den ursprünglichen Daten ohne Zwischenstufen.

### Résumé

On présente un programme d'ordinateur pour calculer les coefficients de sédimentation, dépendant de la concentration. On fait des arrangements pour rejeter les points expérimentaux à l'écart. La méthode donne des résultats extrêmement rapides et précises à partir des données originales sans procédés intermédiaires.

*Received by editor April 11, 1967*

*Submitted for publication August 22, 1967*