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MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

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MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

FOR

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MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

for

Period Ending December 31, 1953

A. S. Householder, Chief
W. C. Sangren, Editor

DATE ISSUED

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ERRATA

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p. v, line 35

for Parameters of KD_2 as O_4 *read* Parameters of KD_2AsO_4

p. 15, column 2, line 28

for PARAMETERS OF KD_2 AS O_4 *read* PARAMETERS OF KD_2AsO_4

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MATHEMATICS PANEL SEMIANNUAL PROGRESS REPORT

INTRODUCTION

THE ORACLE

After two years of design and construction at the Argonne National Laboratory, the ORACLE arrived at Oak Ridge National Laboratory on October 8, 1953. The physical size and complexity of the computer, as well as its delicate construction, made the installation in Building 4500 a major undertaking. Exceptional care was exercised in the installation to provide adequate protection and controlled environment for the machine during operation. A 40-ton air-conditioning system was installed for computer and room cooling. The permanent installation involved the construction of features that were not necessary for the temporary operation at Argonne. Testing of the ORACLE is now in progress, and the computer will be ready for actual problem operation within the next few weeks.

Design of the control for the magnetic tape storage unit is being done at Oak Ridge National Laboratory, while fabrication of the frame and tape drives is continuing at the Argonne National Laboratory. The design and development of a photographic output device are under way to provide fast output information in either graphical or digital form. A fast punch and a Ferranti tape reader are to replace the temporary, standard teletype units.

The ORACLE remained at the Argonne National Laboratory for a longer period of time after completion than was expected; consequently, time was available for problem solution, as well as for the testing program. During July, August, and September a total of 218 hr of computer time was used for the solution of problems that are described elsewhere in this report.

LECTURES

Members of the Mathematics Panel presented the following lectures on the Traveling Lecture Program.

A. W. Kimball, *A Stochastic Model for a Biological Growth Process*, Louisiana State University, December 9, 1953; *L. D. 50 Estimation Without Iteration*, Tulane University, December 7, 1953.

A seminar series under the direction of C. P. Hubbard has been initiated for studying the logical design of the ORACLE.

A. C. Downing, Jr. presented a joint paper with R. C. F. Bartels of the University of Michigan at a meeting of the American Mathematical Society in Kingston, Ontario, on September 4, 1953 entitled *On Surface Waves Generated by Travelling Disturbances with Circular Symmetry*.

J. Z. Hearon, *Thermodynamic Efficiency*, Symposium on Human Performance, National Institute of Health, Bethesda, Maryland, October 29, 1953; *Enzyme Distribution and Reaction Rate*, Biology and Medicine Seminar, Argonne National Laboratory, November 27, 1953.

A. S. Householder, *Vacuum Tubes, Neurons, and Computations*, Meeting of Mathematics Section, Tennessee Education Association, Nashville, Tennessee, October 23, 1953; *Generation of Errors in Digital Computation*, Meeting of Southeastern Section of American Mathematical Society, Spartanburg, South Carolina, November 27, 1953; *Preparation of Problems for Digital Computers*, Meeting of American Institute of Chemical Engineers, St. Louis, Missouri, December 16, 1953.

A. S. Householder and A. W. Kimball, *A Stochastic Model for the Selection of Macronuclear Units in* Paramecium *Growth*, annual joint meeting of the Biometric Society, the Institute of Mathematical Statistics, and the American Statistical Association in Washington, D. C., December 27-30, 1953. At this same meeting, J. Moshman discussed *A Two-Sample Procedure for Linear Discrimination in Normal Samples*.

J. Moshman presented a discussion on *Generation of Pseudo-Random Numbers on a Decimal Calculator* at a meeting of the Institute of Mathematical Statistics in Kingston, Ontario, August 30 to September 4, 1953.

LIST OF PUBLICATIONS

G. E. Albert, *A General Theory of Stochastic Estimates of the Neumann Series for the Solutions of Certain Fredholm Integral Equations and Related Series*, ORNL-1508 (Aug. 28, 1953).

J. Z. Hearon, "Comments on the Approximate Solution of the Diffusion Equation. II," *Bull. Math. Biophys.* **15**, 111 (1953).

J. Z. Hearon, "The Kinetics of Linear Systems with Special Reference to Periodic Reactions," *Bull. Math. Biophys.* **15**, 121 (1953).

J. Z. Hearon, "A Note on the Integral-Equation Description of Metabolizing Systems," *Bull. Math. Biophys.* **15**, 269 (1953).

A. S. Householder, "Can Machines Think?" *Computers and Automation* **2**, No. 9, 14 (December 1953).

A. S. Householder, *Principles of Numerical Analysis*, McGraw-Hill, New York, 1953.

M. E. Gaulden, M. Nix, and J. Moshman, "Effects of Oxygen Concentration on X-Ray Induced Mitotic Inhibition in Living Chortophaza Neuroblasts," *J. Cellular Comp. Physiol.* **41**, 451 (1953).

J. Moshman, "Critical Values of the Log-Normal Distribution," *J. Am. Stat. Assoc.* **48**, 600 (1953).

J. Moshman, *A Two-Sample Procedure for Linear Discrimination in Normal Samples*, ORNL-1582 (Aug. 28, 1953).

W. C. Sangren, *Differential Equations with Discontinuous Coefficients*, ORNL-1566 (Oct. 21, 1953).

S. D. Conte and W. C. Sangren, "An Asymptotic Solution for a Pair of First Order Equations," *Proc. Am. Math. Soc.* **4**, No. 5, 696 (October 1953).

R. R. Overman, W. S. Wilde, C. W. Sheppard, and W. C. Sangren, "The Disappearance of K^{42} from the Nonuniformly Mixed Circulation Pool in Dogs," *Circulation Research* **1**, No. 4, 284 (July 1953).

The following chapters of the ORACLE Manual, ORNL CF-53-12-2, have appeared for distribution: "Basic Operations of the ORACLE," by A. S. Householder; "Flow Charts and Coding," by J. Moshman; "Electronic Digital Computers," by C. L. Perry.

EMPLOYEE CHANGES

J. H. Fishel and P. J. (Brown) Sweeton terminated during this period. New members of the Panel are S. G. Campbell, formerly of Syracuse University, C. L. Gerberich of Johnsville Naval Air Development Center, Johnsville, Pennsylvania, and M. F. Todd of Colorado College.

M. E. Dailey, who transferred to the Panel in August, died as the result of an automobile accident on October 9.

R. A. Willoughby from the Georgia Institute of Technology has joined the staff as a research participant. The research participants, L. P. Burton, Nathaniel Macon, and W. F. Spragens, have completed their work and returned to their respective universities. Also, B. M. Drucker, recipient of an ORINS fellowship, has completed his work, received the doctorate degree from the University of North Carolina, and is now teaching at the Georgia Institute of Technology. J. F. Elliott, also an ORINS fellow, has finished his work at the Laboratory, received the master's degree from the University of Tennessee, and returned to his teaching position in Kingsport, Tennessee.

UNCLASSIFIED PROJECTS

TEST ROUTINES FOR THE ORACLE

Participating Member of Panel: C. P. Hubbard

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1588

Background and Status. The test routines for the ORACLE fall into two general categories:

1. *Routines for the Initial Test Program.* These routines were used to test the correctness of the logical design, the engineering design, and the actual construction of the computer. All tests in this category were successfully executed during the ORACLE test program at the Argonne National Laboratory; they are now being repeated at ORNL and, once completed, will not be used again.

2. *Operating Test Routines.* Routines in this category are designed for one or more of the following purposes: (*a*) to determine whether or not the computer operates correctly, (*b*) to evaluate the condition of the memory as to read-around or impurities, (c) to be used during engineering adjustment of machine parameters, (*d*) to diagnose the cause of machine errors. Many operating test routines have already been prepared for the ORACLE and were found to be useful. Additional routines will be devised as the need for them arises.

PROGRESS OF THE ORACLE SUBROUTINE LIBRARY

Participating Members of Panel: A. S. Householder, C. P. Hubbard, A. C. Downing, M. R. Arnette

References: Mathematics Panel Quarterly Progress Reports, ORNL-1498, -1435; Mathematics Panel Semiannual Progress Report, ORNL-1588

Background and Status. At the time this report was written, the ORACLE was being installed at Oak Ridge. During the period that the ORACLE was operating at Argonne, many test routines were written and successfully executed, some problems were run, and several subroutines were machine checked. The test routines and problems are discussed as separate projects.

Over 20 subroutines were checked in on the machine during this period. These included such elementary functions as square root, cube root, sine, cosine, exponential, and logarithm; programmed arithmetic included floating-point arithmetic and floating-point square root; utility programs included input programs, conversion routines (both from decimal to binary and from binary to decimal) for fixed- and floating-point arithmetic, a tape verifying routine, an error diagnosis routine for order-by-order check of a program, and other small utility programs such as a program which packs the addresses for use with the floating-point arithmetic. A list of available subroutines and detailed specifications can be obtained from the Subroutine Library.

When these subroutines were checked at Argonne, they were coded for some fixed location in the memory. Since then they have been recoded relative to cell No. 000, and an input routine has been coded which will put them any place in the memory with the proper changes of addresses. Because of the recoding, new tapes will be made, and the subroutines will be machine checked again. Another version of the floating-point subroutine has been coded for use in some special problems.

An entirely new floating-point subroutine which will be faster and more accurate than the existing one is being written. Various program assembly routines are being investigated; a basic one has been designed but not coded. Also, additional utility programs are planned which will facilitate the coding and checking of problems on the ORACLE.

APPROXIMATE SOLUTION OF THE DIFFUSION EQUATION

Origin: Mathematics Panel

Participating Member of Panel: J. Z. Hearon

Background and Status. In the course of dealing with certain biological problems involving diffusion-limited metabolic systems, a technique has been evolved for obtaining approximate solutions of the diffusion equation. The method is an extension of work previously done in this Panel.[1] With appropriate alterations of the boundary conditions, the method is applicable to the multiregion, multigroup reactor problem. Only a few applications have been made owing to the scarcity of exact solutions against which to check results, and it has not been established that the accuracy of the method can be made to meet the demands of the reactor problem. However, it seems desirable to sketch briefly the general features of the method at this time.

Consider a spherical system consisting of n regions: a central sphere and $n - 1$ concentric spherical shells. Let the regions be numbered 1, 2, . . . , n from the center outward, the interfaces between the regions be located at $r_1, r_2, \ldots, r_{n-1}$, and the outer surface be located at r_n. The regions so defined may be actual regions, each of which exhibits different properties, or several or all of them may be mathematical regions chosen for the purpose of calculation. Denote by $\vec{J}_i = -D_i \text{ grad } \phi_i(r)$ the flux of a chosen diffusing species (group) at any point in the ith region, where D_i and ϕ_i are the diffusion coefficient and the concentration (or density) of the chosen species. If the chosen species is being produced at the rate $Q_i(r)$ at any point in the ith region, the steady-state equations of continuity are

$$\text{(1)} \qquad \text{div } \vec{J}_i = Q_i \ , \qquad i = 1, 2, \ldots, n \ ,$$

[1] Mathematics Panel Quar. Prog. Rep. July 31, 1952, ORNL-1360, p. 5; J. Z. Hearon, *Bull. Math. Biophys.* 15, 15 (1953); *ibid.*, p. 111.

and the boundary conditions are

(2) $$\vec{J}_1(0) \quad , \qquad \text{bounded} \quad ,$$

(3) $$\vec{J}_i(r_i) = \vec{J}_{i+1}(r_i) \quad , \qquad i = 1, 2, \ldots, n-1 \quad ,$$

(4) $$\phi_i(r_i) = \phi_{i+1}(r_i) \quad , \qquad i = 1, 2, \ldots, n-1 \quad ,$$

(5) $$\vec{J}_n(r_n) = h[f(r_n) - \phi_n(r_n)] \quad ,$$

where $f(r)$ is a harmonic function with a prescribed limit, c, at infinity and h is a given constant.

The method consists of formally integrating Eq. 1 and evaluating the constants of integration in terms of space integrals of the Q_i. These space integrals can be expressed in terms of the spatial means,

$$\overline{Q}_i = \frac{3}{\sigma_i} \int_{r_{i-1}}^{r_i} r^2 Q_i(r) \, dr \quad ,$$

where $4\pi\sigma_i/3$ is the volume of the ith region, and in terms of the spatial means of the functions $r^2 Q_i$ and Q_i/r. The mean values of the functions ϕ_i,

$$\overline{\phi}_i = \frac{3}{\sigma_i} \int_{r_{i-1}}^{r_i} r^2 \phi_i \, dr \quad ,$$

are computed, and the space integrals arising in this process are likewise expressed in terms of the means of the functions Q_i, $r^2 Q_i$, and Q_i/r. The final result can be written as

(6) $$\overline{\phi} = (K + \epsilon)\overline{Q} + cu \quad ,$$

where $\overline{\phi}$ and $\overline{Q}$ are column vectors of the ϕ_i and Q_i, respectively, K is a square matrix, the elements of which can be expressed in terms of the D_i, the r_i, and the constant h, u is a column vector of ones, and the scalar c has been defined. The matrix ϵ represents a correction term, and the elements ϵ_{ij} consist of terms proportional to the quantities $1 - \overline{r^2 Q_i}/\overline{r^2}\,\overline{Q_i}$ and $1 - \overline{(Q_i/r)}/\overline{Q_i}\,\overline{(1/r)}$. The approximation consists of neglecting ϵ relative to K. If the Q_i are linear in ϕ_i, Eq. 6 comprises a set of linear equations which may be solved by standard methods. For the reactor problem, $c = 0$ and $h \to \infty$. From Eq. 5, this clearly yields $\phi(r_n) = 0$ since $\vec{J}_n(r_n)$ is bounded. For the one-group problem, $Q_i = k\phi_i$, and Eq. 6 is a homogeneous set of linear equations which has nontrivial solutions only if

(7) $$|K - \lambda I| = 0 \quad ,$$

where $\lambda = 1/k$. If λ_0 is the largest root of Eq. 7, then $k = 1/\lambda_0$ is the first eigenvalue. Similarly, if ϕ_i^j is the jth species in the ith group, then Q_i^j is a linear combination of the Q_i^s, $s = 1, 2, \ldots, n$. One coefficient in these linear combinations remains to be determined from an eigenvalue equation similar to Eq. 7. In any case, the eigenvalue

problem is reduced to that of solving a polynomial, the degree of which is equal to the number of regions (real or fictitious) containing fissionable material. The elements K_{ij} are such that for given s, $K_{1s} = K_{2s} = \ldots = K_{s-1,s}$. Moreover, K may be written as σK^*, where K^* is symmetric and $\sigma = [\delta_{ij}\,\sigma_i]$. Thus, of the n^2 elements K_{ij}, basically only $2n - 1$ have to be computed.

The results in biological problems have been exceptionally good because the permeability coefficient h in Eq. 5 is such that $h << D_i$, and the matrix ϵ is truly negligible. For the one-region, one-group reactor problem, the three-region approximation gives the first eigenvalue with 5% accuracy.

INVERTING MATRICES OF HIGH ORDER

Participating Member of Panel: V. C. Klema

Status. A general-purpose routine for inverting matrices of high order is being programmed for the ORACLE. The routine uses floating-point operations and the method reported by von Neumann and Goldstine,[2] which involves factoring of a symmetric matrix A into B^TDB, where B is a triangular matrix, and D is a diagonal matrix. Subsequently, the inverse X of B is determined, and $A^I = XD^IX^T$. As now coded, the routine can invert matrices of order up to 40 in the internal memory of the ORACLE. For matrices of higher order, external storage will be used. It is planned that this routine will be checked when the ORACLE is in operation at ORNL.

METHODS OF COMPUTATION FOR USE WITH A HIGH-SPEED AUTOMATIC COMPUTER

Participating Members of Panel: W. Givens, V. C. Klema

References: Mathematics Panel Quarterly Progress Reports, ORNL-1498, -1574;
Mathematics Panel Semiannual Progress Report, ORNL-1588

Problem 3: Numerical Computation of Characteristic Values

Status. A report[3] on the numerical computation of characteristic values of a real symmetric matrix is in the process of being distributed at this time. Flow diagrams and codes for reducing a matrix to the Jacobi form and subsequently finding the characteristic values within an assigned tolerance of 2^{-38} were put on the ORACLE and checked with matrices of order up to 89. These codes will be put in the Mathematics Panel Subroutine Library.

BASIC STUDIES IN THE MONTE CARLO METHOD

Participating Member of Panel: G. E. Albert

Reference: Mathematics Panel Quarterly Progress Report, ORNL-1498

Background and Status. The report entitled, *A General Theory of Stochastic Estimates of the Neumann Series for the Solutions of Certain Fredholm Integral Equations and*

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[2] J. von Neumann and H. H. Goldstine, *Bull. Am. Math. Soc.* **53**, 1021 (1947).

[3] W. Givens, ORNL-1574 (to be published).

Related Series, discussed in ORNL-1498, was issued on August 13, 1953 as ORNL-1508.

The participant has given some attention to two important but difficult problems posed in the above-mentioned report. In particular, the variance analysis on pages 20-21 and the relationship between the two types of estimate described in sections 3.2 and 4.3 of the report have been studied with refinement as an object. Little or no progress in that direction has been made.

In view of the difficulties inherent to further theoretical studies on this project, it has been decided that some experimental work should be done on the project on the ORACLE. A variety of types of Monte Carlo processes will be coded for the machine in the near future. These will include the simplest possible estimating process, a stratified process, and a process based upon the importance function (approximately zero variance) notion of H. Kahn. All processes will be arranged for the integral equation

$$Q(x) = \Phi(-x - \Delta) + \int_0^A Q(y)\, \phi(y - x - \Delta)\, dy \quad ,$$

where A and Δ are parameters and

$$\phi(x) = (2\pi)^{-1/2} \exp\left(-\frac{1}{2}x^2\right) \quad ,$$

$$\Phi(x) = \int_{-\infty}^{x} \phi(y)\, dy \quad .$$

The choice of this integral equation for the experiments was based upon the importance of the equation in a certain statistical problem and upon the fact that the participant has been able to devise a good importance function process for the equation. Also, good upper and lower bounds for the solution to the equation are known. The results of the experiments should provide information on the relative merits of the various types of Monte Carlo processes and upon the degree of accuracy that is feasible from a Monte Carlo process on the ORACLE.

FERMI AGE CALCULATIONS

Origin: R. A. Charpie, Research Director's Division

Participating Member of Panel: C. L. Gerberich

Background and Status. In order to characterize the properties of a multiplying system, it is often convenient to compute certain integral quantities which conceal the details of the complicated processes going on within the medium. One such property is the Fermi age, which measures the root-mean-square distance which a neutron travels in slowing down from fission energy to thermal energy. The age is easy to calculate from first principles for single elements but is rather more difficult for mixtures of elements.

The computational technique which is being used is the Monte Carlo method. The fission spectrum for a typical neutron is sampled, and the progress of this neutron is then traced through the medium in detail, taking proper account of scattering, fission, and the absorption process. The distance which the neutron travels between collisions and the angle at which it emerges from a collision are chosen randomly from the appropriate probability distributions. Since the scattering angle is correlated to the scattered energy, the neutron's history through phase space can be traced. When the neutron being studied is either slowed to thermal energy or is lost in an absorption process, its position is recorded and another neutron is selected from the fission distribution. A running average of the total crow-flight distance traveled by each neutron is retained. When this average remains sufficiently stationary to satisfy some preassigned convergence criterion, the calculation is completed.

In order to calculate the age in a mixture, it is necessary to supply the computer with only the atomic concentrations of the various atoms in the mixture. All the microscopic cross sections which are needed in the calculation will automatically be supplied to the machine, so the human labor involved in performing an age calculation is very small.

NUMERICAL INTEGRATION OF CERTAIN SINGULAR INTEGRALS

Origin: A. M. Weinberg, Research Director's Division

Participating Members of Panel: R. C. Weaver, A. C. Downing

Background and Status. The functions $F_1(x)$, $F_2(x)$, and $F_3(x)$ defined recursively by the relation

$$F_i(x) = \int_{-R/2}^{R/2} F_{i-1}(\xi)\, E_1(\sigma|x - \xi|)\, d\xi \qquad (i = 1, 2, 3) \quad ,$$

where $F_0(x) = \cosh kx$ and $E_1(x)$ is the exponential integral, were evaluated over the interval $-R/2 \leqq x \leqq R/2$. Because of the singularity occurring in the integrand at $\xi = x$, the contribution to the integral from ξ in a neighborhood of x was obtained by performing the integration in this neighborhood analytically. The remainder of the interval of integration was handled in the customary manner by using Simpson's rule.

The calculation was carried out for $R = 1$, 2, and 5 with $k = 0.6$ and $\sigma = 0.2$ in each case.

RADIOSENSITIVITY CURVES FOR CYTOLOGICAL AND GROWTH STUDIES WITH MOUSE ASCITES TUMORS

Origin: A. D. Conger, Biology Division

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

Background and Status. Ascites tumors were studied in mice which had been exposed to varying doses of x radiation in atmospheres containing from 0 to 100% oxygen. For cytological evidence, samples of from 150 to 400 anaphase cells were examined and

classified as normal or abnormal. In another phase of the experiment, tumor growth was measured by obtaining a total cell count for each animal.

Each effect was plotted linearly against log dose. The curves were fitted by least squares, and for a given oxygen percentage, the slope of the fitted curve was taken as a measure of radiosensitivity for that atmosphere. Each slope was expressed in units of the slopes for 0% oxygen, and the resulting ratios, when plotted against the per cent of oxygen, yielded the curve of radiosensitivity. Radiosensitivity curves were computed for both the cytological and the growth measurements, and confidence limits were computed by means of Fieller's theorem.

A TEST FOR RADIATION SENSITIVITY OF UNLINKED MARKERS IN BACTERIOPHAGE T4

Origin: A. H. Doermann, Biology Division

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

Background and Status. In the experiments on radiation sensitivity, a parent containing unlinked markers *m*, *r*, and *tu* was irradiated and mated to the wild-type parent, thereby producing eight classes of offspring. In one burst containing N' offspring, let a_i be the number of offspring in the *i*th class with the following associations:

Class	Number	Class	Number
m r tu	a_1	+ + *tu*	a_5
+ *r tu*	a_2	+ *r* +	a_6
m + *tu*	a_3	*m* + +	a_7
m r +	a_4	+ + +	a_8

Clearly,

$$N' = \sum_{i=1}^{8} a_i$$

The markers are assumed to be unlinked, and a test is needed for the equality of radiation sensitivities among the three markers.

If p_1, p_2, and p_3 are defined as the probabilities of sublethal hits in the vicinity of markers, *m*, *r*, and *tu*, respectively, the sample probability is given by

$$P'(S) = k'(q_1q_2q_3)^{a_1}(p_1q_2q_3)^{a_2}(q_1p_2q_3)^{a_3}(q_1q_2p_3)^{a_4} \times (p_1p_2q_3)^{a_5}(p_1q_2p_3)^{a_6}(q_1p_2p_3)^{a_7}(p_1p_2p_3)^{a_8} ,$$

where

$$q_j = 1 - p_j \qquad (j = 1, 2, 3)$$

and where

$$k' = \frac{N'!}{a_1!\, a_2! \ldots a_8!}$$

Because of the presence of both parent classes in every burst, these two classes are artificially augmented unless, of course, the experimenter has been successful in providing the two parent types in exactly the right ratio. Accordingly, only the six nonparental classes may be included in any test of hypothesis concerning the p's.

The null hypothesis is $p_1 = p_2 = p_3 = p$, and the probability of the reduced sample under the null hypothesis is

$$P(S) = \frac{k}{(1 - p^3 - q^3)^N} (pq^2)^{a_2 + a_3 + a_4} (p^2 q)^{a_5 + a_6 + a_7} ,$$

where

$$q = 1 - p,$$

$$N = \sum_{i=2}^{7} a_i ,$$

$$k = \frac{N!}{a_2!\, a_3! \ldots a_7!} .$$

The maximum likelihood estimate of p, obtained from the solution of the equation $d \log P(S)/dp = 0$, is

$$\hat{p} = \frac{a_5 + a_6 + a_7}{N} .$$

With the use of this estimate to compute expected frequencies in the usual manner, a χ^2 with four degrees of freedom provides the desired test of the null hypothesis.

TEST FOR INDEPENDENCE OF SINGLE AND DOUBLE CHROMOSOME BREAKS IN NEUROBLASTS OF *CHORTOPHAGA VIRIDIFASCIATA* EMBRYOS

Origin: M. E. Gaulden, Biology Division

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

Background and Status. After exposure to x or beta radiation, both single and double chromosome breaks can be seen in neuroblasts of grasshopper embryos. Before comparisons between beta- and x-ray effects can be made, something should be known about the relationships between the two types of breaks. In particular, if the breaks can be assumed to be independent, the data can be pooled and thereby provide a more sensitive comparison between beta- and x-ray effects.

If x is the number of single breaks and y is the number of double breaks, independence of the two events will exist if and only if

$$\text{Prob}\ \{x, y\} = \text{Prob}\ \{x\} \cdot \text{Prob}\ \{y\}$$

for any given cell. The marginal distributions were first tested for Poissonality. Although there is some evidence of a slightly super-Poisson variation, only one out of twelve χ^2 tests was significant at the 5% level. Thus it may be assumed that the joint probability

distribution is something like a bivariate Poisson; such a distribution has been discussed by Kendall.[4] It has three parameters; λ_x and λ_y are the means of the marginal distributions, and λ_{xy} is such that the correlations coefficient is $\rho = \lambda_{xy}/\sqrt{\lambda_x \lambda_y}$.

In this distribution, it happens that independence and zero correlation are equivalent a property not possessed by all bivariate distributions. Hence, if the maximum likelihood estimates of λ_x, λ_y, and λ_{xy} are obtained, a likelihood ratio test for independence could be constructed, at least in principle. Actually, in this case there is no hope of obtaining such a test. However, Kendall shows that the distribution asymptotically approaches bivariate normality. Since the sample sizes in the grasshopper data range from 120 to 196, a reasonably good test of independence should be given by the usual product-moment correlation coefficient. These tests have been carried out, and the six sample correlations range from –0.083 to +0.191. The largest correlation is just significant at the 5% level, but all are so small in magnitude that independence of single and double breaks may be assumed without serious error. After pooling the two types of breaks, radiation effects were evaluated by conventional methods.

A STOCHASTIC MODEL FOR THE SELECTION OF MACRONUCLEAR UNITS IN *PARAMECIUM* GROWTH

Origin: R. F. Kimball, Biology Division

Participating Members of Panel: A. W. Kimball, A. S. Householder

Background. Experimental evidence obtained by various research workers has provided interesting information about the existence and behavior of macronuclear units in *Paramecium*. All paramecia of the same stock probably have about the same number of macronuclear units. Before division takes place, each macronuclear unit doubles, and each daughter cell presumably selects one-half of the macronuclear units present at the time of division. In this way, the number of units per animal is kept constant in a manner analogous to the behavior of chromosomes. Unlike chromosomes, however, the macronuclear units do not separate into homologous sets, and, as yet, very little is known about the macronuclear unit selection process. The originator of this problem is interested in a mathematical formulation of selection mechanism which would aid in the interpretation of certain experiments.

Status. A stochastic model based on the theory of finite Markov processes has been constructed. After certain extensive calculations have been carried out, probably on the ORACLE, evidence will be available which is expected to show good agreement between the theory and the experimental data. The results of this investigation are in manuscript form and will be submitted soon for publication in the open literature.

[4] M. G. Kendall, *The Advanced Theory of Statistics*, 2d ed. revised, Vol. I, p. 133-134, 136, Charles Griffin, London, 1945.

CORRECTION FACTORS FOR VOLUME CALCULATIONS IN CELL-DIVISION STUDIES

Origin: H. S. Roberts, Biology Division

Participating Member of Panel: A. W. Kimball

Background and Status. In quantitative studies of dividing cells, a slight flattening of the cell against the cover slip enhances visibility of internal structures. Such flattening introduces an error into calculations of cell volume, and the error depends on the degree of flattening. A method of correcting for this error is desired.

Assume that the cell is a spheroid whose equation is

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{b^2} = 1 \quad .$$

Its volume is $V = 4\pi ab^2/3$. Assume further that the flattened cell is a truncated spheroid in which the flattening has taken place in a direction perpendicular to the x axis and by an amount ϵ on both sides of the cell. Then the volume of the truncated spheroid is

$$V_\epsilon = \frac{2\pi b^2}{a^2}\int_0^{a-\epsilon}(a^2 - x^2)\,dx = \frac{2\pi b^2(a - \epsilon)}{3a^2}[3a^2 - (a - \epsilon)^2] \quad .$$

Hence the ratio of the two volumes is

$$\frac{V_\epsilon}{V} = \frac{1}{2a^3}\left\{(a - \epsilon)[3a^2 - (a - \epsilon)^2]\right\} \quad .$$

Furthermore, if p is the proportion of flattening on either side, that is, $\epsilon = pa$, the ratio reduces to

$$\frac{V_\epsilon}{V} = 1 - \frac{p^2}{2}(3 - p) \quad .$$

This result is also obtained if flattening occurs perpendicular to either the y axis or the z axis or if the cell is assumed to be a sphere. Thus, the correction would hold for cells in prophase or anaphase. Since a dumbbell-shaped solid may be approximated as two connected spheres, the correction factor probably applies also to cells in telophase.

ESTIMATION OF THE RBE AND GAMMA CONTAMINATION FROM BIOLOGICAL DATA IN WEAPONS TESTS

Origin: W. L. Russell, Biology Division

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

Background and Status. In weapons tests, the calculation of an RBE (relative biological efficiency of neutrons compared with gamma or x rays) is often complicated because neither the total dose nor the gamma contamination is known very accurately. When certain assumptions are made, however, the RBE for the weapon can be estimated by least squares. Likewise, if the RBE's are known or can be assumed, an estimate of the gamma contamination can be obtained.

Let

u_c = biological effect, cyclotron,
u_w = biological effect, weapon,
R_c = total dose (rep), cyclotron,
R_w = total dose (rep), weapon,
G = gamma dose (rep), weapon,
B_c = RBE, cyclotron,
B_w = RBE, weapon.

Then if the logarithm of the biological effect is linearly related to dose and if the gamma contamination in the cyclotron is assumed to be 10%,

$$\log u_c = \alpha_c + \beta[0.9R_cB_c + 0.1R_c]$$

(1)

$$\log u_w = \alpha_w + \beta[(R_w - G)B_w + G] ,$$

which can be rewritten as

$$y = a + bx_1$$

(2)

$$z = c + dx_2 + bx_3 ,$$

where

$$y = \log u_c , \qquad c = \alpha_w ,$$
$$a = \alpha_c , \qquad d = \beta B_w ,$$
$$b = \beta , \qquad x_2 = R_w - G ,$$
$$x_1 = 0.9R_cB_c + 0.1R_c , \qquad x_3 = G .$$
$$z = \log u_w ,$$

If the biological effect is measured at n doses in the cyclotron and m doses in the weapon and if at each weapon dose relatively correct estimates of R_w and G are available, the constants in Eqs. 2 may be estimated from normal probability theory, which, in this case, is equivalent to least squares. B_c must be assumed to be known. The probability of the sample is

$$P(S) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^{m+n} \exp\left\{-\frac{1}{2\sigma^2}\left[\sum_{i=1}^{n}(y_i - a - bx_{1i})^2 + \sum_{j=1}^{m}(z_j - c - dx_{2j} - bx_{3j})^2\right]\right\}$$

and the maximum likelihood (M-L) estimates are obtained by maximizing $\log P(S)$ with respect to the four constants. If $\hat{b}$ and $\hat{d}$ are two of the M-L estimates, an M-L estimate of B_w is given by $\hat{B}_w = \hat{d}/\hat{b}$.

On the other hand, an estimate of the weapon gamma contamination can be obtained if $B_w = B_c = B$, for example, and if B is assumed to be known. Equations 1 can then be written as

$$\log u_c = \alpha_c + \beta[0.9B + 0.1] R_c$$

(3)

$$\log u_w = \alpha_w + \beta[(1 - g) B + g] R_w ,$$

where g is the fraction of the total weapon dose which is gamma radiation. Then Eqs. 3 can be rewritten as

$$y = a + bx_1 ,$$

$$z = c + \lambda x_2 ,$$

where y, z, a, c, and b are defined as before and where

$$x_1 = (0.9B + 0.1) R_c ,$$

$$x_2 = R_w ,$$

$$\lambda = \beta[(1 - g) B + g] .$$

If $\hat{\lambda}$ and $\hat{b}$ are M-L estimates of λ and b, the M-L estimate of g is given by

$$\hat{g} = \frac{B - \frac{\hat{\lambda}}{\hat{b}}}{B - 1} .$$

DESIGN AND INTERPRETATION OF SAMPLE SURVEYS IN PROCESS AREAS AT Y-12

Origin: W. H. Baumann, Health Physics Division, Y-12

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

Background and Status. In connection with solvent-vapor contamination in certain process areas at Y-12, a question arose concerning the representation of existing sampling techniques. The methods now in use were established with no systematic consideration given to possible variations in concentrations throughout working areas. The originator asked for assistance in designing a sampling experiment which would provide definitive answers to the problem of representativeness.

One floor of one process building was selected for the initial experiment. The area was divided into 18 approximately equal sections, and air samples at three heights above the floor were taken at the centers of these sections once a day for a period of one week during which the process was in operation. On the following Monday, when the process was shut down, another sample was taken. While this special sample survey was in progress, the regular sampling continued as usual.

The data from both the special sample and the regular sample were treated by the method of analysis of variance. The concentrations found in about 40% of the special sampling areas were significantly greater than the concentrations found in the regular

sampling areas. This is a clear indication that present sampling methods are not representative. Other information obtained from the analysis indicated a slight tendency for concentrations to be lower when the process is not in operation. More complete details are contained in a memorandum.

In another process area, smear samples for uranium contamination are taken regularly in different locations and from different types of surfaces. Samples from the same surface taken at the same time are frequently in poor agreement. If such errors are large enough, they would completely mask any real differences among working areas or among types of surfaces. In this case, the smear-sample technique would be of no value.

A survey-sample method was designed which provided for repeated samples from various locations and working surfaces over a period of one week. A statistical analysis of the results indicated definitely that significant differences could be established in spite of the large internal sampling error. Working surfaces were found to be most highly contaminated, whereas the contamination of floors and settled-dust areas was somewhat lower. A memorandum covering the entire survey has been prepared.

DAMAGE TO TISSUE FROM NEUTRON DISTRIBUTIONS WITH MAXIMUM ENERGIES RANGING FROM 1 TO 300 kev

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

References: Mathematics Panel Quarterly Progress Report, ORNL-1453;
Mathematics Panel Semiannual Progress Report, ORNL-1588

Participating Members of Panel: M. R. Arnette, N. M. Dismuke, C. P. Hubbard

Status. The following Monte Carlo problem was computed on the ORACLE in August: An isotropic source of 300-kev neutrons irradiated a cylindrical tissue phantom with a radius and thickness of 30 cm. From 2500 neutron histories, the average energy loss and the thermal collision density were recorded as functions of the penetration and the radial dimension of the cylinder.

ENERGY LOSS IN TISSUE AS A FUNCTION OF PENETRATION

Origin: W. S. Snyder, Health Physics Division

Participating Members of Panel: J. Moshman, J. H. Vander Sluis

Background. Previous calculations have provided estimates of the energy loss in tissue from various monoenergetic neutron beams for each of several elements found in tissue. By weighting each element by its relative biological effectiveness, total effective energy loss may be estimated at 1-cm intervals in tissue. It was desired to obtain a confidence interval for the maximum energy loss. A cubic polynomial appeared to give a reasonable fit over the interval of tissue penetration of interest. The energy loss, E, is expressed as

$$E = a + bx + cx^2 + dx^3 ,$$

where x is the penetration in centimeters.

The maximum E corresponds to one of the solutions of

$$\frac{dt}{dx} = b + 2cx + 3dx^2 = 0 ,$$

and the corresponding E_{max} may be determined. The least-squares fitting process provides estimates of the variance of the fitted coefficients. The approximate variances of x_{max} and the corresponding E_{max} can be calculated in a straightforward manner.

Status. Eight polynomials were fitted on IBM equipment, and the desired confidence intervals were obtained.

CONSTRUCTION OF A NOMOGRAM

Origin: C. P. Straub, Health Physics Division

Participating Member of Panel: J. Moshman

Background. The maximum permissible concentration of a radioactive substance in an organ may be obtained from the expression

$$(MPC) = \frac{KWmX}{N(\Sigma E)\, fTT_r} ,$$

where

(MPC) is the maximum permissible concentration,

K is a constant depending on the medium,

W is the dose,

m is the mass of the organ,

X is a function of the radioactive isotope,

N is a number proportional to the uniformity of deposit,

(ΣE) is the effective energy,

f is the per cent deposited or carried,

T is the effective half life,

T_r is the physical half life.

The range of the variables is given below:

Variable	Lower Limit	Upper Limit
K	10^{-11}	10^{-6}
W	10	10^3
m	1	10^5
X	1	10^9
N	1	10^2
(ΣE)	10^{-3}	10^2
f	10^{-5}	1
T	10^{-5}	10^5
T_r	10^{-5}	10^{12}

Status. The nomogram was constructed.

FITTING OF CROSS-SECTION CURVES

Origin: W. E. Kunz, Physics Division

Participating Members of Panel: J. Moshman, J. H. Vander Sluis

Background. In a He^3 and deuterium reaction experiment, the cross section, σ, is given by the expression

$$(1) \qquad \sigma = \frac{f(E)\ \gamma\Gamma}{[E_r + \gamma\Delta(E) - E]^2 + \frac{1}{4}[\gamma g(E) + \Gamma]^2},$$

where $f(E)$, $g(E)$, and $\Delta(E)$ are known functions of the energy, E; Γ is the reaction width; γ is the reduced width for scattering; and E_r is the resonance energy. It is desired to obtain estimates of γ, Γ, and E_r based upon observed experimental values of σ corresponding to known values of E.

By keeping linear terms,

$$(2) \qquad \sigma \approx \sigma^0 + \left(\frac{\partial\sigma}{\partial\gamma}\right)^0 (\gamma - \gamma^0) + \left(\frac{\partial\sigma}{\partial\Gamma}\right)^0 (\Gamma - \Gamma^0) + \left(\frac{\partial\sigma}{\partial E_r}\right)^0 (E_r - E_r^0),$$

where the superscript refers to an evaluation of the expression with approximations γ^0, Γ^0, and E_r^0. Equation 2 may be treated as a linear function of $\delta\gamma = \gamma - \gamma^0$, $\delta\Gamma = \Gamma - \Gamma^0$, and $\delta E_r = E_r - E_r^0$. Estimates of the three δ terms, obtained in the usual manner, may be used to obtain better approximations to the parameters; the iterative process is continued until satisfactory convergence is obtained.

Status. Various sets of experimental data have been satisfactorily processed in this manner by the use of IBM equipment.

BETA-DECAY SPECTRUM OF RADIUM E

Origin: M. E. Rose, Physics Division

Participating Members of Panel: A. C. Downing, R. C. Weaver

Background. The providing of a suitable explanation for the energy spectrum of the beta rays emitted by an unstable nucleus has attracted the attention of physicists for two decades. In order to evaluate a particular theory for the radium E spectrum, the Panel was requested to fit a set of experimental points (W_i, y_i) with a curve of the form

$$(1) \qquad y = \lambda[x^2 K_p(W) + xK_{pt}(W) + K_t(W)]\,(W_0 - W)^2,$$

where λ and x are parameters to be adjusted in obtaining a best fit, say in the sense of least-square deviations. In this equation, y is related to the probability that an electron will be emitted with energy W per dW, and the K functions are the interaction coefficients for pseudoscalar (p), tensor (t), and mixed (pt) coupling. W_0 is the energy lost by the nucleus during the beta-decay transformation; hence, this term provides an upper limit for the energy of the emitted beta ray, and it may therefore be evaluated by extrapolation from

the experimental data. For physical reasons, the parameters x and λ are subject to the additional conditions that x be real and that λ be positive.

Status. Let σ be the sum of the squares of the deviations between the experimental and the theoretical values for y, that is, let

$$\sigma = \sum_i \left\{ y_i - \lambda[x^2 K_p(W_i) + x K_{pt}(W_i) + K_t(W_i)] (W_0 - W)^2 \right\}^2 .$$

The standard technique for producing a least-squares fit is to minimize σ by solving the normal equations $\partial\sigma/\partial x = 0$ and $\partial\sigma/\partial\lambda = 0$ for x and λ – perhaps by eliminating one of the variables. The side conditions on x and λ are ignored in the above statement because the introduction of Lagrangian multipliers would seriously complicate the procedure. It happens, nevertheless, that the procedure described is not feasible because of the properties of the functions K_p, K_{pt}, and K_t.

When the three K functions were computed, it was found that they were closely proportional to each other. In fact, the ratio of any two of them remains constant to within 4% over the energy range of the experimental data. It can be seen that if these three functions were exactly proportional for all values of W, then no fit could be better than that obtainable by picking an arbitrary x and by varying λ. In actual computation, the difficulty arising from the similarity of these functions takes the form of a loss of significant figures. For when λ is eliminated from the normal equations, the result is a fourth-degree polynomial in x in which each of the coefficients is the difference of two expressions involving the K's. For example, the coefficient of x^4 is

$$\left(\sum_i y_i K_{pt}\right)\left(\sum_i K_p^2\right) - \left(\sum_i y_i K_p\right)\left(\sum_i K_p K_{pt}\right) .$$

These two terms agree to about three significant figures. Unfortunately, the K's involve the Fermi functions which have been tabulated only to four significant figures.

Further investigation indicates that any direct analytical method for solving the normal equations will lead to the same type of difficulty. The following numerical scheme was therefore applied. Given a fixed value of x it is possible to minimize σ with respect to λ without loss of significance in λ. A sequence of minimum values for σ corresponding to a sequence of real x values was computed in this manner until the absolute minimum with respect to x had been located.

The comparison of the experimental data and the "best" theoretical curve was not good. In fact,

$$\sqrt{\sigma_{\min}} = 0.14 \sqrt{\sum_i y_i^2} ,$$

which indicates an average deviation of 14%.

It appears that a better result may be obtained by using a different value for W_0. For when Eq. 1 was solved for $(W_0 - W)$ and when the experimental points were substituted

into the resultant expression for $W_0 - W$ and plotted vs. W, the best line through these points did not intersect the W axis at W_0. Ideally, the minimization of σ should be carried out with x, λ, and W_0 as parameters, but this is impossible because of the very complicated manner in which the K's depend upon W_0 and W.

CALCULATION OF INTERNAL-CONVERSION COEFFICIENTS WITH SCREENING

Origin: M. E. Rose, Physics Division

Participating Members of Panel: S. G. Campbell, N. D. Given

References: Mathematics Panel Quarterly Progress Reports, ORNL-1290, -1360, -1498, -1588

Background and Status. Work on the calculation of internal-conversion coefficients with screening is continuing at The National Bureau of Standards, Washington, D. C., on the SEAC. The possibility of completing the most complex stages of the computation on the ORACLE is being examined in terms of the problems involved in recoding for the ORACLE. An investigation has been made of available numerical methods to determine which would be most suitable to this computation if it is to be programmed for the ORACLE.

Although it was planned to do this computation on the UNIVAC, the large backlog of UNIVAC problems with higher priority eliminated this possibility.

THREE-REGION, THREE-GROUP REACTOR CALCULATION

Origin: M. C. Edlund, Physics Division, L. Cooper, Reactor Experimental Engineering Division

Participating Members of Panel: S. E. Atta, W. C. Sangren, R. C. Weaver

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1588

Background and Status. The three-region, three-group reactor calculation was successfully coded for and run on the UNIVAC. Unfortunately, the iterative method used led to poor results in the outer region. It is believed that this is due primarily to round-off error. Since it is known that the iterative scheme used for the other multigroup calculations discussed in this report converges well in all regions, it has been decided to incorporate this problem with the other multigroup calculations.

RANDOM COINCIDENCES IN MULTIPLE-CHANNEL COINCIDENCE COUNTERS

Origin: T. A. Love and F. C. Maienschein, Aircraft Nuclear Propulsion Division

Participating Member of Panel: G. E. Albert

Background and Status. The following is a brief statement of the problem of random coincidences in multiple-channel coincidence counters. N counters (N is usually 2, 3, or 4) generate pulses of carefully controlled shape and duration, one pulse for each recorded event. The pulses from all N counters are observed simultaneously in a coincidence counting circuit. An overlap of pulses, one from each of the N counters, is recorded as

a coincidence. Some of the coincidences are genuine in the sense that they arise from a physical process that produces coincident records in the N separate counters. The observer wishes to count the number of such genuine coincidences occurring in a given time interval; this number will be termed the "signal." Other coincidences occur because of chance overlapping of pulses. The number of such chance coincidences will be called a "noise." The ultimate statistical problem is to estimate the signal in the presence of the noise by observation of the total record of coincidences of both types and the records of total counts recorded in the individual counters. Also, a measure of the reliability of the estimated signal is needed.

Before the solution of the ultimate statistical problem can be effected, the probability distribution of chance coincidences must be found. To the best of the participant's knowledge, this distribution has not been found to date. The references cited[5,6,7] contain the major mathematical contributions that have been made to the problem. In no case have the dead times of the individual counter channels been taken into account. In every case it has been assumed that the products $\lambda_i\tau$, $i = 1, 2, \ldots, N$, are much smaller than 1. Here the λ_i are the counting rates of the individual counters and τ is the duration of the pulses that produce coincidences. Schroedinger and Jánossy[5] have shown by elementary methods that the coincidence rate is approximately $N\lambda_1\lambda_2 \ldots \lambda_N\tau^{N-1}$ to within higher order terms in the $\lambda_i\tau$. This paper[5] exposes an unsettled argument between these two authors concerning the nature of correction terms for a better approximation. Feather[6] and Domb[7] utilize successively more refined mathematical methods on the problem for the case in which $N = 2$. According to Domb, the coincidence counting circuit is assumed to have a dead time following each recorded coincidence, but no dead times are ascribed to the individual counter channels. The Laplace transform (with some errors that are easily corrected) for the complete distribution of coincidences in two counter channels is obtained by Domb but is not inverted.

It should be clear from the above remarks that two mathematical problems remain open in the theory of the distribution of chance coincidences. First, Domb's technique should be generalized to handle more than two counter channels, and second, the dead time and resultant counting losses for individual counters should be taken into account. As remarked by Feller in his review,[7] these problems are very difficult and require very delicate handling. The participant has attacked both problems mentioned by using three quite different methods.

If counting rates and dead times are small, it seems reasonable to ignore the dead-time effect as was done by Schroedinger and Jánossy[5] and by Domb.[7] Two of the three

[5]E. Schroedinger and L. Jánossy, *Nature* **153**, 592 (1944).

[6]N. Feather, *Proc. Cambridge Phil. Soc.* **45**, 648 (1949).

[7]C. Domb, *Proc. Cambridge Phil. Soc.* **46**, 429 (1950); reviewed by W. Feller, *Math. Reviews* **12**, 114 (1951).

methods used by the participant involve that approximation. The first method is similar to that of Schroedinger and Jánossy and involves further approximations to the physical model; it is difficult to assess the effects of the several approximations used. For the purposes of this report, it should suffice to mention that the approximation given[5] was checked and that correction terms were obtained that were different from either Jánossy's or Schroedinger's. Pursuit of this method has been dropped by the participant.

The second method to be tried is exact under the assumption of zero dead times for the individual counters and for the coincidence circuit. This method involves some general theorems on Poisson processes which the participant expects to publish at some later date. The mathematical details are too involved for presentation here. In essence, the method consists in showing that certain random variables defined on a Poisson process have distributions for which the moment generating functions satisfy integral equations of the Volterra type. The integral equations appropriate to the coincidence problem for twofold ($N = 2$) coincidences have been solved to obtain exact formulas for the moment generating function and moments of a distribution which, on specialization, gives the moments of the distribution of chance coincidences. The integral equations appropriate to the study of coincidences in more than two channels have defied solution. Work on this second method has been discontinued temporarily.

The third method is under investigation at present. It involves a generalization of the method used by Domb to take into account the effect of individual counter dead times. To date, progress on this method has been insufficient for any report here.

To sum up, the participant has been unable to provide any substantially new contributions to the coincidence problem. Some interesting and perhaps publishable theorems on Poisson processes have been achieved by the second method mentioned above.

KINETIC CONDITIONS FOR THE ISHR

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

Participating Members of Panel: L. P. Burton, C. L. Gerberich, F. W. Stallard

Background and Status. Nine differential equations and one algebraic equation were used to represent the kinetic conditions of a reactor of the ISHR type. During the time covered by this report, the equations were analyzed, and the algebraic equation was found to be extremely unstable for machine calculation. It was modified by P. R. Kasten and returned to the Mathematics Panel. While looking over data from a preliminary hand computation of the equations, it was found that one of the differential equations did not represent completely the conditions desired, and it too was modified for better results.

The problem was then coded for the UNIVAC; the system of solution was the Heun method. At present, the problem is completely coded and has been partially checked by hand.

STABILITY OF BOILING REACTORS

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

Participating Members of Panel: A. S. Householder, V. C. Klema

References: Mathematics Panel Quarterly Progress Reports, ORNL-1435, -1498

Status. Work on the problem concerned with the stability of boiling reactors is awaiting the operation of the ORACLE.

KINETICS EQUATIONS FOR THE HRE

Origin: V. Paré, Reactor Experimental Engineering Division

Participating Member of Panel: M. E. Dailey

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1588

Status. The reactor period of the HRE was recalculated with one group and with six groups of delayed neutrons by using a new set of values for the fraction of neutrons which are delayed.

ANALYSIS AND INTERPRETATION OF LIQUID-LIQUID CONTACTOR DATA

Origin: A. C. Jealous, Chemical Technology Division

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

Background and Status. The description of the analysis and interpretation of liquid-liquid contactor data and the statistical analyses pertaining to this problem are contained in a special memorandum.

REFINING THE STRUCTURAL PARAMETERS OF KD_2AsO_4

Origin: H. Levy, Chemistry Division

Participating Members of Panel: J. Moshman, R. C. Weaver, N. Macon

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1588

Status. Hand calculations for a particular, small, linear system (10 independent variables) have been completed. The general procedure has been coded for the ORACLE and now awaits debugging on the computer.

DETERMINATION OF FAST-NEUTRON FLUX IN THE ORNL GRAPHITE REACTOR

Origin: D. K. Holmes, Solid State Division

Participating Members of Panel: J. Moshman, S. E. Atta, N. D. Given

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1588

Status. All UNIVAC calculations on the determination of fast-neutron flux in the ORNL Graphite Reactor have been completed. A detailed description has been prepared for issuance as a project report.

SECRET PROJECTS

MULTIGROUP REACTOR CALCULATIONS

Origin: R. A. Charpie, Research Director's Division

Participating Members of Panel: S. E. Atta, N. M. Dismuke, J. H. Fishel, N. D. Given, W. C. Sangren

Reference: Mathematics Panel Semiannual Progress Report, ORNL-1588

Background and Status. The two-region multigroup computations are now in final form and are being operated on a routine basis. Starting with a flat source, three to five iterations are needed for convergence of the source. In this program, approximately 7 min are used in obtaining the macroscopic cross sections and other constants from the microscopic cross sections. In each iteration, it takes about 4 min to calculate a new set of fluxes and sources. The total time per reactor therefore varies from about 18 to 28 minutes.

Two other multigroup computations have been prepared. One of these allows up to five regions and sixty space points, while the other allows up to nine regions and sixty space points. In both cases, the general method developed for the two-region problem has been followed, although the five-region case has been prepared with the objective of saving more machine time than would be saved by the direct extension of the two-region code. The same thirty fast groups and possible four thermal groups are used in these calculations as were used in the two-region case. At present, the five-region problem is being debugged at the UNIVAC. The nine-region problem, under the code name Medusa, has been checked out on the UNIVAC and is now being used for running nine-region fireball-type reactors.

COMPUTATION OF Pa^{233} CAPTURE CROSS SECTION

Origin: R. A. Charpie, Research Director's Division

Participating Members of Panel: A. C. Downing, R. C. Weaver

Background and Status. Since the neutron balance in a thermal breeding system is very delicate and the possibility of breeding hangs in the balance on every source of neutron losses, it is necessary to evaluate each neutron loss as accurately as possible. For a long time there has been in the literature a moderately low value for the capture cross section of Pa^{233}, an isotope which is intermediate between the fertile material thorium and the breeding material U^{233}. Irradiations at Hanford of thorium in connection with U^{233} production always revealed a surprisingly large amount of U^{234} which could come only from neutron capture in Pa^{233}. In order to measure the protactinium cross section as accurately as possible, data from a series of experiments were carefully analyzed. Mathematically, this involved the solution of a system of three transcendental equations and one algebraic equation in which the unknowns were the desired cross section of Pa^{233} and the concentrations of Pa^{233}, U^{233}, and U^{234}.

ESTIMATION OF DOSE INSIDE CREW SHIELD

Origin: F. Maienschein, Aircraft Nuclear Propulsion Division

Participating Members of Panel: J. Moshman, R. C. Weaver

Background. The estimation of dose inside the crew shield falls into three general categories:

1. *Radial Beam.* The basic relationship giving the dose per unit power, D_{kpn}, inside the crew shield is

$$(1) \qquad D_{kpn} = \frac{1}{\gamma(E)} \Phi_{kpn} \exp \left\{ - \sum_{i=1}^{2} d_i \csc \beta_p \mu_i(E^*) \left[1 - \epsilon_i(E, \beta)\right] \right\} ,$$

where

γ is the conversion factor from flux to dose,

k, p, n are indices for source angle α, receiver angle β, and initial energy E^*, respectively,

Φ_{kpn} is the scattered flux per unit power,

E is the scattered energy,

i is an index for material ($i = 1$ indicates lead; $i = 2$ indicates plastic),

d_i is the shield density,

$\mu_i(E)$ is the absorption coefficient,

$\epsilon_i(E, \beta)$ is the buildup factor.

For each combination of k, p, and n, the values of Φ_{kpn} and E are tabulated. Values of β are the angles 10°(10°)180°. The d_i ($i = 1, 2$) are given explicitly. Values of the different functions of E, $\mu_i(E)$, $\gamma(E)$, and $\epsilon_i(E, \beta)$ are available in graphical form.

For the side wall, the value of D_{kpn} is desired for 970 combinations of the parameters in which Eq. 1 will be used.

For the front wall, csc β_p is replaced by –sec β_p, and about 485 values of D_{kpn} are needed.

2. *Skew Beam.* Index p in Eq. 1 is replaced with an index m that refers to the distance from the reactor shield to the point of scattering. The receiver angle β is now dependent on all three indices, namely, β_{kpn}. Values of Φ_{kmn} and β_{kmn} are available in tabulated form from previous UNIVAC calculations.

For the side wall, values of D_{kmn} are required for about 320 combinations of the parameters.

For the front wall, csc β_{kmn} is replaced with –sec β_{kmn}, and another 320 values of D_{kmn} are desired.

3. *Direct Beam.* The fundamental equation now takes the form

$$(2) \qquad D_{kn} = \prod_{i=1}^{2} \left[B_i(E) \frac{1}{\gamma(E)} \Phi_{kn} \exp \left\{ -d_i \sec \beta_k \mu_i(E) \right\} \right] ,$$

where $B_i(E)$ is a buildup factor given in graphical form and

$$\beta_k = \theta_k - \bar{\alpha}_k ,$$

in which

$$\theta_k = \arcsin \left\{ \frac{1716}{H_k} \sin \alpha_k \right\} ,$$

and

$$H_k^2 = (1716)^2 + r_k^{\star 2} - 3432 r_k^\star \cos \bar{\alpha}_k ;$$

α_k, $\bar{\alpha}_k$, and $r_k^\star$ are tabulated as a function of k. D_{kn} is desired for 36 combinations of the parameters.

Status. All graphical input data have been converted to analytical form by interpolating curves. The procedure is being programmed for IBM equipment.

FLUID FLOW THROUGH A SPHERICAL VESSEL CONTAINING DISTRIBUTED HEAT SOURCES

Origin: D. H. Fax (Johns Hopkins University), Reactor Experimental Engineering Division

Participating Members of Panel: J. Moshman, N. D. Given, J. H. Vander Sluis

References: Mathematics Panel Semiannual Progress Report, ORNL-1588; ORNL CF-53-9-75

Background. Given the following system of equations:

$$D^2\psi = \frac{\partial^2 \psi}{\partial R^2} + \frac{\sin\theta}{R^2} \frac{\partial}{\partial \theta}\left(\frac{1}{\sin\theta} \frac{\partial \psi}{\partial \theta}\right) = -ZR^2 \sin^2\theta , \tag{1}$$

$$\frac{\partial(\psi, T)}{\partial(\theta, R)} = \frac{3}{2} qR^2 \sin\theta , \tag{2}$$

$$\frac{\partial(\psi, Z)}{\partial(\theta, R)} = -N_B \left(R \sin\theta \frac{\partial T}{\partial R} + \cos\theta \frac{\partial T}{\partial \theta}\right) , \tag{3}$$

a solution is desired subject to the boundary conditions

$$\begin{aligned} \psi &= 0 \text{ for } \theta = 0, \pi , & 0 \leqq R \leqq 1 , \\ \psi &= 1 \text{ for } R = 1 , & 0 \leqq \theta \leqq \pi , \\ T &= 0 \text{ at } R = 1 , & \theta = \pi , \\ Z &= 0 \text{ at } R = 1 , & \theta = \pi . \end{aligned} \tag{4}$$

The method of integrating the temperature equation (Eq. 2) as suggested by Fax was to let subscripts 1, 2, 3, 4 refer to the grid points of a rectangular lattice and 0 denote the center and then to solve a succession of algebraic equations of the form

$$T_2 - T_4 = \left[\frac{2F_0(\Delta\theta)(\Delta R) - (\psi_4 - \psi_2)(T_3 - T_1)}{\psi_3 - \psi_1}\right](1 - E_0) , \tag{5}$$

where $F_0 = 3/2\ qR_0^2 \sin\theta_0$ and E_0 is the error of the approximation. Neglecting E_0, it is possible to start at one corner of the region and successively "march" across the region in one pass without iterating. However, E_0 is of order

$$\frac{(\Delta R)^2}{6}\left(\frac{\dfrac{\partial^3\psi}{\partial\xi^3}}{\dfrac{\partial\psi}{\partial\xi}} + \frac{\dfrac{\partial^3 T}{\partial\eta^3}}{\dfrac{\partial T}{\partial\eta}}\right), \tag{6}$$

where ξ and η are a pair of auxiliary coordinates. Subsequent analysis revealed that the higher derivatives increased rapidly as $R \to 1$ and $\theta \to 0$ so that the error per step increased and was accumulated in the "marching" process.

The above numerical analyses were performed on the UNIVAC.

Status. The integrating scheme was revised by Fax to one which was self-checking and iterative across the field. He revised the programs and tried the new procedure on the UNIVAC; the system still failed to converge.

FLUORIDE-LOOP CALCULATION

Origin: M. T. Robinson, Solid State Division

Participating Members of Panel: S. E. Atta, R. C. Weaver

Background. The numerical values of y, T_1, T_2, T_a, and T_f were calculated on a hand calculater at intervals of $\Delta s = 10$ cm, from $0 \leqq s_n \leqq S$. The constants (γ_1, γ_2, α_1, α_2, α_3, β_1, a_1, and a_2) were calculated for 20 reactor combinations and were used in the following equations to obtain the desired values of y, T_1, T_2, T_a, and T_f.

$$y = \left[y_0 e^{a_1 s_n}\int_0^{s_n} e^{-a_1 s}\,\phi(s)\,ds\right] + y_0 e^{a_1 s_n},$$

$$T_a = \frac{\alpha_3}{\alpha_1} y_0\left(e^{a_1 s_n} - e^{a_1 S}\right) - \beta + T_a^0,$$

where $\beta = \alpha_3 \int_0^S \Delta y\ ds$,

$$T_f = T_f^0 + \left[\beta_1\int_0^{s_n}\phi(ds)\right] - \left[\alpha_2\int_0^{s_n}\Delta y\,ds\right] + \frac{\alpha_2 y_0}{\alpha_1}\left(e^{a_1 s_n} - 1\right),$$

$$T_1 = T_f + \gamma_1 y,$$

$$T_2 = T_1 + \gamma_2 y.$$

Status. The problem with the above parameter values has been completed.