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MATHEMATICS DIVISION ANNUAL PROGRESS REPORT

FOR PERIOD ENDING DECEMBER 31, 1964

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MATHEMATICS DIVISION
ANNUAL PROGRESS REPORT
for Period Ending December 31, 1964

A. S. Householder, Director
H. P. Carter, Assistant Director

MARCH 1965

OAK RIDGE NATIONAL LABORATORY
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Mathematics and Computing

Research

L. L. Bumgarner
J. A. Carpenter
G. K. Haeuslein
A. S. Householder
L. R. Shenton
F. W. Stallman[1]
L. Turner[1]

MATHEMATICS AND NUMERICAL ANALYSIS

A new class of methods of successive approximation for computing characteristic roots and vectors of normalizable matrices has been mentioned previously[2]. These methods had been under investigation by Clanton for his doctoral dissertation, and the dissertation has now been completed[3]. It is shown there that limit points other than characteristic roots do exist, and that any method of the class could lead to such a point. However, this happens only in rather special situations, and sufficient conditions for convergence to a root are given for normal matrices. However, the problem calls for a considerable amount of further investigation, including numerical experiments to test the effectiveness of the algorithm and to compare different methods of the class.

An inclusion domain for roots of a matrix is a domain in the complex plane known to contain at least one root of the matrix. An inclusion domain for the vectors would be a domain in complex Euclidean n-space known to contain at least one vector. Presumably this would be in the form of a cone above a given vector as axis. Knowledge of such a domain would, for example, provide a measure of the error in a computed characteristic vector. Wielandt communicated privately an unpublished theorem, valid only for Hermitian matrices, which he had obtained perhaps as early as 1950. In 1961, Swanson[4] obtained

[1]Consultant.

[2]*Math. Panel Ann. Progr. Rept. Dec. 31, 1961*, ORNL-3264, pp. 3–4.

[3]D. H. Clanton, *Some Algorithms for the Calculation of the Characteristic Roots and Vectors of a Normalizable Matrix*, ORNL-3688 (October 1964).

[4]C. A. Swanson, "An Inequality for Linear Transformations with Eigenvalues," *Bull. Am. Math. Soc.* **67**, 607–8 (1961).

independently what amounts to an extension of this theorem to the case of normal matrices. Both theorems made use of Euclidean norms. It turns out that Swanson's result can be extended to provide a result of great generality that (1) applies with arbitrary absolute norms to (2) matrices that are normalizable and not necessarily normal and (3) provides both inclusion domains for roots and inclusion domains for vectors.[5]

OPTIMIZATION OF REACTOR POWER SYSTEMS

Suppose a certain power $P(t)$ is required at any time in the next T years, $0 \leqq t \leqq T$. This is to be produced by combinations of n available reactor types Each reactor is characterized by three parameters:

k_i = cost of construction and operation per unit time per unit power produced,
m_i = mass of the fuel inventory per unit of power produced,
b_i = fuel bred per unit time per unit power produced,

for $i = 1, 2, \ldots, n$. Thus if $P_i(t)$ is the power output of the reactor (m_i, b_i, k_i), then $M_i = m_i P_i(t)$ is the fuel inventory, $k_i P_i \, \Delta t$ is the cost of operating in the period $[t, t + \Delta t]$, $b_i P_i \, \Delta t$ is the net fuel bred by this reactor, $\Sigma m_i P_i = M(t)$ is the total fuel inventory at time t, $\dot{M} = \Sigma b_i P_i + \dot{q}$, where $\dot{q}$ is the rate at which fuel is purchased from mines.

The cost function will be modified by charging interest so that $k_i P_i \, \Delta t$ is replaced by $k_i P_i \, \Delta t \, e^{\gamma(T-t)}$, where γ is approximately the rate of interest. If $F(q)$ is the cost of q units of fuel, the total cost over T years is

$$J = F(q_0)e^{\gamma T} + \int_0^T [(h_1 P_1 + \ldots + k_2 P_2) + \dot{q}] e^{\gamma(T-t)} \, dt .$$

The problem is to find $P_1(t), \ldots, P_2(t), q(t)$ on $0 \leqq t \leqq T$ which minimizes J and such that

$$P_1 + P_2 + \ldots + P_n = P ,$$

$$\frac{d}{dt}(m_1 P_1 + m_2 P_2 + \ldots + m_n P_n) = b_1 P_1 + b_2 P_2 + \ldots + b_n P_n + \dot{q} , \qquad \dot{q} \geqq 0 .$$

The reactors (m_i, b_i, k_i) all lie in two octants of three-space as $h_i > 0$, $m_i > 0$, while b_i can have either sign. Any time a fixed proportion of the power P is produced by each reactor, we may define $m = (\Sigma m_i P_i)/P$, $b = (\Sigma b_i P_i)/P$, $k = (\Sigma k_i P_i)/P$, so that the operation of n reactors in the ratios $(P_1/P, P_2/P, \ldots, P_n/P)$ is equivalent to the operation of one reactor (m, b, k). Thus, instead of n reactor points we have all the infinitely many points in the convex hull of the original n points.

This convex hull K of operating points is bounded and lies in two octants. If we think of k being the vertical axis, we may speak of the upper and lower boundaries of K. With given values of m and b, obviously the least possible k should be used; so the operating point (m, b, k) is always on the lower boundary of K. Thus several reactors (m_i, b_i, h_i) can be ruled out immediately as uneconomical,

[5] A. S. Householder, "Localization of the Characteristic Roots of Matrices," pp. 39–60 in *Recent Advances in Matrix Theory*, The University of Wisconsin Press, Madison, 1964.

independently of $P(t)$. Moreover, any point on the boundary of K is a convex combination of three points (m_i, b_i, h_i), so no more than three reactor types should be used at any one time. Actually, if the lower boundary is projected onto the (m, b) plane, it may be shown that the operating point should always be such that its projection lies on the boundary of the projection of K. Thus only two reactor types should be used at any one time.

Work is continuing in an effort to predict more exactly which reactors should be used, depending on $P(t)$, $F(q)$, γ, and the convex body K.

MATHEMATICAL MODELS FOR RECOMBINATION KINETICS OF FREE RADICALS

Electron spin resonance was measured in glycine after exposure to radiation in order to determine the decay of free radicals. A first attempt has been made to fit these data to functions which describe a second-order kinetics model. This gave reasonable fits in some experiments but failed to converge to a solution in others.

This failure to converge may be due to the computational procedure, which does not necessarily converge for nonlinear parameters. Changes in the computer program may eventually yield a satisfactory fit. This possibility is under investigation.

The failure in convergence may, however, indicate that the proposed model does not describe adequately the underlying process. There is some experimental evidence that in the initial stage there may be more than two different types of radicals or there may be interaction between them. A differential equation governing such general second-order kinetics has been investigated. Results obtained so far show that substantial effort in programming and computation is required in order to obtain functions that describe this more general model. Because of this an attempt in this direction seems indicated only if other possibilities have failed.

MILLS'S RATIO AND THE PROBABILITY INTEGRAL FOR A PEARSON TYPE IV DISTRIBUTION

The Pearson system of curves does not have general application in specifying distributions, but there can be little doubt that its uses, in one form or another, in approximating distributions by moments leave it without a serious rival. For this reason tabulations of the percentage points of Pearson curves against $\sqrt{\beta_1}$ and β_2 have recently received considerable attention.[6]

A particularly wide region of the Pearson β_1-β_2 chart belongs to type IV distributions, and little work has been done on methods of approximating (numerically or analytically) a type IV probability integral. Now in the case of the normal and type III distributions it has been convenient to study the so-called Mills ratio of "tail" area to bounding ordinate,[7] for this has asymptotic expansions for small and large arguments and also rational fraction approximations convergent in the limit. These classes of expansions cannot be sustained for the type IV distribution, mainly because sooner or later one has

[6]See, for example, N. L. Johnson *et al.*, *Biometrika* **50**, 459 (1963).

[7]The ratio is generally attributed to Mills [*Biometrika* **18**, 395 (1926)], but it seems to have been introduced by B. H. Camp in *Biometrika* **16**,163 (1924).

to assume the existence of moments of all orders; the type IV distribution has only a finite number of finite moments. A clue to a completely different approach is found in the Mills ratio for the normal integral,

$$R(t) = \int_t^\infty g(x)\, dx/g(t) \qquad (t > 0)\ , \tag{1}$$

where $g(x) = \exp\,(-\frac{1}{2}x^2)/\sqrt{2\pi}$, for there is the Laplace rational fraction approximation to it,

$$R(t) \sim \chi_s(t)/\omega_s(t)\ ,$$

with the properties

$$\omega_s\, R(t) - \chi_s = (-1)^s \int_t^\infty (x - t)^s\, g(x)\, dx/g(t)\ , \tag{2a}$$

$$\omega_s = (-1)^s \int_{-\infty}^\infty (x - t)^s\, g(x)\, dx\ . \tag{2b}$$

Starting with (2*a*) as a remainder formula, we could set up a recursive scheme for $R(t)$, and this would in fact generate the Laplace continued fraction. Moreover, by saddle-point methods one could show that $R(t) - \chi_s/\omega_s \to 0$ as $s \to \infty$.

The way is now clear foı developing approximations to the type IV probability integral

$$P(v) = \int_v^\infty f_m(y)\, dy\ ;$$

corresponding to (2*a*), we use

$$\mathcal{R}_m^{(s)} = \int_v^\infty \left(\frac{y - v}{1 + y^2/a^2}\right)^s f_m(y)\ dy/f_{m-1}(v)\ , \tag{3}$$

where

$$f_m(y) = c_m(1 + y^2/a^2)^{-m} \exp[-k \arctan\,(y/a)]\ ,$$

$$(ac_m)^{-1} = \int_{-\pi/2}^{\pi/2} e^{-kx} \cos^r x\, dx \qquad (r = 2m - 2)\ .$$

A second-order recursive scheme can be derived from (3), and we find in Pringsheim's notation for a continued fraction,

$$\mathcal{R}_m^{(0)} = \frac{ac_m}{c_{m-1}} \left[\frac{r_0}{q_0}\ ,\ \frac{sr_s p_s}{q_s}\right]_1^\infty\ , \tag{4}$$

where p_s, q_s, r_s are polynomials in s involving r, k, and the "point" of truncation. The expression (4) is a new expansion for the type IV curve and includes in it, as degenerate cases, the normal and Student's

t distributions. Convergence questions can be settled by an appeal to a theorem of Van Vleck and also by the use of saddle-point approximations. It turns out that the error in using the sth convergent of (4) in approximating the probability integral tends to zero as rapidly as $[\tan(\frac{1}{2}\theta - \frac{1}{4}\pi)]^{2s+r+1}$, where θ $(0 < \theta < \frac{1}{2}\pi)$ refers to the truncation point.

Further work includes a search for simple effective approximations to the complete integral for the type IV distribution.

SIMULATION OF A CROSS-COUPLED PERCEPTRON

The perceptron concept was introduced by Rosenblatt[8] in 1957, and since then results on the properties of simple perceptrons and multilayer non-cross-coupled perceptrons were obtained. In order to gain insight into the efficiency of cross-coupled perceptrons, a program was written simulating a five-layer perceptron with cross connections within each layer. It turned out that most reinforcement rules soon generate trivial states (either no excitation at all or each association unit at its topmost excitation). Best results were obtained if the cross connections were reinforced more weakly than the other connections.

THE CONTROL DATA CORPORATION 1604-A ALGOL COMPILER

The ALGOL project[9] for the CDC 1604-A was completed. Cooperation with Control Data Corporation was continued in the form of assistance with completion of the documentation and consultations with regard to modifications. The latter were directed toward bringing the compiler in line with the specifications of SUBSET ALGOL 60.

THEORY OF ALGOL TRANSLATION

The design of the CDC 1604-A ALGOL compiler stimulated revisions and extensions of previous theory. An earlier document[10] was completely rewritten, and much new material was added, especially regarding storage allocation and procedures. Details may be found in the new document.[11]

---

[8]F. Rosenblatt, *The Perceptron, a Perceiving and Recognizing Automaton (Project PARA)*, Cornell Aeronautical Laboratory Report No. 85-460-1 (January 1957).

[9]*Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, pp. 6–7.

[10]A. A. Grau, *The Structure of an Algol Translator*, ORNL-3054 (Jan. 23, 1961).

[11]A. A. Grau and L. L. Bumgarner, *An Approach to Algol Translation*, ORNL-3592 (April 1964).

Computing Services

ANALYTICAL CHEMISTRY

G. J. Atta
Judy J. Eatherly
D. C. Ramsey
R. P. Rannie
R. L. Shively

Stationary Electrode Polarography

The theoretical expression for the current-voltage relation at a stationary spherical electrode is

$$i = nFAC_o^* \left[\sqrt{aD_o\pi}\, \chi(at) + \frac{D_o}{r_o} \Phi(at) \right],$$

where i is the current, at is a dimensionless parameter proportional to time (and involving voltage), $\chi(at)$ and $\Phi(at)$ are dimensionless functions of at, and the other parameters may be treated as constants in this consideration.

The function $\Phi(at)$ is defined explicitly, but $\chi(at)$ is defined in the integral equation

$$\int_0^{at} \frac{\chi(z)\, dz}{\sqrt{at - z}} = \frac{1}{1 + \gamma\theta\, S(at)},$$

where $\gamma\theta$ can be treated as a constant and the function $S(at)$ is given. It has been shown[1] that this integral can be transformed into a Riemann-Stieltjes integral and replaced by a finite sum to give

$$2\sqrt{\delta} \left\{ \chi(1)\sqrt{n} + \sum_{i=1}^{en-1} \sqrt{en - 1}\, [\chi(i+1) - \chi(i)] \right\} = \frac{1}{1 + \gamma\theta\, S(\delta n)},$$

where $at = \delta n$. Successive χ's can now be evaluated for any number, n, of steps of size δ. The functions $\chi(\delta n)$ and $\Phi(\delta n)$ are thereby available in step form.

Three computer programs were written in connection with this work. The first program calculates and stores on magnetic tape a set of χ's and Φ's as a function of δn (or at) and other physical parameters. The second program utilizes the χ's and Φ's and other parameters to calculate the electrode current as a function of voltage. This program also calculates the first, second, and third derivatives with respect to voltage of the current for both flat and spherical electrodes. Finally, the currents and their derivatives are stored on magnetic tape. The third program utilizes the currents to produce plots of the currents and their derivatives vs voltage.

Portions of this work have been used in subsequent publications.[2]

---

[1] R. S. Nicholson and I. Shain, "Theory of Stationary Electrode Polarography," *Anal. Chem.* **36**, 706–9 (1964).

[2] S. P. Perone and T. R. Mueller, "Application of Derivative Techniques to Stationary Electrode Polarography," *Anal. Chem.* **37**, 2–9 (1965).

Polarographic Diffusion Coefficients

A computer program was written to calculate diffusion coefficients for use in polarographic research. The coefficients were calculated from the Ilkôvic equation and from the more accurate Koutecký equation. This program made use of the VIETA subroutine that solves the cubic equation.

Porosimetry Through Mercury Intrusion

Mercury is injected into the pores of various materials at different applied pressures. A computer program was written to calculate pore diameters, pore volumes, and pore surface areas for a distribution of absolute pressures. The program produces for each set of data both a tabular output and a graphical output. The graphical output takes the form of a bar chart which shows the distribution of pore volumes as a function of pore diameters.

Time and Cost Distributions

Two programs mentioned previously[3] have been converted from the IBM 7090 to the CDC 1604-A. Additional subroutines were added to the programs to provide summaries of the information in the reports produced by the programs.

BUDGET AND PROGRAM PLANNING

Judy J. Eatherly M. T. Harkrider

Work Order Estimates

Information is recorded in numerical form on punched cards by the Central Work Order Office concerning the funds committed by work orders to support divisions (e.g., Plant and Equipment). Data recorded are: (1) originating division; (2) executing division; (3) type of work (fabrication, engineering, inspection, maintenance, construction, etc.); (4) field engineer; (5) estimate of the percentage of total cost needed for labor and the actual percentage of total cost used for labor; (6) original estimate of cost and revisions; (7) final cost; and (8) date opened, requested completion date, and actual completion date. A program has been written for storing this information on magnetic tape for subsequent analysis.

A program is being written to obtain basic statistical information showing the accuracy of the estimated factors mentioned above. This program will be used to compare dollar estimates to actual costs and time estimates to actual completion dates, and to indicate areas where improved estimation procedures are necessary. The program should help to supply information to the support divisions on how to handle the work by using the least amount of money and manpower.

---

[3] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962,* ORNL-3423, p. 24.

CHEMICAL TECHNOLOGY

G. J. Atta
C. W. Dyche
Manuel Feliciano
A. R. Jenkins
R. P. Rannie
R. L. Shively

Chloride Volatility Processing of Nuclear Fuels

Various chemical processes are being developed for recovering uranium from spent nuclear fuels.[4–6] The effects of temperature, inert gas, carbon monoxide, and pressure on the chemical reactions were investigated in detail. The following five programs were written to perform thermodynamic calculations relating to chloride volatility processing of nuclear fuels:

1. a program to calculate the equilibrium yields of solid UCl_3 from the reduction of gaseous UCl_4,
2. a program to calculate the equilibrium capacity of chlorine gas to carry plutonium as $PuCl_4$ during the reaction of U_3O_8-PuO_2 with carbon tetrachloride,
3. a program to calculate the equilibrium amount of chlorine needed to keep uranium chloride in the pentachloride and hexachloride forms during the reaction of U_3O_8 with carbon tetrachloride,
4. a program to calculate the equilibrium yield of $PuCl_3$ from the reduction of $PuCl_4$, and
5. a program to calculate the equilibrium yield of solid UCl_4 from the reduction with carbon monoxide of UCl_5 and UCl_6 in the gas produced by the reaction of U_3O_8 with carbon tetrachloride.

All the calculations were based on standard free-energy data obtained from the literature.

Cylindrical Pellet Dissolution

Cylindrical pellets of nuclear reactor fuel are dissolved during the reprocessing of this fuel. A computer program was written that calculates the surface area of the pellets as a function of the fraction of the pellet that has dissolved. This program made use of the VIETA subroutine that solves the cubic equation.

Catch Pan Volume

An irregularly shaped catch pan is located beneath several storage tanks of enriched uranium solution in order to catch any solution leakage. Because the solution contains enriched uranium, it was necessary to make sure that no critical configuration of fluid would occur in the catch pan. A computer program was written to calculate the volume of the catch pan as a function of fluid height. The program also plotted these data.

---

[4]T. A. Gens and G. J. Atta, *Thermodynamic Calculations Relating to Chloride Volatility Processing of Nuclear Fuels. I. The Gas-Phase Reduction of Uranium Tetrachloride to the Trichloride with Carbon Monoxide*, ORNL-TM-829 (Apr. 22, 1964).

[5]T. A. Gens, *Thermodynamic Calculations Relating to Chloride Volatility Processing of Nuclear Fuels. II. The Capacity of Chlorine for Transporting Plutonium Tetrachloride Vapor During Reaction of U_3O_8-PuO_2 with Carbon Tetrachloride*, ORNL-3693 (October 1964).

[6]T. A. Gens, internal memorandum (Aug. 20, 1964).

Digital Spectroscopic Data

Spectroscopic data are obtained in digital form on punched cards. Prior to analysis of these data they must be smoothed to remove instrument noise, cell balances (zero corrections) must be subtracted, and beam attenuation factors must be added as needed.

One computer program was prepared to add beam attenuation factors to the spectrum. The beam attenuation factors are prepared by another program that performs least-squares fitting of beam attenuation measurements to a low-order polynomial.

Another computer program has been developed that smooths the spectrum data using an n-point least-squares convolute[7] where n may run from 5 through 15. This program also subtracts cell balance and can plot the spectrum before and after smoothing. The corrected spectral data are stored on punched cards or magnetic tape for subsequent analysis.

High-Pressure Window Stress

A computer program was prepared to calculate the deflection and stresses in a sapphire window under various loads and types of mounting. The window was used in a high-temperature, high-pressure spectrophotometer.

Induction-Heating Furnace Design

An IBM 7090 computer program used in the design of induction-heating furnaces at Hanford[8] was converted for use on the CDC 1604-A computer. An error in the original program was corrected, and the program was expanded to cover additional aspects of the design problem.

Nomograph Construction

Three programs have been written for the CDC 1604-A computer that draw nomographs using the Calcomp plotter.

One nomograph presents the relation between the surface temperature (T_1) of a nuclear-fuel-element shipping cask, the surface emissivity (ϵ), and the surface heat flux (Q/A); under the conditions of combined radiation and natural convection, heat transfer from the cask surface is shown in Fig. 1. The equation represented by this nomograph is

$$Q/A = \sigma\epsilon[(T_1 + 460)^4 - (T_2 + 460)^4] + 0.19(T_1 - T_2)^{4/3} ,$$

where σ is the Stefan-Boltzmann constant and T_2 is 100°F.

This program also makes use of the STSYMBØL subroutine for the drawing of nonstandard characters with the plotter.

---

[7] A. Savitzky and M. J. E. Golay, "Smoothing and Differentiation of Data by Simplified Least Squares Procedures," *Anal. Chem.* **36**, 1627–39 (1964).

[8] G. Jansen, Jr., *Design of Induction Heating Coils for Cylindrical Charges*, HW-74093 (July 16, 1962).

ORNL-DWG 65-328

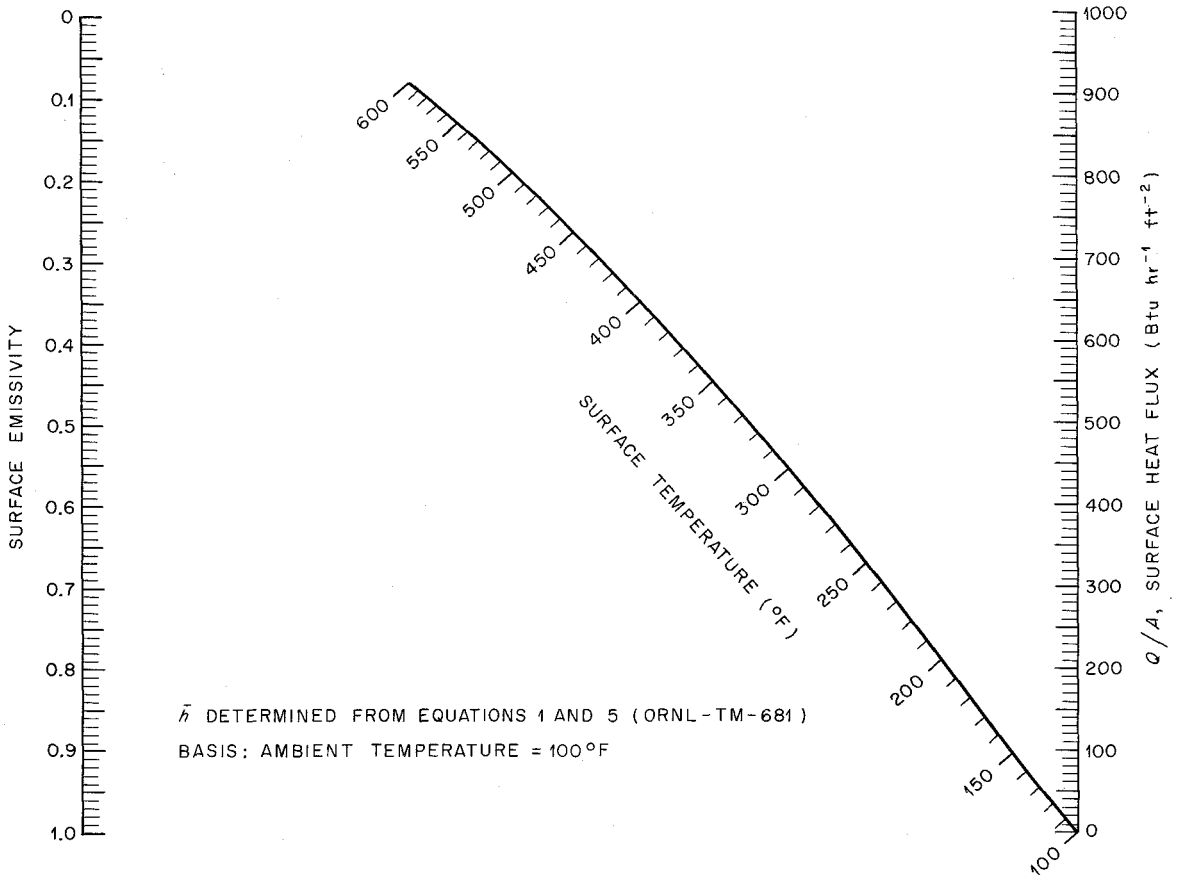

Fig. 1. Cask Surface Temperature in Still Air Based on the Surface Heat Flux and Emissivity. L. B. Shappert, *A Guide to the Design of Shipping Casks for the Transportation of Radioactive Material*, ORNL-TM-681 (to be published).

The other nomographs provide correlations between such variables as mass and volume as functions of specific gravity and instrument readings, and liquid level as a function of specific gravity.

Multivariable Screening

A multivariable screening program[9] had been written for the Burroughs 220 digital computer at the Georgia Institute of Technology Research Institute. Assistance was provided in the conversion of this program to a FORTRAN 63 program for use on the CDC 1604-A.

The FORTRAN 63 program is called FACSCREN, and it may also be used as a subroutine under certain conditions. This program screens the response of one variable to changes in other factors and

[9]H. M. Wadsworth and N. G. Hardie, "A Screening Procedure for the Empirical Exploration of Response Surfaces," paper presented at the American Statistical Association Meeting, Cleveland, Sept. 4, 1963.

ranks these factors according to the variation in the response which is removed when the effects of each factor are removed.

CHEMISTRY

G. J. Atta
Susie E. Atta
Judy J. Eatherly
A. R. Jenkins
Sharron P. King
R. P. Rannie
R. L. Shively

Central-Force Scattering

This problem deals with the classical-mechanical description of elastic scattering of potassium atoms by iodine atoms.

The solution is in terms of the classical deflection function, x, as a function of the impact parameter, b, given an interatomic potential. The behavior of x indicates most of the dynamic properties of the system and tells the experimenter what to expect in a beam scattering experiment.

A computer program was written to compute the classical deflection. The results of the calculation imply that there may be a significant difference between the potassium-iodine molecule scattering system and the potassium-iodine atom scattering system; this difference is of physical interest.

Hydration Structure in Aqueous Electrolytes

In the experimental studies of the hydration of alkali ions in solution, measurements have been made of the density and of the viscosity of salt solutions. This has been done with sufficient precision and with a sufficient number of points that mathematical tests may be made of the reality of effects that could be caused by solvent structure. These mathematical tests have been made. This required the numerical evaluation of a large set of integrals by using standard techniques.

Reaction Rates in Porous Electrodes

The distribution of reaction rates in porous electrodes was numerically approximated for additional[10] sets of parameters.

Thermal-Diffusion-Column Filament Temperatures

In an ^{17}O thermal-diffusion column an electrically heated filament is centered within an externally cooled tube. Heat is transferred from the filament to the tube by the combined mechanisms of radiative heat transfer and conduction heat transfer through the oxygen gas. The overall heat-transfer equation for this process was formulated.

In this equation the thermal conductivity of the gas was expressed as a polynomial in the gas temperature, and the filament emissivity was expressed as a linear function of the filament temperature.

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[10] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567.

Estimates of tube and filament emissivities were obtained from experimental data, but it was necessary to estimate the thermal conductivity of oxygen at high temperatures (2200°K) by means of the Eucken equation and Lennard-Jones parameters. The resulting overall heat-transfer equation was a polynomial in the filament temperature, and a computer program was written to determine the filament temperature as a function of power input to the filament. This program made use of the PØLYRT subroutine that solves polynomial equations. Another program plotted the filament temperature as a function of power input.

Least-Squares Plane

Yields have been obtained for the decay of short-lived rubidium isotopes obtained from the fission of ^{235}U as a function of separation time. These yields may be represented by an expression of the form

$$y = \alpha e^{-\beta t} ,$$

which may be linearized by taking the natural logarithm of both sides to obtain

$$\ln y = \ln \alpha - \beta t .$$

Since the separation times are subject to errors, it is necessary to use a least-squares procedure that allows for errors in the independent variable. A program has been written, based on a method[11] for determining a least-squares plane through a set of points when all variables are subject to error.

Volumetric Dose Rate

A computer program was written that evaluates the total dose rate produced within a spherical volume by an external point source of radiation as a function of the radius of the sphere and the distance from the source to the sphere.

Simultaneous and Consecutive Chemical Reactions

A computer program has been written that provides numerical solutions to a system of seven simultaneous differential equations.

The differential equations arise in the kinetics of the system of simultaneous and consecutive second-order chemical reactions,

$$A + B \xrightarrow{k_1} C + D ,$$

$$B + D \xrightarrow{k_2} C ,$$

$$D + E \xrightarrow{k_3} F ,$$

$$B + F \xrightarrow{k_4} E + C ,$$

$$A + F \xrightarrow{k_5} G + D ,$$

where the k's are estimated reaction rate constants.

[11] W. C. Hamilton, "On the Least-Squares Plane Through a Set of Points," *Acta Cryst.* 8, 185–89 (1961).

The concentration of each component is calculated as a function of time from initial to equilibrium concentration by using the RKLDEQ subroutine for Runge-Kutta-Gill numerical integration.

This program checks for material balance and concentration at each step and changes step size as required to maintain an adequate material balance and nonnegative concentrations.

Work on this project is continuing in order to develop a program that will compare experimental results with results calculated by the existing program and to use least-squares techniques to obtain better values for the reaction rate constants. Also, the original program will be extended to include more chemical reactions.

A Computer-Controlled Diffractometer

Construction of the computer-controlled x-ray diffractometer that has been described elsewhere[12] is now in progress. Programs are being written for the PDP-5 computer,[13] which is a major component of this system. In addition, two experimental programs, coded in FORTRAN for use on the CDC 1604-A computer, have been used to test the methods proposed for calculating diffractometer angles and for refining the parameters that define the crystal unit cell and the sample orientation.

Three-Dimensional Multiparameter Pulse-Height Analyzer

During the past year, considerable experience has been gained in applying to studies of nuclear disintegration schemes a multiparameter pulse-height analyzer[14] with a 20,000-word ferrite-core memory and a storage capacity of 10^6 counts per channel. The basic configuration of 100×200 channels can be rearranged into other arrays, all with provision for subgrouping and dynamic routing into desired subgroups. The output data (entire memory) of the analyzer can be written on a magnetic tape unit for later processing on a computer. A general description of the analyzer has been published elsewhere.[15]

Nuclear spectroscopy with a multiparameter analyzer involves many exploratory aspects; therefore, setup time may often exceed the actual data acquisition time by a large factor. Further, much of the setup time actually may arise from the inherent complexity of multiparameter experiments themselves. For these reasons, it is necessary that the data be stored in a sorted array and that both the raw and processed data be displayed so the experimental situation may be assessed at any time from setup to completion.

The CDC 1604-A computer is used to process the output data. Magnetic tapes are written by the analyzer, the information is processed in the computer, and the computer output magnetic tapes are listed or plotted or both.

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[12] W. R. Busing *et al.*, *Chem. Div. Ann. Progr. Rept. June 20, 1964*, ORNL-3679, pp. 100–101.

[13] Manufactured by Digital Equipment Corp., Maynard, Mass.

[14] Model MP-204 RT, Victoreen Instrument Co., Cleveland.

[15] G. D. O'Kelley, D. A. Bromley, and C. D. Goodman, "The Role of Multiparameter Pulse-Height Analyzers in Radioactivity Studies," *Proceedings of the Conference on the Utilization of Multiparameter Analyzers in Nuclear Physics, Grossinger, N.Y., November 12–15, 1962*, pp. 49–56.

Computer programs have been written to convert the raw data of the analyzer to computer format, to correct the raw data for background counts and store the corrected spectra on magnetic tape, and to sum a specified number of planes of a three-dimensional corrected spectrum and plot the results.

EDUCATION

G. J. Atta A. R. Jenkins

Flat-Plate Thermometer

This investigation was concerned with the temperature distribution in the laminar boundary layer on a flat-plate thermometer placed in a steady, incompressible flow field in which the velocity and heat source are uniform. The solution is intended to apply to regions in actual systems where the plate is not too near a solid boundary and where the velocity and heat source are approximately uniform over distances of the order of the length of the plate.

When the problem is formulated mathematically, one obtains a second-order differential equation with two prescribed boundary conditions, that is, a two-point boundary-value problem. This differential equation was solved numerically by transforming the problem into an initial-value problem and using the Runge-Kutta method for the numerical solution of the initial-value problem; the extra initial condition was approximated and adjusted to satisfy the prescribed boundary conditions. Estimates of errors were obtained by using a scheme devised by Richardson.[16]

HEALTH PHYSICS

G. J. Atta	A. M. Craig	A. R. Jenkins	J. E. Schmith
G. A. Bogar	Judy J. Eatherly	C. T. McCracken	L. R. Shenton
R. T. Boughner	Manuel Feliciano	D. C. Ramsey	R. L. Shively
E. E. Branstetter	M. T. Harkrider	R. P. Rannie	V. R. R. Uppuluri

Trace Elements in Human Tissue

Spectrographic analyses of human tissue, made in connection with a joint project between the University of Tennessee and ORNL, have provided samples from some 30 organs of 250 subjects from the United States. A program has been written to facilitate a study of observed differences in concentration between different organs and between subclasses of similar tissue, such as diaphragm as opposed to other muscles and vertebra as opposed to other bones. The program tests such hypotheses as equality of mean concentration, that the means differ by an additive term, and that the means differ by a multiplicative factor. At present the study is being expanded to include data from foreign sources such as Switzerland, Africa, the Near East, and the Far East. For this reason the program is being revised.

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[16]Anthony Ralston and H. S. Wilf, *Mathematical Methods for Digital Computers*, p. 117, Wiley, New York, 1960.

The Distribution of Sr in Body Tissue

As an adjunct to the study of trace elements in body tissue, a study of the distribution of Sr in the body is being conducted. In conjunction with this study, a program has been written to compute statistical information to test hypotheses that the distribution of the parent population from which the sample data have been taken is neither normal nor log normal. The present program makes use of subroutine NORMAL that computes Geary's ratio for testing kurtosis and two other ratios of high-order moments of the data; one is used to test kurtosis and the other is used to test symmetry. The input data are transformed to normal deviate form using two different methods, one proposed by W. S. Snyder and the other by J. W. Tukey.

Atomic Bomb Hypocenter

A program has been written to approximate in a least-squares sense the hypocenter of the blast of the atomic bomb exploded in Nagasaki in 1945. Shadow lines created by concrete and marble monuments and gravestones were measured with respect to their position from a predetermined location and their angle to magnetic north. By extending these shadow lines along their direction angle, one should be able to determine the center of the blast or the point where all such lines cross. The center has been selected as the point which minimizes the sum of the squares of the perpendicular distances from these lines to the point.

Two-Species Population Studies

P. J. Wangersky

The rates of change of two competing animal populations, $\dot{x}$ and $\dot{y}$, may be described as

$$\dot{x}(t) = A_x\, x(t) \left[1 - \frac{x(t - \tau_{2x}) + \alpha\, y(t - \tau_{2y})}{K} \right]$$

and

$$\dot{y}(t) = A_y\, y(t) \left[1 - \frac{\beta x(t - \tau_{2x}) + y(t - \tau_{2y})}{K} \right],$$

where A is a function of τ_1, gestation period; τ_2, reaction delay time; τ_3, maximum life span; b, birth rate; and p, death rate. The competition effectiveness of the two species is given by α and β, and K is a constant.

A computer program has been written that calculates numerical solutions of these differential-difference equations by Euler's method.

The distribution functions for the parameters τ_1, τ_2, τ_3, b, and p, for both x and y, are given, and parameter values can be chosen at random. The frequency with which these parameters are randomly changed for any species varies as a function of the population of that species.

The program also allows various starting populations and competition efficiencies for each species.

A second computer program has been written that plots the populations as a function of time. This program uses a subroutine PREPPLØT that provides the conventional linear plot requirements such as size, position, labels, numbers, etc. The program also uses a subroutine SIMPLØT3 that provides a convenient means of plotting linear functions. This subroutine automatically scales data, plots forward or backward, with solid or dashed lines, with or without symbols, checking or not as required for off-scale points, and providing folded scale plots as required.

Data Processing for Ecological Studies

A CDC 1604-A computer program was written that is being used to store a large volume of data on magnetic tape. These data will be used in systems ecology analyses.

Environs Data

A CDC 1604-A computer program has been written to produce weekly a year-to-date report on the fallout data as detected by air filters, gum paper, and rainwater collection at Health Physics stations located around ORNL. The stations are of three types depending upon their proximity to ORNL, namely, (1) local air monitors, (2) perimeter air monitors, and (3) remote air monitors. Health Physics personnel visit the stations weekly to gather the air filters, gum paper, and rainwater measurements. These measurements are recorded on cards from which input to the program can be keypunched directly. From the weekly input and the stored input on magnetic tape for previous weeks during the year, the program produces the report.

The program reports weekly measurements, monthly averages, quarterly averages, semiannual averages, and year-to-date averages for each type of measurement made at each of the stations. It also produces a system average of each type of measurement for each of the three systems of stations.

Competition Among Plants as It Influences Spatial Relationships

System ecologists have accumulated abundant data concerning the natural occurrence of plants in various environments. One method of collecting such data is that of dividing the terrain into a rectangular grid of equally spaced points and recording those plants which occur at these points. A record is formed each time a certain number of consecutive plants have been recorded. A computer program has been written to analyze records of length 10. All records for a given terrain are processed simultaneously. The program consists of three phases.

The first phase scans the entire data to form a list of distinct plant names and to record the length, L, of the list. Thus a three-dimensional array A of dimensions $L \times L \times 12$ is determined.

The intermediate phase reprocesses the data, handling each record individually. All possible plant-pair comparisons are made within each record, and a count is entered into the A matrix for each comparison. The matrix element to be incremented is a function of the plants compared and their separation.

The final phase analyzes matrix A by computing certain variables for each plant pair. These are total comparisons, chi-square value, and percentage comparisons at each distance. Finally, a plot of percentage vs distance is made if the chi-square value indicates a plant pair not to be distributed at random.

Interaction of a Plasma with a Helical Electron Beam

The interaction of a stationary plasma and an electron beam in the presence of a static magnetic field B has been investigated theoretically. It was assumed that the electrons in the beam have helical trajectories coaxial with B.

The interaction of a plasma with a helical beam is of relatively frequent occurrence in astrophysics, geophysics, thermonuclear research, etc. In the early stages of the development of radio astronomy it was thought that nonthermal radio emissions from the sun were due to beams of electrons produced at the sunspots and directed at an arbitrary angle to the magnetic field. These helical beams spiral out of the sunspots into surrounding plasma which forms the polar corona. Similar types of interactions occur under terrestrial conditions in the outer regions of the ionosphere. They are caused by helical beams composed of electrons and protons gyrating around the earth's magnetic field and are believed to produce auroral effects. These beams interact with the plasma in the ionosphere and generate very-low-frequency electromagnetic radiations which are detected at the earth's surface.

The plasma-beam system is examined for instabilities which result in growing transverse electromagnetic waves aligned in a direction parallel to that of the field B. The behavior of such a system can be described by the dispersion equation for the system.

The dispersion equation for the plasma-beam system investigated was a sixth-degree polynomial equation, which in some cases was approximated very well by a quartic polynomial equation. The dispersion equation was analyzed numerically, and some of the results of the investigation were presented in graphical form.

The coefficients of the dispersion equation were functions of many parameters of the system, and much precision was needed in finding the roots of the equation for various ranges of the parameters. It was found that double-precision arithmetic was necessary in the coding of the solution to give the accuracy required to make the graphical analysis of the system.

Capture Probability of Electrons for Contaminant Gas

Experiments on the diffusion of electrons in gases in the presence of applied electric fields have yielded considerable data with which to study energy levels of atoms and molecules in the gaseous state. One problem encountered in these experiments is that electrons diffusing through a gas are not monoenergetic but have a distribution which depends upon the electric field, the composition of the gas, and the temperature of the system.

The distribution of energies may be considered well defined when electrons diffuse in a uniform electric field in one of the inert gases at energies below the first excitation level in the gas and when

the pressure is such that the electron mean free path is less than the container dimensions. Thus one may add small quantities of contaminant gases to the inert gases and determine average cross sections for the contaminant gas. If the amount of contaminant gas is such that the electron distribution function is essentially unaffected by its presence, one may infer the actual energy dependence of the cross section in question from the variation of its averaged cross section within the applied electric field.

The integral equation presented by this problem is

$$\bar{\alpha}(E/P) = \int_0^\infty \alpha(\epsilon)\, f_0(E/P,\ \epsilon)\, d\epsilon\ ,$$

where $\alpha(\epsilon)$ is the capture probability of electrons on a contaminant gas per centimeter measured in the field direction, $\bar{\alpha}(E/P)$ is the expected value of $\alpha(\epsilon)$ over the energy range, $f_0(E/P,\ \epsilon)$ is the equilibrium distribution function for elements in a given gas, and E/P is the electric field strength per unit pressure.

The evaluation of the distribution function $f_0(E/P,\ \epsilon)$ is the subject of a previous report.[17] Experimental results yield values for $\bar{\alpha}(E/P)$ for different E/P. The desired quantity is $\alpha(\epsilon)$.

To solve for $\alpha(\epsilon)$, it is necessary to restrict ϵ to the common energy range of the data. The energy range is then subdivided into ten intervals, and the variance for each E/P is calculated in each subinterval. The subinterval of least variance is selected, and the process of subdivision is continued in this subinterval until the variances of the end points differ by less than a given positive number. The average energy of this final interval is selected for $\alpha(\epsilon)$, and the above integral is evaluated for each E/P thus:

$$\int_0^\infty \alpha(\epsilon_1)\, d\epsilon_1 = \frac{\bar{\alpha}(E/P)}{f_0(E/P,\ \epsilon_1)}\ .$$

A program to solve this equation for $\int_0^\infty \alpha(\epsilon_1)\, d\epsilon_1$ is currently being written.

Electron Time-of-Flight Studies

Electron swarm experiments in which electrons were allowed to diffuse in a gas and in which a Geiger-Mueller counter was used for a detector have been performed to determine the diffusion coefficient and the drift velocity of the electrons. The number of electrons entering the detector in a time interval between t and $t + \Delta t$ was automatically recorded by an analyzer during several minutes of operation. It was shown[18,19] that the distribution of the time of arrival of the electrons at the detector aperture is

$$E(t) = \frac{aNw\ \Delta t}{(4\pi Dt)^{1/2}} \exp\left[-\frac{(L - wt)^2}{4Dt} - \beta wt\right]\ ,$$

[17] R. H. Ritchie and G. E. Whitesides, *Equilibrium Electron Distributions in Elastically Scattering Gases*, ORNL-3081 (June 2, 1961).

[18] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, pp. 27–28.

[19] G. S. Hurst *et al.*, *J. Chem. Phys.* **39**, 1341 (1963).

where a is the area of the aperture, N is the total number of electrons per unit area available at time $t = 0$, D is the diffusion coefficient, w is the drift velocity, and βw is the capture rate of the electrons. Estimates for the values of N, D, and w for the case $\beta = 0$ and for the gases C_2H_4 and CO_2 were obtained[20] by fitting the measured data to the analytical expression for $E(t)$. Owing to error fluctuations in instrumentation, it was felt that this method for determining the diffusion coefficient and drift velocity was inadequate. Therefore a model to account for these error fluctuations was sought.

If $T_0(t)$ represents the error fluctuations, it has been mentioned[20] that, in measuring $E(t)$, actually the convolution integral

$$E'(\tau) = \int_0^{\tau} E(t)\, T_0(\tau - t)\, dt$$

was measured. Consequently, a least-squares fit of the experimental data to this function for the case $\beta = 0$ and the gas C_2H_4 was made to obtain estimates of aN, D, and w. As an analytical expression for $T_0(t)$ was not assumed, the measured data for $T_0(t)$ were used to integrate the function $E'(\tau)$ and its partial derivatives with respect to aN, D, and w. The trapezoidal rule was used for all integrations, since the values of the integrands were obtained from tables.

High-Energy Proton Dosimetry

A program was written to calculate the distribution of energy losses by isotropically incident monoenergetic protons in a proposed high-energy proton dosimeter. The distribution function $n(\epsilon, E)$, where E is the energy of the incident proton and ϵ is the total energy lost in passing through the dosimeter, was obtained for each of several incident energies. The generalized concept of dosimetry developed by Hurst and Ritchie[21] can then be applied to determine the operator $O(\epsilon)$ that converts the energy loss distribution $n(\epsilon, E)$ to a radiation dose $D(\epsilon)$.

An Application of the Generalized Concept of Dosimetry to Space Radiations

The study of dosimetry of high-energy protons is of extreme importance to manned space flight. High-energy proton radiation is very harmful to human tissue and is a very common space radiation. Recent studies in this area have led to the generalized concept of dosimetry described by Hurst and Ritchie[22] and its application to space radiations. Further investigations have led to the conceptual design of a high-energy (0–400 Mev) proton dosimeter.

The detector used for this dosimeter consists of an array of lithium-drift silicon detectors. The particular array geometry used was that of a cubic crystal whose edges are 1 cm long and which is bounded on each of its faces by a side crystal of dimensions $0.1 \times 1 \times 1$ cm.

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[20] R. D. Birkhoff *et al.*, *Health Phys. Div. Ann. Progr. Rept. July 31, 1964*, ORNL-3697, p. 134.

[21] G. S. Hurst and R. H. Ritchie, *Health Phys.* **8**, 117 (1962).

[22] G. S. Hurst and R. H. Ritchie, *Health Phys.* **8**, 117 (1962).

Protons entering the detector array may penetrate the entire array or may stop within the array. Since the dimension of the detector array is approximately equal to the range (1.18 cm) of a 50-Mev proton in silicon, it is convenient to separate the protons into two energy groups: the high-energy group of energy greater than 50 Mev and the low-energy group of energy less than 50 Mev.

Various kinds of paths can be traversed by protons passing through the detector array. The electronic circuitry connected to the seven crystals of the detector will make the appropriate energy selection (high-energy group or low-energy group) and signal routing for every proton passing through the detector. For example, a proton entering a side crystal and penetrating the opposite side crystal would be counted in the high-energy group by the circuitry. A proton entering a side crystal and penetrating an adjacent side crystal would be counted in the low-energy group. Therefore, every proton that hits the detector and deposits some energy is counted in one of the two energy groups.

The energy lost by protons in passing through the detector can be calculated from the relativistic stopping-power formula.[23] Although a few nuclear collisions will occur within the detector, they will usually be rejected by the electronic circuitry and have been neglected in the calculation of energy loss within the detector.

A FORTRAN program has been written that will calculate the energy distribution of energy losses resulting from the radiation of the above array of silicon detectors by isotropically incident monoenergetic protons. The program generates randomly and for each incident proton records a history that consists of:

1. the point of penetration,
2. the direction of travel,
3. whether the proton stopped within the detector array,
4. the component of the array in which the proton stopped if indeed it did stop,
5. whether the proton penetrated opposite side crystals, adjacent side crystals, or neither,
6. the amount of energy lost by the proton in each component of the detector array.

Using these histories, the bombardment of the detector array by an isotropic source of monoenergetic protons can be simulated. Ultimately the program will be able to calculate the distribution of energy losses in the detector array exposed to an isotropic flux of protons of selected incident energies up to 400 Mev.

The distribution function $n(\epsilon, E)$, where E is the energy of the incident proton and ϵ is the total energy lost by the proton in passing through the detector array, was obtained for each of several incident energies in the high-energy group. Each distribution indicated a range of energy losses. However, the distribution function $n(\epsilon, E)$ obtained for the selected energies E in the low-energy group did not have a range of energy losses, because all protons counted in this group lost all of their energy within the detector array.

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[23]See, for instance, U. Fano, "Penetration of Protons, Alpha Particles and Mesons," *Ann. Rev. Nucl. Sci.* **13**, 1 (1963).

The fundamental principle involved in the generalized concept of dosimetry is based on an operator $O(\epsilon)$ which will transform an energy-loss distribution function $n(\epsilon, E)$ into a radiation dose function $D(E)$. An operator which is particularly suited for this illustration is a matrix of weighting coefficients. Finding the operator $O(\epsilon)$ consists simply of solving a matrix equation to find the weighting coefficients corresponding to the dose function $D(E)$. This is done for each energy group separately.

The dose curve $d(E)$ to be approximated by the response of the dosimeter will vary depending on the dose received from exposure which contributes to a specific effect on the body. In fact, the output from a single exposure of the dosimeter can be used to fit any number of dose curves $d_i(E)$ and thus to determine the dose received for a given exposure as related to any number of different effects.

The dose as computed by using the operator $O(\epsilon)$ is identical with the dose-curve value when the incident proton energy is one of the selected incident energies. Otherwise, the dose computed by using $O(\epsilon)$ will only approximate the $d(E)$ dose-curve value. However, any number of distributions $n(\epsilon, E)$ with incident energy $E \leqq 400$ Mev can be calculated, and theoretically it is possible to obtain any desired degree of accuracy.

It is interesting to note that the calculation of dose received from high-energy protons using the generalized concept of dosimetry assumed the energy spectrum was completely arbitrary except that the total energy range was 0 to 400 Mev. Therefore, it is conceivable that a dosimeter of a type similar to the one described here could relay pulses corresponding to the high-energy data to a remote data processor which could perform the necessary calculations and relay back immediately the dose a man would receive at that point.

Monte Carlo Analyses

Monte Carlo methods have been used in the following problems.

Several programs were written in connection with a study of linear energy transfer distributions and energy deposition in "tissue-like phantoms." The phantoms were subjected to a monoenergetic broad beam of neutrons in order to determine the above quantities resulting from a unilateral exposure situation. These results were transformed analytically to get estimates for bilateral and multilateral exposure situations.

A code for gamma-ray analysis was written to compute dose deposition resulting from photons emitted from an ^{125}I source located in the thyroid region of the phantom. Two phantom sizes were used, one representing an adult and another representing an infant.

A program was written to simulate irradiation of a hollow boron sphere with neutrons from a Godiva spectrum source. The program computes the expected number of fission neutrons produced in each of three metal foils suspended in the sphere per neutron introduced into the system as a function of incident neutron energy.

Liquid Injections into Permeable Formations

If water containing radionuclides is injected into a porous medium, subsequent movement of the radionuclides is mainly due to the movement of the transporting water, but it is also affected by the ion exchange properties of the medium. A program was written to compute and plot analytic solutions for streamlines, equipotential contours, and speed of water movement in sandstone under conditions of an "inverted five-spot" system of injection and relief wells. The results of a calculation for the movement of water and radiostrontium through a slab of sandstone were in good agreement with experimental data.

Analysis of Column Data

Sodium-saturated hydrobiotite was used to fill ion exchange columns. Hydrobiotite exists as a mixed-layer mineral having a rather random mixing of collapsed biotite-type layers with no interlamellar water. The spacing between the charged faces of the sodium-saturated vermiculite layers is 5.55 A;[24] thus Donnan membrane theory can be used to describe the chloride exclusion from the interlamellar region.

The columns were preequilibrated with untagged NaCl solution of the desired concentration. Tritiated water solutions of NaCl of the same concentration and tagged with ^{36}Cl were passed through the column at a constant flow rate. Each run consisted of a saturation and a leaching step, and the same column was used for all runs. Samples were counted simultaneously for ^{3}H and ^{36}Cl, using a Packard Instrument Tri-Carb counter.

A computer program was written to correct the overlap of the two beta spectra and to fit the experimental data to a chromatographic breakthrough curve of the type[25]

$$C/C_0 = 1/2 \left[1 - \mathrm{erf} \left(\sqrt{P} \frac{v - \bar{v}}{\sqrt{v\,\bar{v}}} \right) \right],$$

where C/C_0 is the fraction breakthrough of the tracer, P is the Peclet number for the column, v is the throughput volume, and $\bar{v}$ is the equivalent column volume.

In addition to this study of anion exclusion by soils, the program will also be useful for analyzing the data for other column studies, using single- or double-tracer techniques.

Stochastic Models for the Distribution of Radioactive Material in a Connected System of Compartments

A simple model for the distribution of radioactive material in an organism has been described by Bernard and Uppulluri.[26] They considered the radioactive material retained in animals (dogs, etc.) by

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[24] R. E. Grim, *Clay Mineralogy*, p. 74, McGraw-Hill, New York, 1953.

[25] I. Hashimoto *et al.*, "Peclet Numbers and Retardation Factors for Ion-Exchange Columns," *Ind. Eng. Chem., Fundamentals* 3, 213–18 (1964).

[26] *Health Phys. Div. Ann. Progr. Rept. July 31, 1964*, ORNL-3697, pp. 193–98.

introducing an open system consisting of two compartments S and B, which refer to the blood stream and bone structure respectively.

Initially (time $t = 0$ or stage $m = 0$), compartment S holds unit mass of radioactive material and compartment B holds zero mass, and the connecting valve is closed. At the end of a unit time interval Δt (stage $m = 1$), there occurs a random event which determines the opening or closing of the valve connecting the two compartments. If the valve at the end of time Δt is closed, then the amount of material in S is reduced by a factor a (the attenuation or decay factor); thus in this case the amount in S at the end of the first interval of time would be $a \times 1 = a$, whereas the amount in B is still zero. If, however, the valve opens at the end of time Δt, then the total amount in the two compartments is reduced by a factor a and reapportioned in equal amounts between S and B. Thus if the system has initially unit material in S and zero in B, then at the end of time Δt there will be a in S and zero in B with probability p, or $\frac{1}{2}a$ in S and $\frac{1}{2}a$ in B with probability $1 - p$. Similarly, the state of the compartments with respect to the amount of material held at the end of the second time interval Δt can be constructed and will be seen to consist of four possibilities as shown in Table 1.

Table 1. State of the System at the End of Time $2\,\Delta t$

State of System:				
At end of Δt	Closed	Closed	Open	Open
At end of $2\,\Delta t$	Closed	Open	Closed	Open
Probabilities	$(1-p)(1-p)$	$(1-p)p$	$p(1-p)$	pp
Amount in S	a^2	$\frac{1}{2}a^2$	$\frac{1}{2}a^2$	$\frac{1}{2}a^2$
Amount in B	0	$\frac{1}{2}a^2$	$\frac{1}{2}a^2$	$\frac{1}{2}a^2$

The scheme in Table 1 could be continued so as to show the possible amounts of material in S and B at the end of m intervals of time Δt. Denoting the amounts in S, B at the end of $m\,\Delta t$ by $C_{S,m}$, $C_{B,m}$, these are random variables given by the stochastic recursive equations:

$$C_{S,m} = X_m \frac{a}{2}(C_{S,m-1} + C_{B,m-1}) + a(1 - X_m)C_{S,m-1}\,, \tag{1a}$$

$$C_{B,m} = X_m \frac{a}{2}(C_{S,m-1} + C_{B,m-1}) + (1 - X_m)C_{B,m-1}\,, \tag{1b}$$

$$m = 1, 2, \ldots\,; \qquad C_{S,0} = 1\,; \qquad C_{B,0} = 0\,.$$

In these equations X_m is a random variable associated with the state of the valve at the end of the mth time interval. If the valve is open, then X_m takes the value unity with probability p, whereas if the valve is closed, X_m takes the value zero with probability $1 - p$. From (1) the sample space of the random amounts in the system is given by

$$\begin{bmatrix} C_{S,m} \\ C_{B,m} \end{bmatrix} = J_m J_{m-1} \cdots J_1 \begin{bmatrix} C_{S,0} \\ C_{B,0} \end{bmatrix}\,, \tag{2}$$

where

$$J_i = \begin{bmatrix} \frac{1}{2}aX_i + a(1 - X_i) & \frac{1}{2}aX_i \\ \frac{1}{2}aX_i & \frac{1}{2}aX_i + 1 - X_i \end{bmatrix}.$$

It does not seem possible to simplify the matrix product in (2), which may be regarded as a random branching process or as linear iterations of an initial vector. However, the lower-order moments of the variates can be found, since the random quantities occurring in the matrix product in (2) are independent. Moreover, a functional equation can be set up for the joint characteristic function of $C_{S,m}$, $C_{B,m}$.

The two-compartment system just described can be generalized in several ways. Clearly, a connected system of j compartments suggests itself, and this could consist of peripheral compartments, in series, connected to a central compartment, or a "catenary" system in which the peripheral compartments are connected to each other but only one of which is connected to the central compartment.[27] Another generalization concerns the probability complex associated with the communicating valves. This could be such that each valve operates independently, in which case the probability structure would be that of strictly independent random variates. On the other hand, the opening of one valve could preclude the opening of any other valve in the system; in this case the random variates associated with the valves would be mutually exclusive. Another generalization concerns the "mixing" principle which is invoked for the apportionment of material in compartments that happen to become connected.

Each of these generalizations has been considered, and expressions have been derived for the mean amounts in the compartments of the system. In general, covariances for the amounts in the system are more complicated. For example, for a "mammillary" system, it turns out that the covariance matrix (uncorrected second-order moments) Q_m at the mth stage is given in terms of that at the previous stage by the relation

$$Q_m = \sum_{i=1}^{j-1} p_i A_i Q_{m-1} A_i' \qquad (m = 1, 2, \ldots) ,$$

where the A_i's are certain matrix operators related to the probability structure of the communicating valves.

The sample space for each of these generalized systems can be readily defined; however, the problem of finding closed expressions for it remains unsolved. If, however, the "decay" factor a is unity, then the sample space for a three-compartment system reduces to evaluating the binomial expansion $(p_1 A_1 + p_2 A_2)^m$, where m is a positive integer and A_1, A_2 are idempotent stochastic matrices. This has been accomplished by reference to classical occupancy theory.

Solutions for the models considered consist of linear expressions in damped exponentials, and feasibility studies have been undertaken. Further problems related to model identification remain for consideration.

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[27] Reference may be made to C. W. Sheppard and A. S. Householder, *J. Appl. Phys.* **22**, 510–20 (1951) and to C. W. Sheppard, *Basic Principles of the Tracer Method*, Wiley, New York, 1962.

Core Adjustment and Correlation Analysis

The sediment in the Clinch River below White Oak Lake contains varying amounts of low-level radioactive substances. Core samples of this sediment have been taken at several locations on the river, and the activity of the core has been measured in 2-in. sections of sediment. Since the sediment is of varying thickness due to the structure of the river bed, rate of flow, and other factors, direct correlation of the activities of several cores is not possible. However, it is obvious from examination of plots of activity vs depth in the core that there is a similarity between many of the samples. Therefore, a means of adjusting the core lengths and segments of core lengths before correlation seems feasible. Owing to the large amount of data involved, a computer program has been written to adjust these core lengths and perform the correlations. The cores to be correlated are chosen for their similarity in plots, and a base or main peak and a secondary peak are chosen for each core. The core lengths are then adjusted to the same length between peaks, and excess portions of either core are discarded. The segment lengths are then normalized and the correlation performed. The results of the code are: (1) correlation coefficients between cores, (2) regression coefficients between cores, and (3) scale factors necessary to adjust the core lengths.

To date, very high correlations have been found not only between core samples from the river bed but also between these samples and plots of the release of radioactive materials from the White Oak Lake.

Stepwise Regression

A stepwise regression program, BMDO2R, has been converted to operate on the CDC 1604-A computer in a manner approximating as closely as possible the description of the original program as published in *Biomedical Computer Programs.*[28] The program computes a sequence of multiple linear regression equations, adding one variable at each step on the basis of greatest reduction in the residual sum of squares. There are two differences in operation which are the result of program revisions by the original programmers for which the program description was not revised. If the program user enters F-level or tolerance-level values of zero, the program sets them to predetermined values. Secondly, if the user requests a printer plot of residuals, the x-axis labels start at the minimum value of the independent variable rather than at zero as indicated in the BMD publication.

Clinch River Safety

Additions have been made to the program for the analysis of Clinch River safety[29] to permit the results of the calculations to be plotted on the Calcomp plotter.

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[28] W. J. Dixon (ed.), *Biomedical Computer Programs*, p. 233, University of California, Los Angeles, 1964.
[29] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 13.

Quarterly Bioassay Sample Report

A computer program has been written to produce a quarterly report on the bioassay samples processed by the Health Physics Division. The program lists the samples processed (1) alphabetically, (2) by divisions, and (3) by Health Physics areas. Several summaries of certain information concerning the samples are also reported by the program.

Stationary-Instrument Service Data

In order to study stationary-instrument service data more efficiently, a computer program was written. The program sorts and reports the instruments, along with pertinent service information, according to (1) instrument type codes, (2) division numbers, (3) components, (4) property numbers, and (5) building numbers. The program also lists those instruments whose service data meet certain conditions that warrant special attention. These instruments are reported according to (1) instrument type codes and (2) property numbers. In addition to this information, the frequency of repairs, classified according to the type of instrument and the technician who serviced it, is tabulated.

INSTRUMENTATION AND CONTROLS

G. J. Atta

Electrical Network Design

An attempt is presently being made to design an electrical network which may replace the present networks in the Q2069 pulse amplifier. Essentially, a network design is being sought that will yield a desired transient response and steady-state frequency response. The transient response of the network is important because it carries the information, while the steady-state frequency response is important because it is a measure of the capability of the network to reject noise.

The transient response may be obtained from the solution of a differential equation by use of the Laplace transform.[30] The frequency response may be obtained from the solution of an integral by use of the calculus of residues.[30]

A program was written to calculate and plot the transient response for various network designs; another program was written to determine the steady-state frequency response.

ISOTOPES

G. J. Atta A. R. Jenkins

Radioactive Isotopes

Two computer programs have been written. The first program calculates the fraction of a radioactive isotope remaining after a specified period of time. As many as five tables in different units of time can

[30] R. V. Churchill, *Modern Operational Mathematics in Engineering*, McGraw-Hill, New York, 1944.

be generated to give this information. The second program calculates the activity of a radioactive daughter isotope of a radioactive parent isotope by various formulas and plots this activity as a function of time.

Yield for (n,γ) Production of Radioactive Isotopes

This program[31] has been extended so that calculations that involve radioactive as well as stable parent isotopes may be performed. The program calculates the irradiation time in a reactor that is necessary for maximum yield of a radioactive daughter isotope from a parent isotope. The specific activity of the daughter and the combined activity of both the daughter and the parent are also computed.

The program can also be used in two other ways. It can calculate the product activity yields which are produced by simple decay, allowing for decay of the daughter as well as the parent. It can also calculate the activity of the daughter and the combined activity of both parent and daughter after an arbitrary time in the reactor.

Details have been published elsewhere.[32]

CRUNCH Modifications

The original CRUNCH[33] program for the IBM 704 computer was reprogrammed for the CDC 1604-A computer. Details have been reported elsewhere.[34]

LIBRARY

G. K. E. Haeuslein J. G. Sullivan, Jr.

Book Circulation Control System

Books being charged out are recorded on two lists: the charge-out list, the entries of which are sorted by the book's call number, and the borrower's list, the entries of which are sorted by the borrower's badge number. Each book contains a punched book card containing the book's call number, author, and title. If the book is charged out or returned, the IBM 357 Data Collection System is used to generate a turnover card containing information copied from the book card and the borrower's badge number. The turnover cards are put on tape, sorted by call number, and merged into a tape containing the old charge-out list. Then the turnover records are sorted by the borrower's badge number and merged into a tape containing the old borrower's list. The charge-out list, the borrower's list, and overdue notices in mailable format are printed. The daily updating procedure takes place in one run. Other programs generate book cards, maintain the shelf list, and update the user's address list.

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[31] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 15.

[32] C. W. Friend and A. R. Jenkins, *ISOTOPES – a Program for Neutron Product Yields and Decay Calculations Using a Control Data 1604-A Computer*, ORNL-3673 (in press).

[33] M. P. Lietzke and H. C. Claiborne, *CRUNCH – an IBM 704 Code for Calculating N Successive First Order Reactions*, ORNL-2958 (October 1960).

[34] C. W. Friend and J. R. Knight, *ISOCRUNCH – Modification to the CRUNCH Program for the IBM 7090*, ORNL-3689 (in press).

Book Catalog

For each book or report, one group of cards is keypunched which contains information on corporate authors, title, subjects, and isotopes. From these cards are generated 3 × 5 in. index cards and four lists showing all publications entered. These are sorted by corporate author, author, subjects, and isotopes respectively. The above procedure is performed with the aid of programs written in COBOL and the Control Data SORT program. The present input format is that required by the KWIC Index program; a future improvement may be to switch to the card format used by the AEC for report announcements.

MEDICAL – ORINS

Ruth B. Hofstra R. L. Shively

NASA Retrospective Studies in Irradiation Response

Medical research is being done for the anticipation of radiobiological problems for manned space flight. Hospital records in the Medical Division, Oak Ridge Institute of Nuclear Studies, are being taken as a source of data for people receiving total-body irradiation therapeutically. Other sources of data will also be used for conclusions about the effects of accidental or therapeutic irradiation.

Cases being studied will be in groups according to the amount of irradiation received. Procedures of discriminant analysis, analysis of variance, and different special kinds of correlations will be applicable. Bioassay involves all-or-none responses, as in nausea and vomiting, and measured responses, as in hematologic and biochemical considerations.

The project is being carried forward for the National Aeronautics and Space Administration.

Amino Acid Studies

Work has been done on the CDC 1604 computer in the study and nonparametric correlation of corrected concentrations among groups of amino acid chromatograms. Analysis of variance has also been applied, considering differing types of treatments and different types of tissues.

METALS AND CERAMICS

G. J. Atta C. T. McCracken
E. E. Branstetter G. S. McNeilly
R. B. Bullock D. C. Ramsey
Manuel Feliciano R. P. Rannie
R. L. Shively

Preferred Orientation of Crystallographic Planes

A large system of algebraic linear equations has been solved to determine numerically the orientation distribution function on a solid angle. A knowledge of this function is needed for a quantitative study of preferred orientation in polycrystalline materials.

Resistivity Tensor Components

Additional subroutines have been written for this program[35] to permit the plotting of certain properties in polar coordinates and to permit the fitting of a polynomial in terms of magnetic field strength to the tensor components for fixed values of magnetic field angle.

Density of States

A method[36] that does not rely on perturbation theory has been developed which determines the density of states of a random one-dimensional two-atom alloy in the limit as the length of the crystal approaches infinity. James[37] obtained solutions of the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi = E\psi ,$$

where

$\hbar = h/2\pi$, h is Planck's constant,

m = mass of electron,

$V(x)$ = potential encountered by the electron, and

E = energy of the electron.

James's solutions were valid for each atom, and he joined them, while maintaining the continuity of ψ and ψ', to form the complete solution for finite crystal lengths. Two programs have been written by using these methods to calculate the density of states for Dirac delta function and square-well potentials.

Randomly generated sequences of A and B atoms for concentrations of 50, 20, and 10% of the A atoms were used in the calculations. Strings of up to 1500 atoms are used.

For both potentials, the method of James is used to count the number of nodes (zeros of the one-electron Schrödinger wave function) in the atom string. These results are compared with the theoretical predictions of Faulkner.

Both the theoretical and calculated density of states are obtained as a function of energy and then printed and plotted.

X-Ray Intensity Contour Plots

The distribution of diffusely scattered x-ray intensities in reciprocal space may be described by a Fourier series. A program has been written to evaluate this series for given Fourier coefficients at nonrandom lattice positions (in real space) of atoms in a binary alloy. For a constant value of the

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[35] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 16.

[36] J. S. Faulkner and J. Korrinja, *Phys. Rev.* **122**, 390 (1961).

[37] H. M. James and A. S. Ginzbarg, *J. Phys. Chem.* **57**, 840 (1953).

space variable z, a contour map of the function is plotted in the x-y plane. The results are to be compared with previous calculations in which the distribution of intensities was known and the positions of the atoms were obtained.

Anisotropy Factors for Pyrolytic Carbons

A computer program has been prepared to calculate anisotropy factors for pyrolytic carbons using data from x-ray diffraction studies of these materials. The data are fitted by least-squares methods, using three different functions. The functions are $\cos^m \theta$, a Gaussian, and a polynomial. The anisotropy factor is σ_{oz}/σ_{ox}, where

$$\sigma_{oz}/\sigma_{ox} = z \frac{\int_0^{\pi/2} f(\theta) \cos^2 \theta \sin \theta \, d\theta}{\int_0^{\pi/2} f(\theta) \sin^3 \theta \, d\theta},$$

and $f(\theta)$ is the function used. The integral is evaluated numerically when necessary.

The program can plot any or all of the functions and the data in plots of any convenient size, as $8\frac{1}{2}$ by 11 in.

Coating by Rotating Drum

A mathematical analysis was made to determine the feasibility of coating nuclear particles by blowing a coating gas into a horizontal rotating drum. The purpose of the study was to determine numerical values of such constants as the most suitable angular velocity for the rotating drum, the optimum charge to be introduced into the rotating drum, and the physical characteristics of the drum. The study has shown that for best results horizontal drums with fins should be used.

Vapor Deposition

Vapor deposition is being investigated as a method of fabricating reactor components. This includes fuel element cladding, tubing, and special parts. It is difficult to fabricate fuel element materials by standard metallurgical techniques. Vapor deposition requires that metal halides such as WF_6 react with hydrogen to produce a metal deposit. This process is not well understood. As an important aid in the problem of investigating this process, numerous arithmetic calculations have been made to obtain parameters for the most favorable deposition.

Estimation of Fuel Fabrication Costs

Two computer programs, FABCØST 5 and FABCØST 6, were written for use in predicting the cost of fuel element fabrication for various nuclear reactor types. In the FABCØST 5 program, fabrication costs are computed for fuel elements in the form of rod bundles, that is, clusters of small-diameter metal-clad fuel rods, and nested fuel elements consisting of concentric metal tubes filled with fuel material. A

variety of flowsheets, fuel compounds, and cladding and operating conditions can be treated. In the FABCØST 6 program, similar calculations are done for advanced high-temperature gas-cooled reactor fuel elements consisting of graphite bodies filled with carbon-coated fuel particles. The effects of geometry, fuel particle size, and coating thickness are among the variables manipulated by the program.

The programs have been used for calculation of fuel fabrication costs in several reactor evaluation studies.[38]

Cost Control and Manpower Allocation

A program has been written which is to be used for cost control within the Metals and Ceramics Division. This program provides a summary of cost data and compares the cost to date with budgeted standards by man-year-dollars, man-month-dollars, and total cost vs time expended.

Two new programs have been written and an old program has been revised that report the allocation of manpower in the Metals and Ceramics Division. One of the new programs deals with sorting information received from the division. The other program plots the financial plan and costs of different projects.

NEUTRON PHYSICS

Nancy A. Betz
R. T. Boughner
Arline H. Culkowski
Margaret B. Emmett
Manuel Feliciano
M. T. Harkrider
R. L. Shively
J. G. Sullivan, Jr.

Response Functions of an Organic Scintillator to Fast Neutrons

A knowledge of the neutron response of organic scintillators is needed over a wide range of energies and scintillator sizes in order to provide the response functions required for unfolding measured neutron pulse-height distributions obtained with such detectors, as well as to furnish a convenient means for determining the efficiencies of organic detectors used in time-of-flight spectrometry. A method for obtaining the response function of organic scintillators using experimental calibrations and Monte Carlo calculations has been devised and applied to a 2-in. by 2-in.-diam NE-213 scintillator.[39] Good accuracy over a wider range of pulse heights than has been heretofore possible has been achieved.

SNAP Reactor Shield System

A preliminary calculation of the unscattered and scattered neutron dose has been made for a SNAP reactor shield design of simple geometry. Work is under way on the problems of the scattered dose calculation and of determining the shape of shield that provides adequate shielding with the least weight of shielding material.

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[38] M. W. Rosenthal *et al.*, *A Comparative Evaluation of Advanced Converters*, ORNL-3686 (in preparation).

[39] Nuclear Enterprises Ltd., Winnipeg, Manitoba, Canada.

Applications of O5R Monte Carlo Code to Neutron Shielding and Scattering Problems

A comparison of the effectiveness of a conical shell shield vs disk shields for the SNAP program has been made. The results show, for shields of the same weight, that the disk shield will provide greater attenuation.[40]

A program has been written to calculate neutron flux and dose at various distances from a point source in an infinite or a finite medium. The program was written as a first step in calculating the neutron field in air from a point source above the ground interface, finding the perturbations caused in that field by the presence of certain shielding structures, and, finally, finding the shielding value of several of these structures in the perturbed field. This work is being done for the BREN project.

A measured source angular distribution of neutrons and a collimated detector have been incorporated into the lithium hydride slant slab program in an attempt to bring the programmed model closer to the experimental model.

Much assistance, especially to those working on the DASA project, has been given to people wishing to use O5R[41] for various neutron calculations.

Monte Carlo Calculations on Intranuclear Cascades

MECC (Modified Energy Cascade Calculations) Code. – This project has been reported previously.[42] All subroutines involved in the recoding and revision have been written and checked out. At present, tests are being run to compare the machine language code with the codes written in FORTRAN for the IBM 7090 computer. Comparisons between the last-mentioned code and the code written in FORTRAN for the CDC 1604-A computer are also under way. The results of these efforts show good correspondence.

The tests also showed that parts of the original code needed revisions. These revisions have been made.

Isobar Code. – An analysis code to allow comparisons to be made between predictions of the isobar model used in the MECC code and experimental data has been written. All data generated will be in the laboratory system. A method of obtaining center-of-mass system quantities from laboratory system quantities is available and will be coded in the near future.

Isobar model calculations were extracted from the cascade calculation code and altered to meet the situation of an incident particle (proton, neutron, π^+, π^0, or π^-) in space striking a nucleon at rest. All reactions are either single production, double production, or both, and the output is tagged to distinguish between the different types of reactions.

Four distinct types of data are calculated, along with the statistical errors for all quantities. The four types of data are (1) energy spectra, (2) angular distributions, (3) multiplicities, and (4) invariant mass distributions.

These data will be used for the above-mentioned comparisons. For every spectrum, quantity, or distribution, except the invariant mass distributions, there is a version of the code pertaining to the

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[40] Abstract of TM-981 (in press).

[41] ORNL-3622 (to be published).

[42] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 17.

type of production and type of product, recoil, or decay. Histograms for all data will also be obtained.

A short code was also written to check the isobar model calculations for conservation of energy, momentum, and charge.

Miscellaneous Codes

The OGRE[43] system of Monte Carlo gamma-ray codes has been modified. The subroutines which were previously written in FAP have been rewritten in FORTRAN with the exception of the random number generator. The system has also been adapted to the CDC 1604-A.

OGRE-S, a Monte Carlo gamma-ray code with spherical symmetry and an extended source having an energy spectrum resembling a fission spectrum, has been written, and results produced by it have been compared with results of an Sn code which is under development at Los Alamos.

The general geometry routine, GEOM, of the O5R[44] system has been revised for use in a preliminary version of a general geometry Monte Carlo gamma-ray code.

OGRE-H, a Monte Carlo code, has been written using this revised general geometry routine. A comparison between O5R, OGRE-H, and a code written at another installation was made with a problem having a complex geometry and a simple medium. Several different geometries were tried for a particular problem in order to determine which geometry, as well as which code, was more efficient as far as computer time was concerned.

Some statistical estimation routines have been written for use within the O5R system. These routines are for use either with the version of O5R that generates tapes or with a version which bypasses the use of tapes and immediately processes the data. Neutron distributions in water[45] and concrete were produced using these codes.

A group of numerical integrations was done for the DASA weapons-shielding handbook.

Gamma-ray fluxes calculated at Los Alamos were processed to produce heating results in iron.

A system for reporting the computer costs accounts of the Neutron Physics Division has been set up. Reports are made on an individual basis as well as on an account basis, and a summary sheet of all division accounts is given to those in charge of the division's budget.

Radiation Shielding Information Center

A system for selective dissemination of information by the Radiation Shielding Information Center[46,47] is in use, and the necessary computer codes have been written. This system operates along with the updating of the tapes of the RSIC. The abstracts of the documents being placed in the system are on

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[43] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 39.

[44] R. R. Coveyou *et al.*, *O5R, A General Purpose Monte Carlo Neutron Transport Code*, ORNL-3622 (to be published).

[45] D. K. Trubey and M. B. Emmett, *A Comparison of First- and Last-Flight Expectation Values Used in an O5R Monte Carlo Calculation of Neutron Distributions in Water* (to be issued as ORNL-RSIC-3), presented at American Nuclear Society meeting in San Francisco, December 1964.

[46] *Neutron Phys. Div. Ann. Progr. Rept. Aug. 1, 1964*, ORNL-3714, vol. 1, p. 68.

[47] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 14.

magnetic tapes as well as the names, addresses, and fields of interest of the people on the RSIC distribution list. Whenever documents are added to the system, a search is done to determine which people are interested in the individual documents. An abstract of the document, together with the information on how to obtain this document, is sent immediately to the interested persons. This operation is aimed at aiding the individual researcher who would like to have this information at a larger frequency than the bibliographies would provide.

Some special edits have been written for the RSIC system. All logical combinations of three, four, or five categories may be used to produce these special edits. For example, suppose *A*, *B*, *C*, and *D* represent category numbers; further assume that the interested party wants to know what documents are available that contain categories *A*, *B*, and *C or* that contain only *D*; then, this can be determined by using the special edit for four categories. Another special edit allows an edit of any group of categories taken one at a time and listed only if a certain emphasis indicator applies. These emphasis indicators appear with each category of each document to reveal the importance of that document in relation to the particular category. In other words, an edit of only the more important documents can be produced.

An operations manual for the RSIC retrieval system has been prepared and will soon be published.

PHYSICS

G. J. Atta
G. A. Bogar
R. T. Boughner
A. M. Craig
M. T. Harkrider
Ruth B. Hofstra
A. R. Jenkins
C. W. Nestor, Jr.
M. F. Patterson
D. C. Ramsey
R. L. Shively
J. G. Sullivan, Jr.
T. C. Tucker

Monte Carlo Analyses

A study of the transmission of neutrons through a hollow cylindrical shield of ^{6}LiH was accomplished by means of a computer program. Isotropic monoenergetic neutron sources of from 1 Mev to 10 ev were located at the center of the longitudinal axis of the shields. Shield thicknesses of from 0.5 to 4 cm were used.

A program was written to compute the flux distribution of neutrons escaping from a carbon block irradiated by a monoenergetic broad-beam neutron source, and the spread in path length l as a function of emission energy was computed, where

$$l = \sum_n \frac{l_n}{\sqrt{E_n}} \sqrt{E_f} .$$

Here l_n is the track length between the $(n-1)$st and nth collision of a given neutron, E_n is the neutron energy before the nth collision, and E_f is the neutron's escape energy.

Fast-Chopper Measurements

A multichannel analyzer is used to measure the number of neutrons detected in a particular time interval and to record this information on punched paper tape in a hexadecimal format. A CDC 160-A program was written to convert the data into a BCD format and store it on magnetic tape for subsequent analysis.

Multiple Scattering Corrections to Neutron Capture Data

In determining resonance parameters from neutron-capture measurements, it is frequently necessary to correct the capture data for the energy-dependent multiple scattering which takes place near the resonance energy. A program was written for the CDC 1604-A computer to calculate the neutron scattering over the energy region of an isolated Breit-Wigner resonance, using the complex probability integral technique[48] to compute the Doppler-broadened resonance and interference terms. A calculation of the secondary capture in 0.001, 0.002, and 0.005-in. tungsten samples has been made for the 18.8-ev resonance in ^{186}W, and these calculations have been applied to correct the capture data obtained at the RPI linac. These corrected data have been combined with ORNL transmission data (WASH-1048) to obtain a radiation width of $(53 \pm 3) \times 10^{-3}$ ev, where the error of $\pm 3 \times 10^{-3}$ ev is essentially determined by the statistical fluctuation in the resonance capture areas and is relatively independent of the error in the transmission measurements. For these calculations, where the secondary capture was comparable to the primary capture, a cost of $2.50 per 1000 neutron histories was obtained.

Charged-Particle Cross Section

A number of programs have been written for the purpose of using magnetic tape in a storage and retrieval system for data on charged-particle-induced nuclear reactions.

More specifically, these programs provide for the transfer of data from punched cards to magnetic tape and for the retrieval of these data in the form of lists and plots of several specified types. Retrieval may be accomplished either directly through the use of identification numbers or indirectly by specifying certain parameter ranges. Auxiliary programs were also written to delete, replace, or reproduce any desired records.

These and other programs previously reported[49,50] comprise the storage and retrieval system used by the CPX Data Center located at ORNL. This system is used to provide the lists and plots for published editions such as ORNL-CPX-1.

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[48] S. E. Atta and J. A. Harvey, *Numerical Analysis of Neutron Resonances*, ORNL-3205 (Dec. 26, 1961).

[49] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 43.

[50] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 23.

Nuclear Matter

A program was written to determine the parameters in two velocity-dependent potential functions such that a least-squares fit could be made to (1) the energy and density of nuclear matter, (2) the effective ranges and scattering lengths for each potential, and (3) experimental nucleon-nucleon phase shifts at elected energies. The major programming problem was the development of an efficient subroutine for the solution of the second-order ordinary differential equation for the radial wave function. A subroutine in the library using Gill's modification of a fourth-order Runge-Kutta procedure[51] was reprogrammed in FORTRAN 63 for the CDC 1604-A and has been used satisfactorily. Thus far no parameters have been found which give an adequate fit to both the energy density of nuclear matter and the phase-shift data, but this is owing to deficiencies of the model rather than the program. A new version is being written using more realistic potentials.

Neutron Cross Sections

Work is being done in the Physics Division to use the CDC 1604-A computer to process neutron time-of-flight transmission data from a 4096-channel time-of-flight analyzer. The computer receives, as original data, raw counts per channel taken from the analyzer, and proceeds to apply dead-time corrections, average the counts (if desired), and compute the neutron total cross section as a function of neutron energy. It also computes neutron-capture cross section as a function of energy from the counting data of the 4096-channel analyzer.

Fission-Fragment Data

The gamma-ray spectrum fitting program described previously[52] has been modified for use in the analysis of fission-fragment energy and yield distributions. The major change is the incorporation of an improved iterative procedure[53] in the nonlinear least-squares section of the program.

A program has been written to carry out a simple iterative calculation to unfold a Gaussian response function from an observed spectrum and to list and plot the input spectrum and the final estimate of the unfolded spectrum.

Several programs were written to study fission-fragment data taken with a three-parameter multichannel analyzer. Data from an experiment in which two fission-fragment kinetic energies and a gamma-ray energy are measured simultaneously were analyzed to obtain the average gamma-ray energy per fission fragment and the number of gamma rays per fragment, both as functions of fragment mass.

A program to study two-parameter multichannel analyzer data was modified to include a calculation of the variance of the distribution of the energy per fragment. Some explanatory calculations were made to investigate the effect of small correction terms in the analysis.

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[51] Anthony Ralston and H. S. Wilf (eds.), *Mathematical Methods for Digital Computers*, chap. 9, pp. 110–20, Wiley, New York, 1960.

[52] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 19.

[53] T. G. Strand, D. A. Kohl, and R. A. Bonham, *J. Chem. Phys.* **39**, 1307 (1963).

Electrical Conductivity of Ferromagnetic Materials

A program was written to calculate the temperature variation of the electrical conductivity of a ferromagnetic material, based on Mott's model. The program can be used for binary alloys as well as pure metals. A set of parameters was found which gave fair agreement between calculated values and experimental data for pure nickel.

Relativistic Hartree Calculations

A preliminary version of a program for the calculation of electron energies and wave functions using a relativistic Hartree model[54] was completed and checked. A comparison of the energy eigenvalues for the ground state of neon with the results of an earlier nonrelativistic calculation showed satisfactory agreement, and the $2P_{1/2} - 2P_{3/2}$ splitting was of the proper sign and order of magnitude. Since for a large atom the amount of data to be used during a calculation exceeds the available space in core storage, a revised version of the basic code was written using buffered tape handling, so that data may be transferred to and from core storage while the calculation proceeds with little if any loss of time for tape handling.

Gamma-Ray Spectra

A program was written for the analysis of gamma-ray spectra obtained from targets exposed to a beam of oxygen ions in the Tandem Van de Graaff accelerator. Operations to be performed on the data include normalization according to beam density or collection time, subtraction of background spectra, addition of selected data from the observed spectrum, and plotting the data with an indication of statistical error.

PLANT AND EQUIPMENT

R. T. Boughner M. T. Harkrider

Use of Building Space

An inventory of the present use, by division, of assigned building space has been taken in Building 4500. The object of the inventory is to obtain a divisional comparison on a cost basis of the use of space, and to provide economical guidelines for the assignment of building space in the future.

Building space has been divided into six classes, each class having been assigned a cost per square foot. The program reports the use, by division, of all six types of space, and then gives a comparison, by division, for each type of space. A division may be checked as a unit or against other divisions in its use of building space.

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[54] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963,* ORNL-3567, p. 20.

Results of the Building 4500 survey indicate that similar studies of other office and laboratory buildings in the ORNL complex are needed. It is expected that as the original inventories are completed a program of yearly revisions will be started.

REACTOR

G. J. Atta
R. B. Bullock
Judy J. Eatherly
Manuel Feliciano
M. T. Harkrider
C. T. McCracken
J. E. Schmith
T. C. Tucker

Deposition of Fission Products from Gas Streams

A program[55] for the calculation of the rate of deposition of fission products from gas streams onto conduit walls was revised to allow treatment of more complicated systems. In an isothermal region the deposition $D(z)$ as a function of z, the normalized length of the region, is given by

$$D(z) = e^{-z} .$$

A multiplier P is evaluated by the Program such that e^{-Pz} is equal to the experimental value of the deposition.

Statistical Analysis of Graphite

A program has been written which performs a statistical analysis of data received from graphite specimens. The data consist of experimental stress and strain information obtained from the testing of graphite specimens in uniaxial tensile and compressive tests and flexural tests. The mean and standard deviation, and certain confidence intervals, are calculated from these data.

Generalized Stress-Strain Thick-Walled Cylinder (GUSS)

This program calculates stress-strain distribution in long thick-walled cylinders. The code is equipped with subroutines that allow a variety of loading conditions, a variety of stress-strain relationships, and time-dependent displacements. Integral equations in terms of nonelastic strains were formulated from the compatibility and equilibrium equations. The code first calculates the elastic deformation, then iterates to determine the total strain from the stress-strain relationships. Once the total strains are determined, the stresses are calculated.

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[55] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963,* ORNL-3567, p. 24.

Likelihood Estimates of the Weibull Parameters

The Weibull probability function

$$f(x;\, X_u,\, X_0,\, m) = \left(\frac{m}{X_0}\right)\left(\frac{x - X_u}{X_0}\right)^{m-1} \exp\left[-\left(\frac{x - X_u}{X_0}\right)^{m}\right]$$

is widely used in statistical theories of failure. The present methods of estimating the three parameters, X_u the location parameter, X_0 the scale parameter, and m the scatter parameter, have several undesirable properties, one of which is that it gives no information as to the quality of the estimates. The maximum likelihood method would improve the efficiency of the estimates and allow adequate tests to be developed. The likelihood equations have not yielded to analytic efforts. The present effort is therefore directed toward developing adequate numerical methods for determining these parameters and their variances.

A computer program has been written which solves three equations for the three parameters. Also the variances and the standard deviations are calculated by using the gamma and the psi functions. Newton's method and the method of direct search were first used in solving for the parameter. After some difficulty was encountered in using these methods, a modified Newton's method was devised. The latter method has given good results.

General Statistical Program

A program has been written which calculates certain statistics and plots a histogram and frequency curve for a table of data. Included in the program is the calculation of the mean, standard deviation, skewness, kurtosis, significance level of skewness, and the significance level of kurtosis. This program has been written to handle many different forms of input data.

91-Rod Boiling-Water Test

The 91-Rod Boiling-Water Test is an electrically heated mockup of a Rankine-cycle system using potassium as the reactor coolant. The water mockup is hydraulically similar to the potassium-cooled system. The major components of the system are the boiler, the vapor separator, the turbine pump, the condenser, and the jet pumps that provide boiler recirculation and scavenging of liquid from the condenser. Data are obtained from several instruments that monitor these major components during operation of the system.

A program has been written to extract from these data information concerning the flow characteristics of the jet pump, the performance of the turbine pump, and the quality of vapor in the boiler. These results will be used in the design of components and control schemes for the potassium-cooled systems.

Computer Monitoring of the MSRE

A Bunker Ramo 340 process-control computer will be used to monitor the Molten Salt Reactor Experiment. The primary purpose of the computer is to serve as a high-speed data logger and to relieve reactor operators from routine computations.

Signals from 274 instruments are available to the analog-to-digital converter of the computer. These signals, process variables, will be scanned and stored by the computer at least once every 5 sec. A permanent log of reactor performance is to be obtained by converting all the stored signals to engineering units and recording the results on magnetic tape every 10 min.

For the most part these operations use the input-output equipment; the central processor can be used for other purposes. Several subroutines will be executed during this time. These subroutines can be divided into two categories: those that make routine calculations and those that respond to interrupts.

The subroutines in the first category will be activated periodically, or by operator demand, or both. They calculate variables that are functions of process variables. The second class of routines are activated by interrupts occurring when process variables or computed variables fall out of prescribed limits. In general, response routines type alarm messages or increase the frequency of the scanning and logging of process variables.

Nondissipative, Vortex-Like, Magnetohydrodynamic Flow

The stability criterion for nondissipative, vortex-like, magnetohydrodynamic flow in an annulus, under an externally applied axial magnetic field, leads to an equation for the perturbation velocity which involves two coefficients and Bessel functions of the first and second kinds of real or imaginary order and real arguments. The boundary conditions of zero velocity on the annular walls lead to a transcendental equation of the Bessel functions. The first positive root of this transcendental equation is proportional to the magnetic flux for transition between stable and unstable flow.

An algorithm for calculating two real Bessel functions of imaginary order and real argument was devised. Programs were written to obtain the transition flux and to calculate and plot the perturbation velocity.

Fluid Flow Parallel to Rod Clusters

Laminar fluid flow parallel to clusters of rods enclosed in a cylinder occurs in some nuclear reactor fuel elements. The boundary conditions are such that no analytical solution for the velocity distribution has been possible. However, a satisfactory semianalytical method of solution has been found.

A general solution of the partial differential equation is determined first. Then as many coefficients as possible are determined by analytical means from conditions of boundaries coinciding with the coordinate system. Finally, the remaining infinite series is truncated to an arbitrary number of terms, and coefficients are determined that satisfy the remaining boundaries at arbitrary points.

Programs have been written to calculate the empirical coefficients and plot velocity profiles for clusters of rods with one rod concentric with the containing cylinder and the others at equal angles on a constant radius. Figure 2 is typical of the results obtained. The semicircular and lower radial boundaries were fitted analytically. Thirteen empirical coefficients were used for the remaining boundaries. The boundary conditions are zero velocity on the walls and zero velocity derivation normal to lines of radial symmetry.

Further work is planned for clusters with rods on as many as four concentric circles.

ORNL-DWG 65-329

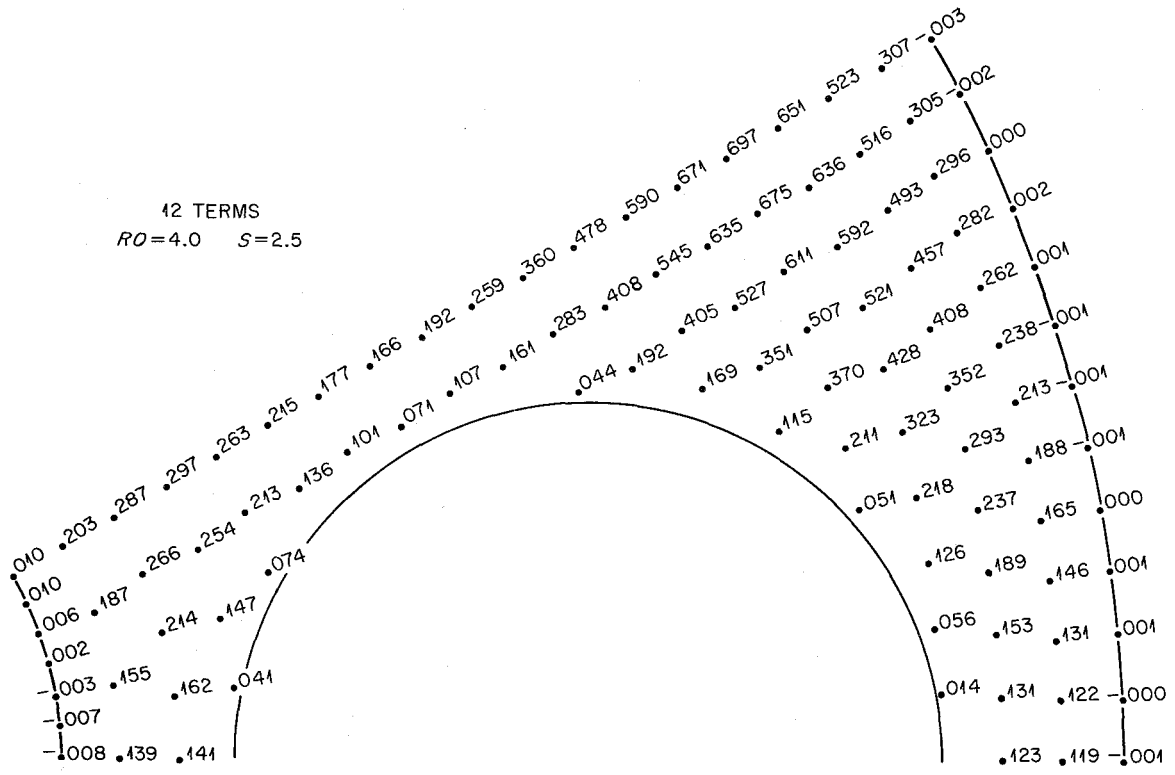

Fig. 2. Semianalytical Velocity in a Septafoil Cluster.

REACTOR CHEMISTRY

G. J. Atta
E. E. Branstetter
A. M. Craig
Judy J. Eatherly
M. T. Harkrider
Ruth B. Hofstra
A. R. Jenkins
R. L. Shively

Characterization of Volatile Radioactive Species by Composite Diffusion Tubes

A project has been undertaken in the Reactor Chemistry Division in the characterization of volatile radioiodine species by composite diffusion tubes. It centers around the automatization of certain parts of the data handling and the analysis of the results. Computer programs have been prepared to analyze and to resolve the radioactivity profiles resulting from deposition of iodine and iodine compounds in composite diffusion tubes. The depositions are from gas flowing through the tubes under laminar conditions. The composite diffusion tubes consist of consecutive segments of tubing having differing inner surfaces to distinguish among various iodine species. The overall objective is to identify and measure the different vapor forms of radioiodine encountered in certain problems connected with nuclear safety.

Linear Combinations of Exponentials

Diffusion tube data collected in the Reactor Chemistry Division may be represented by linear combinations of exponentials of the form

$$f(x) = \sum_{k=1}^{p} \alpha_k e^{-\beta_k x} .$$

If the empirical values of $f(x)$ are specified at n ($n \geqq p$) equally spaced points, then Prony's method[56] can be used to estimate the parameters α_k and β_k ($k = 1, 2, \ldots, p$). A computer program for this procedure has been written and checked out.

Physical Chemistry Studies for the MSRE

A study of the physical chemistry of the molten LiF-BeF_2 system (solvent in MSRE) included measurement of the formation of hydrolysis products and removal of these products by sparging with HF. Transpiration experiments were conducted in which H_2O or HF, or both, were passed through the melts in an H_2 carrier gas.

The experimental quantities measured were: influent pressures of HF and H_2O, $P_i(HF) = a$, $P_i(H_2O) = c$, and effluent pressures of HF and H_2O, $P_e(HF) = x$, $P_e(H_2O) = y$, at specified values of W (a function of volume of gas through melt and weight of melt). These quantities were measured at temperatures from 500 to 700°C and from 27.3 to 60 mole % BeF_2.

The expected hydrolysis products were oxide ions and hydroxide ions. Since these quantities cannot be directly determined by existing analytical chemical methods, a mathematical model was developed for their indirect determination from the experimental quantities measured.

Oxide and hydroxide could be formed by the following independent reactions:

$$H_2O\ (gas) + 2F^-\ (solution) = 2HF\ (gas) + O^{2-}\ (solution)$$

and

$$H_2O\ (gas) + F^-\ (solution) = HF\ (gas) + OH^-\ (solution).$$

Other reactions that might occur involving oxide and hydroxide can be shown to be combinations of these two. Equilibrium quotients for the above reactions are given by:

$$Q_0 = x^2 r/y \text{ and } Q_A = xs/y ,$$

where r = oxide concentration and s = hydroxide concentration.

According to the above reactions, the difference between the amounts of water entering and leaving the reaction system corresponds to the amounts of oxide and hydroxide added to the system (if reactions are

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[56]E. T. Whittaker and G. Robinson, *The Calculus of Observations*, pp. 369–71, Blackie and Sons Limited, London and Glasgow, 1944.

considered to be instantaneous). Expressed as an incremental change this would be

$$(c - y)\, dW = dr + ds\ .$$

Formation of hydroxide in the melt results in the removal of a corresponding amount of hydrogen from the gas stream. Expressed as an incremental change this would be

$$[(a + 2c) - (x + 2y)]\, dW = ds\ .$$

Estimates of the initial concentrations of oxide and hydroxide in the melt and for the reaction equilibrium quotients were made for each experiment and the above equations used in a least-squares fit of the data. The improved values of Q_0 and Q_A obtained from this treatment are further correlated as functions of temperature and composition of the LiF-BeF_2 system.

Release of Fission Gases

An active project of the Reactor Chemistry Division is the study of the kinetics of releases of fission gases.

A monocrystal of UO_2 is oscillated inside the ORR, and the transfer functions of the fission-gas release with respect to changes of both temperature and fission density level are measured.

A substantial part of the project is heavily dependent on the use of numerical results. To analyze the experimental data a Fourier analysis program has been developed which fits the sinusoidal temperature or flux input, as well as the fission-gas release, to a truncated Fourier series. The output of the program consists of the amplitudes and phase shifts of the various waves; this allows the study of the kinetic behavior of the fission-gas release.

In a parallel development several theoretical models to describe the observed phenomena have been programmed.[57] Much effort has been exerted on this aspect of the problem owing to the complication of the model. Therefore, a highly flexible set of codes that allow parameter studies have resulted.

Preliminary work has also been done in setting up a completely automatic process of data collecting and analyzing in order to cope with the expected increase in the amount of data to be analyzed in the near future.

SOLID STATE

C. W. Nestor, Jr.

Electrical Resistivity of Metallic Lithium Vapor

Programs were written to evaluate the momentum-space matrix elements of a pseudopotential describing a neutral lithium atom, to perform the numerical Fourier transform required to obtain the pseudopotential as

[57] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963*, ORNL-3567, p. 26.

a function of radial distance, and to solve the Schrodinger equation for the wave function of an electron in this pseudopotential. The scattering amplitude obtained from this wave function is then used in the calculation of the resistivity. In addition, by numerical solution of the radial Schrodinger equation containing the appropriate screened pseudopotential, a relation between scattering length and density may be found, which then can be used to estimate the density at which the system transforms from the metallic to the atomic phase.

SPECIAL ROUTINES

Susie E. Atta	C. T. McCracken
Margaret B. Emmett	J. E. Schmith
Manuel Feliciano	T. K. Teague
G. K. E. Haeuslein	T. C. Tucker

Subroutine INTRIGUE

An IBM 7090 subroutine package[58] has been written to facilitate the plotting of curves and points on linear, logarithmic, and semilogarithmic graphs using the Calcomp plotter. The subroutines accomplish the necessary computations and prepare a magnetic tape for use by the plotter. It has the same features as previously described for a 1604-A package.[59] The CDC 1604-A package can be supplemented by a subroutine which makes use of GREEK,[60] a subroutine for plotting Greek letters. Additional changes which have been made are explained elsewhere.[60]

A general-purpose program for making semilogarithmic plots for any set of data points has been written. It makes use of the plotting package described in ORNL-3447.[59]

Basic Plotting Package

The basic plotting package[60] was written in CODAP2 for the FORTRAN 63 library tape. Error diagnostics were incorporated, as well as features to accept the more flexible FORTRAN 63 language. The resulting subroutines are shorter and more efficient than their CODAP1 counterparts. This was accomplished by packing character-defining tables and deleting options rendered unnecessary by the compatibility of the two plotting systems. A significant effort was expended in aiding ORNL personnel of other divisions in changing FORTRAN 62 programs with plot-generating capability to the FORTRAN 63 language.

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[58] M. B. Emmett, *INTRIGUE, an IBM-7090 Subroutine Package for Making Linear, Logarithmic and Semilogarithmic Graphs Using the Calcomp Plotter*, ORNL-3581 (March 1964).

[59] D. K. Trubey and M. B. Emmett, *A CDC-1604 Subroutine Package for Making Linear, Logarithmic and Semilogarithmic Graphs Using the Calcomp Plotter*, ORNL-3477 (June 10, 1963).

[60] ORCID Memo No. 10 (revised) (Sept. 22, 1964).

A Subroutine for Plotting Greek Letters

A subroutine was written to enable users of the CDC 1604-A–Calcomp plotting package to call for Greek letters. The subroutine contains all lower-case Greek letters and those upper-case letters which are not identical to Latin letters.

Multiple Regression and Correlation

A general multiple regression and correlation program described in the BMD report[61] was converted for the CDC 1604-A computer. This program can handle up to 60 variables and gives summary statistics on the input variables as well as correlation and regression analyses. The program allows several options, among which is that of graphic output by means of the Calcomp plotter.

Special Functions

Several special functions have been coded and are now available in the computer library. The routines coded are: Romberg integration for single, double, and triple integration; Lagrangian interpolation for functions of single variables and Lagrangian bivariate interpolation; the exponential integral $[E_n(x)]$ for complex x and integer $n \geqq 1$; the Fourier transform of functions of pure parity with finite limit values at points of discontinuity; and evaluation of the generalized sine and cosine integrals $[S_i(x)$ and $C_i(x)]$ for real x. These routines were coded with the objective of minimizing the time used in computation while maintaining a sufficient degree of accuracy. In general, the user may supply the degree of accuracy needed for his computation.

Solution of Linear Equations

Subroutine MATQ, which solves systems of linear equations using the Gaussian pivot method, was rewritten in CODAP. This resulted in a reduction of execution times to a third of those used by the original FORTRAN version.

Subroutine for Solving Simultaneous Linear Equations

A program using Householder's[62] method for the numerical solution of the matrix equation $Ax = b$ and the value of the determinant of A was written in the FORTRAN language as a library subroutine.

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[61] *BMD Biomedical Computer Programs*, School of Medicine, University of California, Los Angeles (January 1964).

[62] A. S. Householder, "Unitary Triangularization of a Nonsymmetric Matrix," *J. Assoc. Comput. Mach.* **5**(4), 339 (1962).

COMPUTER OPERATIONS

C. S. Williams

The CDC Computers. – With the exception of the seasonal decline at the end of the year, use of the 1604-A computer increased steadily during the year, and the total hours of use was more than double the 1963 figure. Over 300 different users ran problems that required over 5500 hr of computer time.

Twice during the year (in June and September), the work load on the computer approached the saturation point, and additional shifts of operation on an overtime basis were frequently required throughout the year in order to meet the demand. In light of this situation, considerable study is being given to extending the scheduled operation from its present 15 shifts per week, and to the acquisition of a new computer with larger storage capacities and faster internal compute speeds.

The 1604-A computer has been "down," that is, unavailable for use because of machine malfunction, for a total of only 74.6 hr for the entire year. This total is only 1.2% of the scheduled productive time, and is an indication of the excellent performance and reliable operation experienced. Once again this year, the failure of a memory stack accounted for the largest single stretch of downtime, a 24-hr period in August. Figure 3 shows 1604-A productive time and downtime for the year. Experience for 1963 is

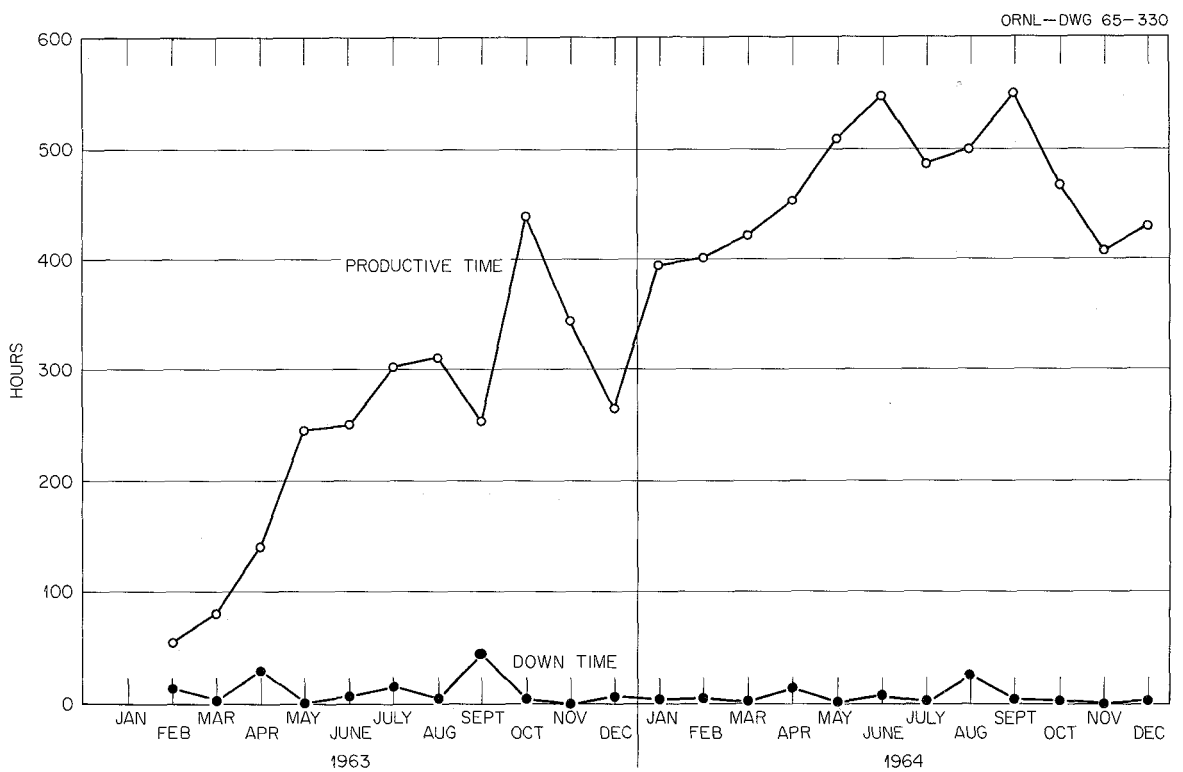

Fig. 3. CDC 1604-A Productive Time and Down Time.

included on the graph for comparison purposes. Figure 4 shows use of the 1604-A computer by various divisions.

The 160-A peripheral computer systems continued to function well. Almost all the downtime charged against the systems could be attributed to breakdown of electromechanical input/output devices rather than to any of the electronic components. Productive time and downtime for the two systems are shown in Table 2.

As more experience was gained in the use of the two peripheral systems, it became evident that both systems would not be required to stay abreast of the input/output requirements of the 1604-A. Even when the 1604-A ran continuously for 24 hr, the combined use of the 160-A systems did not approach three-shift operation. This can be attributed to the speed and input/output capabilities of a 160-A computer, and to the peripheral processing program which was written to take advantage of these capabilities. As was reported in the last report, this program allowed card-to-tape or tape-to-card operations to be performed simultaneously with tape-to-printer operations.

The conclusion was drawn that a single 160-A system, with the additional printer from the second system, would be capable of doing all peripheral processing. In July a modification was purchased which

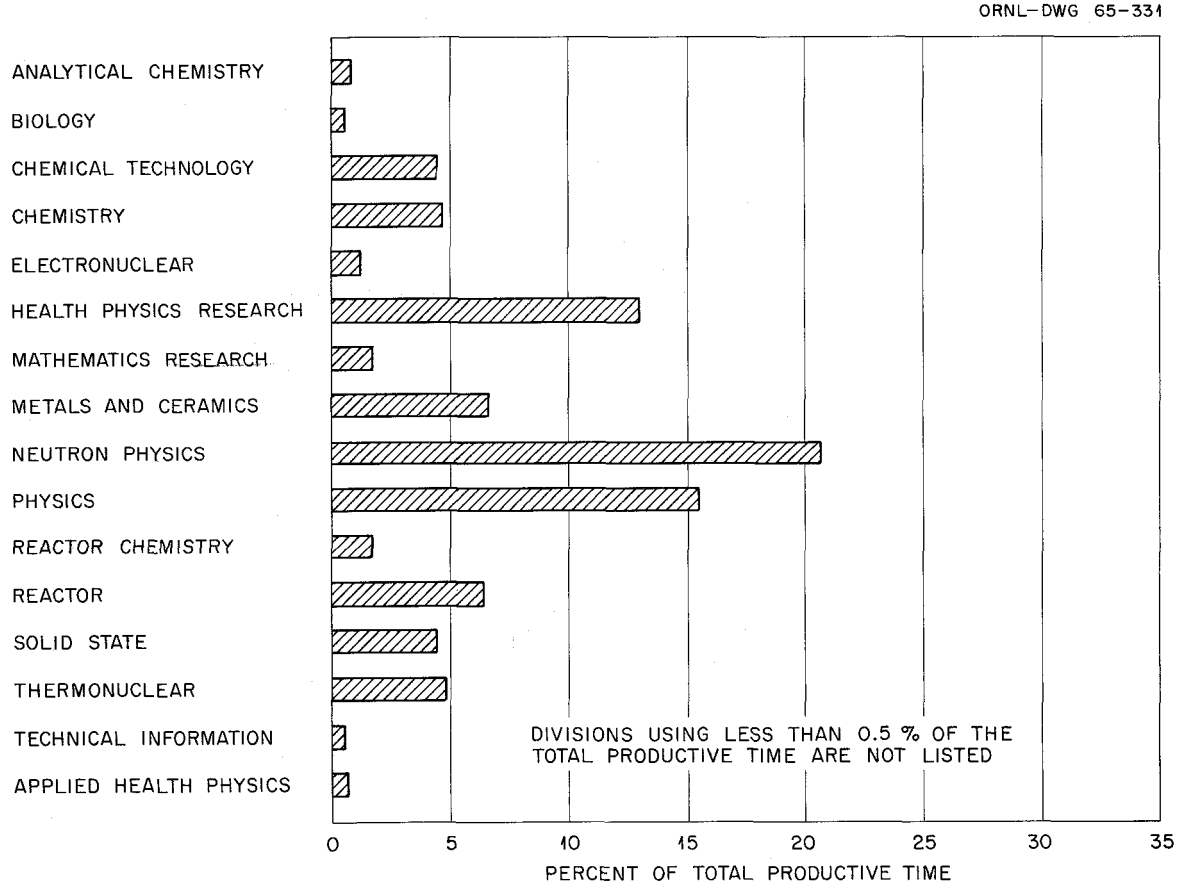

Fig. 4. CDC 1604-A Use by Divisions.

Table 2. Productive Time and Downtime for the CDC 160-A Peripheral Computer Systems

Month	System No. 1		System No. 2	
	Productive Time (hr)	Downtime (hr)	Productive Time (hr)	Downtime (hr)
January	189.7	10.4	172.8	0.7
February	179.9	5.7	119.6	2.8
March	213.4	6.4	126.0	0.0
April	240.8	1.3	85.0	0.0
May	238.1	1.0	121.6	4.1
June	228.6	2.3	149.1	6.9
July	298.5	5.1	88.3	0.0
August	333.7	2.9		
September	338.7	9.1		
October	326.0	0.5		
November	299.8	0.5		
December	308.3	0.1		

permitted a single 160-A computer to drive both printers; at the same time a 160-A computer, a 161 typewriter, and a 162-2 tape control unit were released. Since the released items had been rented, the release resulted in a reduction in operating costs and permitted a corresponding reduction in the rates charged for use of this equipment. The peripheral processing program was modified and extended so that a single 160-A can now print on both printers and, at the same time, perform a card-to-tape or tape-to-card operation. As the program now stands, any two peripheral operations may be performed simultaneously at full speed, while simultaneous printing on both printers plus a card operation proceeds at approximately 80% of the rated speeds. It is felt that the single CDC 160-A computer is now being utilized in a highly efficient manner, and at a lower cost to the user.

A great deal of maintenance has been required on the punches attached to the peripheral system. These units are quite old, and punching from them has at times been unreliable. Since Control Data Corporation has announced a new punch unit that is faster and more reliable than the present units, the decision has been made to rent one of these new punches and to release both the old 523 punches, the 088 reader, and the control unit for these devices. Delivery of the new punch is expected early in 1965. When the old card equipment is returned, there will be still a further reduction in operating costs for the peripheral system.

The monitor system in use at the ORNL Computing Center continues to give excellent service, permitting the "batching" of jobs to reduce the necessity of operator intervention. The principal compilers in use with this system are FORTRAN 63 and ALGOL. FORTRAN 62 is also available, and

some work is being done with the COBOL compiler. An average, for the year, of about 248 jobs per day flow through the center. Figure 5 shows this daily average by month.

The Digital Plotters. – The two Calcomp plotters discussed in last year's report continue to give satisfactory service, and their use has increased by at least a factor of 2, with a total of 5331 hr of use being accumulated during the year. Figure 6 shows use of the Calcomp plotters by month.

Operating Services. – All three operating sections were expanded during the year in order to provide more and better service to users at the Laboratory.

The setup section assumes responsibility for preparing and running computer problems of a routine nature for users at the Laboratory. In addition, this group handles all incoming work at the Computing Center, and expedites, as much as possible, the processing of work through the center.

The operating section operates the computer and associated peripheral equipment 24 hr a day, five days a week. Consideration is being given to extending this coverage by at least two additional shifts per week.

The key-punch section continues its function of providing keypunching and EAM services for the Laboratory.

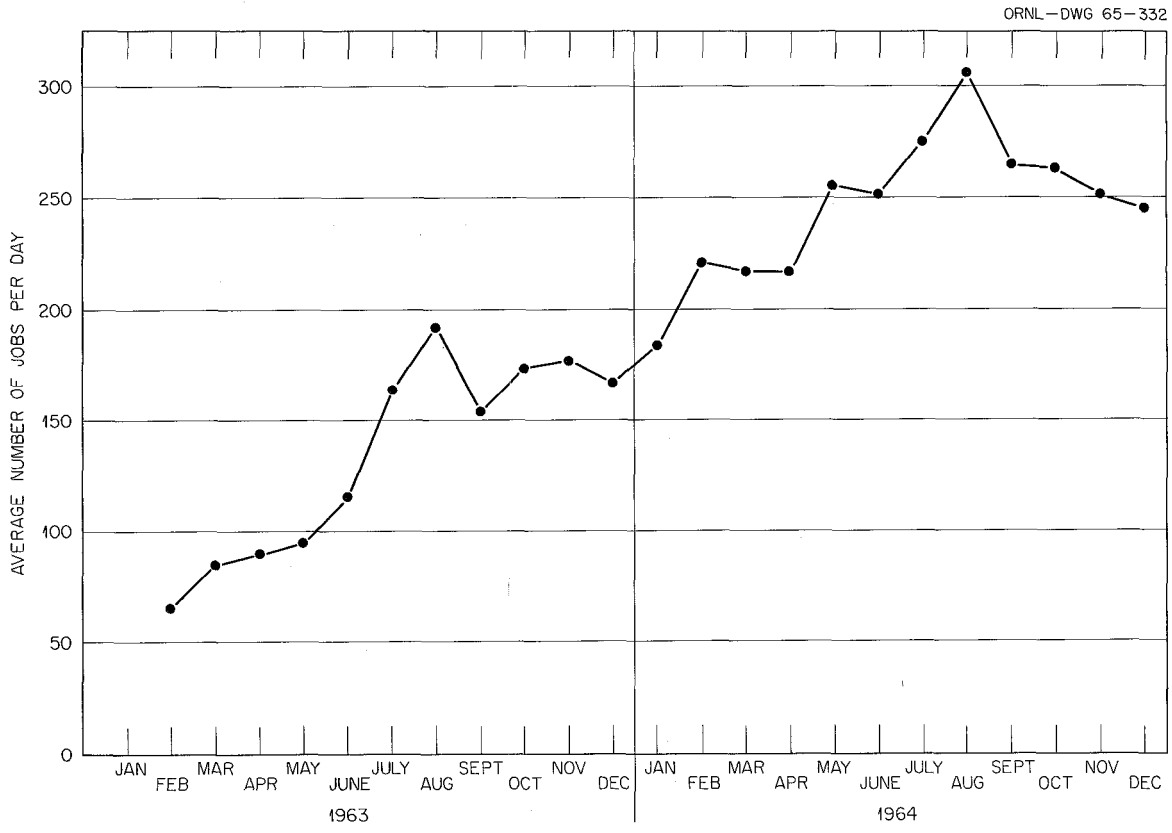

Fig. 5. Work Load at ORNL Computing Center.

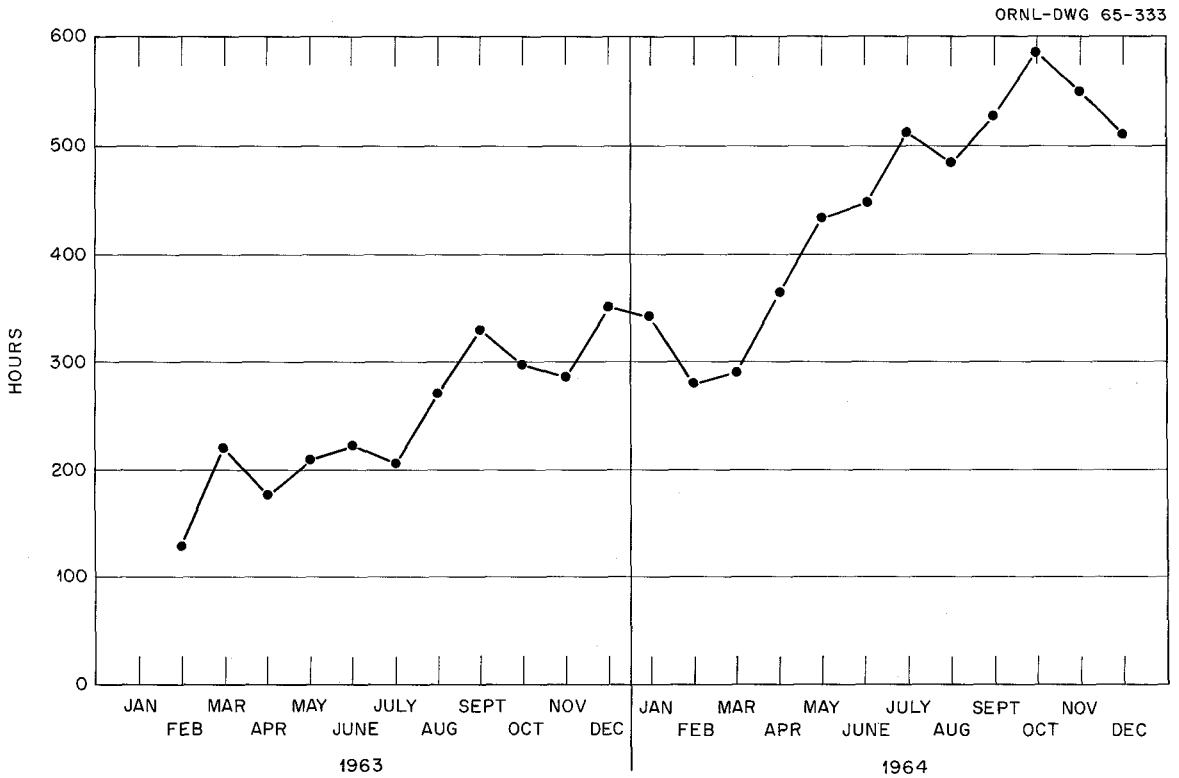

Fig. 6. Digital Plotter Use.

Mathematical Statistics

Barbara F. Bombay
D. A. Gardiner
D. G. Gosslee
T. L. Hebble
D. G. Hoel[1]
Norma C. Hull
D. R. Jensen[2]
M. A. Kastenbaum
E. Leach
H. L. Lucas[3]
F. L. Miller[4]
J. E. Parham
V. R. Rao Uppuluri
L. R. Shenton
F. W. Stallman[3]

[1]Temporary summer employee.
[2]Research participant.
[3]Consultant.
[4]On leave of absence.

Introduction

This report is a compendium of the more important projects participated in by members of the Statistics Group during the past calendar year. The Statistics Group, which has the responsibility for writing this report, is made up of five professionally trained statisticians, three persons qualified to program high-speed computers, a supervisor for a Data Recording Section, and three key-punch operators. The functions of this group and its history are covered in an earlier annual report.[1] The problems discussed in this report emanate in general from projects which have been undertaken by some of the divisions of ORNL. The report is therefore arranged alphabetically by division, by section within each division wherever possible, or by project within each division. Divisions included this year are Biology, Health, Health Physics, Metals and Ceramics, Reactor, and Reactor Chemistry.

The extent to which each project is reviewed depends on the amount of progress made during this report period. Discussions may include a statement of the physical problem as well as conclusions based on the statistical analysis of data. Alternatively, the physical problem may be formulated mathematically, and its implications may be discussed in terms of future investigation. In some instances where experiments have been planned, a brief review of the experimental design may accompany the conclusions. Wherever possible, statements concerning avenues and areas for future study are included.

Though the report is rather extensive, it does not touch on many of the projects in which the group participated. Careful documentation is not always desirable or possible even when a project is initiated and concluded to the complete satisfaction of both the principal investigator and the statistician. For example, projects which involve the numerical reduction of large quantities of data by standard computing techniques may not be reviewed. Moreover, many projects which require extended mathematical or probabilistic formulation may not have been pursued because of time considerations.

[1]*Math. Div. Ann. Progr. Rept. Dec. 31, 1963,* ORNL-3567, p. 33.

Many hours of thought and discussions were devoted to the study of stochastic processes by the senior members of this group. A concentrated study of this area of statistical research was needed because of the increasing number of Laboratory projects to which stochastic processes could be applied. As a result, a 16-hr lecture series on this subject was conducted by one member of the Statistics Group. Two specific topics in this area were emphasized: time series and finite Markov chains. Applications of some of the subjects covered in the lecture series may be found in the report.

Finally, a section on statistical programming is part of this report. Included in this section is a list of statistically oriented programs completed during this report period. A brief description accompanies each program title.

Statistical Research

FURTHER RESULTS IN THE COUNTERCURRENT DIALYSIS MODEL (A FINITE MARKOV CHAIN WITH ONE ABSORBING STATE)

The problem of separation of peptides from contaminating amino acids, sugars, and salts by countercurrent dialysis may be embedded in a Markov chain model as indicated by Kastenbaum.[2] He has also determined the probability distribution of the presence of the particle in any stage, given that it was initially in a certain stage.

Further results, which may also be applicable in the optimal design of any experimental setup of a separation problem, depend on the "fundamental matrix" of this absorbing Markov chain. This matrix was determined in a closed form, and the following random variables were studied:

1. n_j, the total number of times that the process is in state s_j,
2. t, the number of steps in which the process is in a transient state (or time to absorption),
3. M, the total number of transient states the process will ever be in, and
4. the probability that the process will ever go to transient state s_j starting in transient state s_i.

For systems with m stages ($m = 2, 3, 4, 5$), a numerical study was made with $p = 0.05\ (0.05)\ 0.95$, where p is the probability that a particle will remain in the dialysis sac. Moreover, certain interesting recursive relations between stages for a given time and between times for a given number of stages were studied in the case of two of the above random variables.

DECAY RATE AS A RANDOM VARIABLE

The decay rate in a model describing the disintegration of a radioactive element is treated traditionally as a nonrandom variable or as a parameter of the system. An entirely different complexion is thrown

[2]M. A. Kastenbaum, "The Separation of Molecular Compounds by Countercurrent Dialysis: A Stochastic Process," *Biometrika* 47(1&2), 69 (1960).

upon the problem when decay rate is considered to be a discrete random variable. Under this condition the limiting behavior of the mean and variance of the amount of the radioactive element in the system has been determined. This has immediate applicability to the two-compartment system considered recently by Bernard and Uppuluri.[3]

WEIGHTED LINEAR REGRESSION

Weighting by the inverse of the variance can cause problems in weighted regression analysis of mutation rate on radiation dose. Let a_i be the number of mutations observed among n_i animals at dose X_i, and let π_i be the true, but unknown, mutation rate at this dose. Assume that a_i is a Poisson random variable with expectation and variance equal to $\alpha_i = n_i\pi_i$. If $y_i = a_i/n_i$ estimates π_i, then its expectation $E(y_i) = \alpha_i/n_i$ and its variance var $(y_i) = \alpha_i/n_i^2$.

Weighted averages and weighted regressions of the random variable y_i have good statistical properties if the weights used are the inverses of the variances of the observations. Thus, $W(y_i) = n_i^2/\alpha_i$ would be the true weight associated with y_i. Unfortunately, in most practical problems the true values of the parameters are unknown. In the case of mutation rates, one might use the actual observations as estimators of the parameters, that is, $E(y_i) \doteq a_i/n_i$, var $(y_i) \doteq a_i/n_i^2$, $W(y_i) \doteq w_i = n_i^2/a_i$. However, if $a_i = 0$, this procedure leads to the unacceptable condition that $w_i = \infty$.

An alternative procedure is to use a set of weights each equal to the inverse of the variance of $\hat{y}_i$, where $\hat{y}_i = b_0 + b_1X_i$ is the mutation rate at dose X_i as estimated from the fitted regression. Starting with an arbitrary set of initial weights w_i^0, one estimates $\hat{y}_i^1 = b_0^1 + b_1^1X_i$ by weighted least squares. The second set of weights is formed by taking $w_i^1 = n_i/\hat{y}_i^1$. In general, after the jth iteration $w_i^j = n_i/\hat{y}_i^j$. The iteration continues until the weights in the $(m + 1)$st iteration are the same, to a desired degree of accuracy, as the weights in the mth iteration.

Statistical Applications

BIOLOGY

Cytology and Genetics

Paramecia subjected to radiation may have certain genetically controlled mechanisms permanently altered. In particular, the mechanisms under consideration are survival and growth, and temperature sensitivity. Following radiation treatments, autogamous reproduction is induced in each specimen, which then is subjected to environmental conditions favorable to asexual reproduction.

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[3]S. R. Bernard and V. R. R. Uppuluri, "A Two-Compartment Model with Random Variable Flows," *Health Phys. Div. Ann. Progr. Rept. July 31, 1964,* ORNL-3697, p. 193.

Genetic sites controlling the two mechanisms of interest are known to exist within each of two similar micronuclei within the one-celled animal. With a given radiation dose, alternations (mutation) of sensitive genetic sites within the micronucleus are assumed to be Poisson random variables. Similarly, mutations affecting the survival and temperature-sensitivity mechanisms are assumed to be Poisson.

With respect to survival and thermal mechanisms, one may recognize four exhaustive and mutually exclusive classes of outcomes. Then for n exautogamous descendants, the conditional probability of x_i (i = 1, 2, 3, 4) progeny of type i is a multinomial density function. Though the form of the joint marginal density function is intractable, expressions for the first and second factorial moments have been derived. Further study of this problem is contemplated. The objective is to make inferences about the parameters of the specified distributions. Work is continuing toward this end, along a route of indirect inference which has been proposed.

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The lack of interaction between x-ray- and neutron-induced chromosome breaks in *Vicia* has been attributed to the spatial relationships of chromosomal strands and the LET values of the radiations. Experiments were performed to demonstrate this interaction with combined x-ray and neutron irradiation. Regression analyses of data representing the proportion of aberrations as a function of dose indicated that x-ray data followed a quadratic model, $Y = b_0 + b_2X^2$, and neutron data followed a linear model, $Y = b_0 + b_1X$, "best." The adequacy of these models was gaged by tests of goodness of fit, and by whether or not the regression coefficients were significantly different from zero. Hypotheses of additivity (no interaction) were expressed in such a way that rejection implied nonadditivity (interaction), and acceptance implied additivity.

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Forward-mutation experiments on wild-type 74A *Neurospora* after treatment with different mutagens were carried out for the purpose of characterizing the purple colonies recovered by the direct method. The data collected in these experiments were numbers of *ad-3A* and *ad-3B* mutants resulting from treatments with different mutagens. One of the hypotheses tested was that the ratio of *ad-3A* to *ad-3B* mutants is the same regardless of mutagenic origin. Chi-square and partitioned chi-square tests were performed on the contingency table data. In general, the null hypothesis could not be rejected. Of further interest was a closer study of the degree of complementation among the *ad-3B* mutants. Tests applied to these data indicated that the proportion of noncomplementing *ad-3B* mutants differed with mutagenic origin.

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Chi-square tests of interaction in three-dimensional contingency tables were applied to data involving leaky *ad-3A* mutants in *Neurospora*. The application of this particular type of statistical technique has been hampered, until recently, by the need to solve simultaneous fourth-degree equations. A computer program to handle the numerical solutions for this problem was written several years ago for the Oracle. Unfortunately, no program exists for the modern generation of computers. Alternative tests of the same

hypothesis have appeared in the statistical literature in recent months. At least one of these requires very little numerical manipulation, and was therefore easily applied to the data on leaky mutants. It is important, however, that a computer program be written which, for any given set of data, will calculate the necessary test statistics using all the new techniques which have recently been proposed in the literature. Such a project will be undertaken by the Statistics Group during the next calendar year.

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The proportion of *ad-3* mutants of *Neurospora* has been observed to increase with increased doses of x radiation. Plots of these data on logarithmic paper suggested that the proportion of *ad-3* mutants was related to dose as $Y = \alpha X^{\beta_1}$ or $\log Y = \beta_0 + \beta_1 \log X$, where X is the dose in kiloroentgens. Preliminary plots further suggested that the value of β_1 was near unity. It was proposed, therefore, that the data be fitted by least squares for the purpose of testing the hypothesis $\beta_1 = 1$. Moreover, a value of $1 < \beta_1 < 2$ would suggest that mutants were being formed by both a one-hit and a two-hit mechanism. If so, a reasonable approximation to the dose-response relationship might be achieved with the model $Y = \beta_0 + \beta_1 X + \beta_2 X^2$. Least-squares estimates of the parameters in both these models were obtained by standard techniques of weighted regression analysis.

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Regression analyses were performed on data representing the proportion of *ad-3 Neurospora* mutants (reparable and irreparable) as a function of x-ray dose. The proposed model was $Y = \alpha X^{\beta_1}$, where X is x-ray dose in kiloroentgens and Y is the proportion of mutants. It was expected that the estimate of β_1 for reparable mutants would not differ significantly from 1, and that estimates of β_1 for irreparable mutants would not differ significantly from 2. Such conclusions would confirm the notion that reparable mutants result from one-hit events, and irreparable mutants from two-hit events. Analyses of the data generally confirmed these conclusions.

On the basis of these results, one could speculate that the proportion of reparable mutants would plot linearly with dose ($Y = \beta_0 + \beta_1 X$), and that the proportion of irreparable mutants would plot as a function of the square of the dose ($Y = \beta_0 + \beta_2 X^2$). These speculations were further confirmed by the data.

Finally, with the information that the proportion of irreparable mutants increases proportionately as the square of the dose ($Y = \beta_2 X^2$; β_0 is not significantly different from zero), it was reasonable to expect that the square root of the proportion of mutants increases linearly with dose. This point was also verified by the data.

Drosophila Cytology and Genetics

It has been conjectured that certain mutations observed in offspring of female *Drosophila melanogaster* result from alkylations on the DNA (deoxyribonucleic acid) strands in the zygote, which are induced by radiation or by chemicals. These alkylations remain with the strand on which they appear through each replication; that is, through each nuclear division of the zygote. It is known that after eight or nine divisions, some of the nuclei cluster at one pole, and that some of these pole cells develop into gonadal

cells. If the gonadal cells do in fact follow this pattern of development, then the observed proportion of mutants in the offspring should be related in some way to the number of mutations which result from alkylation-induced misreplications in the first eight or nine divisions of the zygote. It is important therefore to know initially the frequency distribution and the expected number of mutant cells in the zygote after the first n divisions.

Preliminary study of this question with the following set of definitions has already yielded some interesting results:

1. Generation "zero" represents the zygote. Thereafter, generation r consists of those nuclei which result from the rth division ($r = 1, 2, \ldots, n$). Thus, there will be 2^r nuclei in the rth generation.
2. A DNA strand with an alkylation may or may not misreplicate. If misreplication occurs in generation r, one hybrid will appear in generation $r + 1$, and one mutant will result in generation $r + 2$. The implication is that a misreplication in generation $n - 1$ will not produce a mutant in generation n. One hybrid will appear in generation n, but we *do not* propose to call it a mutant.
3. q is the probability of a misreplication at any division ($0 \leqq q \leqq 1$; $p = 1 - q$), due to an alkylation on one of the two DNA strands. If an alkylation appears on each of the two DNA strands in the zygote, then designate the probabilities of misreplication as q_1 and q_2 respectively ($0 \leqq q_1, q_2 \leqq 1$).

With these definitions, the expected number of mutations after n divisions is $(2^{n-1} - 1)q$, for an alkylation on a single DNA strand, and $(2^{n-1} - 1)(q_1 + q_2)$, for an alkylation on each of two DNA strands.

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In dealing with mutations in *Drosophila melanogaster*, it is of interest to know how one would test for differences in mutation rates if mutations occur in clusters. The inherent difficulty in this problem lies in estimating the variance of the mutant proportion. If m is the observed number of mutants, and f_i is the number of clusters of size X_i, then $m = \Sigma f_i X_i$, and var $m = \Sigma X_i^2$ var f_i. H. J. Muller has suggested that var f_i may be approximated by $f_i(1 - p)$, where p is the observed proportion of mutants. As might be expected, this approximation yields estimates of variance of the mutation rate which are higher than those for binomial rates. As a result, hypotheses concerning differences in mutation rates are less likely to be rejected, all other things being equal.

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A study was undertaken to investigate the response surface (percent survival) of *Drosophila* larvae as a function of dose of x ray and age. Little was known about the nature of this surface, other than the possible range of doses and ages which might yield the desired information. Consequently, a series of experiments was designed to be used in a sequential fashion in such a manner as to permit a decision before all the experiments had been completed. The series consisted of sets of points in the factor space selected so that the adequacy of the following responses to dose and age could be studied sequentially:

1. a linear function

$$Y = b_0 + b_1 D + b_2 A ,$$

2. a quadratic function

$$Y = b_0 + b_1 D + b_2 A + b_{11} D^2 + b_{22} A^2 + b_{21} DA ,$$

3. a cubic function

$$Y = b_0 + b_1 D + b_2 A + b_{11} D^2 + b_{22} A^2 + b_{12} DA + b_{111} D^3 + b_{222} A^3 + b_{112} D^2 A + b_{122} DA^2 ,$$

where $Y = \text{arc sin} \sqrt{p}$, p is proportion of larvae surviving, D is dose of x ray, and A is age of larvae.

The idea was to proceed sequentially as follows:

1. Fit the linear function. If the fit is adequate, stop; if not,
2. fit the quadratic function. If this fit is adequate, stop; if not,
3. fit the cubic function. If this fit is adequate, stop; if not, reexamine the experimental results to see if a more appropriate model is suggested by the data.

Third-order rotatable designs are a class of factorial designs. The property of rotatability, first advanced by Box and Hunter,[4] is desirable because the variances of least-squares estimates of the responses are constant on circles or spheres about the center of the design. In the present experiment, the range of doses was 600 to 1300 r of x ray, with center point at 950 r, and the range of ages was 1 to 5 hr, with center point at 3 hr. The three stages of the experiment were to be carried out sequentially at the following points in the factor space:

	Dose (r)	Age (hr)
Stage 1	600	3.0
	950	1.0
	950	3.0
	950	5.0
	1300	3.0
Stage 2	702	1.6
	702	4.4
	950	3.0
	1197	1.6
	1197	4.4
Stage 3	670	3.0
	729	1.7
	729	4.3
	950	1.4
	950	4.6
	1171	1.7
	1171	4.3
	1230	3.0

[4]G. E. P. Box and J. S. Hunter, "Multi-Factor Experimental Designs for Exploring Response Surfaces," *Ann. Math. Statist.* **28**, 295 (1957).

At each point in the factor space the number of surviving larvae out of 100 in each of three groups was to be determined. The analysis was then to be carried out on the inverse sine of the square root of proportion survival. This procedure allows for an independent measure of the variance based on the assumption of a binomial distribution of the variables. If radian measure is used for the angular transformation, the expected variance is $\sigma^2 = 25 \times 10^{-4}$.

Although the experiment was designed to be carried out sequentially in three stages, the investigator chose to complete all three stages before examining the adequacy of any of the successive models. In spite of this oversight, the data were analyzed as if they had been presented one stage at a time. The following conclusions could be drawn:

1. Stage 1: The estimate of the error mean square, with eight degrees of freedom, was 21.78×10^{-4}. This value is not significantly different from $\sigma^2 = 25 \times 10^{-4}$ (Prob. = 0.55). The theoretical variance was therefore used to test the goodness of fit of the linear model. This test indicated that the observations deviated significantly (Prob. < 0.001) from a linear model. Thus, it was decided that the data from the second stage of the experiment would be analyzed.

2. Stages 1 and 2: The estimate of the error mean square, with 18 degrees of freedom, was 29.41×10^{-4}, which is not significantly different from $\sigma^2 = 25 \times 10^{-4}$ (Prob. = 0.20). The test of goodness of fit using the theoretical variance indicated that the observations deviated significantly (Prob. $\cong 0.005$) from a quadratic model. It was decided, therefore, that the data from the third stage would be analyzed.

3. Stages 1, 2, and 3: This time the error mean square, with 33 degrees of freedom, was estimated to be 66.71×10^{-4}. This value is very definitely significantly different from the theoretical variance (Prob. $< 10^{-4}$). What has happened is that a source of variation other than binomial has been introduced into the data in the third stage of the experiment. That this is so is apparent in the variation among the proportions surviving at the same dose-age level of stage 3.

4. If the age of parents might be affecting the results in the third stage, as suggested by the investigator, then the third stage of the experiment should be completely repeated, controlling this extraneous source of variation. One wonders, however, why this variation was not apparent in the first two stages of the experiment.

5. A supplementary analysis was carried out on the data after three of the apparently aberrant observations in stage 3 of the experiment were discarded. Aside from the fact that a considerable amount of extra-binomial variation was eliminated by this procedure, the results of this analysis suggested that the response surface might not deviate from the proposed cubic function.

6. On the basis of these results, it is proposed that stage 3 of the experiment be repeated using the points listed below as experimental points in the factor space.

Proposed repetition of stage 3: Because of the slight error in arithmetic, the experimental points chosen in the first attempt at stage 3 were wrong. A slight change in the coordinates of these points, as well as the addition of a point at the center, may be noted in the proposed list of new points as follows:

Dose (r)	Age (hr)
618	3.0
715	1.7
715	4.3
950	1.1
950	3.0
950	4.9
1185	1.7
1185	4.3
1282	3.0

Pathology and Physiology

Young adult female mice were exposed to 14-Mev neutrons from a Cockcroft-Walton accelerator. Five groups totaling 1765 mice were exposed to 0, 50, 100, 200, and 400 rads respectively. The mice were returned to the colony and maintained until natural death, when they were necropsied and all pathological findings were recorded.

The age of death was also recorded, and mortality curves were estimated by least squares for each exposure group, as well as for subgroups divided on the basis of pathological findings.

Tests of hypotheses were also made on the effect of exposure to mean age of death and to the incidence of various conditions according to the pathological findings. Analysis of the hematology data is in progress.

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The maturation process of megakaryocytes, the cells of the bone marrow from which blood platelets arise, is not well understood. It is generally accepted that nuclear division occurs without cytoplasmic division during megakaryocyte maturation, with the result that nuclei of mature megakaryocytes contain several times the normal diploid chromosome complement of the species. Since it has been difficult to group megakaryocytes into maturation stages based on their appearance under the light microscope, it seemed that measurement of the amount of DNA (deoxyribonucleic acid) in each megakaryocyte might provide a systematic means of classification. With such a method, additional insight into the maturation process of megakaryocytes may be gained, and a clearer assessment of effects of various experimental or

disease-related perturbations of the megakaryocyte-platelet system may be possible. The DNA of 1383 megakaryocytes from seven animals has therefore been measured microspectrophotometrically.

The data thus consist of estimates of DNA content in each of several hundred megakaryocyte cells for each rat. The estimates of DNA for these animals were analyzed as a series of four Gaussian distributions. Since the DNA content is expected to double from stage to stage, and the variance is assumed to be constant in each distribution, six parameters determine the function:

$$F = b_3 \exp\left[-(X - b_1)^2/b_2\right] + b_4 \exp\left[-(X - b_1 - 0.3)^2/b_2\right] + b_5 \exp\left[-(X - b_1 - 0.6)^2/b_2\right] + b_6 \exp\left[-(X - b_1 - 0.9)^2/b_2\right],$$

where $X = \log \text{DNA}$, $b_1 = \log$ (mean of the first distribution), $b_1 + 0.3 = \log$ (mean of the second distribution), $b_2 = 2 \times$ variance, and b_3, b_4, b_5, and b_6 are proportional to the areas under the corresponding distributions. The parameters were estimated by nonlinear search techniques.

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The RNA (ribonucleic acid) chain is formed by repetition of four basic units (mononucleotides) into a chain several thousand units in length. The ordered sequence of the units contains the information necessary for the synthesis of proteins and ultimately the function of the cell. These nucleotide sequences, or codes, cannot be determined directly, but the relative proportion of several di- and trinucleotides and the percent of each nucleation in the RNA chain can be determined. It was of interest to discern if the observed frequencies of several di- and trinucleotides differed from predicted frequencies.

The sequence, u_n, u_{n+1}, u_{n+2}, of three units is defined as the nth trial in a Markov chain, and is classified as one of the states of the system.

A Markov chain with four states was derived from a model based on biological information relating to cell messenger RNA, viral RNA, and ribosomal RNA. The predicted frequencies differed considerably from the observed frequencies. Therefore, a model based on more than four states will be derived considering additional biological information. That is, additional restrictions will be placed on the occurrence of certain sequences.

An illustration of the four-state model will be given for only one of the sequences of three units of interest. Let a, b, c, and d be known proportions of the total number of units of the nucleotides guanine (A), adenine (B), uracil (C), and cytosine (D). The sequence CBD could not be distinguished from the sequence DBD. It is convenient to let $E = C \cup D$ and also let $F = A \cup B$ and $X = E \cup F$ and consider the occurrence of the sequence EBD. Then the following four states are disjoint and complete: (1) EBD, (2) $XXE - EBD$, (3) XEB, and (4) $XXF - XEB$.

The transition matrix is

$$A = \begin{bmatrix} 0 & c+d & b & a \\ 0 & c+d & b & a \\ d & c & 0 & a+b \\ 0 & c+d & 0 & a+b \end{bmatrix},$$

and for $n > 2$,

$$A^n = \begin{bmatrix} bd(c+d) & (1-bd)(c+d) & b(c+d) & a+b(a+b) \\ bd(c+d) & (1-bd)(c+d) & b(c+d) & a+b(a+b) \\ bd(c+d) & (1-bd)(c+d) & b(c+d) & a+b(a+b) \\ bd(c+d) & (1-bd)(c+d) & b(c+d) & a+b(a+b) \end{bmatrix}.$$

Thus, the probability of being in state 1 at trial n is $bd(c+d)$, when $n > 2$. If N is the length of the chain, the numbers of occurrences at $n = 1$ and $n = 2$ are of order $1/N$ and can be ignored. Thus, the expected number of occurrences of EBD can be expressed as $Nbd(c+d)$.

The occurrences of other sequences, such as ABC, EAC, and XED, were predicted in a similar manner.

Cell Growth and Differentiation

In an effort to observe the mechanism of primary embryonic induction, RNA synthesis occurring in the ectoderm of *Triturus pyrrhogaster* was studied with autoradiography. The ectoderm was isolated from the early gastrula and separated into two halves. One half of the ectoderm was fused to a piece of the dorsal mesoderm to serve as the experimental explant; the other half was used as a control. The explants were placed in ^{3}H-uridine for 3 hr, after which they were fixed for autoradiography. This experiment was replicated several times. Grain counts per unit nuclear area were made in both the experimental and control ectoderm for each replicate.

In testing the hypothesis of equal average grain counts in the control and experimental groups, the data were handled in two ways. For each replicate, an analysis was made on the grain count data as if they were observations on continuous Gaussian variables. Then a similar analysis was made using the square roots of the grain counts on the more tenable assumption that they were more likely to be Poisson variables. In all cases, the results of the tests of hypothesis were the same for the transformed data as for the untransformed grain counts.

Mammalian Genetics

Mammalian geneticists have been concerned for many years with the question of radiation-induced mutations in mice. Studies of seven specific loci have revealed that the mutation rate for unirradiated mice is approximately 5×10^{-5}. Thus, the number of mutations which occur spontaneously or which are induced by radiation may be considered to be a Poisson random variable. Experimentation has yielded a range of mutation rates for differing doses of radiation. These mutation rates may be looked upon as the expectation of Poisson variables. It is therefore of interest to the experimenter to know how to test the hypothesis of equality of two Poisson means.

Three approaches, all of which are asymptotically equivalent, have been suggested for analyzing these data:

1. A chi-square test for data in a 2×2 contingency table. The observations are classified as mutants or nonmutants in each of two samples. The square root of chi-square with one degree of freedom is a normal deviate, so that tabulated values are available for this test.
2. The normal approximation to the binomial. Here, the probability of interest is that of observing a_1 or more mutations in a total of $(a_1 + a_2)$, given that the true proportion of mutations is $n_1/(n_1 + n_2)$.
3. The "Birnbaum test."[5] If complete tables of the binomial distribution are not available, this procedure could entail several approximations. Therefore, a short computer program has been written which will evaluate the quantity

$$\alpha = \sum_{r=0}^{a} C_r^n (1-p)^r p^{n-r} = \sum_{r=n-a}^{n} C_r^n p^r (1-p)^{n-r} ,$$

for values of $0 < a \leqq n \leqq 1000$, and $0 < p < 1$.

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Skeletons of n_1 unirradiated and n_2 irradiated mice were examined for class-2 abnormalities. Totals of a_1 and a_2 skeletal abnormalities were observed in these respective groups. If the occurrence of abnormalities is equally likely in both groups, then one might expect the proportion of abnormalities in the irradiated group (say) to be equal to the proportion of irradiated animals in the experiment. The "Birnbaum test" was used to test the hypothesis that the proportion of abnormalities was the same in the irradiated and unirradiated groups.

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The relative biological effectiveness (RBE) of neutrons to x rays was estimated by the relative survival of type A spermatogonia in mice. The routine estimate of RBE was complicated by contamination due to gamma rays and by deviation of the response from an exponential survival curve. A correction for contamination in the total dose due to gamma rays was derived. A preliminary analysis of the data was obtained by estimating RBE's and their confidence limits at specific survival points.

A statistical method of estimating a general RBE for this situation was suggested in discussions with the investigator. The survival curves are indicative of a sum of exponentials rather than a single exponential. Even though the basic definition of the RBE is rather complicated in this situation, research on a method of estimating it should be conducted.

Cytochemistry and Cell Reproduction

The spatial distribution of cells which divide and synthesize DNA (deoxyribonucleic acid) in mouse epithelium was investigated by utilizing ^{3}H-thymidine autoradiography and colchicine techniques. To derive the statistical distribution, it was first assumed that every cell in the germinal layer of an epithelium

[5]Allan Birnbaum, "Statistical Methods for Poisson Processes and Exponential Populations," *J. Am. Statist. Assoc.* **49**, 254–66 (1954).

has the same probability of being in division. This assumption leads to a random spatial distribution of dividing cells in the plane of the germinal layer and in cross sections of that layer. The distribution of distances between dividing cells in a cross section would thus be described theoretically by the geometric distribution. The distance between dividing cells is measured by the number of intervening nondividing cells. This discrete measure accounts for the use of the geometric distribution in place of the corresponding continuous "waiting time" distribution, the exponential.

The class with zero distance between dividing cells is inflated by the failure of the cells to separate after division with a probability equal to 1. This separation is actually assumed to occur according to the binomial distribution. Thus, a complete model would be a compound distribution of a binomial and a geometric distribution. A truncated geometric distribution, omitting the zero class, has been fitted to the data in order to test hypotheses concerning the investigation and as a step toward formulation of the complete model.

Human Cytogenetics

In a study involving human karyotypes, data on the length of chromosome arms were collected in an effort to estimate the errors of measurement attributable to various sources. A total of 11,040 measurements were made by three technicians, using two different methods of measurement on the four arms of 46 chromosomes in each of ten leukocytes of one human female. A detailed analysis of variance was done for the primary purpose of estimating the components of variance. Because of the large numbers of observations available in this experiment, it is reasonable to assume that "good" estimates of certain of the variance components were achieved. Moreover, this analysis confirms the suspicion that almost all sources of variation, such as chromosomes, cells, technicians, methods, etc., and their interactions, contribute significantly to the differences in the means of chromosome lengths.

Further analyses of these data are being contemplated so that a simultaneous confidence region may be placed on the mean lengths of the long and short arms of each chromosome in a cell. This confidence region takes the form of an ellipse in the plane of the long-arm and short-arm means. There will be one ellipse for each chromosome, with center at the point specified by the mean length of the long arm and mean length of the short arm. When all ellipses are plotted on the same graph, the overlap will be some indication of the inability (using present techniques) to tell one chromosome from another solely on the basis of length measurements.

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Chromosome-type aberrations induced by 2.5-Mev neutrons in humans have been observed to be functionally related to the dose of neutrons. Irradiated blood samples from five humans were analyzed for deletions, rings, and dicentrics. These data were examined for homogeneity among the five humans; the deletion data and the data on rings and dicentrics were then fitted by least squares to the model $Y = \alpha + \beta D$, where Y is the number of aberrations per cell, and D is the dose of neutrons.

The same dose of radiation of different types may affect living organisms with varying degrees of severity. It is important, therefore, to define a term such as "relative biological effectiveness" (RBE), which

is merely the number of units of type I radiation which yield the same response as *one* unit of type II radiation. The RBE is usually estimated from the ratio of slopes of two fitted linear regressions. If the doses of the two types of radiation are known precisely, and the dose response curve is linear, there is no difficulty in estimating the RBE. Because of the physical limitation of certain radiation sources, however, the apparent total dose of type II radiation may be a mixture of both type I and type II radiation. For instance, a dose of 100 rads of neutrons from a neutron source might really be 90 rads of neutrons and 10 rads of gamma rays. If an estimate of the RBE of neutrons to gamma rays is being sought, such a confounding of radiation types may cause some difficulties. Several techniques have been developed to overcome these difficulties.

Mammalian Recovery

A series of experiments has been designed to determine the possible interaction of variables that have been known or suspected, in the past, to have an influence on mortality from secondary disease. Preliminary discussions of the details of these experiments are available elsewhere.[6–8]

The first series of experiments was designed as $\frac{1}{2}$ replicates of 2×2^3 factorials with two center points. Each treatment combination was applied to three cages of approximately five animals per cage, and the whole experiment was repeated four times. The total number of mice in the experiment was approximately 600.

By the nature of the experimental design, all sums of squares involving curvature were confounded. With appropriate adjustments, however, orthogonal partitions of the sums of squares could be achieved. Results of the analysis indicated:

1. 30-day mortality: A highly significant difference between the 0- and 90-day groups and between the 10 and 50×10^6 levels of dose, as well as a highly significant interaction of age and dose. Mortality at 30 days was higher in the low-dose group than in the high-dose group. Mortality at 30 days was higher in the group receiving younger donor tissue than in the group receiving tissue from 90-day-old donors. The interaction is evidenced by a sharper increase in mortality between 90-day donors and 0-day donors for a cell dose of 10×10^6 than for a cell dose of 50×10^6. A highly significant curvature effect results from the fact that the lowest mortality was observed at the center point of the experiment.
2. 60-day and 90-day mortality: Although the significant effects due to age of donor which were observed at 30 days disappeared, significant differences in 60-day and 90-day mortality were apparent in the effects due to dose, age $\times$ dose interaction, and curvature.

The second series of experiments was designed as a 2×2^3 factorial laid out in two blocks with four center points. The analysis of data representing five animals per cage and six cages per treatment combination indicates that the variability from cage to cage is more than might be expected on the assumption

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[6]C. C Congdon, *Biol. Div. Semiann. Progr. Rept. Feb. 15, 1964,* ORNL-3601, p. 116.
[7]C. C Congdon, *Biol. Div. Semiann. Progr. Rept. Aug. 15, 1964,* ORNL-3700, p. 101.
[8]*Math. Div. Ann. Progr. Rept. Dec. 31, 1963,* ORNL-3567, p. 41.

that the number of animals dying in a cage is purely a binomial variable. That is, the variation in mortality among cages within the same treatment group is more than might be expected by chance. We may conclude, therefore, that there is a "cage effect" in the sense that the death of a mouse in a cage is not completely independent of whether his cage mates are alive or dead. This condition is apparent at 30, 60, and 90 days; the probability associated with the test of hypothesis is less than 10^{-4}.

Having arrived at this conclusion, one further concludes that the among-cages mean square with 100 degrees of freedom is the appropriate estimate of error variance for this experiment. Variance-ratio tests based on this conclusion yield the following results:

1. There is significant interaction effect of cell dose and day of injection on 30-, 60-, and 90-day mortality. Examination of the means indicates that 10×10^6 cells injected on the third day results in a higher mortality than the same dose injected on day 0. Conversely, 50×10^6 cells injected on day 0 results in a higher mortality than the same dose injected on day 3.
2. There is a significant increase in mortality at 90 days when the age of donor is increased from 7 to 91 days. One may not conclude, however, that this increase is linear or even monotonic. In fact, the center point of the design indicates that under different conditions of cell dose and day of injection, the 30-, 60-, and 90-day mortality at the 45-day-old-donor point is smaller than at the 7- and 91-day-donor points. This is reflected in the significant effect of curvature in the 60- and 90-day mortality analyses.
3. No other significant effects on mortality of the factors considered in this experiment or of their interactions are indicated.

In the third series of designs, two new levels of age of donor (14 and 21 days) were considered; the levels of the other factors were the same as in the second series. These data were then combined with the 7-day data from the second series to make up a $2 \times 2^2 \times 3$ factorial with two center points. Each treatment combination involving the new levels of age was applied to three cages of about 5 animals per cage, for a total of approximately 270 mice. The total number of mice, including 7-day data, was about 510.

As was the case with the second series of experiments, analysis of the data from the third series indicated that the cage-to-cage variability was significantly higher than might be expected on the assumption that the number of animals dying in a cage is purely binomial. Therefore, the among-cages mean square with 76 degrees of freedom was taken as the estimate of the error variance for this series. Variance-ratio tests yielded the following results:

1. A significant effect of curvature on 30-, 60-, and 90-day mortality. This effect, which is consistent in all three series of experiments, indicates that there is evidence of reduced mortality when a cell dose of 30×10^6 cells is injected at 1.5 days. Indications are that the "best" response (in terms of reduced mortality) occurs when 30×10^6 cells from a 14-day-old donor are injected at 1.5 days. Perhaps further investigation of this segment of the factor space is in order.
2. There is a significant interaction effect of sex and age of donor on 30-, 60-, and 90-day mortality. For males, mortality is low for 7- and 21-day-old donors and high for 14-day-old donors, whereas for females, mortality is high for 7- and 21-day-old donors and low for 14-day-old donors. This phenomenon would show up as an interaction of sex and age on mortality.

3. There is a significant interaction effect of cell dose and day of injection on 60-day mortality. This might be attributed to a difference in percent mortality resulting from 10×10^6 cells given at 0 and 3 days after injection, which is not evident when the cell dose is 50×10^6 cells.
4. There is a significant effect of age on 90-day mortality. The data indicate that mortality at 90 days increases sharply as the age of donor increases to 21 days.

Proposals for future experiments and analyses:

1. A complete analysis of all the data from the second and third series of experiments might be carried out. This analysis would be considerably simplified if the observations at the center points are eliminated. The experimental design, consisting of all points aside from the center points, is a $2 \times 2^2 \times 5$ factorial.
2. Further studies of the response (mortality) in that segment of the factor space which was taken as the center point are suggested by the reduced mortality which was consistently observed for 30×10^6 cells injected at 1.5 days.
3. An examination of the standard deviations measuring cage-to-cage variability at the several points in the experimental design might cast some light on this consistently occurring phenomenon.

Chemical Co-Carcinogenesis

Discussions continued concerning the required sample for the co-carcinogenesis study. The phase of the overall study which was discussed deals with the induction of virus in mice of a resistant strain which have been subjected to various insults of radiation or chemicals. The total number of mice to be studied in this experiment was predetermined by the extent of available facilities. These facilities include six chambers, each with a capacity for housing approximately 440 mice in 44 cages of 10 mice per cage.

The factors under consideration include three atmospheric conditions (ozone gas, dust, and clear air), presence or absence of radiation, and presence or absence of a specific virus.

The resulting 12 treatment combinations will be assigned to the six chambers as follows:

Chamber	Treatment Combinations
1	Ozone gas Ozone gas plus radiation
2	Ozone gas plus virus Ozone gas plus virus plus radiation
3	Dust Dust plus radiation
4	Dust Dust plus virus plus radiation
5	Clear air Clear air plus radiation
6	Clear air plus virus Clear air plus virus plus radiation

There will be 22 cages of 10 mice per cage for each of the 12 treatment combinations.

In discussing the serial studies of the 2640 mice in this phase of the experiment, it was agreed that

1. a sample of one animal per cage, chosen at random and replaced in his cage after examination, would be adequate for determining the degree of bacterial and parasitic infection in each chamber; the frequency of this type of sampling and examination would be once in 4 to 6 weeks,
2. a sample of two animals per cage, chosen at random and replaced after examination for viral infection (mouth swab), is necessary to estimate a 50% incidence of viral contamination within ±10%,
3. no decision was made concerning serial sacrifice studies for tumor induction or viral infection.

Biophysics

Radiation of a particular substance may produce as many as three radical species (denote concentrations by X, Y, and Z) with measurable electron spin resonance (ESR) properties. Reactions occur among these radical species, forming new molecular species without the ESR property. Thus the total number of particles with the ESR property diminishes through time as the reactions proceed.

Consider a system in which two radical species X and Y are produced. Suppose $X + Y = N$, the total number of particles with ESR property. Possible reactions are

$$X + X \longrightarrow M_1 \text{ and } Y + Y \longrightarrow M_2 ,$$

where M_1 and M_2 are new stable molecular species. In the case of these reactions, the concentrations are known to change with time (t) according to the laws

$$dX/dt = aX^2 \text{ and } dY/dt = cY^2 ,$$

where a and c are negative rate constants. Solutions of these differential equations are

$$1/X = -at + \alpha_1 \text{ and } 1/Y = -ct + \alpha_2 ,$$

where α_1 and α_2 are arbitrary constants. Rate constants are generally known to be exponential functions of temperature. Therefore, the following relationship suggests itself:

$$N = X + Y = (\alpha_1 + \beta_1 te^{-\alpha_1/\theta})^{-1} + (\alpha_2 + \beta_2 te^{-\alpha_2/\theta})^{-1} ,$$

where θ is temperature and $a = -\beta_1 e^{-\alpha_1/\theta}$, $b = -\beta_2 e^{-\alpha_2/\theta}$. This model failed to adequately describe the observed relationship between N, t, and θ. This fact tends to discount assumptions made concerning the mode of the reaction.

Suppose the following reactions occur simultaneously:

$$X + X \longrightarrow M_1,\ Y + Y \longrightarrow M_2,\ X + Y \longrightarrow M_3 .$$

Then the following differential equations are known to characterize time rates of change of radical species X and Y:

$$dX/dt = aX^2 + bXY, \; dY/dt = bXY + cY^2 .$$

Simultaneous solution of this pair of equations is a key to the form of the function $N(t)$. Work is progressing in this direction.

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A "spot" theory has been proposed to explain degradation in irradiated DNA strands. Suppose random spots of two types are placed on each of two DNA strands with equal probability. The first type, black, occurs with probability p, and the second type, red, with probability $(1 - p)$. After the spots are randomly placed on the two strands, degradation occurs in a fixed direction along a strand from each black spot until a red spot is encountered. The problem is to find the total expected amount of degradation.

This problem has been solved for two cases, that is, for a pair of linear strands and for a pair of circular strands. If N is the total number of spots on the two strands, then the expected fraction of degradation is

$$p\left[1 - \frac{2}{N+1} + \frac{1}{2^N(N+1)}\right] \text{ for linear strands,}$$

and

$$p\left[1 - \left(\frac{1}{2}\right)^N\right] \text{ for circular strands.}$$

As $N \longrightarrow \infty$, the expected fraction tends to p in both cases.

Biomedical Data Recording

During this report period major emphasis was placed on establishing a method for recording and processing the anticipated large volume of data that will result from the study in the Biology Division of low-level, long-term effects of radiation on mice. The initial problem was to handle the breeding data from this experiment. As the experiment progresses, it will be necessary to add to the system other forms of data which will be collected by the Pathology and Physiology Section.

One of the most difficult aspects of data storage and retrieval in the low-level study has to do with the encoding of pathological findings. Experience in this area is rare, but it does exist at some medically oriented institutions in this country. One such school is Western Reserve University, where computer techniques have been devised for automatic retrieval of autopsy diagnoses. A cooperative program has been instituted with members of this university to determine if their techniques will satisfy the needs of the Biology Division.

Aside from the technical aspects of the experiment, there are many mundane logistical problems. These will include expansion from a few breeder animals to several tens of thousands of animals, which

will be maintained behind a limited-access barrier in a relatively pathogen-free environment. Not only is information to be kept on the progeny, but data about the progenitors must be maintained. At some stage of the experiment, mice will be taken from the breeder colony and moved to other rooms to become experimental animals. Factors affecting the development of the experiment are average litter size, date of delivery, fertility, mortality, and sacrifice of mice in litters.

As the experiment continues, the investigators will want reports informing them of the status of active breeders to include animal number, date of birth, mating date, room number, number of litters born, number of animals born and weaned by sex, average number per litter born and weaned, and average weight at weaning. Also, historical information is desired about the retired and dead breeders. The records system should provide data concerning potential breeders.

It is expected that annual summaries will also be required summarizing such information as variation of litter size with month of the year, variation of litter size with parity, and variation of productivity with maternal parity, year of birth, generation, and location or room number.

A decision was made toward the end of 1963 to install, on a trial basis, an IBM 357 data collection system to record the large volume of data being generated in the Biology Division. The system, at the present time, consists of an IBM 026 card punch, an IBM 358 input control unit, and two IBM 357 input stations. The first two pieces of equipment are located in the Biomedical recording area and the two input stations are two floors above in the Pathology and Physiology Section. Input to the system is by punched cards, punched badges, and manual entry devices. Output from the system is punched cards. Transactions being made routinely are for mating, birth, weaning, cage assignment and weighing, room change for breeders, radiation, missing mouse, death, kill, take out of laboratory, and terminate record. A considerable amount of computer programming has been done, but the programs are incomplete at this time.

An input station has been ordered for the Cooperative NIH-AEC Chemical Co-Carcinogenesis Inhalation program. This experiment is discussed above in the section entitled "Chemical Co-Carcinogenesis."

Input stations are contemplated for the Mammalian Recovery Section and the Experimental Animal Facility, provided the operational experience with the system is satisfactory.

HEALTH

A pilot study was undertaken several years ago to evaluate the cancer frequency at ORNL. Although the likelihood of obtaining significant results from it was small, this study was justified on the theory that the experience and techniques developed through it would be useful for future, more extensive studies at other atomic energy installations.

The acquisition of data from employees who were currently on the payroll presented no problem. However, pertinent information about former employees was not readily available. To get this information would require assistance from the local payroll department as well as cooperation from state and federal agencies.

It was hoped that the Bureau of Old Age and Survivors Insurance (BOASI) could indicate if a person with a specific social security number were alive or dead. If dead, this agency would have some record about the particular state public health department in which the death certificate had been filed. With this type of information, a reasonably good study could be made of the death rate from cancer among former employees. The individuals under consideration in this study were to be those employees with at least one year of company service credit at ORNL since 1951.

This study has been under way for three years. Very little information on cancer deaths among former employees has been collected. Much knowledge, however, was gained and has been applied in the use of payroll records as source material for surveys of this type. Indeed, the maintenance of personnel records, including those involving medical and payroll histories, and social security numbers in large private and public installations is a subject worthy of far more attention than is being given it at present.

Cooperation with the payroll department at the Oak Ridge Gaseous Diffusion Plant and with the BOASI in Baltimore has been excellent throughout this study. Social security numbers and other pertinent information were obtained locally and forwarded to the BOASI. By the end of the calendar year, a list of all the known deaths among former employees will be in the hands of the Health Division. Using the information in this list, contacts will be made with state departments of public health for the purpose of determining causes of death. It is hoped that sufficient information will be available by the end of the next report period for a final report on this project.

HEALTH PHYSICS

Waste Pit Studies

Investigators in the Waste Disposal Section of the Health Physics Division planned to sample the waste pits in the local AEC area by boring into the pits and extracting cores of solidified wastes. To accomplish the sampling efficiently and economically, they requested an experimental design. We recommended a design which could be performed in three stages (a sequential design). This will allow useful information to be obtained at the end of each stage, with the additional information obtained at the end of each stage augmenting the previous information in an orthogonal manner.

According to the design, sample cores would be obtained on three ellipses concentrically located around the center of the pit. Eight cores were to be obtained at points symmetrically spaced on each ellipse, and one core was to be obtained from the center of the pit. Each ellipse represents a different stage in the sequential sampling process. The outer ellipse circumscribed the waste pit, so that estimates of seepage from the pit could also be obtained.

Salt Deformation

A series of experiments are being performed in which small pillars of salt are subjected to a constant pressure. The deformation of the salt is then measured on two gages. The gages are read frequently over the first 2 hr and then less frequently for the next 1000 hr or more.

We have been asked to assist in processing and analyzing the data. First we shall attempt to find a suitable asymptotic function to describe deformation as a function of time. From this, estimates of the derivative of the function for selected points in time may be computed.

When this is satisfactorily completed, we shall attempt to analyze the combined results of several experiments performed under different temperature conditions.

Ecology

We were requested by investigators of the Ecology Section to recommend an experimental design to pursue further the uptake of strontium and calcium in the shells of snails and Asiatic clams. The first experiments in this area were reported in last year's annual report.[9]

The factor space was redefined on the basis of this previous experience, and a new experiment was designed. We recommended a rotatable design in the factor space of strontium concentration and calcium concentration in the medium. The design points are located on two randomly oriented concentric ellipses. Each ellipse contains six design points symmetrically placed. There are six replications of a point in the center of the ellipses. This latter will assure a relatively flat information contour over the design region.

METALS AND CERAMICS

Inspection of HFIR Fuel Plates

Many statistical problems are involved in the examination of the fuel plates manufactured for the High Flux Isotope Reactor (HFIR). One of these is a description of the uranium density contour specified by the designers of the reactor. As it is written, this consists of a table of uranium surface densities for about 50 discrete distances across the width of the fuel plates. Although there appears to be no known reason why the contour should follow any specific mathematical form, we discovered that the specified

[9] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963,* ORNL-3567, p. 45.

density follows the equation

$$Y = \alpha(X + \beta)^{\gamma} e^{\delta(X+\beta)+\lambda(X+\beta)^2} ,$$

in which Y is uranium surface density and X is distance from the edge of the plate. The coefficients in the equation are:

	Inner Annulus Plate	Outer Annulus Plate
α	17.64	182.11
β	1.02	1.17
γ	1.70	4.49
δ	0	−2.06
λ	−0.10	0

The maximum deviation of the density calculated from the equation and the density specified by the designers is 0.71% for the inner-annulus plate and 1.75% for the outer-annulus plate. Thus the fit is quite satisfactory. The equation is much more convenient to use than a table of 50 densities in problems resulting from fuel plate inspection, especially those involving interpolation.

Before installation, each fuel plate will be thoroughly inspected by means of an x-ray-attenuation scanner. Equations have been derived to facilitate the conversion from the digital printout of the x-ray-attenuation scanner to uranium surface density. This is a problem in calibration which was solved quite satisfactorily by use of the model

$$Y = \exp\,(\alpha + \beta X + \gamma X^2 + \delta X^3) ,$$

in which Y stands for uranium surface density and X is the output from the scanner.

The output from the scanner is being examined to determine if there are any dependencies in the measurements of uranium surface density along the length of the plates. An outer-annulus plate, selected at random from those on hand, has been subjected to spectral analysis. The analysis on 3 of the 48 scans obtained from this plate has revealed no consistent pattern of periodicities. The data are now being subjected to an autoregression analysis.

The boron content of HFIR fuel plates has been studied from samples punched out of six randomly selected plates. The experimental design was a 3×5 factorial in six replications. Fifteen samples forming a 3×5 lattice were punched out of six plates, and the boron content of each sample was obtained by chemical analysis. Important conclusions were that there was considerable variation from plate to plate and that there was an unexpected curvature in boron content in the lengthwise direction.

Although the present specifications for the manufacture of the HFIR fuel plates include manufacturers' tolerances, these tolerances have been set quite arbitrarily. We have begun an extensive program of inspection of the fuel plates on hand to study the problem of setting satisfactory but realistic tolerances for a vendor to meet. This will involve a much greater volume of the data than we have used to date.

Powder Metallurgy

We have designed an experiment to study the effects of four factors on the efficiency of blending powders of uranium and aluminum. The recommended design was a $3^2 \times 2^2$ factorial experiment with three differently shaped blending containers comprising the levels of one factor, three grades of fineness of the powders comprising the levels of a second factor, and two levels of moisture of the aluminum and uranium powders forming the levels of the remaining two factors. The experimental results have not yet been submitted for analysis.

REACTOR

We were asked to analyze the results from two experiments which had been performed in the Nuclear Safety Pilot Plant. In each case 72 stainless steel coupons were suspended in the pilot plant containment vessel. Then, UO_2 cylinders were partially vaporized by a plasma torch, and the resulting aerosol was swept through the vessel. The experimental observations were the quantities of uranium deposited on the coupons.

The coupons were suspended in pairs at 36 locations in the containment vessel. There were 12 locations on each of three planes (upper, middle, and lower). In each plane, the samples were located on three concentric circles with four locations equally spaced on each circle.

In the first experiment, the coupons on the inner circles had been wrapped with Scotch tape. This resulted in a confounding of the effect of Scotch tape with the inner circle position effect. Also, one observation was lost. We analyzed the data using techniques of the General Linear Hypothesis, examining several orthogonal and nonorthogonal contrasts. There was a significant difference in uranium deposition between the middle and lower planes. The average effects for the three concentric circles also showed significant differences, with the most significant contribution coming from the coupons on the inner circle.

In the second experiment, all of the coupons were wrapped with tape, and no observations were lost. The estimate of experimental error (as measured by the difference between coupons in the same pair) was about half as large as the estimate of error from the first experiment. Probability tests using this estimate of error revealed significant differences among planes and among circles and a significant interaction between circles and planes.

REACTOR CHEMISTRY

Last year's annual report[10] contained a description of an unsolved problem concerned with fractionation of radionuclides. A tenable solution to this problem has now been found.

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[10] *Math. Div. Ann. Progr. Rept. Dec. 31, 1963,* ORNL-3567, p. 43.

Let A represent a proportion of the total amount of a radionuclide released in the simulation of a reactor incident. Similarly, let B and C represent proportions of two other radionuclides. The chemists suggest that these proportions are related by the equation

$$\log (A/C) = \alpha + \beta \log (B/C) .$$

In measuring log A, log B, and log C it is reasonable to assume that the errors of measurement have the same variance (σ^2) and that the measurements are independent. Thus, if $Y = \log A - \log C$ and $X = \log B - \log C$, we may write

$$Y = \eta + \epsilon ,$$
$$X = \zeta + \delta ,$$

where η and ζ are random variables, and ϵ and δ are random variables involving errors of measurement. It follows then that

$$\text{var } (\epsilon) = 2\sigma^2 ,$$
$$\text{var } (\delta) = 2\sigma^2 ,$$
$$\text{covar } (\epsilon, \delta) = \sigma^2 .$$

The model in which the chemists are interested may be written

$$\eta = \alpha + \beta\zeta ,$$

but in terms of what we can observe, the model is the structural relations model,

$$Y = \alpha + \beta(X - \delta) + \epsilon .$$

Empirical evidence and theoretical considerations support the contention that η and ζ follow normal distributions. Under this assumption and the assumption of equal variance of measurement errors, the theory of maximum likelihood yields five equations:[11]

$$E(\zeta) \doteq \overline{X} ,$$
$$\alpha + \beta E(\zeta) \doteq \overline{Y} ,$$
$$\text{var } (\zeta) + 2\sigma^2 \doteq s_x^2 ,$$
$$\beta^2 \text{ var } (\zeta) + 2\sigma^2 \doteq s_y^2 ,$$
$$\beta \text{ var } (\zeta) + \sigma^2 \doteq s_{xy} .$$

This is a consistent set of equations affording a solution to the problem.

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[11]Here, $E(\zeta)$ is the expectation of ζ, and $\doteq$ means "is estimated by." The quantities on the right are sample means, variances and covariance.

Statistical Programming

ANALYSIS OF VARIANCE

An ALGOL procedure called *THREE WAY ANOVA* was written to perform analyses of variance. It will perform analyses of variance on one-way, two-way, or three-way classifications. The output consists of a complete set of two-way tables of means, an analysis of variance for a cross classification, and an analysis of variance for a hierarchal classification.

YATES performs an analysis of a 2^N factorial experiment by the method known as the "Yates calculation." Several problems may be run, one behind another. The number of factors is limited to 7, that is, $N \leqq 7$. The program can handle 2^N factorial designs with or without multiple observations. The output includes:

1. an analysis of variance table,
2. a table of five columns containing the pertinent information of the Yates calculation:
   a) a column identifying the effects,
   b) a column of the means of the responses for the 2^N factor combinations,
   c) a column which is the result of performing the successive additions and successive subtractions in the Yates method N times,
   d) a column of estimates of the effects,
   e) a column containing the sums of squares attributable to each effect,
3. the sum of squares of deviations from the experiment mean,
4. a graph of the Cuthbert Daniel half normal plot.

The program is written in FORTRAN-63.

FREQUENCY DISTRIBUTIONS

DNA is a program which constructs a frequency distribution from a set of data using class intervals specified by the user. The output consists of the frequency distribution table in printed form and on punched cards, and of a plot of the frequency polygon. The program is written in FORTRAN-63.

The expected values in each class of a geometric distribution are computed by *PQTOX*, where $f(x) = pq^x$, and $q = 1 - p$. The parameter, p, is estimated from input data by the method of moments. A chi-square test of goodness of fit is calculated. The output includes a plot of the expected and the observed values for each class on the same graph as well as a listing. In addition, the above procedure is repeated for the truncated geometric distribution obtained by omitting the class for $x = 0$.

STOCHASTIC PROCESSES

Three subroutines useful in spectral analysis have been written in the ALGOL language. One computes the autocovariance function for a given number of lags, another computes autoregression coefficients, and a third computes the spectral density function using the "hammed" cosine transform.

CDFMAT is a program designed to compute numerically the "Fundamental Matrix" of the absorbing Markov chain resulting from the countercurrent dialysis model described earlier. The required input parameters are m, the number of stages in the system, and p, the probability that a particle will remain in the dialysis sac. Numerical results for $m = 2, 3, 4, 5$ and $p = 0.01, 0.05\ (0.05)\ 0.95, 0.99$ were achieved. The output includes a complete numerical specification of the "Fundamental Matrix," a matrix of variances, and several vectors, one of which denotes the expected number of steps in which the process is in a transient state, given that it starts in a particular transient state. This vector and the vector of its variances are specified by $E_i(t)$ and $\mathrm{var}_i\ (t)$. Two graphs are included for each value of m. The first plots $E_1(t)$ for $p = 0.01, 0.05\ (0.05)\ 0.85$; the second plots $\sum_i E_i(t)$ for $p = 0.01, 0.05\ (0.05)\ 0.85$. This program is written in FORTRAN-63.

DATA DISPLAY

Research into the somatic effects of radiation has resulted in the accumulation of large quantities of biological data from experiments performed during the past 15 years. Among the variables of interest are such things as survival time, mortality intensity, and multiple causes of death. Manipulation of these variables has, until recently, been done on desk calculators. Several computer programs have been written during this report period which calculate and plot (1) mortality intensities as a function of age using several alternative methods; (2) survival probability as a function of age and dose, and mean survival times; (3) the probability of dying of a specific cause when other causes are operating concurrently; and (4) the intensity of cataract induction by dose as measured by the degree of opacity of the lens.

The study of somatic effects due to low-level radiation will require the use of more than 80,000 mice over an extended period of time. The logistics of treating, housing, and boarding these animals is a formidable problem. Equally important, however, is the logistics of raising so many animals in such a way that they are available when space and other facilities are ready for handling them. Such things as litter size and sex are known to be influenced by age of mother, parity of litter, mother's parity, location of cage, and year of experiment. To better understand what the requirements of the low-level study will be, several computer programs were written which collate and summarize in tabular form all the available breeding information from prior experiments in the Biology Division. These programs have served as models for new programs which are being written to provide regular reports of the progress of the low-level study.

LOOK AT THE DATA is an ALGOL procedure which produces a 10- by 10-in. graph of a set of points in a two-dimensional space. It was written to provide the statistician with a picture of his data. Scaling

is accomplished automatically with scale labels which are divisible by 1, 2, 4, or 5. Another version of this procedure will connect the data points in the order in which they are provided to the routine.

DATANAL is a program which enables the statistician to examine data through the use of transgenerations and graphical displays. Eighteen different transgenerations are offered with the total number of original and transgenerated variables being limited to 20. The option is given to graph any of the variables as the dependent or the independent variable. The option of listing the original and transgenerated data also is allowed.

If the option to graph is exercised, the means and standard deviations of the two variables and their coefficient of correlation are included in the output. Other output includes the means and standard deviations of all variables (original and transgenerated) and the lower half of the correlation matrix. The program is written in FORTRAN-63.

New IBM 1401 programs written by the group are as follows:

1. list data for Mammalian Genetics Section,
2. Reactor Division work orders,
3. cumulative mortality calculation for Mammalian Recovery Section,
4. Chinese hamster breeding data for the Human Cytogenetics Section.

REGRESSION

An ALGOL program has been written that contains three methods for computing estimates of parameters for a nonlinear model. There are no specified limits on the number of data points, number of independent variables, or the number of parameters. All arrays are dynamic. The number of data points is computed at execution. The user specifies one of the following methods for searching the sum-of-squares surface: Direct Search, Fibonacci Search, or Gauss-Newton Search. The estimates obtained from either Direct Search or Fibonacci Search are refined by the Gauss-Newton method. If Gauss-Newton, as the specified method, fails to converge because of a singular matrix of normal equations, the flow of the program is directed to the Direct Search method. This flow is also taken if the parameters do not converge before the limit for iteration is passed. Because the program contains several paths of flow, we refer to this program as the *RUBE GOLDBERG MACHINE*.

The Direct Search[12,13] is accomplished by an ALGOL procedure called DS Minimum. In this procedure, the parameter space is scaled so that all axes are measured in the same units. Thus steps parallel to an axis in the parameter space are proportional to the magnitude of the initial estimate of that parameter.

A Fibonacci Search is performed by another procedure, which is a one-parameter-at-a-time adaptation of the Fibonacci method for searching single-parameter functions. In the single-parameter case, this

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[12]Robert Hooke and T. A. Jeeves, "'Direct Search' Solution of Numerical and Statistical Problems," *J. Assoc. Comput. Mach.* **8**(2), 212–39 (1961).

[13]A. F. Kaupe, Jr. "Algorithm 178," *Communs. Assoc. Comput. Mach.* **6**(6), 313–14 (1963).

method has been proved optimal in that a fixed size interval containing the point of the minimum of the function can be found in fewer steps than by any other method of direct search.

CORRELATION is an ALGOL program which computes the simple correlation coefficient from a set of bivariate data and tests the hypothesis of zero correlation at the 5% level of significance. Included in the output is a graph of the data using the *LOOK AT THE DATA* procedure.

An ALGOL procedure called *TRANSGENERATE* performs transformations on a column of a two-dimensional array of real numbers. Nineteen different transformations, ranging from simple addition and subtraction to calculation of the hyperbolic arc cosine, may be performed with this procedure. The operational symbols recognized by the procedure are mnemonic and are simple English words or abbreviations. For example, the expression "6 = 4 over 3" would be interpreted by *TRANSGENERATE* to mean "Store in the sixth column the result of dividing each element of the fourth column by the corresponding element of the third column."

Included in the list of transformations is a unit transformation, which records a column of ones in the array, and a weight transformation, which copies a column of the array into another column for possible use as a column of weights. This is an especially useful procedure for regression programs.

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Gardiner, D. A., "Structural Relations Versus Regression," Chemical Division, American Society for Quality Control, Gatlinburg, Tennessee, November 1964.

Gosslee, D. G., "Some Applications of Statistics at a Modern Research Laboratory," U.T.-A.E.C. Agricultural Research Laboratory, Oak Ridge, Tennessee, January 1964; Department of Statistics, University of Florida, Gainesville, February 1964.

Gosslee, D. G., "The Analysis of Variance for Nonorthogonal Data," Institute of Statistics, University of Georgia, Athens, February 1964; Department of Statistics, Florida State University, Tallahassee, February 1964.

Gosslee, D. G., "Some Experiences in Fitting Nonlinear Models," Department of Mathematics, Clemson College, Clemson, South Carolina, February 1964.

Harkrider, M. T. (with Peter Mazur), "Flow of Water in Multicompartmented Cells and Tissues During Freezing," Eighth Annual Meeting of the Biophysical Society, Chicago, Illinois, February 26–28, 1964.

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Householder, A. S., "The Kantorovic and Related Inequalities," Case Institute of Technology, Cleveland, Ohio, March 30, 1964.

Householder, A. S., "Inclusion Theorems for Characteristic Roots and Vectors of Matrices," Auburn University, Auburn, Alabama, August 14, 1964.

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Kastenbaum, M. A., "Countercurrent Dialysis – a Finite Markov Process," Oklahoma State University, Stillwater, April 1964; Kettering Institute, Yellow Springs, Ohio, May 1964.

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Uppuluri, V. R. Rao, "Probability Density Functions with Maximum Entropy," Indian Science Congress, Calcutta, India, December 1964.

Training Courses

Four nine-day lecture series by Nancy B. Alexander and R. P. Leinius, intended to give audiences a working knowledge of FORTRAN 63 for the CDC 1604-A, were offered during 1964. Material covered in each series included a discussion of building blocks, basic statements (of input and output in particular), and declarations. In addition, the concepts of program, subroutine, and fractions were treated.

Throughout the series attention was given to the actual steps required to prepare, check out, and run a program in the local computing facilities. These lecture series were attended by 235 persons.

A seven-day lecture series in Advance Programming Techniques was offered to personnel of the Mathematics Division. Facilities available from the Computer Operations Group; the monitor system and better ways of using FORTRAN; converting ALGOL to FORTRAN; and several general-purpose library subroutines were discussed. These lecture series were attended by 28 persons.

A series of 16 seminars on the Theory and Applications of Spectral Analysis was conducted by V. R. Rao Uppuluri during the period March through August 1964. Statisticians in the Oak Ridge area were invited to participate.

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