UNCLASSIFIED

ORNL-2037
Progress

c.5

MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

FOR

PERIOD ENDING DECEMBER 31, 1955

OAK RIDGE NATIONAL LABORATORY
OPERATED BY
UNION CARBIDE NUCLEAR COMPANY
A Division of Union Carbide and Carbon Corporation
UCC
POST OFFICE BOX P • OAK RIDGE, TENNESSEE

UNCLASSIFIED

ORNL-2037

COPY NO. 3

Contract No. W-7405-eng-26

MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

for

Period Ending December 31, 1955

A. S. Householder, Chief

Edited by
A. S. Householder

DATE ISSUED

FEB 20 1956

OAK RIDGE NATIONAL LABORATORY
Operated by
UNION CARBIDE NUCLEAR COMPANY
A Division of Union Carbide and Carbon Corporation
Post Office Box P
Oak Ridge, Tennessee

ORNL-2037
Progress

INTERNAL DISTRIBUTION

1. C. E. Center
2. Biology Library
3. Health Physics Library
4. Reactor Experimental Engineering Library
5-7. Central Research Library
8-14. Laboratory Records Department
15. Laboratory Records, ORNL RC
16. A. M. Weinberg
17. L. B. Emlet (K-25)
18. J. P. Murray (Y-12)
19. J. A. Swartout
20. R. R. Dickison
21. E. D. Shipley
22. E. J. Murphy
23. F. C. VonderLage
24. A. S. Householder
25. A. H. Snell
26. E. H. Taylor
27. A. Hollaender
28. W. H. Jordan
29. D. W. Cardwell
30. M. T. Kelley
31. K. Z. Morgan
32. E. M. King
33. C. E. Winters
34. L. Nelson
35. E. O. Wollan
36. E. P. Blizard
37. R. S. Livingston
38. C. P. Keim
39. G. H. Clewett
40. C. D. Susano
41. G. C. Williams
42. R. A. Charpie
43. V. C. Klema
44. N. M. Dismuke
45. C. P. Hubbard
46. A. W. Kimball
47. M. R. Arnette
48. D. D. Cowen
49. P. M. Reyling
50. A. C. Downing, Jr.
51. J. Z. Hearon
52. S. G. Campbell
53. C. L. Gerberich
54. J. A. Lane
55. R. W. Johnson
56. M. J. Skinner
57. J. L. Gabbard
58. G. E. Boyd
59. S. J. Cromer
60. E. C. Long
61. C. L. Bradshaw
62. J. P. Kelly (K-25)
63. S. E. Atta
64. ORNL – Y-12 Technical Library, Document Reference Section

EXTERNAL DISTRIBUTION

65. R. F. Bacher, California Institute of Technology
66. Division of Research and Development, AEC, ORO
67-401. Given distribution as shown in TID-4500 under Physics category

DISTRIBUTION PAGE TO BE REMOVED IF REPORT IS GIVEN PUBLIC DISTRIBUTION

Mathematics Panel progress reports previously issued in this series are as follows:

ORNL-345	December, January, February, 1948–1949
ORNL-408	Period Ending July 31, 1949
ORNL-516	Period Ending October 31, 1949
ORNL-634	Period Ending January 31, 1950
ORNL-726	Period Ending April 30, 1950
ORNL-818	Period Ending July 31, 1950
ORNL-888	Period Ending October 31, 1950
ORNL-979	Period Ending January 31, 1951
ORNL-1029	Period Ending April 30, 1951
ORNL-1091	Period Ending July 31, 1951
ORNL-1151	Period Ending October 31, 1951
ORNL-1232	Period Ending January 31, 1952
ORNL-1290	Period Ending April 30, 1952
ORNL-1360	Period Ending July 31, 1952
ORNL-1435	Period Ending October 31, 1952
ORNL-1498	Period Ending January 31, 1953
ORNL-1588	Period Ending June 30, 1953
ORNL-1662	Period Ending December 31, 1953
ORNL-1751	Period Ending June 30, 1954
ORNL-1842	Period Ending December 31, 1954
ORNL-1928	Period Ending June 30, 1955

CONTENTS

MATHEMATICS PANEL SEMIANNUAL PROGRESS REPORT

INTRODUCTION

THE ORACLE

From July through December, a total of 2360 hr of computing time was used by programers for "debugging" and running problems. The computer is scheduled to run 24 hr per day, with 5 hr used daily for engineering maintenance and installation of new equipment.

The curve plotter was completed and placed in operation. Facilities are provided for temporary visual observation and for permanent photographic reproduction in the form of graphs or lettered sheets. Special circuitry has been incorporated which provides semiautomatic letter plotting at a maximum speed of 2000 letters per second.

Arrangements have been made with the ORNL Photographic Section to process film from the curve plotter at the rate of approximately 200 photographs per day.

Modification to the Oracle involving the 8-12 partial substitution is complete.

LECTURES

ORINS Lectures. – The following lecture was given under the Traveling Lecture Program:

A. C. Downing, *Convergence and Stability Criteria for Hyperbolic Systems of Equations,* Georgia Institute of Technology, October 31, 1955.

Other Lectures. – Other lectures given during the report period are as follows:

A. S. Householder, five lectures on *Errors in Digital Computation* and one lecture on *Report from Users of Digital Computers,* two-week summer session on digital computers sponsored by the University of Michigan, August 1–8, 1955; *Convergence of Matrix Iterations,* Technical High School, Stockholm, Sweden, November 2, 1955, University of Notre Dame, December 14, 1955, and University of Michigan, December 15, 1955.

A. W. Kimball, *A Survey of Statistical Methods Used in the Biology Division,* Biology Division Seminar, December 22, 1955.

The Computation Laboratory of Wayne University gave four special summer sessions in order to further train personnel in the field of computers and programing for these computers. J. W. Givens, a consultant to the Mathematics Panel, participated in the fourth session, which was on Numerical Methods and Advanced Programing Techniques. His course was entitled *Direct Methods for Solution of Problems of Matrix Algebra.*

PAPERS PRESENTED AT MEETINGS

American Mathematical Society Meeting, University of Michigan, August 30 – September 3, 1955

T. W. Hildebrandt, ORINS Fellow, *Self-Adjointness in One-Group Multiregion Diffusion Problems.*

A. C. Downing, *A Finite Difference Net Applicable to Multiregion Problems.*

A. C. Downing and R. C. F. Bartels (University of Michigan), *Note on the Stability and Convergence Criteria for Hyperbolic Systems of Equations.*

American Mathematical Society Meeting, University of Maryland, October 22, 1955

C. L. Bradshaw, with W. R. Mann and J. G. Cox (University of North Carolina), *Improved Approximations to Differential Equations Using Low Order Differences.*

Annual Meeting of the Association for Computing Machinery, University of Pennsylvania, September 14–16, 1955

A. S. Householder, *Presidential Address* and *The Convergence of Iterative Methods for Solving Linear Systems.*

C. L. Gerberich and W. C. Sangren, *Codes for the Membrane Problem.*

S. G. Campbell, *Numerical Integration for the Digital Computer.*

E. C. Long, *Pipe Stress Calculations on the Oracle.*

A. C. Downing and A. S. Householder, *An Inverse Characteristic Value Problem.*

J. W. Givens, consultant to the Mathematics Panel, *Numerical Computation of the Characteristic Vectors of a Real Symmetric Matrix* and *Codes for the Solution of Systems of Linear Algebraic Equations.*

N. M. Dismuke was also in attendance at this meeting.

International Meeting on Electronic Digital Computers and Information Processing, Institut fur Praktische Mathematik, Darmstadt, Germany, October 25–27, 1955

A. S. Householder, invited paper on *Numerical Mathematics from the View-point of Electronic Digital Computers.*

Joint Meeting Sponsored by Several Mathematical Societies, New York, December 27–30, 1955

A. W. Kimball, *Approximate Confidence Intervals for Specific Locus Mutation Rates,* in section sponsored by the Biometric Society (Eastern North American Region).

R. G. Cornell, ORINS Fellow, *A New Estimation Procedure for a Linear Combination of Exponentials,* in section sponsored by the Institute of Mathematical Statistics.

A. W. Kimball also participated in a round-table discussion of *Unpublished Mathematical Tables of Interest to Statisticians.*

PUBLICATIONS

A. S. Householder, "Terminating and Nonterminating Iterations for Solving Linear Systems," *J. Soc. Indust. Appl. Math.* **3**, 67 (1955).

A. S. Householder, "Digital Computers in Eastern Europe," *Computers and Automation* **4**, 8 (1955).

A. S. Householder, "Mathematics, Schools and the Oracle," *Computers and Automation* **4**, 6 (1955).

A. S. Householder, "The Generation of Error in Digital Computation," ORNL-1983 (Oct. 11, 1955).

J. Z. Hearon and R. F. Kimball, "Tests for a Role of H_2O_2 in X-Ray Mutagenesis, I. Estimations of the Concentration of H_2O_2 Inside the Nucleus," *Radiation Research* **3**, 283 (1955).

J. Z. Hearon, R. F. Kimball, and N. Gaither, "Tests for a Role of H_2O_2 in X-Ray Mutagenesis, II.," *Radiation Research* (to be published).

PERSONNEL CHANGES

R. L. Plunkett, G. E. Medlin, and J. S. Rosen spent the summer quarter with the Mathematics Panel as research participants, and M. D. George and R. C. F. Bartels were with the Panel as temporary employees. W. D. Howe, an ORINS Fellow from the University of North Carolina, completed his doctoral dissertation and passed the examination for his degree. Terminations during the period were W. C. Sangren, N. D. Given, J. Z. Hearon, and M. O. Gill. B. M. Helton transferred to the Mathematics Panel from the Health Physics Division.

RESEARCH AND PROBLEMS

SUBROUTINE LIBRARY

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1928

Status. – During the last six months many changes have been made in the subroutine library. The number of routines has almost doubled. In addition to the normal basic subroutines, such as floating-point, input, output, and matrix codes, attention has been placed on transcendental functions.

Efforts have been made to obtain writeups, flow diagrams, and operating instructions for all available subroutines. Many such writeups are still not complete, but are expected to be in the next report period.

The library was revised because of the new substitution orders discussed in the last semiannual report, and a few of the routines have been rewritten for magnetic tape. Many more are in the process of being brought up to date.

A number of magnetic-tape and curve-plotter routines have been written and are in use. It is now possible to write the Roman alphabet, most of the Greek alphabet, and a great many mathematical symbols on the curve plotter by just using the subroutines that are available. Also, a routine to plot the X and Y axes for a graph is ready for use.

The subroutine library is now being revised for use with the magnetic-tape compiler. All new routines are being written with this in mind. A full-time subroutine librarian has been appointed and is in charge of preparing all new routines for reproduction and distribution.

VECTOR-BLOCK MATRIX CODES

Origin: J. W. Givens, consultant, Mathematics Panel

Participating Members of Panel: M. R. Arnette, V. C. Klema

Background. – A complex of codes to perform the basic operations of matrix algebra is being developed with the intent to satisfy the following criteria:

1. *Uniform treatment of data.* – To this end, each column vector (or row vector) of a matrix is written on a separate block of magnetic tape. The (i,j)-th element of the matrix is recorded in word i of block j. The inefficient use of tape for matrices with a small number of rows is, in part, compensated for by the simplification of codes. The primary use of the codes is intended to be for matrices of orders 100 to 255.

2. *Accuracy of method.* – When nontrivial scaling and round-off problems are involved, the first codes written will use methods expected to be effective for a large class of problems. Thus the solution of linear equations and the calculation of inverses are done by a new method, which involves more multiplication time than does the straightforward successive elimination but which is somewhat more accurate.

3. *Intermediate speed.* – The requirements of both accuracy and uniformity of treatment of data tend to reduce speed, but neither slow floating-point arithmetic nor long iterative procedures are required. Matrices will be scaled to permit fixed-point arithmetic in the first codes written in this category.

A number of the codes already written were designed for the dual purpose of providing suitable tests for other codes and of facilitating numerical experiments on accuracy as affected by round-off. The major codes written to date, however, were all intended to be of use in calculating the inverse of a specific matrix of order 190 (see p 10, this report), in addition to being of general use.

Codes already prepared include several for manufacturing test matrices with known inverses, for converting a matrix already on tape in standard form but with known errors present, and for converting from decimal to binary form with column scaling. The computation proper will be described briefly.

Solution of Linear Systems. – The solution of a single system of linear equations and the calculation of the inverse of a square matrix are special cases of the algebraic problem which is solved in these three codes. The equations to be solved for s sets of k variables, x_{pj}, are

$$\sum_{p=1}^{k} a_{ip} x_{pj} = \sum_{q=1}^{h} b_{iq} y_{qj} + c_{ij} \quad ,$$

where $i = 1, 2, \ldots, m$, $j = 1, 2, \ldots, s$, and the number of equations, m, is assumed to be at least equal to the number, k, of variables $x_{1j}, x_{2j}, \ldots, x_{kj}$ in each of the s disjoint systems. The limitations on size are:

$$0 < k \leqq m \leqq 255, \quad 0 \leqq h, \quad \text{and } n = k + h + s \leqq 4095,$$

so that each of the n columns of the matrix

$$M = (A \quad B \quad C)$$

will go (with index word) in a single block of magnetic tape and all blocks (including an identification block) will be addressable with three sexadecimal digits.

When the equations are written in the matrix form

$$AX = BY + C \quad ,$$

the case $h = 0$, $k = m$ gives $AX = C$, which yields $X = A^{-1}C$. Then for $s = k = m$, with C the identity matrix, $X = A^{-1}$, and for $s = 1$, X and C are vectors; thus the solution of a single system of linear equations is obtained.

An optional by-product of the coding is the computation of the determinant of a square matrix of order $\leqq 255$. The code calculates a matrix RM, where R is proper orthogonal,

$$RM = \begin{pmatrix} T & U & V \\ O & W_1 & W_2 \end{pmatrix} ,$$

and T is $k \times k$, with zeros below the diagonal. For $m = k$, the W_1 and W_2 are missing. If $m > k$ and the systems are solvable for $x_1, \ldots, x_k$ in terms of arbitrary $y_1, \ldots, y_h$, then W_1 and W_2 must be zero to within round-off error, and the diagonal elements of T must be different from zero. Where k is not known in advance, k is set equal to m, and the number of rows of $RM = (T \;\; U \;\; V)$ which can be regarded as zero (to within the accuracy justified by the problem) is used to determine $m - k$.

A limited number of time tests gives a figure of about $2.5 \times 10^{-3}\ m^2 n$ sec for operation of this code with a 1024-word memory. For calculation of the inverse of a matrix of order m, about $5 \times 10^{-3}\ m^3$ sec are required, or about 1 hr for order 90.

Additional codes perform back substitution, copying, and transposition, and assist in proofreading.

Planned Codes. – Input, output, and checking codes will be developed as the need for them is demonstrated. As availability of magnetic tape permits storing more complex codes on tape, it is planned to rewrite presently available codes for the calculation of eigenvalues and eigenvectors of a real symmetric matrix to deal with larger matrices. The more general eigenvalue problem, det $(A - \lambda B)$, with A and B real symmetric and B positive definite, should also be made available in automatic form and for larger matrices.

Other possible extensions are as follows: the calculation of the characteristic equation of a nonsymmetric real matrix and the solution of various problems for matrices with complex elements.

MATRIX INVERSION AND/OR LINEAR-EQUATION-SOLVER PROGRAM

Origin: J. W. Givens

Participating Member of Panel: S. E. Atta

Reference: "Vector-Block Matrix Codes," this report

Background and Status. – A routine has been programed for solving systems of equations and/or inverting matrices of small order. The method employs the rotational triangularization discussed by Givens. All the arithmetic operations are in unpacked floating point. In addition to obtaining an inverse, the routine subtracts the product of the matrix times its calculated inverse from the identity matrix and records the maximum absolute value of the differences along with its row and column index. The entire matrix and its identity are stored in the internal memory. The largest matrix which can be inverted by this routine in the single memory is a 14×14, and the largest single system is an order 19.

CALCULATIONS FOR SHELL-TRANSMISSION EXPERIMENT

Origin: R. L. Macklin, A. V. H. Masket, and H. W. Schmitt, Physics Division

Participating Members of Panel: S. G. Campbell, M. D. George

Background and Status. – During July and August several programs were run on the Oracle in connection with the shell-transmission experiment. The eventual result of the experiment was the calculation of the absorption cross sections of various materials. The programs which have been completed are described below.

1. It was desired to calculate the activation of a cylindrical detector (NaI crystal) being irradiated by an isotropic point source anywhere outside the cylinder. The activation is given by

$$\left(\frac{Q}{4\pi}\right)\left(\rho\,\frac{N}{A}\,\sigma\right) I \ ,$$

where

$$I = \iiint \frac{r\,dr\,d\theta\,dz}{r^2 + d^2 + z^2 - 2rd\cos\theta} \quad .$$

By integrating twice analytically, the following expression was obtained for I, where L is the height of the crystal, r is the distance of the source point from the crystal axis, and the cylinder is of unit radius:

$$I = \pi \int_{z=0}^{L} \ln \left[\frac{\sqrt{1 + 2(z^2 - r^2) + (z^2 + r^2)^2} + (z^2 - r^2) + 1}{2z^2} \, dz \right] .$$

Since this expression was derived on the assumption that the source point lay in the base plane of the crystal, it was desired to compute $I(L_1) - I(L_2)$ for $0 \leqq r \leqq 7$, where $L_1 - L_2 = 2$ and also where $L_1 - L_2 = 3$. This corresponds to the activation of the cylinder by a point source located in region A of Fig. 1. In addition, for the range $1 \leqq r \leqq 7$, it was desired to compute $I(L_1) + I(L_2)$, where $L_1 + L_2 = 2$ or $L_1 + L_2 = 3$, corresponding to the activation of the crystal from a point whose projection on the crystal axis would lie within the crystal, that is, a point in region B of Fig. 1. The desired values of I were computed for 55 r's in the range $0 \leqq r \leqq 7$ and with 56 L's in the range $0 \leqq L \leqq 12$. The values of I were then normalized by

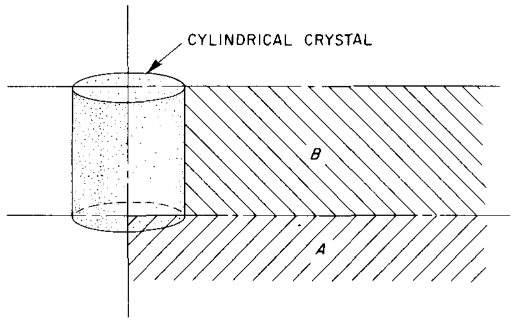

Fig. 1

$$\frac{(L_2 \pm 1)^2 + r^2}{2\pi}$$

for a crystal of height 2 and by

$$\frac{(L_2 \pm 1.5)^2 + r^2}{3\pi}$$

for a crystal of height 3.

2. Next, it was desired to compute the activation of the crystal by secondary (fission) neutrons produced in a spherical shell surrounding the crystal when this assembly was irradiated from a point source located on the cylinder axis. The activation integral, J_1, is

$$J_1 = \int_{R=r_i}^{R=r_0} dR \int_{\theta=0}^{\pi} \frac{R^2 I(R,\theta) \sin\theta \, d\theta}{R^2 + d^2 - 2Rd\cos\theta} ,$$

where R is the radial distance from the center of the crystal to a point in the shell. The inside radius of the shell, r_i, was 1.564, and the outside radius, r_0, was 2.359. The angle θ is the angle between the crystal axis and R, and $I(R,\theta)$ is the integral from program 1, where $r = R \sin\theta$ and I is either

$$I(1 + R\cos\theta) + I(1 - R\cos\theta)$$

or

$$I(1 + |R \cos \theta|) - I(|R \cos \theta| - 1) ,$$

depending on whether $|R \cos \theta| < 1$ or $|R \cos \theta| \geqq 1$; that is, whether a projection of the point in the shell onto the crystal axis would lie inside or outside the crystal.

3. The next phase of the problem was to calculate the activation of the crystal detector as a result of spontaneous fission in the shell material, with no external source point. In this case the shell is considered to be a uniform source surrounding the crystal. This activation integral, J_2, is given by the following expression, where the parameters are the same as in program 2:

$$J_2 = \int_0^{\pi} d\theta \int_{R=r_i}^{R=r_0} I(R,\theta)\, R^2 \sin \theta\, dR .$$

4. In connection with the calculation of the I's, it was desired to calculate the solid angle subtended by the crystal detector from the point source, which might be anywhere outside the crystal. By using a new line-integral method, the solid angle, Ω, is given by

$$\Omega = 2L \int_0^{\text{arc sin } a/r} \frac{d\phi}{\sqrt{L^2 + \rho^2}} ,$$

where

$$\rho^2 = (r^2 + a^2) \cos^2 \phi - (r^2 - a^2) \sin^2 \phi - 2r \cos \phi \sqrt{a^2 - r^2 \sin^2 \phi} ,$$

a is the radius of the crystal (in this calculation a is set equal to 1), r is again the distance from the point to the cylinder axis, and L is the height of the crystal. This expression is also based on the assumption that the source point lies in the base plane of the cylinder, so that the same combination of Ω values must be made as was made for the I calculations, and also the solid angle subtended by a circular disk must be added in certain cases. (The latter calculations have not been completed.) The program was run for the same values of r and L as for the I calculation, except that r was restricted to the range $1 < r \leqq 7$.

5. In order to compare the activation of the cylindrical detector with that of a spherical detector of the same mass, another program was run based on the experimental situation of the J_1 integration; that is, the detector is encased in a spherical shell, with an external source point isotropically emitting neutrons. The activation of a spherical detector of radius a, with the same mass, and of the same material as the cylindrical detector is given by

$$J_3 = 2\pi \left(\int_{r_i}^{r_0} \frac{a}{d}\, r \ln \frac{d + r}{d - r}\, dr - \int_{r_i}^{r_0} \frac{r^2 - a^2}{2d} \ln \frac{r + a}{r - a} \ln \frac{d + r}{d - r}\, dr \right) ,$$

where r_i, r_0, and d have the same values as in the J_1 calculation. A total of 30 cases was calculated on the Oracle for $0 \leqq a < 3$ at intervals of 0.1. It was found that a sphere with the same volume as that of the cylinder is not equivalent as a detector but that the sphere must be expanded. By plotting the J_3 values vs a and by comparing them with the value of J_1, the radius of the sphere which would be equivalent to the cylinder could be calculated.

6. The next phase of the problem was the calculation of J_1, with a correction added for the absorption of the source neutrons as they passed through the shell material. This activation of the cylinder is given by

$$J_1' = \int_{r_i}^{r_0} dr \int_{\theta=0}^{\pi} \frac{R^2 I(R,\theta) \sin\theta \exp(-\Sigma t)\, d\theta}{R^2 + d^2 - 2Rd\cos\theta} \ ,$$

where Σ is the macroscopic absorption cross section of the shell material, t is the distance of traverse through the shell material by the source neutron, given by

$$t = \sqrt{x^2 + r_0^2 - R^2} - x - y \ ,$$

in which

$$y = 2\sqrt{r_i^2 + x^2 - R^2} \ ,$$

$$x = \frac{Rd\cos\theta - R^2}{\sqrt{R^2 + d^2 - 2Rd\cos\theta}} \ .$$

In the range $0 \leqq \Sigma \leqq 1$, J_1' was computed for each of 40 values of Σ.

7. As an outgrowth of the line-integral method set up to calculate the solid angle subtended by the crystal from the source point, a program was set up to calculate the solid angle subtended by a circular aperture from a point source. The method used appears to be superior to previous methods for making this calculation, and it is hoped that eventually a complete table of the solid angles subtended by a circular aperture can be set up. The expression for this solid angle is given by

$$\Omega = 2\pi - 2h \int_0^{\pi} \frac{d\phi}{\sqrt{h^2 + \rho^2}} \ , \qquad \text{for } \lambda \leqq a \ ,$$

and

$$\Omega = -\int_0^{\arcsin a/\lambda} \frac{h\,d\phi}{\sqrt{h^2 + \rho_2^2}} + \int_0^{\arcsin a/\lambda} \frac{h\,d\phi}{\sqrt{h^2 + \rho_1^2}} \ , \qquad \text{for } \lambda > a \ ,$$

where

$$\rho^2 = (a^2 + z^2)\cos^2\phi + (a^2 - \lambda^2)\sin^2\phi + 2\lambda\cos\phi \left|\sqrt{a^2 - \lambda^2\sin^2\phi}\right| \ ,$$

$$\rho_1 = \lambda \cos \phi - \left| \sqrt{a^2 - \lambda^2 \sin^2 \phi} \right| ,$$

$$\rho_2 = \lambda \cos \phi + \left| \sqrt{a^2 - \lambda^2 \sin^2 \phi} \right| ,$$

and where b is the perpendicular distance from the point source to the aperture, λ is the distance from the center of the aperture to a projection of the point source on the plane of the aperture, and a is the radius of the aperture. No cases have as yet been run on the Oracle.

INVERSE OF A 190 × 190 MATRIX

Origin: C. J. McHargue, Metallurgy Division

Participating Members of Panel: M. R. Arnette, J. W. Givens, V. C. Klema

Background. – A matrix with integral elements and of order 190 is used as the coefficient matrix in a system of linear equations for a number of values of the constant terms. The inverse of the matrix is wanted for later use in solving the equations, and the solutions for four particular choices of the constants are desired.

Status. – (The general discussion under "Vector-Block Matrix Codes," this report, should be referred to for a description of some of the codes mentioned below.) The data were put on magnetic tape temporarily and punched out on paper tape in condensed form. The print of this tape was proofread by the originator of the problem. Corrections have been prepared and proofread.

Lack of an adequate supply of magnetic tape has prevented the problem from being finished, but coding has been done to carry out the following operations:

1. putting the corrected matrix on magnetic tape,
2. transposing the matrix and adding to it four columns of constants and the identity matrix,
3. converting from decimal to binary and scale,
4. calculating the inverse and four solution vectors.

A code for the scaling and reconversion of answers is being written.

FOURIER INVERSION OF DIFFRACTION DATA

Origin: H. A. Levy, Chemistry Division

Participating Member of Panel: M. F. Todd

Reference: *Mathematics Panel Semiannual Progress Report*, ORNL-1928

Background and Status. – The problem referred to was recoded in a more general form, and cases were run on the Oracle by using neutron diffraction data from molten KCl, molten CsCl, molten LiI, and x-ray diffraction data from aqueous UO_2F_2 solution.

The code has been given to the originator for use in running additional cases.

INTERNAL CONVERSION COEFFICIENTS OF THE *L* AND *M* SHELLS

Origin: M. E. Rose and A. Glassgold, Physics Division

Participating Member of Panel: S. E. Atta

References: Mathematics Panel Semiannual Progress Reports, ORNL-1842, -1928

Status. – Coefficients from all five subshells of the *M* shell have been obtained. Some changes were made in the *M*-shell programs, and coefficients from all three subshells of the *L* shell were obtained.

ECHELLOGRAM DATA REDUCTION

Origin: P. M. Griffin and K. L. Vander Sluis, Stable Isotopes Research and Production Division

Participating Members of Panel: N. M. Dismuke, J. H. Vander Sluis

Background. – Spectra, photographed on an Echelle-Littrow spectrograph, are recorded in a two-dimensional array of wavelengths on the photographic plate, forming an Echellogram.[1] The distribution of wavelengths is expressed by the function:

$$m\lambda = A + \frac{B(\Delta b)}{a + bl + cl^2} + \frac{C(\Delta b)^2}{(a + bl + cl^2)^2} , \tag{1}$$

where λ is the desired wavelength, m is a known integral order of interference, l is the position of the spectrum line along the direction of the Littrow dispersion, and Δb is the position of the spectrum line perpendicular to the Littrow dispersion and along the direction of the Echelle dispersion. The constants A, B, C, a, b, c are plate constants to be determined from measured positions of known $m\lambda$'s.

With the plate constants having been determined, there are two common applications of this information. The first is to calculate unknown wavelengths from a known m and measured Δb and l. The second[2] is the reduction of Zeeman patterns. If the light source giving rise to the observed spectrum is subjected to a magnetic field, each zero field line will give rise to a many-component pattern which is symmetrical about the zero field-line position. The symmetrical differences of the components of this pattern may be expressed as a linear combination of two constants, g_1 and g_2:

$$y_i = a_{i1}g_1 + a_{i2}g_2 . \tag{2}$$

---

[1] P. M. Griffin and K. L. Vander Sluis, *Stable Isotope Research and Production Semiann. Prog. Rep. May 20, 1955*, ORNL-1908, p 7–8.

[2] K. L. Vander Sluis, P. M. Griffin, and J. H. Vander Sluis, *Stable Isotope Research and Production Semiann. Prog. Rep. Nov. 20, 1955*, ORNL-2028, p 6–7.

Here, the differences y_i are wave-number differences, where the wave number σ is found by

$$\sigma = f(\lambda) .$$

For this type of problem it is desired to know the least-squares values of the two constants g_1 and g_2 and also the probable error associated with each.

Status. – The coding of both parts of this problem is nearly completed. The determination of the constants A, B, C, a, b, c will be made by a nonlinear least-squares subroutine, which will eventually be placed in the subroutine library.

EMF IN INDIUM SULFATE SOLUTION

Origin: M. H. Lietzke and R. W. Stoughton, Chemistry Division

Participating Members of Panel: A. C. Downing, E. C. Long

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1928

Background and Status. – In the course of a study of the thermodynamic properties of indium sulfate solutions by means of emf measurements, an attempt was made, by use of the Oracle, to obtain, simultaneously, a least-squares fit of the data for the potential vs temperature and concentration. Even though a high-order polynomial was tried, a satisfactory fit of the data over the entire concentration range could not be made. An alternative method of calculation was then used in which a polynomial least-squares fit of the emf values vs temperature was made at each of the ten concentrations studied. Values of the potential at even temperatures were then read from the plots, and values of a function $E^{0''}$ were calculated on the Oracle for each of the potential values.

The function $E^{0''}$ was defined as follows:

$$E^{0''} = E + \frac{8.6165T}{k_1}\left[\ln k_2 + \nu \ln m - \frac{2.97187 \times 10^6 (DT)^{-3/2} (\Sigma_j \nu_j Z_j^2)^{3/2} m^{1/2}}{1 + k_3 (DT)^{-1/2} (\Sigma_j \nu_j Z_j^2)^{1/2} m^{1/2} + k_4 (\Sigma_j \nu_j Z_j^2)^{1/2} m^{1/2}}\right] ,$$

where E is the potential obtained at an even temperature from the potential vs temperature plot; k_1, k_2, k_3, k_4, ν_j, and the values of $\Sigma_j \nu_j Z_j^2$ are constants for a particular system. In any given calculation, $k_3 = 0$ or k_3^0 when $k_4 = k_4^0$ or 0, m is the solute concentration, and D is the dielectric constant of water given by

$$D = 78.54[1 - 0.00460(t - 25) + 0.0000088(t - 25)^2] .$$

The constant k_3^0 contains a term for the "distance of closest approach," a^0, and values of $E^{0''}$ were calculated for values of $a^0 = 4A^0$ and $a^0 = 5A^0$. Values of $E^{0''}$ were then plotted vs m in an attempt to make an extrapolation to $m = 0$.

THERMODYNAMIC PROPERTIES OF CHEMICAL REACTIONS

Origin: E. E. Litkenhous, research participant from Vanderbilt University; J. T. Long, Chemical Technology Division

Participating Member of Panel: S. E. Atta

Background and Status. – Under suitable conditions, the specific heat, C_p, the entropy, S, the enthalpy, H, and the free energy, F, for a specific chemical reaction may be expressed as functions of temperature by the equations

$$C_p = A + BT + CT^2 + \frac{D}{T^2} ,$$

$$S = A \ln T + BT + \frac{C}{2} T^2 - \frac{D}{2T^2} + I_S ,$$

$$H = AT + \frac{B}{2} T^2 + \frac{C}{3} T^3 - \frac{D}{T} + \Delta H_0 ,$$

$$F = -AT(\ln T - 1) - \frac{B}{2} T^2 - \frac{C}{6} T^3 - \frac{D}{2T} + \Delta H_0 - I_S T .$$

The six coefficients A, B, C, D, ΔH_0, I_S may be estimated from any combination of six suitably chosen (i.e., linearly independent) measurements of the thermodynamic variables at various temperatures.

A routine has been prepared for the Oracle which constructs from any set of six measurements the corresponding system of observational equations. These are linear algebraic equations, and their solution is the desired set of coefficients. By use of these coefficients, a table of values of all four thermodynamic variables is constructed at regular temperature intervals over the range 0 to 1200°K.

The system of equations is solved by triangularization. In the first version of this routine, the triangularization was accomplished by the familiar method of elimination. Unfortunately, the solutions obtained in this manner did not satisfy the original observational equations to the desired accuracy. Therefore, in the final code, the triangularization is obtained by a series of rotations, with a resultant increase in the accuracy of the solutions.

The Oracle program, with operating instructions, has been given to the originators.

DAMAGE TO TISSUE FROM NEUTRON IRRADIATION

Origin: W. S. Snyder and J. Neufeld, Health Physics Division

Participating Members of Panel: N. M. Dismuke, J. H. Vander Sluis

References: Mathematics Panel Semiannual Progress Reports, ORNL-1842, -1928

Status. – The number of neutron histories and the number of gamma-ray histories which have been calculated by using the Monte Carlo programs mentioned in the previous semiannual report (ORNL-1928) are given in Table 1. Approximately 250 hr of

TABLE 1. NEUTRON AND GAMMA-RAY HISTORIES

Source Energy (Mev)	Slab Thickness (cm)	Tabulation Interval (cm)	Angle of Beam Incidence with the Slab Normal (deg)	Number of Histories	
				Neutron	Gamma Ray
10	30	1	0	6,000	24,814
7.5	30	1	0	5,000	11,464
5.0	30	1	0	5,000	11,876
2.5	30	1	0	5,000	12,284
1.0	30	1	0	4,000	8,942
0.5	30	1	0	4,000	9,774
0.1	30	1	0	4,000	8,826
0.02	30	1	0	4,000	8,516
0.005	30	1	0	4,000	17,268
0.0001	30	1	0	7,000	13,539
0.00001	30	1	0	1,000	4,866
Thermal	30	1	0	4,000	7,060
5.0	30	1	60	1,000	
2.5	30	1	75	1,000	
2.5	30	1	60	1,000	
2.5	30	1	45	1,000	
2.5	30	1	30	1,000	
2.5	10	0.5	0	2,000	2,222
2.5	1	0.1	0	3,000	3,835
Thermal	10	0.5	0	2,000	1,773
Thermal	1	0.1	0	10,000	3,928

Oracle time was required to calculate these histories. Computation time for 1000 neutron histories ranged from 10 min for the 2.5-Mev beam irradiating a 1-cm slab to $2\frac{1}{2}$ hr for a 10-Mev beam irradiating a 30-cm slab. For 1000 gamma-ray histories, computing time ranged from 10 min for the 1-cm slab to 20 min for the 30-cm slab.

A report is being written for presenting the results of the computation to the National Committee on Radiation Protection. The primary problem will be complete with the issuance of this report. However, it is expected that the programs will be used in the future to study some related problems, since use has not yet been made of all the generalizations for which the code was designed.

EXPERIMENTAL CODES FOR THE CURVE PLOTTER

Origin: R. J. Klein, Instrumentation and Controls Division

Participating Member of Panel: C. L. Gerberich

Background and Status. – During the time covered by this report, a curve plotter was added to the Oracle. The specifications for a set of codes were drawn up to aid in the checking of this new equipment:

1. *A test to check linearity.* – This code plotted a series of straight lines, both horizontal and vertical, to form a box with a cross, as shown in Fig. 2.

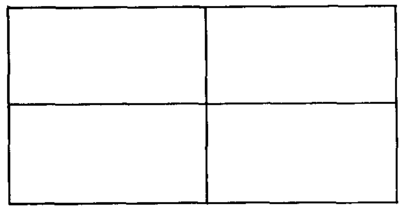

Fig. 2

2. *A test to check focus.* – Code 1 was modified to write the letters *ABCDE* at six places and to have a running index in the lower left corner of the upper right box to identify the particular exposure (see Fig. 3).

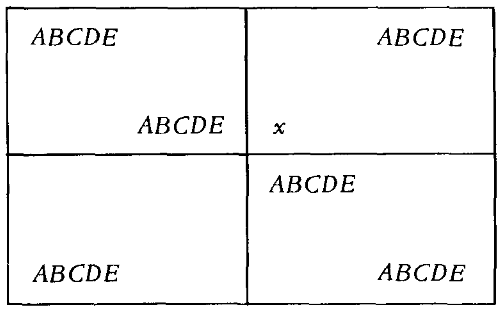

Fig. 3

3. *A test to check readability of characters.* – This code took a list of n characters from a paper-tape input and plotted them 42 characters to a line, with 32 lines required to fill the entire frame.

4. *A test to check the advisability of a background grid.* – This code plots both horizontal and vertical grids on the frame. From eight input parameters (four vertical, four horizontal) it finds the number of points between small divisions, the number of small divisions per large division, the number of points between brightups on the small-division lines, and the number of points between brightups on the large-division lines.

5. *A code to draw axes, with large and small divisions marked off on the axes.* – This code takes ten input parameters and draws axes, as shown in Fig. 4. The parameters are as follows:

a = x coordinate of origin,

b = y coordinate of origin,

c = number of points per small division, x axis,

d = number of points per small division, y axis,

e = number of small divisions per large division, x axis,

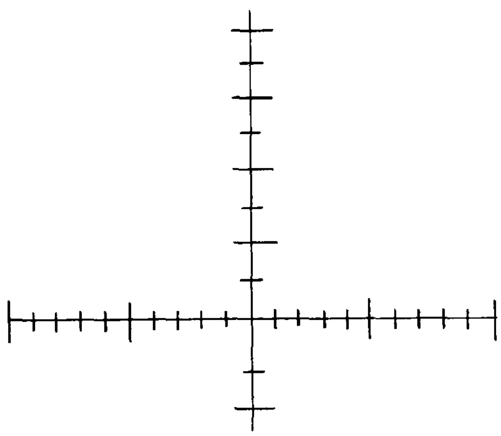

Fig. 4

f = number of small divisions per large division, y axis,

g = number of large divisions on positive x axis,

h = number of large divisions on negative x axis,

i = number of large divisions on positive y axis,

j = number of large divisions on negative y axis.

6. *A code to plot functions.* – This code takes the preceding code with its ten parameters and, with the addition of five more parameters, plots the points of a function on the curve plotter. The added parameters are: n, the number of points to be plotted, and the four values of variables at the ends of the axes.

7. *A format code.* – This code is used to label the graphs or to make more automatic the use of characters. The code uses an input tape as follows:

$$
\begin{array}{c}
[0 \ldots 0n] \\
[m_1 m_1 (xxx)00(yyy)] \\
[AA\ BB\ CC\ DD\ EE] \\
\cdots \\
[\ldots MM0000] \\
\vdots \\
[m_2 m_2 (xxx)00(yyy)] \\
\vdots \\
[m_n m_n (xxx)00(yyy)] \\
\vdots \\
\cdots
\end{array}
$$

where n is the number of different places at which a row of characters may be started, m_i is the number of characters in the ith group, x and y are the coordinates of the first character in the set. There are m pairs of hex digits (five per word) which identify the character to be plotted.

SAFETY CALCULATIONS FOR THE HRT

Origin: P. R. Kasten, Reactor Experimental Engineering Division

Participating Members of Panel: C. L. Bradshaw, C. P. Hubbard

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1751

Background and Status. – The system of four first-order differential equations and one linear algebraic equation, representing the kinetic conditions of the HRT, has been recoded for the revised 8-32 floating-point system. The system is solved by the method of Runge-Kutta to determine maximum power and maximum pressure within the reactor for various values of the parameters involved.

In addition to the one mentioned above, another system of five differential equations has been coded to take into account the effect of gas pressure within the core. This system was also solved by the Runge-Kutta method to determine maximum power and pressure.

Both these codes will use the Oracle curve plotter to plot pressure and power as functions of time. Both codes are completed and will be in production as soon as a curve-plotter subroutine is available for floating-point numbers.

A MULTIGROUP, MULTIREGION, TWO-DIMENSIONAL REACTOR CALCULATION

Participating Member of Panel: C. L. Bradshaw

Background and Status. – Work is progressing on a rather general two-dimensional reactor code, which will allow for several regions and several groups. The code will incorporate several refinements that have been found desirable as a result of experience with two previous two-dimensional reactor codes. In particular, the code will use a refined difference approximation to the differential system. It is hoped that this approximation will permit a considerable reduction in the number of mesh points necessary for a specified degree of accuracy and thus will make the multigroup problem feasible from the standpoint of the computing time.

CALCULATION OF STRESSES IN PIPING SYSTEMS

Origin: M. I. Lundin, Reactor Experimental Engineering Division

Participating Member of Panel: E. C. Long

Reference: *Mathematics Panel Semiannual Progress Report*, ORNL-1928

Background and Status. – A piping system assembled at normal room temperatures and anchored at the ends will undergo certain distortions at temperatures such as those found in nuclear reactors. It is often impractical to engineer systems with loops because of space considerations and material holdup. Because of the noxious nature of the material involved in reactor piping systems it is necessary to know as accurately as possible the stresses in any given part of the system. Therefore, a three-plane pipe stress analysis has been programed for the Oracle.

Recently, the need has arisen for calculating deflections and rotations at any point in the system. The calculation has been programed as the second portion of the pipe stress code.

The third section deals with piping systems with branches, which has also been programed. Up to four branches may be calculated.

All three programs are complete, and the code is routinely in use.

TWO-DIMENSIONAL, THREE-REGION, TWO-GROUP REACTOR CALCULATION

Origin: P. R. Kasten, Reactor Experimental Engineering Division

Participating Member of Panel: C. L. Bradshaw

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1928

Background. – The problem that was solved is indicated by means of Fig. 5, the differential equations, and the boundary conditions. Symmetry is assumed about the z axis (cylindrical coordinates). The differential equations are as follows:

$$D_{f_i}\nabla^2\phi_{f_i} + \frac{k_i}{p_i}\Sigma_{s_i}\phi_{s_i} - \Sigma_{f_i}\phi_{f_i} = 0 \quad ,$$

$$D_{s_i}\nabla^2\phi_{s_i} + p_i\Sigma_{f_i}\phi_{f_i} - \Sigma_{s_i}\phi_{s_i} = 0 \quad ,$$

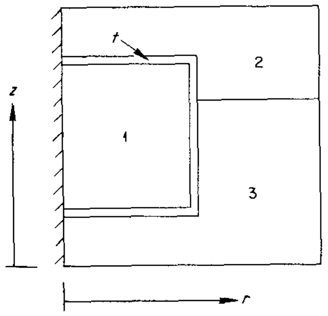

Fig. 5

where $i = 1, 2, 3$ refers to the three regions, and s and f refer to neutron energy groups.

The following are the boundary conditions:

1. The flux vanishes at the extrapolated boundary.
2. The net neutron current and the flux are continuous across interfaces.
3. A thin shell (thickness t) which surrounds region 1 is transparent to fast neutrons and an absorber of slow neutrons. This boundary condition is approximated as follows:

$$D_{s_2}\left(\frac{\partial\phi_{s_2}}{\partial z}\right)_{r<R_0,z=c} = D_{s_1}\left(\frac{\partial\phi_{s_1}}{\partial z}\right)_{r<R_0,z=c} + \Sigma_a t\left(\phi_{s_1}\right)_{r<R_0,\,z=c} \,.$$

The system of differential equations is replaced by a finite difference scheme, which is solved numerically. To avoid the difficulty which arises at mesh points on interfaces and, in particular, at corner points, this code is set up to use a so-called "staggered mesh." This requires that mesh points never fall on interfaces but always must be one-half unit from the interfaces. A mesh system such as this is set up as readily as the ordinary one, and the multiregion point is much easier to handle.

The code assumes that the concentrations of the material in each region are known, and all the constants appearing in the differential system are given as input numbers. The code then computes the effective multiplication for the particular reactor system. When the effective multiplication constant is established, the code will then compute the neutron leakages and absorptions in the different regions so that a neutron balance can be obtained.

Status. – The code is in a production status, and several cases have been run on the Oracle. The code can be run with or without the shell and also as a two-region problem, simply by setting regions 2 and 3 equal. A complete description of the code is to be published in the near future.

PREDICTING THE FREQUENCY OF ISOTOPICALLY SUBSTITUTED MOLECULES

Origin: H. W. Morgan, Stable Isotopes Research and Production Division; E. Mehr and F. Lane, New York University

Participating Member of Panel: M. R. Arnette

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1928

Background and Status. – Several problems have been run for each of the originators named above. The routine for solving the problems involves the calculation of the characteristic values and vectors of the product of two symmetric matrices, G and F, where G is the kinetic energy or mass matrix, and F is the force constants or spring matrix. The routine obtains the characteristic values and vectors, λ's and q's, of the systems $(G - \lambda F)q = 0$. At present, the routine makes use of the magnetic tapes for storage of the codes but has not yet been changed to make better use of the auxiliary memory for storage of intermediate answers. This change is being considered but is not yet completed. The matrices for these originators were of order 5, 7, and 8.

AN INTERPOLATION PROBLEM

Origin: R. Livingston, Chemistry Division

Participating Member of Panel: C. L. Gerberich

Background and Status. – Several sets of experimental data were forwarded to the Laboratory by another establishment. The information was in tabular form for equal steps of the independent variable. The exact equation used to calculate the information was unknown, and there was a need to interpolate for data at points not listed on the table. After some consideration of the problem, it was decided to fit a polynomial through the given points and evaluate it at the values wanted. A program to do this was written for the Oracle, and all cases have been run.

APPLICATION OF STANDARD CODES

Participating Member of Panel: B. J. Osborne

Origin: J. G. Burr, Chemistry Division

Problem. – Characteristic values and vectors of four matrices of order 20, six matrices of order 18, and four matrices of order 16 were obtained by using the Givens codes.

Origin: H. W. Morgan, Stable Isotopes Research and Production Division

Problem. – Several systems of equations of order 15 were solved by using the solver for simultaneous linear equations.

Origin: B. R. Fish, Health Physics Division

Problem. – The inverse of an order-5 matrix was obtained.

Origin: G. J. Atta, Mathematics Panel

Problem. – The inversion of 19 small matrices of order 3 through 9 was obtained.

Origin: K. L. Vander Sluis, Stable Isotopes Research and Production Division

Problem. – A least-squares fit of experimental data to a polynomial of various orders was desired. A program is being set up so that a large number of such problems can be run with a minimum of preparation. It is expected that a large number will be run by using this particular program in the next report period.

HAND COMPUTATIONS

Participating Member of Panel: M. E. Fulmer

The following problems will be reported by the originator in the semiannual progress report of his division.

COMPUTATION OF INTERNAL-CONVERSION RATIOS

Origin: M. E. Rose, Physics Division

COMPUTATION OF THE FERMI FUNCTION OF BETA DECAY FOR MIRROR NUCLEI

Origin: E. D. Klema, Physics Division; R. K. Osborn, Educational Division

SELECTIVITY OF ION-EXCHANGE RESINS

Origin: G. E. Myers, Chemistry Division; J. Z. Hearon, Mathematics Panel

APPROXIMATE CONFIDENCE INTERVALS FOR SPECIFIC-LOCUS MUTATION RATES

Origin: W. L. Russell, Biology Division

Participating Member of Panel: A. W. Kimball

Background and Status. – In this type of experiment, N males are exposed to the same dose of radiation, and each survivor is mated to several unirradiated females, thereby yielding a total of n offspring from each male. Each offspring is examined for mutations at each of k loci, and x_i ($i = 1, \dots, k$) mutations are found at the ith locus among all offspring examined. It is reasonable to assume that the conditional probability distribution of each x_i is of the Poisson form,

$$g(x|m) = m^x e^{-m}/x! \ , \qquad x = 0, 1, \dots \ ,$$

where m is the expected number of mutations at the locus being studied in a sample of Nn offspring. Since m is, itself, a random sample from the population of loci, it will have a probability distribution $h(m)$, $(0 < m < \infty)$, which may be taken to be continuous. Thus the unconditional probability distribution of x is

$$f(x) = \int_0^\infty g(x|m)\, h(m)\, dm \ .$$

An estimate is desired of the mean number of mutations in the population of loci,

$$\lambda = \int_0^\infty m h(m)\, dm \ .$$

It may be shown easily that the expected value of x is λ, irrespective of the form of the probability distributions $g(x|m)$ and $h(m)$. Thus the observed mean number of mutations per locus,

$$\bar{x} = \sum_{i=1}^{k} \frac{x_i}{k} \ ,$$

is an unbiased estimate of λ.

A preliminary study indicated that the gamma distribution

$$\frac{1}{(\alpha - 1)!\, \beta^{\alpha}}\, m^{\alpha-1} e^{-m/\beta}$$

would be a good choice for $h(m)$. This yields

$$f(x) = \frac{\Gamma(\alpha + x)}{x!\Gamma(\alpha)} \left(\frac{\lambda}{\lambda + \alpha}\right)^{x} \left(1 + \frac{\lambda}{\alpha}\right)^{-\alpha} \ ,$$

which is the negative binomial distribution with a mean λ $(= \alpha\beta)$ and exponent α. A study of seven sets of published data indicated that this distribution with an exponent of 1 would provide good fits. In this case $(\alpha = 1)$, the distribution has the form

$$f(x) = \frac{\lambda^x}{(1 + \lambda)^{x+1}} \ ,$$

with mean λ and variance $\lambda(1 + \lambda)$. The goodness of fit was evaluated by means of a chi-square test.

If each x_i has the above distribution, then

$$X = \sum_{i=1}^{k} x_i$$

has a negative binomial distribution with a mean $k\lambda$ and an exponent k. Furthermore, when k is known,

$$y = \sinh^{-1}\left(\frac{X + 3/8}{k - 3/4}\right)^{1/2}$$

will be approximately normally distributed when $k > 2$ and $k\lambda$ is large.[3] The variance of y is approximately $\frac{1}{4}(k - 1)$, which may be used to place confidence limits on y, whereupon the limits so obtained may be transformed back to provide limits for $k\lambda$.

A paper describing this method in detail and illustrating its application has been submitted for publication in *The American Naturalist*.

AN ISOTOPE-EXCHANGE PROBLEM

Origin: G. H. Clewett, Materials Chemistry Division; F. E. Jenkins and G. M. Harris, University of Buffalo

Participating Members of Panel: C. L. Gerberich, J. Z. Hearon; W. C. Demarcus, K-25

Background and Status. – A frequent procedure for determining isotope effect in an exchange of the type

$$AB + B^* \rightleftharpoons AB^* + B$$

is to allow exchange equilibrium to occur and subsequently precipitate out B and B^*. It is then *assumed* that the specific activity of the precipitate gives the equilibrium specific activity of B. If p and q are the equilibrium specific activities of B and AB, the true equilibrium constant is

$$\alpha = \frac{p}{q} ;$$

and the apparent constant, from the above procedure, is

$$K = \frac{p}{z} ,$$

where z is measured, and p is determined from z and the conservation of B^*. This problem consists in solving

$$\frac{dQ}{d\theta} = -s(\alpha Q - P) - \epsilon' Q ,$$

$$\frac{dP}{d\theta} = sre^{-\theta}(\alpha Q - P) ,$$

$$P(0) = \frac{1}{r + \alpha} ,$$

$$Q(0) = \frac{\alpha}{r + \alpha} ,$$

where ϵ' defines the isotope effect in the precipitation reaction, s is the ratio of the rate

---

[3]F. J. Anscombe, *Biometrika* **35**, 246–254 (1948).

of exchange equilibration to the rate of precipitation, and P and Q are normalized variables such that

$$K = r \cdot \frac{P(\infty)}{1 - P(\infty)} ,$$

with r the initial ratio $[B + B^*]/[AB + B^*]$. Computed values of K are compared with the actual value of α.

This problem has been programed for the Oracle. At the present time, a set of 432 cases is being run, and these cases represent all the combinations of six values of r, six values of s, four values of α, and three values of ϵ'. The values of the parameters are tabulated below:

	1	2	3	4	5	6
r	0.5	1.0	2.0	4.0	10.0	100.0
s	0.5	1.0	2.0	4.0	10.0	100.0
α	0.92	0.96	1.04	1.08		
ϵ'	−0.08	−0.04	+0.04			

SOME THEOREMS IN KINETICS OF LINEAR SYSTEMS

Origin: J. Z. Hearon

Participating Member of Panel: J. Z. Hearon

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1842

Background and Status. – In many problems of a rather varied physical nature (e.g., chemical kinetics, isotope exchange, or any system formally equivalent to a system of linearly interacting compartments, see reference, p 31), either the questions directly posed or some aspect of the problem requires a statement of the integrals

$$s_i = \int_0^\infty x_i(t)\, dt \tag{1}$$

in terms of the elements of the coefficient matrix A of the equations

$$\dot{x} = Ax , \tag{2}$$

for which the $x_i(t)$ are solutions. For example, in the referenced problem the dose administered to the *i*th organ is proportional to s_i, and in chemical kinetics a stable product formed from an intermediate whose concentration is $x_k(t)$ has a final concentration proportional to s_k. The main theorem is as follows: If the roots of A are negative, the column vector, s, of the s_i is given by

$$s = -A^{-1} x(0) . \tag{3}$$

The proof follows from direct integration of Eq. 2, since the negativity of the roots of A secure the existence of the s_i and the limits

$$\lim_{t\to\infty} x_i(t) = 0 \ .$$

The other theorems are stated (without proof) in the vocabulary of the referenced problem to show that they can be applied at once from an inspection of the connectivity of the system.

Suppose that a set of compartments can be selected from the system such that, except for one or more irreversible outlets from a given compartment, say the pth, they constitute a closed system. Then $s_p = \sum x_i(0)/\beta$, where the summation runs over the set, and β is the sum of the coefficients associated with the irreversible outlet.

Suppose that the system divides into subsystems I and II such that in I only one compartment, say the rth, receives material from some of the compartments in II or from all of them. Suppose also that the initial values for I are zero, and for II are arbitrary. Then the ratio s_j/s_k in I is independent of the initial conditions and the connectivity in II. Further, $s_j/s_k = A^{\nu}_{rj}/A^{\nu}_{rk}$, provided, first, that the compartments are numbered so that x_i is in I when $1 \leqq i \leqq \nu$, and, second, that A^{ν}_{rj} is the cofactor of a_{rj} in the $\nu \times \nu$ minor of A from the first ν rows and columns.

A PROBLEM IN TRACER KINETICS

Origin: C. J. Collins, Chemistry Division

Participating Member of Panel: J. Z. Hearon

Background and Status. – The rate equations in this problem are

$$\dot{a} = -k_1 a \ ,$$

$$\dot{x} = k_1 a - (\mu + k')x + ky \ ,$$

$$\dot{y} = kx - (\mu + k')y \ ,$$

$$\dot{p}_1 = k'x \ ,$$

$$\dot{p}_2 = k'y \ .$$

It was desired to obtain the ratio $p_2(\infty)/p_1(\infty)$ and to show its independence of k_1. This result follows at once from the last theorem of the preceding problem ("Some Theorems in Kinetics of Linear Systems"). It was further desired to examine, for $\mu = k$, the ultimate constancy of the ratio x/y for large t. Defining $P = x + y$ and $Q = x - y$, it can be shown that

$$P = \frac{k_1 a(0)}{k' - k_1} \left(e^{-k_1 t} - e^{-k' t} \right) \ ,$$

and that

$$Q = \frac{k_1 a(0)}{\lambda - k_1} \left(e^{-k_1 t} - e^{-\lambda t} \right) ,$$

where $\lambda = 2k + k'$. It can then be shown that for the six possible orderings of the parameters, $k_1 < k' < k$, $k_1 < k < k'$, etc., the ratio $x/y = (P + Q)/(P - Q)$ has an asymptotic value identical with $p_1(\infty)/p_2(\infty)$ only if k_1 is negligible relative to k and k'.

A MULTIPLE REGRESSION FIT FOR A CORROSION EXPERIMENT

Origin: D. G. Thomas, Reactor Experimental Engineering Division

Participating Members of Panel: G. J. Atta, A. W. Kimball

Background and Status. – The results of several loop tests with slurries were presented for analysis. Variations in pH, fuel concentration, SO_4^{--} added, etc. were imposed on the tests in order to evaluate simultaneously the effects of five such variables. Some of the variables could not be controlled directly, but they could be measured.

A regression surface was fitted to the data, and the various components of regression were tested for significance.

FITTING OF SURVIVAL CURVES TO SPERMATOGONIA DATA IN MICE

Origin: E. F. Oakberg, Biology Division

Participating Members of Panel: G. J. Atta, A. W. Kimball

Background and Status. – Because of the great radiosensitivity of mouse spermatogonia and because these cells can be followed very closely through several stages of early development, they were chosen for a series of experiments with the new protective compound, *S*,β-aminoethylisothiuronium·Br·HBr (AET). Concurrently, a set of experiments was run in which irradiation took place under hypoxia.

Survival curves were fitted to most of the data from these experiments, and tests of significance were applied to evaluate treatment effects. Wherever the cell counts were too small to justify the fitting of survival curves, chi-square tests were used.

The compound AET was found to be protective, but its effect was not so great as that of hypoxia.

A TEST OF THE MODEL FOR RADIATION-INDUCED CHROMOSOMAL ABERRATIONS IN *TRADESCANTIA*

Orgin: A. D. Conger, Biology Division

Participating Members of Panel: G. J. Atta, A. W. Kimball

Background and Status. – For some time it has been customary to interpret radiation-induced chromosomal aberrations according to target or hit theory. When a cell is scored, the number of exchanges and the number of terminal and interstitial deletions, if any, are recorded. If no aberrations are found, the cell is scored as normal. This is done for many cells at a series of graded doses, and, according to hit theory, the number of exchanges (y_e) and the number of deletions (y_d) per cell should have the following relationships to dose (x):

$$y_e(x) = a_e x + b_e x^2 \ ,$$

$$y_d(x) = a_d x + b_d x^2 \ .$$

Many experiments of this kind have been done, and satisfactory agreement with theory is usually found.

An additional test of the hit theory can be made from the data on the percentage of normal cells at graded doses. Since y_e and y_d have Poisson distributions, the expected proportion of normal cells (N) must be

$$N = e^{-y_e(x)} \cdot e^{-y_d(x)} \ ,$$

so that

$$\log N = -Ax - Bx^2 \ ,$$

where

$A = a_e + a_d,$

$B = b_e + b_d.$

Thus from a fit of log N against x, the parameters A and B can be estimated and tested against their independent counterparts obtained from the aberration data.

This test was performed on several sets of data, and good agreement with the target theory was found.

EFFECT OF AGMATINE ON MITOTIC ACTIVITY IN NEUROBLASTS OF *CHORTOPHAGA VIRIDIFASCIATA*

Origin: G. St. Amand, Biology Division

Participating Members of Panel: G. J. Atta, A. W. Kimball

Background and Status. – Previous experiments had indicated a stimulation of mitotic activity in neuroblasts of grasshopper embryos as a result of adding agmatine to the hanging-drop suspension. In order to evaluate this effect more critically, individual cells were followed from late prophase through mid-telephase, and the time spent in each of four periods was recorded for each cell. This was done with a control group and with a group which had been treated with agmatine.

An analysis of variance revealed that agmatine-treated cells required about 20% less time to pass through this phase of the mitotic cycle than did the control cells. At the same time, however, the existence of a treatment-period interaction was established, and further comparisons showed clearly that agmatine stimulated cells in each of the four periods except the anaphase ($A_1 - T_1$). In this period the times required by both treated and untreated cells were equal. A repetition of the experiment confirmed these conclusions.

ANALYSIS OF A RADIATION EXPERIMENT WITH *ESCHERICHIA COLI* B/r

Origin: A. J. Sbarra, Biology Division

Participating Members of Panel: G. J. Atta, A. W. Kimball

Background and Status. – The lethal effect of long ultraviolet and short visible radiation (3500–4900 Å) on *E. coli* is known to be dependent on the medium in which the organisms are suspended during irradiation. Likewise, recovery after irradiation has been found to depend on the plating medium.

Two $2 \times 2 \times 5$ factorial experiments were carried out in order to ascertain the joint action of these effects. In one experiment, organisms were irradiated in either oxygen or nitrogen and plated out on either basal medium or basal medium plus 2% yeast extract. In the other experiment, organisms were irradiated in either a buffer or a salts solution and plated out on both kinds of media. In both experiments, five separate doses of radiation were used.

Analyses of variance were computed for both experiments. In the first experiment, yeast added to the plating medium resulted in a significant increase in survival in both oxygen and nitrogen, although the survival of organisms irradiated in nitrogen was significantly higher than that of organisms irradiated in oxygen. In the second experiment, the plating medium was found to have the same effect on survival, and organisms irradiated in a salts solution had significantly greater survival than did those irradiated in a buffer solution. In neither experiment was there any evidence of an interaction between the two main effects.

ANALYSIS OF CORROSION DATA FROM IN-PILE LOOP EXPERIMENTS

Origin: J. E. Baker, Reactor Experimental Engineering Division; G. H. Jenks, Chemistry Division

Participating Members of Panel: G. J. Atta, A. W. Kimball

Background and Status. – The details of these experiments and their analyses are contained in a memorandum dated November 10, 1955, to the originators of the problem.