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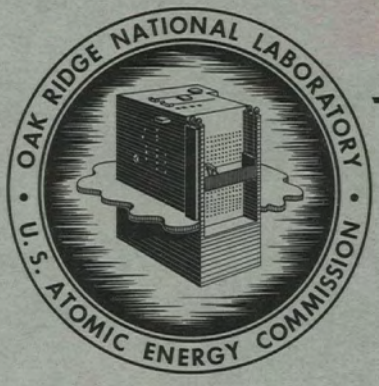
MATHEMATICS DIVISION
ANNUAL PROGRESS REPORT
FOR PERIOD ENDING DECEMBER 31, 1963



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for the
U.S. ATOMIC ENERGY COMMISSION

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ANNUAL PROGRESS REPORT
for Period Ending December 31, 1963

A. S. Householder, Director
A. C. Downing, Assistant Director

MARCH 1964

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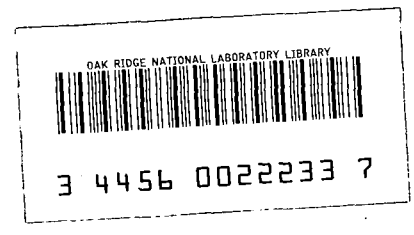

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MATHEMATICS AND COMPUTING

MATHEMATICAL STATISTICS

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Mathematics and Computing

Mathematical Research

A. C. Downing
Walter Gautschi
D. B. Hinton
R. P. Rannie
T. C. Tucker

As a result of a previous study on computational aspects of recurrence relations[1] a package of ALGOL procedures was produced[2] for the calculation of various special functions. Included are Bessel functions $J_{a\pm n}(x)$, $I_{a\pm n}(x)$, $J_{a+n}(z)$, for $0 \leq a < 1$, $x > 0$, z complex, $n = 0(1)N$; Legendre functions $P_a^n(x)$, $P_{a+n}^m(x)$, for a real, $x > 1$, $m \geq 0$ an integer, $n = 0(1)N$; and incomplete beta function ratios $I_x(p+n, q)$, $I_x(q, p+n)$, for $0 < p \leq 1$, $q > 0$, $n = 0(1)N$. These algorithms are being revised and supplemented, to comply with new publication policies of the receiving journal.

* * * * *

Work described earlier[3] on the construction of Gaussian quadrature formulas

$$\int_a^b f(t)\, w(t)\, dt = \sum_{m=1}^{n} \lambda_m f(t_m) + R[f] ,$$

then carried out on the Oracle, was resumed on the CDC 1604-A. The problem was to generate the weights λ_m and the abscissas t_m from the moments

$$\mu_k = \int_a^b t^k w(t)\, dt \qquad (k = 0, 1, 2, \ldots) .$$

After experiments were made with larger values of n, it became apparent that the problem is more delicate, numerically, than anticipated. The major difficulty arose in the attempt to make an accurate determination of the coefficients α_m and β_m appearing in the recursion

$$p_{m+1}(t) = (t - \alpha_m)\, p_m(t) - \beta_m\, p_{m-1}(t)$$

for the associated orthogonal polynomials.

In an effort to understand the reasons for this, the conditioning of the relevant system of equations,

$$\sum_{m=1}^{n} \lambda_m t_m^k = \mu_k \qquad (k = 0, 1, \ldots, 2n - 1) ,$$

was examined. If by "conditioning" is meant the extent to which small changes in the moments μ_k are transmitted into changes in the λ_m, t_m, a natural measure of the condition would be some norm of the matrix $D^{-1}J^{-1}M$, where $D = \mathrm{diag}(\lambda_v, t_v)$, J is the Jacobian of the system, and $M = \mathrm{diag}(\mu_k)$. While numerical values for $||D^{-1}J^{-1}M||$ have not yet been calculated, the values of $||J^{-1}||$ and $||M||$ for a number of common weight functions have been obtained. Some results are shown in Table 1.

In general, we have $J = LT$, where $L = \mathrm{diag}(\lambda_v, 1)$ and T is a certain confluent Vandermonde matrix in the abscissas t_m. The magnitude of J^{-1} depends critically on T, that is, on the location of the t_m. A sharpening of an earlier result has been obtained in the form[4]

$$||T^{-1}|| \leq \max_{1\leq\lambda\leq n} b_\lambda \prod_{\substack{v=1 \\ v\neq\lambda}}^{n} \left(\frac{1 + |t_v|}{|t_\lambda - t_v|}\right)^2 ,$$

[1] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, pp. 2–6.

[2] "Algorithms for Bessel Functions, Legendre Functions, and Incomplete Beta Function Ratios," submitted for publication in *Communications of the Association for Computing Machinery*.

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

[4] Walter Gautschi, "On Inverses of Vandermonde and Confluent Vandermonde Matrices. II," *Numerische Math.* 5, 425–30 (1963).

Table 1. Some Values of $||J^{-1}||$ and $||M||$ for Common Weight Functions

$w(t)$	(a, b)	n	$\|\|J^{-1}\|\|$	$\|\|M\|\|$
1	$(-1, 1)$	6	6.08×10^2	2.0
		12	5.88×10^6	2.0
e^{-t}	$(0, \infty)$	6	77.6	3.99×10^7
		12	2.18×10^3	2.58×10^{22}
e^{-t^2}	$(-\infty, \infty)$	6	14.5	52.3
		12	1.29×10^2	1.19×10^7
$\ln(e/t)$	$(0, 1)$	5	3.49×10^5	2.0

where b_λ is the larger of the two quantities

$$b_\lambda^{(1)} = 1 + |t_\lambda| , \quad b_\lambda^{(2)} = \left|1 + 2t_\lambda \sum_{v\neq\lambda} 1/(t_\lambda - t_v)\right| + 2\left|\sum_{v\neq\lambda} 1/(t_\lambda - t_v)\right|.$$

The bound for $||T^{-1}||$ is assumed, if all $t_m \geqq 0$, and the two expressions whose moduli appear in the definition of $b_\lambda^{(2)}$ are of equal sign for each λ. A procedure to calculate T^{-1} was also obtained.

Further work is required to develop a reliable algorithm for solving the problem. Application of Newton's method to the basic system of equations is contemplated for the purpose of correcting approximations to the λ_m, t_m immediately after they are obtained. Correspondingly, it becomes possible to revise the coefficients α_m, β_m at each step of the recursion. In this way we expect to keep the errors down to the natural level set by the conditioning of the problem.

* * * * *

A one-group, two-dimensional criticality calculation is mathematically equivalent to a vibrating membrane. It is well known that when the region governed by the associated partial differential equation is not convex the convergence of the finite difference solution is slow, particularly in the vicinity of a nonconvex corner. For this reason the L-shaped membrane has been widely studied. The customary handling of this problem is to force points of a regularly spaced grid to fall exactly on the boundary. The fundamental frequencies for the finite difference problems thus defined for various grid spacings form a monotonically decreasing sequence (except for very coarse grids) as more and more grid points are introduced. Each value in this sequence is therefore an upper bound for the desired fundamental frequency of the physical membrane. Sharp lower bounds have not been reported. In recent work at ORNL an alternate approach to handling the boundary condition was tried; this approach forces boundaries to fall midway between two rows of grid points. The condition that the deflection vanish on the boundary can then be approximated by either linear interpolation or quadratic interpolation without departing from the basic five-point approximation for the partial differential equation. It was found that both of these approximations lead to monotonically increasing sequences for the fundamental frequencies as more and more grid points are used. Thus lower as well as upper bounds for the fundamental frequency are now available.

Table 2 shows selected results for the fundamental frequencies of vibration of an L-shaped membrane formed by joining three squares, each one unit on a side. The first column in the table gives the frequencies resulting from the customary method (points on the boundary), and the second and third columns give the frequencies resulting from linear and quadratic interpolation over points nearest the boundary.

Table 2. Fundamental Frequencies of Vibration

Grid Spacing	Method		
	Customary	Linear	Quadratic
3	3.086282	2.934604	3.021805
5	3.111045	3.030382	3.059911
10	3.112602	3.079955	3.087795
20	3.109175	3.096157	3.098705
30	3.107641	3.100053	3.101457
40	3.106846	3.101674	3.102609
50	3.106372	3.102529	3.103220
60	3.106061	3.103048	3.103582
70	3.105845	3.103390	3.103823
80	3.105684	3.103631	3.103992

Similar calculations have been made for the second mode of vibration, but for this mode all three methods lead to monotonically increasing sequences.

Work still remains to fit these data to a suitable analytical expression to permit extrapolation to an infinitely small grid spacing. Letting h be the grid spacing, it appears that an expression of the form

$$V_h = V_0 + a_1 h^{\alpha} + a_2 h^{2\alpha} + a_3 h^{3\alpha} + \cdots$$

will be satisfactory.

* * * * *

A study is being carried out to find which combination of nuclear reactor types, breeders and nonbreeders, will produce nuclear electric power in the most economical manner. A simple model has been formulated, and a more complex model is being prepared. The principal assumptions on which the simple model is based are the following: the total power is prescribed in advance as a function of time; all bred fuels are transferred and consumed within the complex operating the reactors; the operating cost of each reactor is proportional to the power production of that reactor, and so are the breeding rate and fuel inventory.

The simple model assumes two reactor types, breeders and burners, with interchangeable fissile fuels and free fertile materials. In this model the costs of construction and other fixed charges are included in the reactor operating costs. The criterion for optimization is the minimum combined total operating and fuel costs for a period of the order of 75 years. The mathematical problem of minimization is one in the calculus of variations, but somewhat nonstandard, involving variable end points, one-sided variations, and extremals with cusps. Sufficiency conditions are presently being sought.

It is expected that the more complex and complete model cannot be solved by analytical techniques, and the need for digital computer optimization techniques is anticipated.

Programming Research

Nancy B. Alexander
L. L. Bumgarner
Manuel Feliciano
A. A. Grau

THE CONTROL DATA CORPORATION 1604-A ALGOL COMPILER

The ALGOL compiler for the CDC 1604-A[1] completed its first stage of development and was made available for general use by Laboratory personnel. A number of minor errors were reported and have been corrected.

Use of FORTRAN Subprograms

The utility of the ALGOL compiler was significantly increased by the addition of facilities for allowing subprograms written in the FORTRAN language to be incorporated into an ALGOL program. This was especially desirable since the FORTRAN compilers do not have the capability of accepting ALGOL subprograms.

These facilities were introduced through the addition of four standard procedures:

Procedure	Subprograms Accommodated
Fortran	FORTRAN 62 subroutines
Fortranf	FORTRAN 62 functions
Ftn	FORTRAN 63 subroutines
Ftnf	FORTRAN 63 functions

As an example of their use, the following ALGOL statement would cause activation of the function BESSEL written in the FORTRAN 63 language:

x := y + Ftnf(BESSEL(N,A)) .

To provide maximum speed, the compiler was modified to interpret these standard procedure names as sentinels which cause machine code to be generated for the appropriate FORTRAN calling sequence, eliminating the need for an administrative subroutine to perform the linkage.

Workshop

A four-day workshop was held July 15–18 for acquainting other CDC 1604-A installations with the ALGOL compiler. It was attended by 12 persons from 9 companies and institutions. These were given access to the Laboratory's computing facilities for program-testing purposes and received a copy of the compiler for use in their own computing laboratories.

Input-Output

The input-output facilities were improved through the addition of several reserved-name procedures. These include *print, write, punch,* and *page*. *Print* is used to put out numbers in a standard form without the necessity for specifying a format. A *print* statement always puts out at least one line printer image, which may contain up to 6 numbers, each of which is in scientific notation with 10 decimal places. The *write* procedure is used to put out strings. Each string put out appears on a separate line. Again no format is used. The *punch* procedure is used for the special purpose of putting out numbers on punched cards in the particular form required for input by the *read* procedure. The *page* procedure is used to cause a page ejection on the standard output medium.

[1] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962,* ORNL-3423, pp. 20–22.

Intermediate tape-handling facilities were completed, along with a set of Boolean procedures for checking tape conditions. All of these use the available FORTRAN facilities.

Control System

Improvements were made in the compiler's control system to allow unrestricted mixing of ALGOL and assembly language subprograms. The need for additional control cards was eliminated. A PROGRAM card is now permitted at the beginning of the program for identification purposes.

Owing to changes made by the systems group in the master control system, it became necessary to add a facility for specifying a time limit on the compile-and-run mode (ALGO) of the compiler. This was done through an additional control card parameter.

REPRESENTATION IN ALGOL STANDARDIZATION EFFORTS

The American Standards Association is investigating the need for establishing standards for common programming languages. The Association established a working group, ASA X3.4.2, charged with considering the specification of standards for ALGOL. As such standards are certain to exert great influence on the acceptability of an ALGOL compiler, representation in this working group is vital to the interests of those who have invested in the construction of a compiler. CO-OP, the CDC 1604-A users' group, recognized the need for protection of its interests, and since the Laboratory, as the developer of the compiler, had the largest investment in the ALGOL project for the CDC 1604-A, it was agreed that the Programming Research Group would provide a representative. The representation became official on October 24, 1963.

DESIGN OF ALGOL INPUT-OUTPUT

The discussions within the ALCOR group with regard to design of an input-output system for ALGOL[2] were continued. As an indication of widespread interest in this problem, an ALGOL Committee was formed by the Association for Computing Machinery for the primary purpose of developing an acceptable solution. The committee was made aware of the ALCOR effort and accepted many of the ALCOR ideas. Liaison has been maintained between the two groups by a Laboratory representative.

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[2]*Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 23.

Computing Services

ANALYTICAL CHEMISTRY

G. J. Atta H. C. Mullikin
D. C. Ramsey

Radiochemical Analysis Calculations

Analyses are performed daily on samples submitted by customers to the radiochemical laboratory. During analysis the technicians record measurements made on the sample. Routine calculations using these measurements must be made before the result the customer wants is obtained.

A computer program has been written to do these calculations. The technicians record the measurements on cards from which the input for the program is keypunched directly.

Equilibrium Concentrations

Successive metal-anion complexes with stability constants are formed from a solution of a metal ion and a liquid. The fraction of the total metal ion concentration which is present in each complex was calculated and plotted.

BIOLOGY

R. B. Bullock A. M. Craig
M. T. Harkrider

Kinetics of Water Loss from Cells at Subzero Temperatures

This program, reported previously,[1] has been expanded to include not only single cells, but also several cells in layers, such as concentric spheres. From the results so far obtained with the multicell code, it has become apparent that the external layers of cells have a greater percentage of survival when exposed to subzero temperatures. This is easily explained by the fact that the outer cells lose their water to the external medium more quickly than the inner cells; thus the probability of intercellular ice being formed is decreased.

[1] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962,* ORNL-3423, p. 10.

BUDGET AND PERSONNEL

A. M. Craig M. T. Harkrider
J. E. Schmith

Accounting Charts

A series of programs which will graph certain accounting variables is being written. The charts may be generally divided into two types. The first type compares the behavior of the account under consideration with a prescribed control variable; such graphs are designed to warn management of any accounts which are currently out of control and to suggest remedial action. The second type is a breakdown of a given account according to specified criteria; these charts should be particularly useful for emphasizing the relative shares of each division in the Laboratory programs.

Analysis of Frequencies of Dispensary Visits

A statistical study of the relationships between nonoccupational (colds, headaches, etc.) and occupational (minor injuries) dispensary visits made by ORNL personnel during the period 1954–1959 is being conducted. Several programs have been written to assist in this analysis.

CHEMICAL TECHNOLOGY

G. J. Atta
E. E. Branstetter
M. T. Harkrider
H. C. Mullikin

Fission Product Recovery

Separation and recovery of fission products in a waste solution are followed by means of the gamma-ray-emitting isotopes Sr^{85}, Ce^{141}, Ca^{45}, Ba^{133}, and Fe^{59}, which are added in tracer quantities to the waste solution. The separation of strontium and rare earths in the ion exchange step required the collection of hundreds of effluent samples. Data obtained by scintillation spectrometry included the gamma spectra of the background, of identical volumes of the feed solution to the ion exchange column, of the standard solution with the concentration of any tracer, and of the effluent samples with concentrations. Electronic problems produced a nonlinearity of energy vs channel number at the lower end of the energy spectrum and also caused energy-peak shifts during long-term operation of the instrument, wherein the channel number was proportional to energy. The overall effect of these problems was the introduction of greater inaccuracies at the lower end of the energy spectrum where, characteristically, the activity of a gamma peak would span about four or five channels, as compared with the 15 to 20 channels at energies greater than 1 Mev.

The analysis of the data took the form of obtaining sorption and elution curves for each of the five gamma-emitting isotopes. The activity contribution of each isotope at each channel in a spectrum was computed, and the ratio of the individual isotope activities relative to their individual activities in the feed solution to the ion exchange column was plotted as a function of resin volumes of liquid passed through the column.

The resolution of these gamma spectra into individual isotopic activities was done by a least-squares procedure. A correction was made for the channel shift of the energy peaks, proportional to the energy level of the peak. However, the computation assumed linearity over the entire energy spectrum covered, 0 to 1.6 Mev.

A Study of Shipping Costs of Uranium Fuel Elements

The spent fuel elements removed from nuclear reactors ordinarily will be shipped to a fuel reprocessing plant for recovery of the remaining fissionable material or to a disposal plant for the disposition of radioactive fission products. Because of their high gamma radioactivity, the spent fuel elements must be contained during shipment in heavily shielded, sealed casks. A typical cask consists of a steel inner shell, a layer of lead shielding, and a heavy steel outer shell to provide the necessary structural strength. The fuel elements are contained in a box-like array inside the inner shell and are separated from each other by divider plates.

The cost of shipments of fuel elements is an appreciable factor in reactor economics, because of the cost of the casks and the freight, handling, and insurance charges incurred. The problem then is, in a given situation, to arrive at a cask design which will meet specifications and will minimize the shipping costs.

A computer code has been written which does this. Given shipping distance, number of fuel elements, activity of the elements, etc., the code designs a cask and calculates the overall shipping cost of the fuel element.

CHEMISTRY

G. J. Atta
Susie E. Atta
D. C. Ramsey

Calculation of Reaction Rates in Porous Electrodes

Porous electrodes are potentially useful in analysis and separation methods, including electrolysis of saline waters. The distribution of reaction rates in porous electrodes is governed by a system of nonlinear partial differential equations.

A "good" method for obtaining a numerical solution of this system of differential equations was not found, since the system is highly nonlinear. An approximating iterative technique using finite difference steps together with recursion schemes is used successfully to obtain solutions for some of the parameters. A computer program

using these techniques is written, and the program and the techniques were tested with a restricted set of parameters which could be transcribed into functions permitting solution by direct methods.

Since the approximating methods are highly sensitive to any change in some of the parameters, the accuracy, and the technique used for a smooth convergence, as well as the criterion for convergence, are determined for each set of parameters used.

SORT Program

A program was written to sort data collected from an automatic radiation counter. The program also reduces the data to more comprehendible results.

HEALTH PHYSICS

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E. E. Branstetter
R. B. Bullock
H. P. Carter
A. M. Craig
M. T. Harkrider
A. R. Jenkins
R. P. Leinius
D. C. Ramsey

Determination of n and k from Reflectivity Measurements

The response of a substance to bombardment by charged particles or by electromagnetic radiation is characterized by specifying either the dielectric constant ϵ or $n^* = n + ik = \sqrt{\epsilon}$. In a study of the collective behavior of electrons in metals, it has become necessary to know the dielectric constant of metals as a function of the frequency of the incident light. Dielectric data are being obtained from measurements of the reflectivity of opaque vacuum-evaporated foils as a function of angle and of wavelength of the incident light. These measurements are made for both polarized and unpolarized light whenever possible. The Fresnel equations give the reflectivity of a plane surface as a function of the angle of incidence and of n and k for that wavelength. Then, in principle, it is possible to measure the reflectivity at two angles and solve the two resulting equations for the unknowns n and k.

A computer program has been written to compute n and k for measurements taken in the following ways:

1. reflectivities for polarized and unpolarized light at one angle,
2. reflectivities for unpolarized light at two angles, and
3. reflectivities for polarized light at two angles.

This program has been used to calculate n and k for silver. These values for the dielectric constant give better agreement with experimental data than do the values found in the literature. The dielectric constants found by this method are being used in theoretical equations for reflection, absorption, and transmission of light by thin foils, and for transition radiation.

Transition Radiation from a Two-Layered Foil

When a beam of charged particles passes from one medium into another, it may be shown that electromagnetic radiation (called "transition" radiation) will be emitted owing to the change in dielectric properties along the path of the particles. Since the radiation emitted is determined by the electrical properties of the target, this method can be used as a tool to investigate these properties. A study is being made of the collective behavior of electrons in metals by observing light emitted from thin vacuum-evaporated metal foils bombarded by electrons. A theory has been developed to predict the light emission from a single foil, and the resulting equation has been programmed for computer evaluation. The agreement with experimental data is, in general, good.

There are, however, several reasons for having a theory that applies to a two-layer foil.

1. Even with high-vacuum techniques, for some metals it is virtually impossible to produce a single-layer foil without creating an oxide layer.
2. For very thin foils, a substrate may be necessary for support.
3. It may be desired to study the properties of intentionally produced double-layer foils; for example, gold on silver.

With the assumption that the incident particle traverses the foils without slowing down, solving Maxwell's equations in the presence of boundaries yields the equation for light emission from a double-layer foil. The resulting equation contains,

as parameters, the energy and charge of the incident particle, the thicknesses and the real and imaginary parts of the dielectric constants of the two foils, the angle, with respect to the normal to the foil, at which emission occurs, and the wavelength of the light. The computer code calculates, for each incident electron, both the number of photons and the energy emitted into unit solid angle and unit wavelength interval. The comparison of the computer results with experimentally determined values has been good. The code has also been useful in exploring optimum values for foil thicknesses, energies, and angles, in planning experimental tests.

Secondary Electron Cascades in Metals[2]

The process used for the numerical solution of the slowing-down and cascade spectra resulting from electrons of low energy has proven to be quite sensitive to the grid size in energy. Results obtained have agreed very well with experimental data, but at the cost of long running time on the computer. Several methods, including a Monte Carlo scheme, are being studied to increase the speed of obtaining solutions, thereby allowing a greater throughput of cases to be examined.

Corrections to Keplertron Electron Slowing-Down Data

A program has been written to correct measurements made by the Keplertron electrostatic focusing spectrometer of the electron flux for corona discharge at high outer-sphere potential, grid transmissions, gamma background, source activity, and source decay. The corrections have made experimental results comparable to theoretical values.

Spectral Distribution of Electron Flux in a Beta-Radioactive Medium

Two programs were written to calculate and plot the electron slowing-down spectrum using a simplified version of the Spencer-Fano theory. In computing the buildup of secondary electrons in the medium, one program made use of an approximate Möller formula while the other used the complete Möller formula.

Linear Energy Transfer

Four programs have been written to compute the neutron dose distribution as a function of linear energy transfer. Several categories of dose are being studied: dose attributable to collisions with hydrogen nuclei, dose due to interaction with heavy-ion-recoil nuclei, total dose due to protons born of neutron collisions, and dose due to collisions of neutrons at thermal energy. These programs differ mainly in the size, shape, and partitioning of the subject phantom and the size of the neutron beam. At present these programs analyze neutron histories on magnetic tapes which have been generated by a Monte Carlo program (ϕ5R). Efforts are being made to incorporate the Monte Carlo code and the analysis code into one program which will eliminate temporary storage of neutron histories on magnetic tapes.

Monte Carlo Gamma-Ray Program

The OGRE Monte Carlo Code[3] for generating gamma-ray histories is being modified and adapted to the CDC 1604-A. Subroutines to calculate the azimuthal sine and cosine of the particle as it leaves the collision in the scattering frame, Klein-Nishina routines to determine where on the cone in the scattering frame a collision lies, and a rotation routine which performs a transformation from scattering frame to a fixed coordinate system have been revised. Programs for generating, updating, and editing a master gamma-ray cross section tape used by the above program have been completed.

Energy Deposition

Studies in high-energy proton dosimetry are of interest to manned space flight, to biological irradiation experiments, and to radiological

[2] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 30.

[3] *Ibid.*, p. 39.

protection in the vicinity of high-energy accelerators. A program is being written to calculate radiation dose from protons with energies up to 400 Mev.

The basic approach to specifying radiation dose is the determination of a number of physical quantities accompanying the irradiation of a target. The principal quantities of interest are the amount of energy absorbed per unit mass of material, the spatial and temporal distributions of the absorbed energy, and the accompanying values of linear energy transfer (LET) at which energy deposition takes place. The average energy absorbed over some volume in the target is a measure of the rad dose. From the absorbed energy, its spatial and temporal distributions, and a consideration of the LET spectrum, one usually specifies a relative biological effectiveness (RBE) on which rem dose is based for a particular biological effect being studied.

The nature of the problems involved in the determination of high-energy proton dose can be brought out by considering the following special problem. Consider a uniform parallel beam of monoenergetic protons with a flux of ϕ protons/cm^2 incident normally on the surface of a homogeneous tissue slab 30 cm thick and having infinite lateral extent. The problem to be considered is the determination of energy absorbed in a volume element ΔV located at depth X in the slab as a result of the flux ϕ incident upon the slab. This energy divided by the mass of ΔV and by the flux ϕ then leads to the rad dose per unit flux at the depth X in the slab. It can be shown that these results can be obtained by calculating the total energy absorbed in the extended subslab S from a total of ϕ protons incident at a single point P. When the subslab S is located at the same depth X and has the same thickness ΔX as the volume element ΔV, the total energy absorbed in the subslab S from ϕ protons is proportional to the energy absorbed per unit mass in the volume element ΔV from a uniform flux of ϕ protons/cm^2. Therefore, to obtain the rad dose in ΔV for this problem, one calculates the total energy absorbed in subslab S. This technique is utilized in the computer program being written.

For the analysis, a 30-cm tissue slab was divided into a number of subslabs of uniform thickness. Histories of protons normally incident at a given point P were generated by a Monte Carlo technique and were analyzed for absorbed dose, utilizing the technique described above. In general, a proton entering the slab will immediately begin slowing down by electromagnetic interaction with the surrounding medium, and the penetration is calculated in accordance with well-known expressions from stopping power theory. In the course of this slowing-down process, a proton may or may not have an interaction with the nucleus of an atom. Based on the cross sections for interactions with constituent nuclei of the slab, a collision of a given incident proton with a nucleus is decided by a Monte Carlo technique. A number of protons ϕ are "injected" into the slab at P and their histories are generated and stored on tape. The program being written analyzes the physical information stored on this history tape and calculates the total energy deposited in any of the given subslabs. From these results the dose in the slab at that depth from a broad beam of protons of flux ϕ protons/cm^2 can be calculated.

Clinch River Bed Studies

Several codes have been written to assist the U.S. Geological Survey Stable Chemical Studies for the Clinch River. The results from one code are used to estimate the amount of radioactivity contained at different levels in the bottom soil of the river. Core samples were obtained of the bottom soil from several locations along the river. Raw counts were taken at 2-in. intervals along the core. The code makes corrections for both the background activity and contributions to the count from adjacent slabs. Corrections also are made for slabs less than 2 in. thick. Output is in both printed and graphical form. Other codes correlate various chemical levels for degree of sedimentation, plot the concentration of various chemicals on a monthly or weekly basis by sampling station, and perform statistical evaluations of the data from these stations.

Neutron Spectrometer Feasibility Study

A code has been written to make calculations to determine the feasibility of a theory for constructing a neutron spectrometer. This necessitated the evaluation of an integral

$$V(\tau) = \int_{L1}^{L2} f\left(\tau, t(\phi, \psi, L), L\right) dL$$

$$= K \int_{L1}^{L2} \left[\ln\left(1 + \frac{\tau - t}{t_0}\right)\right] (R-L)^{(1-n)/n}\, dL,$$

where

$$t(\phi, \psi, L) = \frac{1}{\alpha^2}[L^2 \sin^2 \psi + 2dL \sin \psi \cos \phi + d^2] + \frac{c}{2M-1}[R^{(2n-1)/2n} - (R-L)^{(2n-1)/2n}] \leqq \tau,$$

$0 \leqq L1 < L2 < R$, and parameters c, d, n, R, t_0, ϕ, ψ, α^2 are positive.

It is desired to evaluate $V(\tau)$ for a set of increasing values of time t for various values of the many parameters involved. Since f is undefined for $\tau < t$, the set of increasing values of τ is dependent on the initial value of τ. Therefore, to calculate the starting values of τ it is necessary to determine the minimum value of t for all values of L in the interval $[0, R]$. After the arguments τ have been calculated, the limits of integration $L1(t, L)$ and $L2(t, L)$ can be computed for each value of τ. For fixed τ, $L1$ and $L2$ are values of L in the interval $[0, R]$ such that for $L1 \leqq L \leqq L2$, $t(\phi, \psi, L)$ is such that $t \leqq \tau$. When the limits of integration are computed, the integral $V(\tau)$ can be approximated with a 16-point Gaussian numerical integration scheme. This method of integration was suggested by the discontinuity of the integrand f and $L = R$.

Weekly Bio-Assay Sample Status Report

A computer program has been written in order to produce a more complete report on the status of bio-assay samples. There are three categories of samples to be considered, namely, (1) those on request, (2) those in laboratory process, and (3) those for which laboratory results have been obtained. The program lists the samples in each category (1) by Health Physics Areas, (2) by departments, and (3) alphabetically. Samples that are not on time within the categories are marked with an identifying word, or listed separately. Health Physics Area totals and Department totals are summarized within each category.

Clinch River Safety Analyses

Men may be exposed to internal and external sources of ionizing radiation due to the discharge of radioactive fluids to the Clinch River. A computer program has been written to allow individuals of various age groups to hypothetically begin consuming Clinch River or Tennessee River water during various years. Based on intake constants, critical organ mass, radionuclide concentration of the water, etc., critical organ burdens and dose received are calculated.

Diffusion into a Platelet

A program was written to compute the diffusion into a platelet by the formula

$$F = 1 - 4 \sum_{n=1}^{\infty} (1/j_{0,n}^2) \exp(-j_{0,n}^2 \tau),$$

where $j_{0,n}$ are the zeros of the Bessel function $J_0(x)$ and τ is a time measurement.

Population Dynamics

The growth curve of a species of field mice is normally cyclic in nature. A relative maximum is obtained at the peak of the breeding season during the warm months, and a relative minimum is observed during the cold winter months. An attempt was begun to construct a mathematical model that would approximate this cyclic growth curve with an additional feature of superimposing a "no-breeding" season on the curve. Various breeding periods used were (1) 12 months breeding, (2) 10 months breeding, 2 months no breeding, (3) 8 months breeding, 4 months no breeding, and (4) 6 months breeding, 6 months no breeding.

One model considered was

$$\dot{X}(t) = b\left[X(t-\tau_1) + \int_0^{\tau_3} S'(z)\, X(t-\tau_1 - z)\, dz \right] \times \left[1 - \frac{X(t-\tau_2)}{K} \right], \quad (1)$$

where $X(t)$ is population at time t, b is birth rate, τ_1 is gestation time, τ_2 is the length of time it takes the animal to mature, τ_3 is the maximum

length of life, and $S(z)$ is the fraction of the population surviving at time z after birth at $z = 0$. The method used in attempting to solve this difference-differential-integral equation was the so-called Euler method. Numerical values obtained eventually turned negative, and this is a troublesome inconsistency.

A possible solution to the problem may be to use a completely different equation to describe the population function $X(t)$. A constant number of animals and an exponentially increasing number of animals have been assumed, but neither supplied the information necessary for the mathematical model to be valid. Another possible solution is a method more sophisticated than the so-called Euler method for handling the given equation (1).

INFORMATION CENTERS

Radiation Shielding Information Center (RSIC)

Margaret B. Emmett

The information retrieval system for the literature examined by the Radiation Shielding Information Center has been designed for utilization of a large digital computer. The most valuable features of the retrieval system are automatic updating and editing directly onto Multilith masters. A feature which has not been fully exploited to date is the possibility of searching the files for information which satisfies some search criterion. This feature will become more and more useful as the holdings of RSIC increase.

Basically, the information retrieval system consists of five magnetic tape files and a set of programs written originally for the IBM 7090 but which could be easily converted for use on the CDC 1604-A. The set of programs consists of three types of programming operations: (1) programs to add new documents to the files (update the files) and check input data; (2) programs to correct a large number of possible types of errors and to make other types of changes, such as altering the major category list; (3) programs to edit the tape files. The operations involved in these programs are sorting and merging with movement of keys, merging fixed fields of binary-coded decimal information by squeezing out unwanted blank characters, as, for example, in names of authors, and alphabetizing by machine with the aid of manual keys.

The retrieval system is now fairly well hardened except for an occasional unforeseen situation.

ISOTOPES

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Inhomogeneous-Sector Magnetic Fields

A program has been written which determines the paths of ions and their points of intersection with predescribed planes where the relevant forces are those of an inhomogeneous-sector magnetic field. The results should be helpful in guiding the design of a sector isotope separator.

Several assumptions were made regarding the field configuration to facilitate evaluation of the magnetic field. First it was assumed that field lines lie in planes parallel to the z axis, even as they fringe away from the face of the magnet. The angle that the field lines make with the reference trajectory was estimated by comparing the ratio of the gradients of the fringing field and the inhomogeneous field. Finally an estimate of the fringing field strength was made from values computed from the complex transformation for a parallel plate capacitor.

Calculation of Ion Trajectories in Experimental Magnetic Fields

The 255° isotope-separator orbit and magnetic-field measurement processing programs[4] have been altered so that other experimental data from new azimuthally varying magnetic shimming systems may be evaluated also. Data smoothing and calculations of the magnetic-field intensity are performed for 1500 polar grid points, which completely covers the entire midplane beam path of the isotope separator. Alterations may be made on this magnetic-field intensity distribution to determine corrections to the field shape for correcting magnetic lens aberrations in the separator. Cal-

[4] *Math. Panel Ann. Progr. Rept. Dec. 31, 1961,* ORNL-3264, p. 49.

culations of the corrections to be made on the magnetic pole pieces may be made from this altered magnetic-field shape. Midplane ion beam orbits are also calculated from the original and from the altered magnetic-field data to evaluate the various magnetic-field intensity distributions.

Two supplementary additions have been made to the basic magnetic-field data-processing program. The first compares the magnetic-field intensity at each data point with a value got from a least-squares interpolation using the neighboring radial and azimuthal points. Any bad data points arising from measuring errors, digital logging errors, or varying experimental conditions are immediately visible on examining the differences from the above interpolation. This process very efficiently verifies the data and provides a measure of its precision.

The second addition performs cubic interpolations in the table of data to provide the coordinates of contours of equal magnetic-field intensity. These data are then hand plotted on large drafting-size paper to aid the evaluation of the various experimental field shapes.

In addition to the above alterations and additions, the 255° isotope separator orbit and magnetic-field measurement processing programs have been converted from the IBM 7090 computer to the CDC 1604-A computer for future use.

Yield for (n,γ) Production of Radioactive Isotopes

A program was written to calculate the irradiation time in a reactor that is necessary for maximum yield of a radioactive isotope daughter from a stable parent isotope. The activity of the daughter product, in curies/g, at the time when this maximum is reached was also calculated. The basic formula for the time at which the number of atoms in the daughter product will reach a maximum (hence its radioactivity will reach a maximum) is derived from a solution of the Bateman equations.[5] The activity formula was adopted from a solution for the number of daughter atoms, N_B, formed after time t whose activity is $0.693N_B/T_p$ (refs. 6,7).

[5]R. D. Evans, *The Atomic Nucleus*, p. 479, McGraw-Hill, New York, 1955.

[6]*Ibid.*, p. 478.

[7]Gerhart Friedlander and J. W. Kennedy, *Nuclear and Radiochemistry*, p. 130, Wiley, New York, 1955.

METALS AND CERAMICS

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Strain Calculations

A program was written to compute the deformation of crystalline lattices subjected to arbitrary strains. The minimum number of slip systems were active, five being required for an arbitrary strain, and the total slip was minimized.

The calculations were simplified by finding each kind of combination that could operate, there being only four for face-centered cubic lattices, and summing the shears for each. The actual system that would operate consistent with the above assumption was the one having the smallest shear.

Water Channel Measurements

In the fuel core for a certain reactor, metal plates containing uranium are placed in two concentric circles with channels between each pair of plates through which the coolant will flow. The width of each channel must meet rigid specifications. Consequently after the plates are installed, three measurements of the channel spacing are made across the width of the plate at various positions along its length. An average channel width is computed and compared with the specifications.

A program was written to compute the average width of each channel at various positions along its length. The program also computes a frequency distribution for each set of measurements and one for the average widths of the channels. Since the size of the channels may vary after welding, data were supplied both before and after the welding was done.

Plastic Deformation of Metals

Crystalline materials can exhibit point, line, or surface imperfections. The line imperfection is known as a dislocation. Among other things dislocation theory has been applied toward the rationalization of the plastic behavior of crystalline materials in terms of elasticity. Under the combined action of thermal fluctuations and applied

stress, a pair of kinks will be produced in the dislocation line.

The shape $y(x)$ of the dislocation line may be obtained from the ordinary differential equation

$$E_0 \frac{d^2y}{dx^2} = \tau_p^0 b \sin \frac{2\pi y}{a} - \tau b \qquad (1)$$

with boundary conditions $y(0) = 0$ and $y(\frac{1}{2}) = y_0$ for L sufficiently large. In Eq. (1), E_0 is the line energy of the dislocation, τ_p^0 is the Peierls stress, τ is the external stress, a is the lattice parameter, and b is Burgers' vector.

The minimum energy required for the nucleation of a pair of kinks can be obtained by inserting the solution of (1) into

$$E(y_0) = 2\int_0^{L/2} \frac{E_0}{2}\frac{d^2y}{dx^2} + \frac{\tau_p^0 ab}{2\pi}\left(1 - \cos\frac{2\pi y}{a}\right) - \tau b y \, dx \qquad (2)$$

and minimizing the resulting expression with respect to y_0.

In previous models the external stress τ was assumed to be zero, and analytical solutions to Eqs. (1) and (2) were found. Since $\tau \gg 0$ in the plastic deformation of metals, the agreement of the experimental with the theoretical results using this model proved to be fortuitous. Hence an effort was made to solve Eqs. (1) and (2) for $\tau > 0$.

An analytical solution of (1) was obtained. Application of Lagrange's method to minimize (2) yielded an integral which could be evaluated numerically to obtain the minimum energy.

It appears that the theory accounts rather well for the experimental results observed.

Resistivity Tensor Components

The galvanomagnetic properties of pure metal crystals at low temperatures and in high magnetic fields are measured in order to determine topographical features of the Fermi surface. An experimental study of this type is being conducted in the Metals and Ceramics Division; electric-field measurements are taken in three noncoplanar directions with the magnetic field oriented perpendicular to the direction of current flow and to the axis of the cylindrical crystal. A program has been written which normalizes the voltage measurements to unit distance and to unit current density, corrects for probe misalignment, and transforms the data from the experimental frame of reference rigidly attached to the crystal to a rotating frame which follows the magnetic field around the crystal. This frame of reference, oriented by the current, the magnetic field, and a direction normal to both, is the standard for comparing with theories of galvanomagnetic effects. It is convenient to separate the tensor relation

$$\vec{E} = \rho \vec{J} \, ,$$

representing Ohm's Law, into symmetric and antisymmetric parts. The computing program does this for the first column and the first row of the pair of 3×3 tensors which are the components that can be determined with the existing experimental geometry:

$$\begin{pmatrix} E_1^e \\ E_2^e \\ E_3^e \end{pmatrix} = \begin{pmatrix} \rho_{xx}^e & \rho_{xy}^e & \rho_{zx}^e \\ \rho_{yx}^e & \rho_{yy}^e & \rho_{zy}^e \\ \rho_{zx}^e & \rho_{zy}^e & \rho_{zz}^e \end{pmatrix} \begin{pmatrix} J_1 \\ 0 \\ 0 \end{pmatrix},$$

$$\begin{pmatrix} E_1^o \\ E_2^o \\ E_3^o \end{pmatrix} = \begin{pmatrix} 0 & -\rho_{yx}^o & -\rho_{zx}^o \\ \rho_{yx}^o & 0 & -\rho_{zy}^o \\ \rho_{zx}^o & \rho_{zy}^o & 0 \end{pmatrix} \begin{pmatrix} J_1 \\ 0 \\ 0 \end{pmatrix}.$$

The output has been arranged in tabular form and in graphs on the Calcomp plotter. The linear graphs of the above components in all combinations as a function of magnetic-field angle, as well as graphs of the angles showing the position of the electric field, $\vec{E^o}$ or $\vec{E^e}$, in the rotating frame of reference are plotted in a flexible and convenient manner. The superscripts o and e refer to odd and even parts of this vector with respect to a reversal of the magnetic-field direction.

It is planned to extend the program to include graphs in polar coordinates and to include a statistical analysis of the tensor components as polynomial expansions in powers of the variable, magnetic-field strength, for fixed values of the magnetic-field angle.

Analysis of Fused-Salt Absorption Spectra

The code[8] for analysis of fused-salt absorption spectra was modified so that it might be processed on the CDC 1604-A computer. Certain portions of the input from magnetic tape were revised, resulting in a considerable reduction of running time.

NEUTRON PHYSICS

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A Smoothing Code for Monte Carlo Output

A code has been written that smooths a histogram representing distribution in light responses (i.e., intensities) that result from a monoenergetic neutron impinging on a cylindrical organic scintillator. The purpose of the code is to obtain a smoothed curve such as would be observed in an actual experiment.

Program LIGHT[9] calculates the data corresponding to the histogram. This output is used as input for the new code. The histogram is smoothed by a prescribed series of Gaussians, the spreading being effected by a Gaussian centered at the middle of each light bin with an empirically determined full width at half maximum as a function of light intensity from experiment.

Monte Carlo Calculations on Intranuclear Cascades

A program is being revised to calculate nuclear reactions on the assumption that these can be calculated on a particle-particle basis. The program used a reasonable nuclear model, recent cross-section data, and an exact statistical sampling technique. Calculations using the original program were performed for incident π^+, π^-, neutrons, and protons on nuclei from lithium to uranium with energies varying from 50 to 350 Mev. The present program will allow the energy range of the incident particles to vary from about 50 Mev to about 2 Gev. The programming is being recoded in FORTRAN for use in the IBM 7090 and CDC 1604-A machines. It is expected that the program can be run in any machine with a "standard" FORTRAN compiler. The code will be expanded to include higher energies.

The technique used in designing the code has been published elsewhere.[10]

Monte Carlo Calculations of Neutron Scattering from Cylinders of Be, C, Al, and Fe

A program was written to perform calculations to help predict the scattering of neutrons for systems proposed in the Space Nuclear Auxiliary Power (SNAP) program. The immediate objectives of the computer program are (1) the computation by Monte Carlo techniques of a sufficient body of data to establish under what circumstances single scattering methods can be successfully used and (2) the development of a means for estimating directional leakage fluxes to give rough predictions for scattering from massive components.

The program uses the O5R[11] code. The geometry is that specified by a parallel beam of neutrons incident on a cylinder in a direction normal to the cylinder axis. The cylinders were originally taken to be made of beryllium, carbon, aluminum, and iron. This was revised to allow for cylinders composed of concrete and $(C_2H_4)_n$.

Details have been published elsewhere.[12,13]

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[8] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 35.

[9] *Neutron Phys. Div. Ann. Progr. Rept. Aug. 1, 1963*, ORNL-3499, vol. II, pp. 56–57.

[10] H. W. Bertini, *Monte Carlo Calculations on Intranuclear Cascades*, ORNL-3383 (Apr. 23, 1963).

[11] R. R. Coveyou, J. G. Sullivan, and H. P. Carter, *Neutron Phys. Div. Ann. Progr. Rept. Sept. 1, 1958*, ORNL-2609, p. 87; for modifications to the code see D. Irving, *Neutron Phys. Div. Ann. Progr. Rept. Aug. 1, 1963*, ORNL-3499, vol. I, p. 177.

[12] F. B. K. Kam, F. H. S. Clark, and Jeuel G. LaTorre, *Neutron Phys. Div. Ann. Progr. Rept. Aug. 1, 1963*, ORNL-3499, vol. I, p. 159.

[13] F. B. K. Kam, R. S. Hubner, F. H. S. Clark, and Jeuel G. LaTorre, "Monte Carlo Calculations of Neutron Scattering from Cylinders of Be, C, Al, and Fe," *Trans. Am. Nucl. Soc.* 6, 424 (1963).

Monte Carlo Calculations of Fast-Neutron Penetration in Lithium Hydride

Several Monte Carlo calculations were made of the penetration of lithium hydride by fission neutrons. The O5R code[11] was used in these calculations. Tabulated lithium nonelastic cross sections[14] were used. Except for necessary interpolations within the tables, no approximation was made and no model was imposed on the data.

The purposes of the calculations were (1) to determine whether certain shield measurements in the earth's environment can be given meaningful application to the free space environment, (2) to study the channels through which neutrons penetrate a configuration similar to, but not typical of a Space Nuclear Auxiliary Power (SNAP) shield, and (3) to determine some of the fundamental neutron-shielding properties of lithium hydride. Details on these calculations have been published elsewhere.[15,16]

Modified Long Counter Analysis

The O5R program was adapted to the analysis of a modified long counter, an instrument under development for dosimetric application. With this analysis the instrument's energy and its angular responses were determined.

Calculation of Pair-Production Cross Section

A program was constructed to calculate the coefficients in the Legendre polynomial expansion of the differential cross section for the production of a pair of Dirac particles by a photon. Calculations performed with the program to date have been used to obtain information about the behavior of the total cross sections as higher angular momentum states are included.

Boron Filters

A CDC 1604-A code was written to compute the neutron transmission of boron filters as a function of energy, as part of a preliminary study to investigate the feasibility of using such filters as a neutron spectrometer.

Reaction Cross Sections

The inelastic scattering of neutrons was considered by Hauser and Feshbach,[17] and a reaction cross section formula was obtained for the process. Competition from other processes was excluded from the formula, since it was developed primarily for application to inelastic scattering of neutrons. A program was written to compute the cross sections when competition from other processes and the possibility of particles other than neutrons as incident and emergent particles were included.

The ANNEX-2 Code

ANNEX-2,[18] a conditional Monte Carlo code for the analysis of neutron scattering from small volumes, was converted for use on the CDC 1604-A.

PHYSICS

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Gamma-Ray Spectrum Fitting

The "direct-search" program for the IBM 7090[19] was modified and placed in service on the CDC

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[14] Louis Rosen and Leona Stewart, *The Neutron-Induced Disintegration of Li^6 and Li^7 by 5- to 14-Mev Incident Neutrons*, LA-2643 (Dec. 22, 1961).

[15] F. H. S. Clark, F. B. K. Kam, and Nancy A. Betz, *Neutron Phys. Div. Ann. Progr. Rept. Aug. 1, 1963*, ORNL-3499, vol. I, p. 116.

[16] F. H. S. Clark, F. B. K. Kam, and Nancy A. Betz, "Monte Carlo Calculations of Fast-Neutron Penetration in Lithium Hydride," *Trans. Am. Nucl. Soc.* 6, 426 (1963).

[17] Walter Hauser and Herman Feshbach, *Phys. Rev.* 87, 366 (1952).

[18] R. S. Hubner, *Analytic Techniques for the Calculation of the ORNL Tower Shield Experiments: Part II, Annex-2*, NAA-SR-8516 (revised) (June 26, 1963).

[19] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, pp. 43–44.

1604-A. The assumed form of the element of the response matrix used in the present code is

$$a_l[F_{li} + cx_i(\partial F_l/\partial\zeta)_i] , \qquad (1)$$

and the "direct-search" procedure[20] is used to determine both the a_l and the gain shift factor c. The form (1) was used rather than the previous one in order to obtain a more realistic approximation to the effect of amplifier gain shift. The "direct-search" procedure was used rather than the previous mixture of direct search and linear least squares to facilitate the incorporation of constraints on all the parameters instead of only the shift factors s_l previously used. In addition, the maximum possible number of gamma rays was increased from 14 to 20 and the maximum possible number of channels was increased to 256.

The nonlinear least-squares program[19] for the IBM 7090 was converted for use on the CDC 1604-A and extensively modified. As many as 20 parameters may be used in the revised version, distributed at the user's option among the following forms:

Ordinary Gaussians

$$y_e = a_i \exp[-(x_j - x_{Gi})^2/2\sigma_j^2] ,$$

Skewed Gaussians

$$y_e = a_i \exp[-(x_j - x_{SGi})^2/2\sigma_i^2][1 + b_i(x_{Gi} - x_j)] , \quad x_j < x_{Gi} ,$$

$$y_e = a_i \exp[-(x_j - x_{Gi})^2/2\sigma_i^2] , \quad x_j \geq x_{Gi} ,$$

Polynomial

$$p(x) = \sum_{n=1}^{NTERM} C_{n-1} x^{m_{n-1}} ,$$

with the number of terms, *NTERM*, and the exponents, m_i, $i = 1, 2, 3, \ldots$, supplied as input and $m_0 = 0$,

Joining Function

$$j(x) = \{1 - \exp[\beta(x_i - x_J)]\}^2 , \quad x_i < x_J ,$$

$$j(x) = 0 , \quad x_i \geq x_J .$$

The form used for the fit is then

$$\sum_{i=1}^{NSG} a_i \exp[-(x_j - x_{SGi})^2/2\sigma_i^2] \times \begin{cases} [1 + b_i(x_{SGi} - x_j)] , & x_j < x_{SGi} \\ 1 , & x_j \geq x_{SGi} \end{cases}$$

$$+ \sum_{i=1}^{NG} a_i \exp[-(x_i - x_{Gi})^2/2\sigma_i^2] + \begin{cases} p(x)\, j(x) , & x < x_J \\ 0 , & x \geq x_J \end{cases} ,$$

where *NSG* and *NG* are the number of skewed Gaussians and the number of ordinary Gaussians, respectively. The nonlinear least-squares procedure is a modified version of the one described by Lietzke.[21] The iterative process used in the previous version can be written as

$$\vec{\beta}_{k+1} = \vec{\beta}_k + \vec{h}_k , \qquad (2)$$

where $\vec{\beta}_k$ is the set of parameters at the kth iteration and h_k is the set of corrections calculated during the kth iteration. In the modified version, the iterative process[22] is given by

$$\vec{\beta}_{k+1} = \vec{\beta}_k + w\vec{h}_k \qquad (3)$$

when the factor w is an input number. It has been found that for some data it is necessary to use $w = 0.05$ to induce convergence.

In connection with the programming of the nonlinear least-squares computation, some of the numerical experiments in the inversion of large symmetric matrices reported by Lietzke *et al.*[23] were repeated on the CDC 1604-A. In general, the results of the CDC 1604-A calculations were

[20] Robert Hooke and T. A. Jeeves, "'Direct Search' Solutions of Numerical and Statistical Problems," *J. Assoc. Comput. Mach.* **8**, 212 (April 1961).

[21] M. H. Lietzke, *A Generalized Least Squares Program for the IBM 7090 Computer*, ORNL-3259 (Mar. 21, 1962).

[22] R. H. Moore and R. K. Zeigler, "The Use of High-Speed Computers in Determining the Parameters of Nonlinear Functions by Iterative Least Squares Methods," *Trans. Am. Nucl. Soc.* 1(2), 128 (December 1958).

[23] M. H. Lietzke, R. W. Stoughton, and Marjorie P. Lietzke, *A Comparison of Several Methods for Inverting Large Symmetric Positive Definite Matrices*, ORNL-3430 (May 9, 1963).

consistent with those of the IBM 7090 calculations, showing smaller error measures (since the length of the floating point mantissa is 36 bits on the 1604, rather than 27 bits on the 7090). The anomalous behavior of the rank annihilation method was again observed.

Fission-Fragment Experiments[24]

It was found that the pulse-height vs energy calibration for semiconductor detectors is mass dependent. As a result, a new code to calculate the mass and total energy has been written to accommodate the more complicated relationships that arise.

Data on time-of-flight vs energy are now being collected by a two-dimensional multichannel analyzer with 256 × 256 channels rather than 128 × 128. This change necessitated major revisions in the codes as originally written. At present, data are being analyzed by the new series of codes.

A multilevel fitting code is being used to permit estimates of the contributions of various resonances to fission at given energies, and a Monte Carlo integration code was written to evaluate the sixfold integral necessary in determination of the electrostatic repulsion of two spheroids.

All past codes which are still in use were rewritten for the CDC 1604-A in an improved form.

Mössbauer Effect in Small-Angle Reflection of Gamma Rays

The IBM 7090 program described previously[25] was converted for use on the CDC 1604-A and modified to provide additional output. In addition to the average reflectivity calculated by the 7090 version, information is obtained about the distribution of the intensity of the reflected photon between the two possible polarization states (parallel and perpendicular to the mirror plane) and about the phase difference between the two components. The complex quantity z is related to the complex index of refraction $\eta = 1 - \delta - i\beta$ by the definition

$$z \equiv \frac{2(\delta + i\beta)}{\theta^2} ,$$

where θ is the angle of incidence. The real and imaginary parts of z, labeled x and y respectively, are calculated for each of the two polarization states, and graphs are prepared with the Calcomp digital plotter; the graphs show the path traced by the point with coordinates x and y as the speed of the gamma-ray source is varied. Additional graphs are drawn; they show the phase difference between the components associated with the two different polarization states and the degree of polarization of the reflected gamma ray.

Mössbauer Spectra

Previously written codes[26] for Mössbauer spectra calculations were revised and improved. A new code was written to calculate the thickness correction for the intensity of the Mössbauer spectra lines.

Relativistic Hartree Wave Functions for Many-Electron Atoms

A program for the CDC 1604-A was constructed to calculate approximate solutions of the Dirac equations for the radial wave functions of a particle in a central potential:[27]

$$\frac{dG}{dr} - \frac{KG}{r} - \frac{1}{\hbar c}[mc^2 + E - e^2\,\phi(r)]F = 0 , \quad (1a)$$

$$\frac{dF}{dr} + \frac{KF}{r} - \frac{1}{\hbar c}[mc^2 - E + e^2\,\phi(r)]G = 0 . \quad (1b)$$

Since the solution is required for a large range of radial distance r, Eqs. (1a) and (1b) were transformed by the substitution

$$\rho = \ln (1000r/r_0) , \quad (2)$$

where r_0 is the radius of the first Bohr orbit of a

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[24] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, pp. 40–41.

[25] *Ibid.*, p. 42.

[26] *Ibid.*, p. 41.

[27] L. L. Foldy, "Relativistic Wave Equations," *Quantum Theory*, vol. III, chap. I in *Quantum Theory*, ed. by D. R. Bates, Academic Press, New York, 1962.

particle of mass m in an atom with nuclear charge Z:

$$r_0 = \hbar^2/Ze^2m \ . \tag{3}$$

Also, since the eigenvalue E of Eqs. (1a) and (1b) represents total (rest + kinetic + potential) energy, Eqs. (1a) and (1b) were further transformed by the substitution

$$\epsilon = 1 - E/mc^2 \ . \tag{4}$$

The potential energy term

$$e^2\,\phi(r) = \frac{e^2}{r}[-Z + V_e(r)] \ , \tag{5}$$

where $-Ze^2/r$ is the nuclear potential and $V_e(r)$ is the potential due to all other electrons in the atom.

With the above substitutions, Eqs. (1a) and (1b) were transformed into

$$\frac{dG}{d\rho} - KG - \left[\frac{2-\epsilon}{Z\alpha}x + Z\alpha - \alpha V_e(\rho)\right]F = 0 \ , \tag{6a}$$

$$\frac{dF}{d\rho} + KF - \left[\frac{\epsilon}{Z\alpha}x - Z\alpha + \alpha V_e(\rho)\right]G = 0 \ , \tag{6b}$$

where $x = r/r_0$ and $\alpha = e^2/\hbar c$, the fine structure constant.

The pair of equations (6a) and (6b), with boundary conditions

$$F(0) = G(0) = 0 \ , \qquad \lim_{r\to\infty} F(r) = \lim_{r\to\infty} G(r) = 0 \ ,$$

constitute an eigenvalue problem, since the energy ϵ is unknown. In the program an iterative procedure is used to obtain approximations to the functions F and G and the eigenvalue ϵ. For a given ϵ, approximate solutions are constructed using a fifth-order predictor-corrector method due to Milne and Reynolds:[28]

Predictor

$$y_{n+1} = y_{n-2} + (3h/8)(7y'_{n-1} + 5y'_{n-2} - y'_{n-3}) + 1944T \ ,$$

Corrector

$$y_{n+1} = (y_n + 7Y_{n-1})/8 + (h/192)(65y'_{n+1} + 243y'_n + 51y'_{n-1} + y'_{n-2}) - 75T \ ,$$

where h is the step size and the truncation error T is given by

$$T = h^5 y^{(5)}/5760 \ .$$

The integration is started near the origin, using power series solutions for F and G to provide the first few values of F, G, $dF/d\rho$, and $dG/d\rho$, and continued outward using equal steps of ρ to a point x_J. A second integration is started at x_L, a large distance from the origin, and continued inward in equal steps of ρ to x_J. Starting values are obtained from the relations

$$\lim_{r\to\infty} \frac{G}{F} = -\sqrt{\frac{2-\epsilon}{\epsilon}} \ ,$$

$$G(r) \cong A \exp\left[-r\sqrt{\epsilon(2-\epsilon)}/r_0 Z\alpha\right] \quad \text{for } r/r_0 \gg 1 \ .$$

The values of $G_{in}(x)$ and $F_{in}(x)$ obtained from the inward integration for $x \geq x_J$ are then multiplied by the ratio $F_{out}(x_J)/F_{in}(x_J)$, and the remaining mismatch in G at x_J is used to calculate a correction η to the eigenvalue ϵ:[29]

$$\eta = Z\alpha\,\frac{F_{out}(x_J)[G_{out}(x_J) - G_{in}(x_J)]}{\int_0^{x_J}(F_{out}^2 + F_{out}^2)\,dx + \int_{x_J}^{x_L}(F_{in}^2 + G_{in}^2)\,dx} \ . \tag{7}$$

The process is repeated using $\epsilon + \eta$ as the new estimate for the eigenvalue, until the mismatch in G at x_J is reduced below a certain fraction of $G(x_J)$.

Phase Shift Analysis of Differential Scattering of Neutrons from Spin-Zero Nuclei

Assistance was given in the construction of a code to compute differential cross sections for neutron scattering from spin-zero nuclei as a function of scattering phase shifts up to $g_{7/2}$.

[28] W. E. Milne and R. R. Reynolds, "Fifth-Order Methods for the Numerical Solution of Ordinary Differential Equations," *J. Assoc. Comput. Mach.* **9**, 1 (1962).

[29] D. R. Hartree, *The Calculation of Atomic Structures*, pp. 85–87, Wiley, New York, 1957, gives the procedure for the nonrelativistic case.

This code was then revised to fit the phase shifts by least squares.[30] Although this code has reduced the handwork and improved the final fits obtained, it is not yet a satisfactory version.

Paper Tape Handling

A code is being written to read an eight-level, binary-coded decimal, paper tape which was punched on a multichannel analyzer in memory dump mode. The code will generate data cards for a CDC 1604-A code, a listing and a printer semilog graph of the events per channel.

Electron Polarization Study

A code was written to calculate the correction for electron polarization due to multiple scattering in thick foils. For this code, a complementary error function subroutine was written, using a rational function approximation given by Hastings.[31]

Shield Efficiency

The O5R Code has been used to calculate the amount of light produced by neutron beams striking various-sized cylinders of Ne-213 (a liquid organic scintillator) and stilbene crystals; to investigate the efficiency of various sizes of shields containing varying amounts of lithium; and to calculate the fraction of multiply scattered neutrons detected at 5° intervals around cylindrical samples of carbon and of holmium.

Calculation of Electron Density in Alloys

The code for calculation of electron density in alloys[32] was incorporated into a larger program. Values that were previously input to the program are now obtained as solutions to a set of equations in two unknowns.

*E*2 Coulomb Excitation Calculations

Two codes originally written for the Oracle[33] were reprogrammed for the CDC 1604-A.

Double *E*2 Thick-Target Integrals

An integration over the energy-dependent terms of the semiclassical double $E2$ Coulomb excitation cross section has been programmed to obtain the relation between thick-target gamma-ray yields and the $B(E2)$'s involved. The $F(\xi_1, \xi_2, J)$ is that given by Douglas[34] for even nuclei. By specifying suitable input parameters, the calculation may be performed for arbitrary incident and target nuclei.

Numerical Analysis of Neutron Resonances

Additional computations and modifications were made in the computer programs described in ORNL-3205.[35] An addendum to this report was written.

Circuits with Superconducting Magnets

Additional proposed electrical networks[36] were numerically approximated. The solutions gave good insight into the proper circuits to be used with superconducting magnets. A laboratory report will be written on this project.

Internal Bremsstrahlung Spectra for He^6

For measuring internal bremsstrahlung (IB) gamma radiation, a scintillation spectrometer is used. This gives a pulse-height distribution, however, instead of the desired energy distribution; for a

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[30] M. H. Lietzke, *A Generalized Least Squares Program for the IBM 7090 Computer*, ORNL-3259 (Mar. 21, 1962).

[31] Cecil Hastings, Jr., *Approximations for Digital Computers*, Princeton University Press, Princeton, N.J., 1955.

[32] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 42.

[33] *Math. Panel Ann. Progr. Rept. Dec. 31, 1960*, ORNL-3082, p. 39.

[34] A. C. Douglas, *Double Coulomb Excitation in Even Nuclei. Tables of Cross-Section Functions*, AWRE-NR/P-2/62 (September 1962).

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

[36] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 44.

monoenergetic gamma ray the pulse-height distribution contains a photoline, a Compton distribution, and perhaps some escape peaks. The IB pulse-height distribution that is observed is, then, an overlapping of such distributions for all energies up to the maximum, combined with their relative intensities. The observed distribution must, therefore, be "unscrambled" to obtain the energy spectrum that is wanted.

If R is a response matrix determined empirically from the geometry of an experiment and n is a vector representing the observed pulse-height distribution, then the energy distribution spectrum, s, is obtained by solving the linear system $Rn = s$. While mathematically exact, this method is inapplicable since the treatment of experimental data may introduce considerable errors into the analysis of the measurements.

Various methods of "unscrambling" the observed pulse-height distribution were investigated. These methods included (1) a least-squares procedure, (2) "normalization without backscatter" of the response matrix, and (3) shifting the columns of the response matrix one column to the right, which is physically equivalent to taking the response matrix always at the beginning of the energy distribution intervals. Method (3) produced satisfactory results, but more sophisticated methods of IB unscrambling are being studied.

Transition Probabilities[37]

A general program for computing transition probabilities from one atomic state to another was written for the CDC 1604-A computer. The program accepts wave functions in tabular form, by means of formulas, or both. The functions supplied in tabular form are read in, whereas a subroutine must be written to supply the program with the formulas for the functions of that type. The intervals for the radii may be varied externally from run to run, so that the mesh used in the integration can be made fine in those areas of the function for which fine mesh is desired.

Gamma-Ray Interactions

A program has been written to compute the probability of interactions in certain sodium iodide crystals from gamma rays emitted by a disk source located along the axis of the crystal. This program failed to produce results consistent with other studies. A second program is being written involving the solution of a fourfold integral in an attempt to solve the same problem.

Correlation Analysis

A study is being made of the interdependence of the cross sections of the excited state and the elastic state of sodium iodide crystals acted upon by gamma rays. A computer program has been written which computes these correlations.

Electron Energy Distributions

Maxwellian and non-Maxwellian free-electron energy distributions were calculated and plotted to help investigate their influence on the steady state de-excitation radiation of incompletely stripped impurity ions persisting in homogeneous plasmas.

Charged-Particle Cross Section Compilation

A plotting subroutine has been written for the program described in ORNL-3423.[38] Also, a more flexible printout was incorporated to allow the computer printout to be used directly in the published compilation.

Because of the large amount of data used as input and its repeated use in different combinations, a data retrieval subroutine is being written. This will allow the data to be stored on magnetic tape. At execution time those cases which meet the requirements specified by input parameters can be read from the storage tape and used as input for the program.

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[37] *Ibid.*, p. 41.

[38] *Ibid.*, p. 43.

REACTOR

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ORR Fuel Inventory[39]

Additional bookkeeping procedures have been incorporated into the program that calculates ORR fuel inventory. They are: (1) an up-to-date fuel inventory which includes all ORR elements in pool and in core with the statistics on each at the present time; (2) a history of each element in inventory showing the statistics on the element each time it went into core, and each time it came out of core. This information is kept on magnetic tape and used by the program at the end of a cycle to compute the burnup. The information is updated when the burnup is computed. New elements are added when received and old ones are removed when spent or when discarded by Operations for some other reason. Upon execution the program reports parts or all of the information mentioned above, as called for by certain input parameters.

These procedures should simplify the paper work of the operations personnel and produce some useful reports.

Deposition of Fission Products from Gas Streams

A computer program was written to illustrate an analytical model[40] for the rate of deposition of fission products from gas streams onto conduit surfaces. It will consider a system denoted as isothermal or a system composed of an isothermal region and a variable temperature region. In each case the effect of thermal diffusion due to a radial temperature gradient is included. The code handles both fully developed laminar flow and fully developed turbulent flow, making use of the standard heat-mass analogy in determining the mass transfer coefficients.

Rankine Cycle Water Test

Tests are being conducted on a small Rankine cycle water test rig to determine overall system stability and methods of control. Measurements of temperature and pressure are made across each loop. These measured data are reduced, and several functional values dependent on these data are calculated.

Stress-Strain Analysis

When a bend specimen is subjected to moment loadings, the surface stresses are given by

$$\alpha_a = \frac{2M + K\, dM/dK}{bd\, d\epsilon_a/dK} ,$$

where

$$K = (|\epsilon_c| + |\epsilon_T|)/d ,$$

and M is the moment, ϵ is the strain, b is the width of the beam, and d is the depth of the beam. Subscripts C and T designate compressive and tensile, respectively, and subscript a is either C or T. Strain-gaged specimens of graphite subjected to moment loadings have been tested to failure, and the strains and moments have been recorded.

A computer program has been written to take the raw data, M, ϵ_C, and ϵ_T, and compute both compressive and tensile stresses. Stress-strain diagrams are plotted, and card output for a statistical analysis is generated.

The statistical analysis is conducted in the following manner. Four programs have been written which give a least-squares fit to the above mentioned stress-strain data using

$$\alpha = \epsilon \sum_{n=1}^{K} \left[a_n \sin \frac{n\pi\epsilon}{\epsilon_f} \right] + \left[\frac{\alpha_f - E\epsilon_f}{\epsilon_f^2} \right] \epsilon^2 + E\epsilon , \quad (1)$$

$$\alpha = \sum_{n=1}^{K} a_n \sin n\pi\epsilon , \quad (2)$$

$$\epsilon = \alpha/E + [\alpha/A]^N , \quad (3)$$

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[39] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 46.

[40] M. N. Ozisik, *An Analytical Model for Fission-Product Transport and Deposition from Gas Streams*, ORNL-3379 (July 26, 1963); *Temperature Effects on Fission Product Deposition* (to be issued); *A Transient Analysis of Fission Product Deposition*, ORNL-TM-650 (Oct. 1, 1963).

$$\epsilon = \alpha/E + [\alpha/A]^N + \left[\epsilon_f - \frac{\alpha_f}{E} - (\alpha_f/A)^N \right] \alpha^2/\alpha_f^2, \quad (4)$$

where α_f and ϵ_f is the last set of data, and E is the slope of a parabola through the origin determined by a least-squares fit of the first four points. The parameters under study are the a_n in Eqs. (1) and (2) and A and N in Eqs. (3) and (4).

Conversion of Reactor Codes

Reactor codes for the IBM 7090 checked out for use on the CDC 1604-A are listed in the following table.

Code Name	Type	Source
TWENTY GRAND[a]	Few-group, two-dimensional diffusion theory	CO-OP[b]
WHIRLAWAY[c]	Two-group, three-dimensional diffusion theory	CO-OP
GTP, THR, IMS[d]	Neutron thermalization	Author
ZORCH[e]	Reactor kinetics	Author
MURGATROYD[f]	Reactor kinetics	Author

[a] M. L. Tobias and T. B. Fowler, *The Twenty Grand Program for the Numerical Solution of Few-Group Neutron Diffusion Equations in Two Dimensions*, ORNL-3200 (Feb. 7, 1962).

[b] CDC users' organization.

[c] T. B. Fowler and M. L. Tobias, *Whirlaway — A Three-Dimensional, Two-Group Code for the IBM 7090 Computer*, ORNL-3150 (Aug. 1, 1961).

[d] C. A. Preskitt, E. A. Nephew, and M. E. Tsagaris, *Neutron Thermalization Programs for the IBM 7090*, ORNL-TM-461 (Feb. 25, 1963).

[e] C. W. Nestor, Jr., *Zorch — An IBM 7090 Program for the Analysis of Simulated MSRE Power Transients with a Simplified Space-Dependent Kinetics Model*, ORNL-TM-345 (Sept. 18, 1962).

[f] C. W. Nestor, Jr., *Murgatroyd — An IBM 7090 Program for the Analysis of the Kinetics of the MSRE*, ORNL-TM-203 (Apr. 6, 1962).

Heat Removal in a Gas-Cooled Molten-Salt Reactor

The problem was to determine feasibility of using a gas coolant for the removal of heat generated within the reactor by nuclear fission. In this heat transfer analysis, tubes passing through the molten-salt core contain the coolant gas. Given the input gas temperature and pressure, the maximum wall temperature, the output gas temperature, and the tube configurations, the program calculates the wall and gas temperatures and the pressure drop along the tubes. The equations involved were based on the standard convection heat transfer and fluid dynamics theories. In addition to the calculations above, the program produces a graph of the wall and gas temperature profiles.

REACTOR CHEMISTRY

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Infrared Data Analysis

Polybutadiene contains an unsaturated group (C=C) which exists in three configurations. Each of the configurations gives a characteristic peak in the infrared spectrum. These unsaturated groups are also readily changed by radiation. It is, therefore, desirable to relate the infrared spectrum to the content of the various configurations of the unsaturated group. The peak arising from the *cis* configuration of the unsaturated group varies in shape according to the content of the other two configurations. A computer program has been written to analyze the data from experimental measurement of infrared absorption by polybutadiene rubber. Areas under the peaks for several model compounds have been computed, and these areas have been fitted to a polynomial as a function of the known concentrations of the unsaturated groups within the model compounds. These equations will make possible the calculation of radiation yields for the unsaturated groups from infrared spectral data.

Changes in these groups are partially responsible for changes in the physical properties of polybutadiene, an essential constituent of many

synthetic rubbers. These studies, then, are of practical as well as theoretical interest.

Fission Escape of UO_2

Calculations were made to investigate a model for the fission escape of UO_2 during irradiation as a function of temperature. Other models are being considered, and calculations to test them should be performed in the future.

Limiting Law of Slopes

A program has been written to compute the values of parameters appearing in the Onsager limiting equation for electrolyte conductance in aqueous solution. A second program was written to compute the Debye-Hückel limiting slopes and activity coefficients of electrolytes at three concentrations. The effects of temperature ranging from 0 to 800°C and densities up to 1 g/cm^3 on the coefficients were studied.

Release of Fission Products

Programming changes were made in a code written to compute release of fission products.[41] An error analysis is performed on the calculations involved with release from fuel specimens and from various volumes of the apparatus. Absolute errors, and in some cases, percentage errors, are given for these calculations. Three additional calculations are made for each isotope: (1) percent penetration; (2) percent downstream based on the total number of fissions; (3) percent downstream based on the number of fissions in the high temperature zone. More options were made available in the plotting subroutines.

Calculation of Transient Temperatures in a Multiregion, Axisymmetric Cylindrical Configuration

A code originally written at Argonne National Laboratory is in the process of being converted from FORTRAN II to FORTRAN 62 for use on the CDC 1604-A computer. The purpose of the code is the calculation of transient temperatures in a concentric cylindrical configuration by finite-difference methods.

SOLID STATE

E. E. Branstetter M. T. Harkrider

Thermal Conductivity Study

A program was written to compare experimental measurements of thermal conductivity of alkali halide crystals as a function of temperature with a theoretical model of thermal conductivity:

$$TC = F(T)$$

$$= At^3 \int_0^{\theta/t} \frac{T^4 (\sinh T)^{-2}\, dT}{Bt^4T^4 + Ct^3e^{-a/t}T^2 + D + E\, f(T)},$$

where $f(T) = (\sin btT)^4/2.5$, and a, A, b, t, θ are given parameters.

Particular values of the parameters B, C, D, and E were sought which would yield in $F(T)$ a function representative of the experimental results. This required repeated evaluation of the integral TC for various values of B, C, D, and E.

The integral was evaluated numerically by Gaussian quadrature.

COMPUTER OPERATIONS

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The CDC Computers

To meet the expanding demand for computing capabilities at ORNL, a Control Data Corporation 1604-A computer was delivered on January 28, 1963. This machine is a transistorized digital computer with 32,768 48-bit words of core memory and an effective cycle time of 4.8 μsec. The control console of the computer is equipped with

[41] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 47.

an input/output typewriter, a paper tape reader, and a paper tape punch; however, the primary input/output devices for the computer are twelve Control Data Corporation 606 magnetic tape units. These units use ½-in. wide magnetic tape with a packing density of 200 or 556 characters per inch of tape. With these units, information may be transferred to or from the computer at rates of 30,000 or 83,400 characters per second. Because of the high data transmission rate of the tape units, preferred operating procedure calls for all input/output on the 1604-A to be via magnetic tape, and for use of a smaller peripheral computer to pre- and post-process these magnetic tapes.

Following installation and checkout by the Control Data Corporation, the 1604-A was put into one-shift operation on February 11, 1963, and has run at least five days per week since that time. It was necessary to begin two-shift operation on June 3, 1963, and three-shift operation on September 23, 1963. From startup of operations to the end of the year, the 1604-A was "down" (unavailable for computing due to machine malfunction) for a total of 116.4 hr. This total represents only 3.3% of the scheduled computing time available, and indicates the quality of computer performance. The longest continuous amount of down time was a 48-hr period in April when a memory stack failed and had to be replaced. Twenty-six hours of scheduled productive time was lost.

In order to handle peripheral operations associated with a large-scale digital computer, a Control Data Corporation 160-A computer was installed at ORNL on the same date as the 1604-A computer described above. This machine is a small-scale transistorized digital computer with 8192 12-bit words of core memory and a cycle time of 6.5 μsec. In addition to the paper-tape reader and the paper-tape punch which are part of the 160-A, the system installed at ORNL included an input/output typewriter, a CDC 1612 high-speed line printer, two CDC 606 magnetic tape units, and a CDC 1610 control unit which controls an IBM 088 card reader and an IBM 523 card punch. With this equipment, all forms of computer input/output media can be processed. The primary function of this computer is to perform the routine card-to-tape, tape-to-punch, and tape-to-printer operations.

A few weeks of operation with the 160-A indicated that a second peripheral system would be required to handle efficiently the flow of work through the large computer. Therefore, a second 160-A peripheral system was installed at ORNL on June 18, 1963. At the time of delivery, the system consisted of a 160-A computer, an input/output typewriter, two CDC 606 magnetic tape units, and a CDC 170 control unit controlling an IBM 523 card punch.

Later in the year, additional peripheral equipment was procured, including one 606 magnetic tape unit delivered in late June 1963, one CDC 405 high-speed reader delivered October 17, 1963, and one CDC 1612 high-speed printer delivered November 11, 1963. These three pieces of equipment were added to the second 160-A, so that there are now two complete 160-A peripheral systems in operation at ORNL.

Both systems have performed satisfactorily. Table 1 shows hours of use and hours of down time for both systems.

Table 1. Productive Time and Down Time for the CDC 160-A Peripheral Computer Systems

Month	System No. 1		System No. 2	
	Productive Time (hr)	Down Time (hr)	Productive Time (hr)	Down Time (hr)
February	134.5	15.5		
March	236.0	0.1		
April	187.2	2.9		
May	263.6	0.3		
June	202.2	5.0	91.2	0.0
July	133.8	2.6	265.2	17.7
August	301.3	5.7	148.2	3.4
September	267.0	1.6	104.7	1.7
October	265.4	9.8	144.5	1.3
November	214.8	4.3	140.5	5.2
December	188.1	8.2	142.3	3.4

Since the startup in February, the 1604-A has been used by some 267 different users for a total of more than 2600 hr. This figure represents computer time used for both problem checkout and

production runs; it does not include time for repairs or machine checking and idle time available but not used. Figures 1 and 2 show use and down time of the 1604-A by month and the percent of total time used by various divisions.

While the computer and peripheral equipment are operated only by Mathematics Division personnel, programming for the computer is on an "open shop" basis; that is, any member of the Laboratory staff desiring to do so may write a computer program for the 1604-A.

For this reason, and in order to use the computer in the most efficient manner, a monitor program for the 1604-A is utilized. This program was written initially by the Control Data Corporation, but was modified extensively by our Systems Programming group. It permits the "batching" of jobs so that several jobs may be run sequentially through the 1604-A with little or no operator intervention.

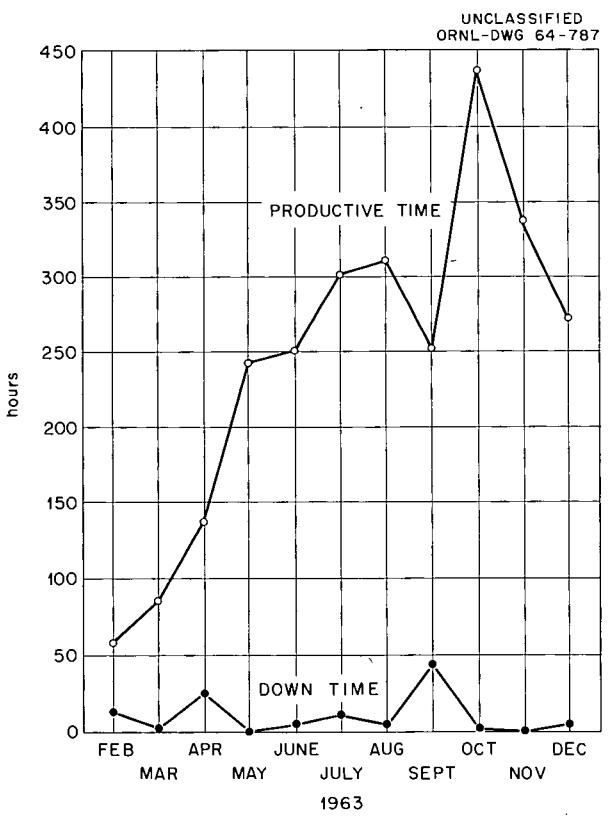

Fig. 1. CDC 1604-A Productive Time and Down Time.

Also included in the monitor system are a FORTRAN compiler and an ALGOL compiler, the latter developed here at the Laboratory (see the chapter "Programming Research," this report). All phases of the monitor appear to be working well, and work flows through the computer at an average rate for the year of 138 jobs per day. Figure 3 shows this daily average by month.

The Digital Plotters

A Calcomp Digital Incremental Recorder and a model 580 magnetic-tape transport were purchased and added to the operation during the year. Not only has this second plotter eased the plotting load on the single plotter already in operation, but it has also provided "backup" in case of breakdown.

The new plotter is similar in operation to the plotter described in the last report; however, two important improvements were included. The tape unit associated with the new plotter requires tape written at a density of 556 bits/in., as compared with the 200 bits/in. requirement of the older plotter. Second, the step size in the x and y directions has been reduced from 0.01 in. on the old plotter to 0.005 in. on the new, thus making possible plots of much higher resolution.

Later in the year, the older plotter was upgraded so that it too would accept 556-bit/in. tape and had a step size of 0.005 in. This was done to make the two plotters completely compatible, so that plotting could continue even if one should break down. Figure 4 shows plotter use by month.

Operating Services

The problem setup group was expanded during the year and continues to assume 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 this work through the center.

The operating staff has been expanded to make possible the operating of the computer and associated peripheral equipment 24 hours a day, five days a week.

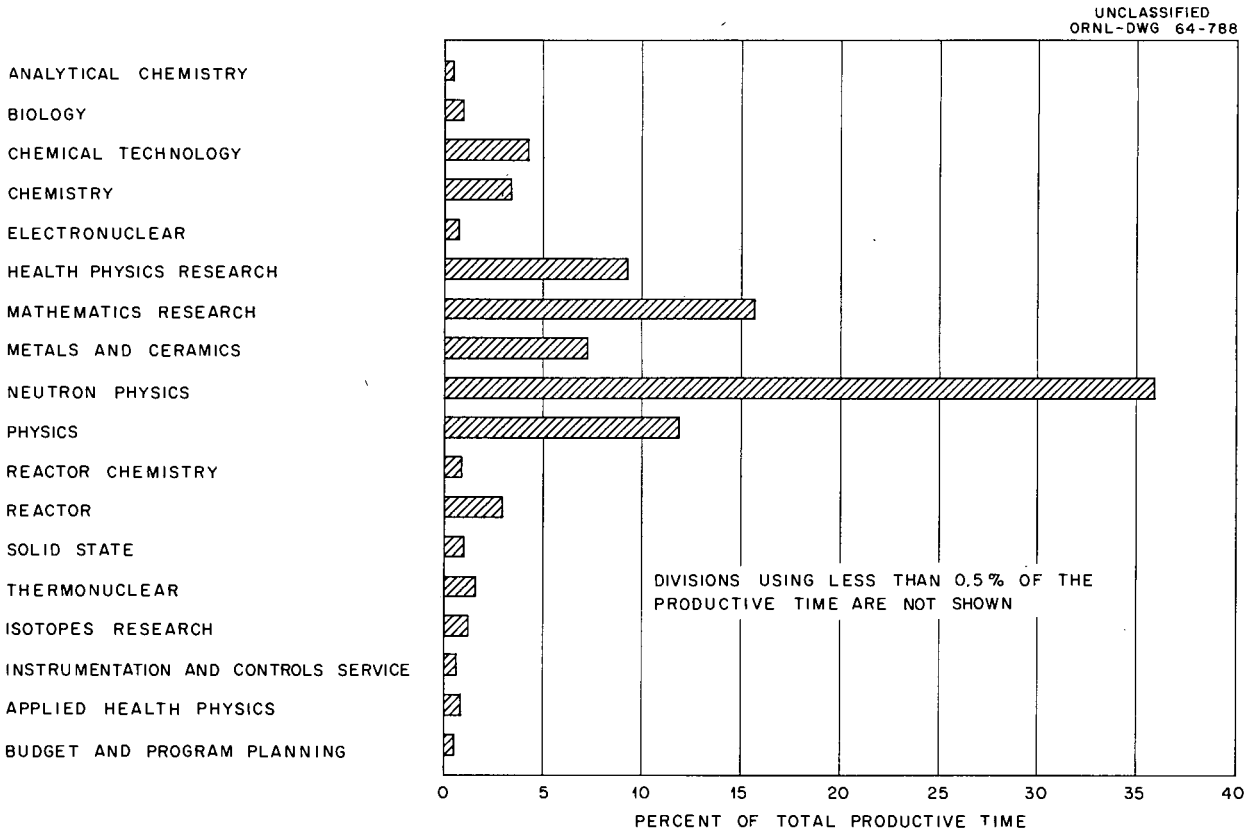

Fig. 2. CDC 1604-A Use by Divisions.

The keypunch section has again been expanded, to accommodate the work load this past year, and continues to provide keypunching service to the Laboratory.

Special Routines

A CDC 1604-A subroutine package[42] 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. This package is more flexible than those previously defined[43,44] for the IBM 7090.

A new version of the IBM 7090 package had to be written when the low-density plotter was replaced, because the original package was produced for low-density tapes only. This version, which incorporates the added features of the CDC-1604-A package, is now ready for use and a description of it will soon be published.

[42]D. K. Trubey and M. B. Emmett, *A CDC-1604 Subroutine Package for Making Linear, Logarithmic, and Semilogarithmic Graphs Using the CALCOMP Plotter*, ORNL-3447 (June 10, 1963).

[43]D. K. Trubey and M. B. Emmett, *An IBM-7090 Subroutine Package for Making Logarithmic and Semilogarithmic Graphs Using the CALCOMP Plotter*, ORNL-TM-430 (Dec. 12, 1962).

[44]D. K. Trubey and M. B. Emmett, *An IBM-7090 Subroutine for Making Linear Graphs Using the CALCOMP Plotter*, ORNL-TM-430 supplement (Feb. 27, 1963).

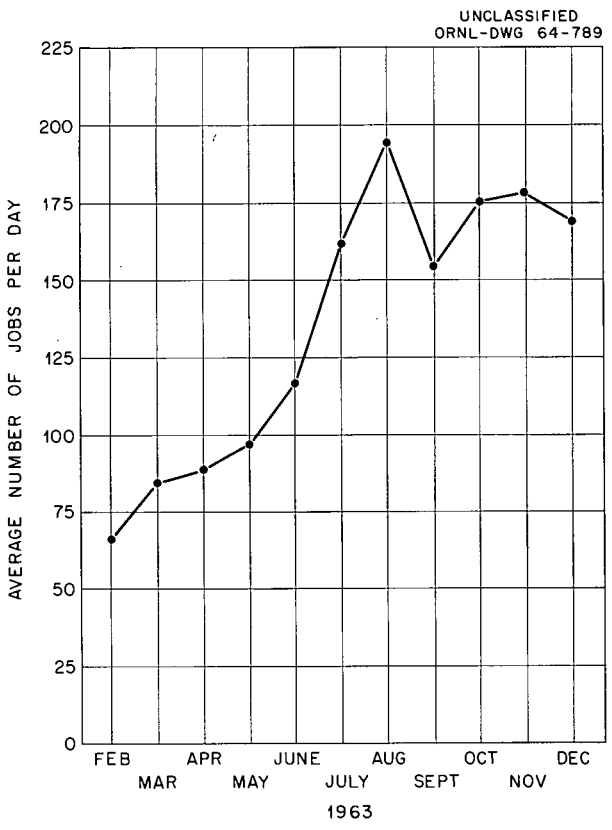

Fig. 3. Work Load at ORNL Computing Center.

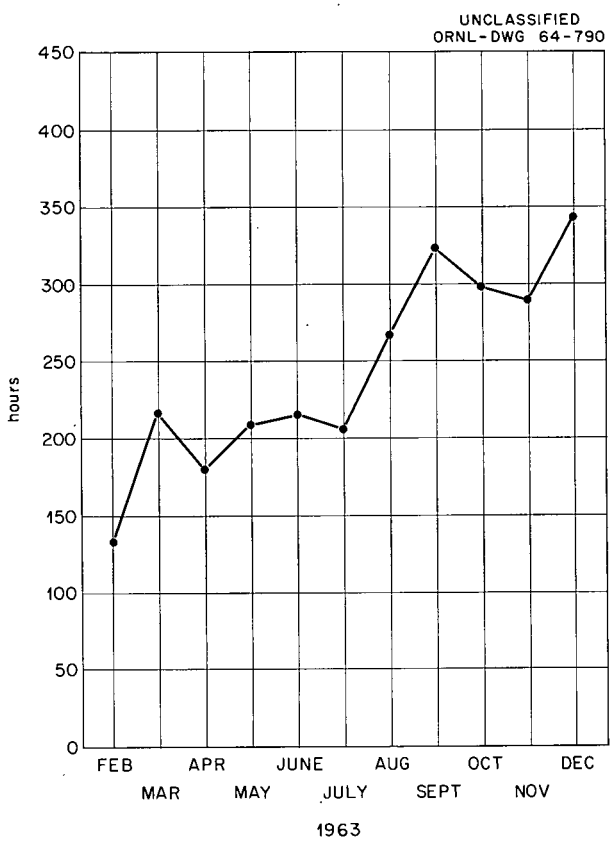

Fig. 4. Digital Potter Use.

Systems Programming

Peripheral processing codes for the CDC 160-A have been revised and to some extent rewritten to allow for the new equipment added to the 160-A systems. Simultaneous peripheral processing on the 160-A has been achieved and has resulted in a considerable saving in processing time. The basic plotting package for the 1604-A was rewritten and improved, taking into account the modification of the Calcomp plotter. Some modifications were made in similar codes for the IBM 7090 in order to preserve compatibility.

Library subroutines provided by the Control Data Corporation for FORTRAN 62 have been examined. Wherever possible they were rewritten to improve speed or accuracy or both.

Debugging of FORTRAN 63 and the ALGOL compiler has proceeded in the sense that each error occurring in compilation or execution was referred to the Control Data Corporation for appropriate action. Many of the library subroutines provided with FORTRAN 63 have been revised in the same fashion as for FORTRAN 62.

The ALGOL monitor system has been modified and made similar to the CO-OP monitor system.

Mathematical Statistics

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Introduction

A function of the Statistics Group of the Mathematics Division is to encourage an atmosphere in which new concepts can be explored and fundamental research carried out using statistics and biomathematics. This group provides consultants who are qualified to assist research investigators in the physical and biological sciences in the development of statistical methods pertinent to their specific areas of interest. The Group also serves as a center within the Laboratory in which basic research in statistics and biomathematics is conducted; consultation is provided on the statistical design and analysis of experiments and on methods for the analysis of experimental data; lectures and training programs are given to Laboratory personnel to acquaint them with statistical techniques; research is conducted in methods of numerical analysis basic to programming data from physical and biological sciences; consultation is provided on certain computing problems; and methods of scaling and coding physical and biological data are developed.

The need for the services of statisticians was recognized in 1950 when the Laboratory employed its first statistician. His primary function was to satisfy the needs of investigators in the various sciences by providing techniques of experimental design and analysis of data. Since that time the Statistics Group has increased in size, fulfilling the needs and demands made upon it for services on the part of Laboratory personnel. At present the staff of the Statistics Group includes five statisticians, two persons qualified to program high-speed computers, a supervisor for a Data Recording Group, and three key-punch operators. Despite the substantial increase in staff during the past eight years the Statistics Group finds that the demands made upon it have continually exceeded its capacity to provide prompt service for everyone.

Some of the specific problems which were handled by the Statistics Group during the past year are discussed elsewhere in this report. Generally it may be said that much emphasis was placed during this period on the use of high-speed computers for handling the large quantities of data which are processed by the Group. Also several areas of investigation such as random sampling studies and testing new mathematical models were attempted, as funds became available for computer use in attacking such problems. Moreover, mathematical models, derived in collaboration with principal investigators, and suggested by a straightforward probability argument, were tested against experimental data by use of the high-speed computers.

In parallel with the increased use of high-speed machines to effect the computations of statistical analysis, there has been a considerable effort spent on the adapting, revising, and construction of computer programs. All of the BIMD programs written by the School of Medicine of the University of California at Los Angeles, with the exception of those few written in machine language, have been adapted to run on the CDC 1604-A or the IBM 7090 in Oak Ridge or on both.

A computer program for nonlinear estimation using the Gauss-Newton iterative technique has been revised to provide automatically a graphic picture of the results by use of the X-Y plotter. As a result of investigations into programming methods of search, a program has been written which will display the sum-of-squares hypersurface in three dimensions in grid form. Also, work continues on the Oak Ridge Linear Regression Program, which is being written in ALGOL. That portion of the program which computes the preliminary analysis of variance is currently in use.

As the Laboratory has added to its history, it has added to the stores of data bearing on the several phases of its research. The aggregate of information pertaining to a subject of research manifests itself by an accumulation of data displaying little comprehensive balance or continuity. This is necessarily so because experimentation is dynamic; its aims change as new ideas are brought forth, and its direction changes as more is learned about the subject. Of late, our scientists are thinking more and more of a comprehensive treatment of the store of data in order to recover that information which might be revealed by an analysis of all the data at hand. Concurrently, new methods and theories for accomplishing such analyses are receiving attention in the literature. The Statistics Group feels a responsibility to adapt and modify these methods to the needs of the Laboratory. However, the pressure of day-to-day consulting makes this difficult.

A continued effort was made to bring investigators in for consultation during the planning stages of an experiment, and before the data had been collected. The common procedure in most research establishments is to approach the statistician after an experiment has been completed. It is only then, perhaps that the investigator may realize that he is in trouble. He may not know, however, that by following such a procedure he is preventing the statistician from applying one of the most useful tools of a statistician's trade, namely, the design of experiments. In an effort to alleviate this condition, the Statistics Group is engaged in a persistent campaign to educate the principal investigators in the best uses which can be made of its staff. As a result of this campaign many more experiments are carried out in the Laboratory according to a plan or experimental design provided by the Statistics Group. The details of several such experiments are discussed in the paragraphs which follow.

Discussions continue with members of the Biology Division concerning the plans for a low-level radiation study. Close contact with the investigators on this study has been maintained in the initial pilot program, which is being carried out at present. The fact that large numbers of animals will be involved and many variables will be studied over a long period of time presents a major problem in the logistics of collecting and analyzing data. Already, information from the breeding studies carried out in the pilot program is available for examination at regular intervals, so that more precise estimates may be made of the specific needs for the different phases of the long-range experiment. It is likely that the data from this experiment will be collected automatically by means of some data collection system. Consequently, several such automatic systems are being examined.

Retrospective studies are being made, in conjunction with the Health Division, of death rates and other vital information collected in the course of dispensary visits and regular health examinations of employees at the local AEC installations during the past ten or twelve years. Health records are maintained at present in 80-column Hollerith cards. It has been proposed that these data be transferred to magnetic tape for processing by high-speed computers. In such processing, more complete studies of both past and current information will be feasible. It is hoped that the results of some phases of these studies will be ready by the end of the next report period.

During the past year the Statistics Group has been called upon several times by the Division of Biology and Medicine of the Atomic Energy Commission to evaluate proposals for funds for experiments in biology. Members of this group have also been asked to review and comment on statistical techniques employed in scientific studies dealing with the effects of radiation on humans. In all cases where such requests were made, an evaluation of the particular experiment or document was presented without delay to the Division of Biology and Medicine.

Also, consultation services were provided, during this report period, to members of the staffs of the Oak Ridge Institute of Nuclear Studies, the University of Tennessee, both at Memphis and at Knoxville, Vanderbilt University, and the UT-AEC Agricultural Research Laboratory. In general, the policy of the Statistics Group of the Oak Ridge National Laboratory has been to provide statistical assistance and consultation to everyone who seeks it. It is the feeling of the Group that the education of investigators in the areas of the physical and biological sciences to statistical methods will serve to minimize the cost of experimentation and maximize the yield from these experiments. Unfortunately, with the small staff available for such services only a limited amount of consultation of this type may be carried out.

Statistical Research

The analysis of variance of nonorthogonal data is commonly performed by one of several exact methods or one of several approximate methods. Since the calculations for the exact methods are more difficult to perform, and to learn, the approximate methods are used by investigators who are not sufficiently familiar with the exact methods. Other investigators use an approximate method when they feel that the results of the approximate analysis would be nearly identical to those of an exact analysis for a specific experiment. Two approximate methods have been investigated in order to determine, more precisely, the experimental conditions under which the methods can be used with little loss in accuracy. In addition, the assumptions under which the two approximate methods and three exact methods are desired have been reviewed and restated.

In the approximate methods the statistics used to test hypotheses are not distributed exactly according to the probability distribution used, the F distribution, except in special cases. Thus, tests of hypotheses are actually conducted at probability levels different from intended levels. The distributions of the statistic and of F are central when the hypothesis under test is true. The distributions are noncentral when the hypothesis is false.

For one of the approximate methods, the method of unweighted means, the central distributions were investigated theoretically and found to be closely approximated by the central F distribution. The noncentral distributions for the same method were examined by empirical sampling studies which indicated that they are not generally well approximated by the noncentral F distribution. Since theoretical and empirical studies would not be practical in specific problems, approximate procedures were developed to judge the degree of aberration from intended levels of probability.

Another method, the method of expected subclass numbers, is biased in addition to being only approximate. The bias was found to be a function of the sample subclass numbers. Thus, the test statistics can be corrected for bias even though their distribution is still only approximated by the F distribution. The aberration of probability levels in the central case was investigated through empirical sampling studies.

Statistical Applications

BIOLOGY AND MEDICINE

Biomedical Data Recording

The services of the Data Recording Group were extended to new users in the Biology Division and to other divisions of the Laboratory. This increased activity created the need for an additional key punch operator, who was added to the staff in February 1963. Also added during this report period were two IBM 026 card punches, one IBM 056 card verifier, one IBM 557 alphabetic interpreter, and one IBM 088 collator.

One new application for the Biology Division this year was the recording of mouse breeding data for the study of low-level, long-term effects of radiation. Machine programs have been written for the statistical analysis of trial data collected in this study. It has been apparent since the inception of this project that conventional methods of collecting and handling the large amounts of data would be extremely cumbersome. Therefore, some means of automating the data collection task is under consideration. Several such systems are being considered at present. No decision has yet been reached as to which system will be used.

New IBM 1401 programs prepared by the Group include:

1. Tissue Culture: Publications listings. Author, title, and reference cards were punched according to the Bell Laboratories BEPIP layout. A program was written for the IBM 1401 to list these cards by the following categories: (*a*) serially by a particular primary author, (*b*) serially by a particular author, either primary or secondary, (c) serially by a particular journal, (*d*) prime author order by a particular journal, (e) serially by reference to two chromosomes, (*f*) author order by reference to same two chromosomes as in e above, (*g*) serially by a particular chromosome in either of two positions, (*h*) author order as in *g* above, (*i*) serially by translocation number, and (*j*) author order by translocation number.
2. Fungal Genetics and *Drosophila* Genetics: A program to write a four-line address on gummed labels for two investigators with rather large mailing lists.
3. Fungal Genetics: The investigator wanted to test all possible combinations of 70 *Neurospora* mutants. A program was written to save the time and labor of writing 70 × 70 combinations of numbers manually. Output was on gummed labels showing mutant No. 1 with mutant No. 2 ... 70, mutant No. 2 with mutant No. 1 ... 70, etc.
4. Physiological and Chemical Effects of Radiation: A program to provide preliminary data reduction of breeding data in the low-radiation-level mouse study. Total number of offspring born to selected female mice and age of mother at first litter are shown. Further statistical treatment is obtained from programs written for the CDC 1604-A.
5. Fungal Genetics: Simple listing of *Neurospora* data punched in cards.
6. Microbial Systems and Mammalian Cell Regulation: The investigator is studying the relationship of amino acids with certain enzymes by using C^{14} and H^3 labeled molecules and counting on a scintillation counter. The C^{14}-H^3 discrimination is calculated by an IBM 1401 program as follows:

$$X = A - \frac{Q(B - AP)}{1 - PQ}, \qquad Y = \frac{B - AP}{1 - PQ},$$

where A = A-channel reading for the unknown, B = B-channel reading for the unknown, $P = H^3$

ratio B/A for standard, $Q = C^{14}$ ratio A/B for standard, $X = H^3$ counts, and $Y = C^{14}$ counts. The X and Y values for each sample, usually about 100 in each run with 2–4 aliquots each, are listed, and on the same line a scaled point is indicated to show graphically the results of the test run. This has proved to be a great time saver for the biologist.

7. Administration: Regular alphabetic listings of personnel with their associated charge numbers.
8. Health Division: The Industrial Hygiene Department conducts a beryllium monitoring program in various divisional areas at ORNL. Both air and smear samples are taken. An IBM 1401 program was written to show the division, sampling point, and other identification. From the total beryllium found by chemical analysis and the volume of air or area surface sampled, the beryllium concentration in milligrams per cubic meter or per 12 sq. in. is calculated. For each sample point a summation is made showing total number of samples, total number of positive results, and number of samples which fall into the three categories: <50% MAC, 50–100% MAC, and >100% MAC. Lists are run monthly and quarterly. Such a tabulation was needed to meet AEC requirements as well as to automate the calculation of results for better management control.
9. Health Physics Division: Tabulation of ORNL visitor films.
10. Instrumentation and Controls Division: Tabulation of instrument inventories.
11. Reactor Division: Listing of surplus materials and parts inventory.

Cost accounting data for the Statistical Services Department continues to be helpful to management. On the average, income for the data recording unit exceeds expenditures.

Much work remains to be done in the area of information retrieval and dissemination. It is suggested that a feasibility study be made to determine the need for establishing an information center for the biomedical field. The Biology, Health, and Health Physics Divisions, the Oak Ridge Institute of Nuclear Studies, the UT-AEC Agricultural Research Laboratory, and the Atomic Energy Commission should all be deeply concerned in this area of study.

Cytology and Genetics

Studies have been made of the action spectra for ultraviolet-induced chromosome aberrations in Chinese hamster cells *in vitro*, pretreated with 5-bromodeoxyuridine (BUdR) or 5-iododeoxyuridine (IUdR). There is reason to believe that the incorporation of thymidine analogues into the cells will modify the action spectrum. Cells exposed to different wavelengths of uv radiation in the presence of IUdR or BUdR or neither were scored for numbers of terminal deletions and exchanges. The number of aberrations per cell was estimated at each wavelength. Then, assuming that the numbers of aberrations were Poisson-distributed and that the number of cells scored was fixed, it was possible to estimate the ratio of aberrations per cell in cells treated with BUdR or IUdR to aberrations per cell in cells not treated in this way, for all levels of uv radiation. At the same time, a confidence interval was calculated for each of the estimated ratios and for each estimated mean of the number of aberrations per cell.

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Mutants of bacteriophage T4D have been isolated and characterized by the fact that they can propagate at low temperatures. Using two-factor cross data for mutations which are uniformly distributed over a large portion of the genome, attempts were made to construct a map which bears a close relation to the "physical map." In principle, one wishes a mapping function which permits conversion of recombination values to map distances. In an effort to arrive at estimates of some of the map distances, 17 observations involving eight intervals on a small segment of the genome were examined statistically. The data, representing recombination distances, were regarded as 17 independent measurements on eight unknown intervals. Then estimates of the sizes of the eight intervals were achieved by the method of least squares. The results are being evaluated for possible extensions to the entire genome.

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Experiments with *Neurospora crassa* have been designed to determine whether 5-fluorodeoxyuridine (FUdR) and structurally related pyrimidine nucleosides are consistent in their effect on the fre-

quency of recombination among four closely linked markers. The effect on recombination in each of three regions is determined by treating a cross of two strains of the genotypes A + *hist-3* + *nic-2* × a *arg-3* + *ad-3B* +. The data resulting from these experiments are in the form of ratios of numbers of recombinants to number of spores in the medium. Inasmuch as the numerator and denominator of each ratio are Poisson counts, confidence limits may be estimated by a method proposed by Birnbaum.[1] Moreover, when the denominators of two ratios are either fixed or equal, the Birnbaum procedure provides a test of the hypothesis that two ratios are equal. This latter approach permits the test of the hypothesis that the proportion of recombinants is the same in treated groups as in the controls.

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An analysis of data from experiments on induction of rings and dicentrics in *Tradescantia* pollen grains by gamma radiation was undertaken in cooperation with members of the Radiobiological Research Unit of the AERE, Harwell, England. The data, which had been collected in England, were transmitted here to be fitted to the two mathematical models:

$$Y_i = N(1 - e^{-kD_i})^2 ,$$

$$Y_i = N\left\{1 - e^{-k_2 D_i}[1 - (1 - e^{-k_1 D_i})^2]\right\} ,$$

where Y_i is the average number of rings and dicentrics at dose D_i and k, k_1, k_2, and N are parameters to be estimated. Successful fits were achieved to the first of these two models, and estimates of the parameters and their standard errors were returned with the data to the research unit in England. A closer study of the second model is still under way.

Drosophila Cytology and Genetics

Experiments were carried out to test the effects of various oxygen and helium tensions applied before, during, and after x-radiation of adult *Drosophila* females on the survival of stage-7 and stage-14 oocytes. The data from these experiments were analyzed in such a way as to compare the parameters of survival curves, where the survival fraction is measured by the ratio of live pupae to total radiated eggs. The "multi-hit" survival model to which the data were fitted is:

$$S_i = k_2[1 - (1 - e^{-k_1 D_i})^n] ,$$

where S_i is the survival fraction at dose D_i, k_2 is the survival fraction at zero dose, k_1 is the expected number of lethal events per unit of dose per target, and n is the number of targets, or "extrapolation number." A subroutine was written to fit this model by means of existing computer programs. In addition, a curve plotter program was written, with options to plot the data from each experiment individually or to plot the results from several experiments on the same graph. The purpose of this latter option was to facilitate the visual comparison of results from several related experiments on the same scale. Data from six experiments were run simultaneously with excellent results. Estimates of the parameters (k_1, k_2, and n) and their standard errors, as well as graphical plots, were produced by the CDC 1604-A computer and its associated curve plotter for all experiments.

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The progeny of irradiated *Drosophila* males are scored for the appearance of linkage between normally unlinked genes in experiments designed to detect translocations. In a study of X-autosome translocations the daughters of irradiated males were utilized. Since crossing-over makes the recognition of translocations difficult, the progenies must be counted. Inasmuch as each of the progeny contains as many as 48 different phenotypes and tests only a single irradiated genome, scoring a large number of treated genomes would involve a vast amount of counting if each of the progeny were counted to completion. To minimize the amount of counting required to score translocations, a procedure of counting and analyzing the data on alternate days was adopted. Each progeny is compared with control progenies, and those showing no difference from control are

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

discarded. Comparisons are made of the proportions of various types of translocations, and the probability that two proportions be drawn from the same population is determined by use of the binomial distribution. The decision to continue counting is based on the total number of flies counted, presence of exceptional progeny, evidence of a sex-linked-recessive lethal, and the various probabilities. The analysis of the data and the decision to continue counting is carried out on alternate days by a suitably programmed high-speed digital computer.

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A nonrandom assortment of nonhomologous chromosomes during meiosis may be induced in *Drosophila* females with high frequency. Inasmuch as marked preferences are shown for nonhomologous pairing when more than two chromosomes are available, experiments were carried out to determine the role of chromosome size and site in determining preference. From data collected in these experiments, estimates and standard errors were calculated for the percent of nondisjunction between X duplications of different sizes and chromosome 4.

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A computer program was written to generate tables of expected frequencies at metaphase I of univalents, bivalents, trivalents, and quadrivalents from a set of four homologous chromosomes which synapsed at prophase as two pairs (*A*) or one quadrivalent (*B*). Two tables were generated for each value of $p = 0.01\ (0.01)\ 0.99$, where p is the probability that any pair of synapsed homologous arms will remain joined together until metaphase I by at least one chiasma. The value of p is estimated directly as the ratio of the mean observed frequency of pairs of arms containing one or more chiasmata to the number of pairs of homologous arms, assuming that chiasmata are randomly distributed among arms. The two tables for each value of p, A and B, were generated on the further assumption that the relative contribution of A and B to observed metaphase pairing depends on the number of independent sites of initiation of synapsis. That is, the probability of A, Pr (A), is equal to $1 - \Pr(B)$.

Cell Growth and Differentiation

In an effort to describe cellular changes during lens regeneration in the adult newt *Triturus pyrrhogaster*, quantitative measurements were made using electron microscopic techniques. Among the variables observed at different times after the removal of the lens were cellular and nuclear areas, sizes of the nucleoli, numbers of nucleoli, and numbers of ribosomes. Although no attempt was made to describe mathematically the functional relationship of these variables with time, estimates and confidence intervals were calculated at different points in time for (1) the average proportion of nuclear area to total cellular area in both dorsal and ventral portions of the iris; (2) the average ratio of nucleoli to nuclei per section of the dorsal portion of the iris; (3) the average size of the nucleoli and the average area of the nucleolar core; and (4) the average number of ribosomes in the cytoplasmic matrix.

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To determine whether or not the enhancement of protein synthesis is connected with the area of the iris involved in tissue transplantation, a comparative autoradiographic study of uptake of H^3-leucine was made of one part of a lens-removed eye which regenerates and another part which does not regenerate in adult *Triturus viridenscens*. The data collected in this experiment represented grain counts in a unit area of tissue from the eyes of several groups of salamanders. The average ratios of grain counts per unit area between regenerating systems and control and between nonregenerating parts and control were estimated, and confidence limits were calculated assuming that the fraction represented the ratio of two independent Poisson counts. The results indicated that the ratios between regenerative systems and control increased considerably with time in days after lens removal, and that no significant change with time was apparent in the ratios between nonregenerative systems and controls.

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The cell metabolism of hair bulb pigment cells in relation to their rhythmic function has been studied. Three groups of labeled compounds were

injected into young agouti mice. In autoradiographic sections, silver grains were counted per unit area. Estimates of the relative grain number for uptake of different labeled compounds were calculated by taking the ratio of the number of grains in the pigment cells to the number of grains in the epidermal cells. Confidence intervals for three estimates were found by assuming that the grain counts in both numerator and denominator of the ratio follow a Poisson distribution.

Pathology and Physiology

The size distributions of blood platelets can be estimated with a 25-channel Coulter electronic particle counter. These distributions are used to study both aging of platelets and aberrations in platelet production due to abnormal conditions. Electronic noise and particles in the diluent cause error in counting platelets of small size. Since these errors occur in channels 1–3, the distributions were truncated to eliminate all counts below channel 4. The distributions are also truncated at channel 25, and procedures for obtaining unbiased estimates of the mean and variance of doubly truncated distributions were used.[2] A method of estimating the number of counts due to the noise and the diluent, separately, has been proposed for future experiments. A more efficient and simpler estimation procedure can then be used.[3] A program for the CDC 1604-A computer has been written for processing the Coulter counter data.

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Hematologic studies were conducted on female mice exposed to 50, 100, 200, and 400 rads of 14-Mev neutrons. Control mice were sham-irradiated. Total leukocyte counts, hematocrit determinations, and differential leukocyte counts were performed on five to ten mice from each treatment group at intervals for 55 days following irradiation. A computer program was written to process the basic data and compute means, variances, and confidence limits for each subgroup of mice. These statistics were used to analyze the effects of radiation during the first weeks following irradiation and the rate of recovery during successive weeks for each group.

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Several physical and biochemical properties of connective tissues have been shown to vary with the age of the animal. Tail tendon fibers from mice exposed at 2–4 months of age to a single 450-r whole-body x radiation were used to investigate age-dependent changes influenced by amounts of ionizing radiation that cause animals to die prematurely with symptoms and signs suggestive of precocious aging in other tissues. The temperature of maximum contraction (TMC) of individual fibers was used as an age-related variable. Regression analyses relating the TMC to the age of the animal were performed for breeding and nonbreeding female mice for irradiated and control groups. These analyses were used to test hypotheses on the effects of aging, x radiation, breeding status, and their interactions on the TMC.

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Adult female mice were acutely exposed to 350–1800 r of 250-kvp whole-body x rays. Some mice at each dose level received 8.8 mg of S,β-aminoethylisothiuronium·Br·HBr (AET) just before irradiation, 10×10^6 isologous bone marrow (IBM) cells just after irradiation, or both AET before and IBM after irradiation. Survivors and unirradiated controls were observed throughout life and examined pathologically after death. Although AET and IBM markedly protected against early lethality and against the induction of thymic lymphomas, protection against life-shortening was less pronounced or equivocal.

The treatment of groups of mice with AET and IBM in the experiment was not orthogonal to variations in levels of x rays. The appropriate statistical analysis was not only more complex, but also less efficient in the sense of requiring more animals than an orthogonal design to obtain the same amount of information.

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Data from experiments on sensitivity to x radiation in terms of mortality of 13 strains of mice

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[2]A. C. Cohen, *Biometrika* **44**, 225 (1957).

[3]D. G. Gosslee *et al.*, *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 29.

were collected and summarized by statistical methods. The data were the results of many different investigators of the Biology Division who use similar radiation conditions. The sources were x rays from 250–300 kvp radiotherapy machines, and dose rates varied from 90 to 165 r/min. Mortality curves, the median lethal dose (LD_{50}), and 95% confidence limits for the LD_{50} were estimated using the probit transformation. The results of these analyses were presented in graphical and tabular form.[4]

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Data from experiments on transplantation of bone marrow cells in mice were submitted for processing and analysis on a weekly schedule. A previously written computer program[5] used to process the raw data was expanded to prepare cards for input for one or more of five programs used to analyze the data. The analyses include regression studies and tests of hypotheses of effects of controlled factors.

Mammalian Recovery

To date, attempts to understand the factors responsible for spontaneous circumvention of secondary diseases or spontaneous cures which favor survival of irradiated mice treated with foreign bone marrow have been unsuccessful. Two approaches which have been suggested as possibly leading to a better understanding of these factors are being investigated by means of statistical techniques.

One attempt is to study retrospectively all bone marrow experiments carried out in a single laboratory of the Biology Division since 1955. Data from these experiments have been recorded on IBM cards for machine processing. The plan is to reexamine 90-day cumulative mortality in all rat and homologous bone marrow chimeras, taking into account such variables as strain, sex, age of donor, amount of cells transplanted, and date of transplantation. It is hoped that some influential factor in spontaneous recovery from secondary disease will be found in the results of such analyses.

The second is a prospective study involving the use of experiments 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. The variables selected for study in the first experiment are bone marrow dose, day of injection, age of donor, and sex. The experimental design chosen for the initial phase of this study was a 2×2^3 factorial design with four center points, laid out in two blocks. The factor levels are: 10×10^6 and 50×10^6 cells of bone marrow, with center point at 30×10^6 cells; injection at 0 and 3 days after irradiation, with center point at 1.5 days; and age of donor 7 and 91 days, with center point at 49 days. The factor of sex is, of course, at the two "levels," male and female. More details and preliminary results of this experiment may be found in ref. 6. Each treatment combination is applied to 15 mice; the mice are caged five to a cage, and the total number of mice in the experiment is 300. The variable being observed is the proportion of mice dead after 90 days out of 15 at each experimental point. If this variable is designated by $p = d/15$, the analysis will be carried out on the transformed variable $\theta = \arcsin \sqrt{p}$, where the variance of $\theta = 54.7$.

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In a study dealing with the quantitative aspects of germinal center dissociation and the migration of germinal center cells in the spleen of normal and autogenically stimulated animals, the germinal cells were labeled and systematically followed at close intervals so that data in terms of grain counts could be obtained on their activity and migration patterns. The factors in the experimental design were five hourly groups, two treatments, and three cell types. In addition four animals were examined within each hour-treatment group, and four germinal centers were counted in each animal. The model proposed for the analysis of variance was

[4]M. L. Davis, G. E. Cosgrove, and D. G. Gosslee, internal memorandum.

[5]D. G. Gosslee *et al.*, *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 18.

[6]C. C Congdon, *Biol. Div. Semiann. Progr. Rept. Aug. 15, 1963*, ORNL-3498, pp. 91–92.

$$Y_{ijklm} = \mu + H_i + T_j + (HT)_{ij} + A_{l(ij)} + G_{m[l(ij)]} + C_k + (HC)_{ik} + (TC)_{jk} + (HTC)_{ijk} + (AC)_{kl(ij)} + (CG)_{km[l(ij)]} ,$$

where Y_{ijklm} is the mean grain count per unit area in the mth germinal center in cell type k of the lth animal in the jth treatment group of the ith hour, and where $i = 1, 2, \ldots, r$ hours; $j = 1, 2, \ldots, s$ treatments; $k = 1, 2, \ldots, t$ cell types; $l = 1, 2, \ldots, v$ animals; and $m = 1, 2, \ldots, w$ germinal centers.

The hours, treatments, and cell types were taken as fixed effects, and the animals and germinal centers were taken as random variables. On these assumptions, the resulting analysis of variance is given in Table 1.

Tissue Culture

Studies with 14-Mev neutrons and with x rays for which RBE = 1 have been undertaken in an effort to make accurate dose estimates from peripheral leukocyte chromosome aberration frequencies in cases of whole-body exposure of humans. Whole blood, freshly drawn from humans, was irradiated with increasing doses of either x rays or neutrons. The leukocytes were then separated, fixed, and stained in such a way that each cell could be scored for chromosome aberrations. Coefficients of aberration production were estimated from the models $Y_{i1} = a_1 + bD_i$ or $Y_{i2} = a_2 + cD_i^2$, where Y_{ij} is the average number of aberrations per cell at dose D_i, a_j is the coefficient of spontaneous aberrations, b is the coefficient of deletion production, and c is the coefficient of ring and dicentric production. The Y_{ij} values were assumed to be

Table 1. Analysis of Variance

Source	Degrees of Freedom	Expected Mean Square
Mean	1	
Hours, H	$r-1$	$t\sigma_g^2 + tw\sigma_a^2 + twvs\sigma_h^2$
Treatments, T	$s-1$	$t\sigma_g^2 + tw\sigma_a^2 + twvr\sigma_t^2$
Hours × treatments, HT	$(r-1)(s-1)$	$t\sigma_g^2 + tw\sigma_a^2 + twv\sigma_{ht}^2$
Among animals in hour-treatment groups, A	$rs(v-1)$	$t\sigma_g^2 + tw\sigma_a^2$
Among germinal centers in animals in hour-treatment groups, G	$rsv(w-1)$	$t\sigma_g^2$
Cells, C	$(t-1)$	$\sigma^2 + w\sigma_{ac}^2 + vwrs\sigma_c^2$
Hours × cells, HC	$(r-1)(t-1)$	$\sigma^2 + w\sigma_{ac}^2 + vwa\sigma_{hc}^2$
Treatments × cells, TC	$(s-1)(t-1)$	$\sigma^2 + w\sigma_{ac}^2 + vwr\sigma_{tc}^2$
Hours × treatments × cells, HTC	$(r-1)(s-1)(t-1)$	$\sigma^2 + w\sigma_{ac}^2 + vw\sigma_{mtc}^2$
Animals × cells in hour-treatment groups, AC	$rs(v-1)(t-1)$	$\sigma^2 + w\sigma_{ac}^2$
Cells × germinal centers in animals in hour-treatment groups, GC	$rsv(w-1)(t-1)$	σ^2
Total	$rstvw$	

Poisson means, and appropriate weights (reciprocal variances) were used in fitting the regression equations. Variances and confidence intervals were calculated for the parameter estimates, and chi-square statistics were computed to test the hypothesis of the goodness-of-fit of the models.

* * * * *

The survival kinetics of HeLa cells allowed to incorporate various amounts of H^3-labeled thymidine into their DNA was discussed in a previous report. The actual model was constructed on the assumption that the probability of survival of a colony of cells is a function only of the probabilities of survival in the first three generations. If then, the probabilities of survival at dose D_i in the first and second generation are

$$\pi_{i1} = \pi_{i2} = 1 - (1 - e^{-kx_i})^n ,$$

and the probability in the third generation is

$$\pi_{i3} = 1 - (1 - e^{-kx_i/2})^n ,$$

then it can be shown that the probability that the colony will survive at dose D_i is

$$\eta_i = 2\pi_{i1}^2(1 - \pi_{i1})[1 - \pi_{i3})^2] + \pi_{i1}^3[1 - (1 - \pi_{i3})^4] .$$

Data collected on H^3-thymidine and H^3-uridine were fitted to this model using an existing nonlinear least-squares program, and estimates of the parameters n and k and their standard errors were found. The results indicated that radiation-induced killing of mammalian cells is largely due to nuclear damage.

Radiation Immunology

The density of cells in a suspension was estimated in several experiments by the dilution series method. In this method successive dilutions are made until a test indicates that there are no longer any cells in a sample of the suspension. If a is the dilution factor and n is the number of successive dilutions for which the test indicated that one or more cells were present, then a^n was used previously as an estimate of the number of cells in the original suspension. This estimate was shown to be biased, and an unbiased method due to R. A. Fisher, which is 88% efficient and easily calculated, was used. The method of maximum likelihood is 100% efficient and unbiased but is not easily calculated. In experiments conducted to compare effects of controlled variables on the density, estimation was not of primary importance. It was found that hypotheses could be tested using n as the basic variable. Furthermore, the tests are 100% efficient and the theoretical variance of the mean of the number of dilutions, $\bar{n}$, of k replicate suspensions is known:

$$V(\bar{n}) = \frac{1}{k \log_2 a} .$$

Biophysics

In an effort to compare several sets of international standards, calibration curves were fitted to data involving determinations of the absolute numbers of electron spin resonances. The data represented observations on the signal for several weights of calibration samples taken on two successive days with the magnetic field in two different directions. Linear regressions of signal (dependent variable) on weight (independent variable) were fitted by least-squares techniques. Then the estimates and standard errors of the regression coefficients were used in determining estimates and confidence limits of the weights of a calibration sample for a given signal.

CHEMISTRY

Fractionation of Radionuclides

Let A, B, and C represent the ratios of the amounts of three radionuclides, found at a single sample location, to the total amounts of the nuclides released. Empirical studies of bomb debris have suggested that for certain nuclides, the proportions are related by the equation

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

Because it is possible that the same phenomenon could take place under appropriate conditions in a

nuclear reactor, chemists at the Laboratory have conducted simulation experiments and have collected data on eight radionuclides from as many as 42 sample locations. Theoretical considerations of the phenomenon suggest particular values for the parameters, α and β. The statistical problem is to determine whether the experimental results support the chemists' hypothesis.

Statistically, this is a problem in structural relations. The model may be simplified to

$$Y = \alpha + \beta X ,$$

in which Y and X are observables which may be written

$$Y = \eta + \epsilon ,$$

$$X = \zeta + \delta ,$$

the ϵ and δ being uncorrelated errors of observation. Under easily defensible assumptions, a joint confidence region for α and β may be constructed if the variances of ϵ and δ are known. Separate confidence intervals may be constructed (and hence tests of hypothesis on α and β, separately), if the ratio of the variances is known. However, we do not know the variances, nor do we know their ratio, although the latter would be easier to come by, conceivably. The problem then is unsolved. Work continues along two lines. One, which is admittedly quite difficult, involves the use of estimates of the variances of ϵ and δ. The other attempts to determine the ratio of the variances from the experience of the analytical chemists.

Impurities in Fuel Pellets

A request was received to analyze a set of data which pertained to what was inelegantly called, "Experiment 8 Crud." The data represented the results of chemical analyses for the quantities of Fe^{55}, Fe^{59}, Co^{58}, and Co^{60} in fuel pellets.

Four samples had been taken from a fuel pellet: one from the top, one from the middle, and two from the bottom. Three solutions were prepared from each sample; the chemical analyses were made from the solutions, one at one time and two at a later time.

The questions to be answered were: What is the distribution of the isotopes throughout the pellet? What is the variability of the analyses? Are there differences between similar samples? Are there dilution differences with and without respect to the time of the analyses?

The questions were put in the form of linear orthogonal contrasts, and estimates of the effects were computed using a general linear hypothesis computing program (UCLA FORTRAN program BIMD 14). There was a definite distribution pattern of the isotopes found in the pellet, with the highest concentrations in the middle section. The two solutions analyzed at the same time showed compatible results. For Co^{58} and Co^{60} the results showed differences over time. Only for Co^{60} were the two bottom samples significantly different.

Oxide Buildup on Aluminum

The thickness of oxide deposited on metal surfaces is postulated to follow the exponential model

$$X = e^{\alpha}\theta^{\beta}e^{\delta/K} ,$$

in which θ is the length of exposure of a specimen and K is the temperature at the surface of the metal. To simulate the buildup of oxides on aluminum as it might be experienced in the High Flux Isotope Reactor and the Advanced Test Reactor, 83 aluminum specimens were exposed in a medium similar to the proposed HFIR coolant and subjected to heat fluxes in the 1×10^6 to 2×10^6 Btu range for varying amounts of time. The thickness of the oxide deposits was then determined by metallographic examination.

From the resulting data, the constants, α, β, and δ, in the exponential model were estimated by linear regression. A short program was written to estimate oxide thicknesses with 95% confidence intervals for 56 selected combinations of θ and K.

Flooding of Pulsed Columns

An attempt is being made to describe a pulsed extraction column mathematically in order to predict flooding. Data have been collected from chemical engineering literature and contain about 1100 data points for several systems such as benzene-water and trichloroethylene-water. At present we are working with eight sets of data, each of which is aqueous continuous, with no mass transfer, and

which comes from pulse columns using metal perforated plates (excluding nozzle plates).

Fifteen proposed models have been fitted to two sets of data by the method of least squares. Work is in progress to fit the other six sets of data to these models. After determining a "best fitting model" by fitting each model to all the sets of data, we plan to remove the restrictions on mass transfer, perforated plates, and continuity of the aqueous phase, and suitably alter the model.

Corrosion Resistance of Aluminum–0.2% Titanium Alloy

An experiment was designed by personnel of the Statistics Group to study the effects of chromium, iron and silicon, manganese, and zinc on the corrosion resistance of aluminum–0.2% titanium alloy. The experiment was designed in sections or modules. Within each section tests can be made on the effects of chromium, iron and silicon, and manganese. A section will be run at each level of zinc, thus allowing tests of the effects of zinc and the interactions of zinc with chromium, iron and silicon, and manganese.

A section consists of 12 measurements, 2 for each of the 6 treatment combinations shown below. The levels of zinc are 5, 10, 15, 20, and 25%. Thus, one section will be run with alloys containing 5% zinc, another section with 10% zinc, and so forth.

Treatments	% Cr	% Fe + Si	% Mn
1	0	0	0
2	.3	0	.3
3	.3	.4	0
4	0	.4	.6
5	0	.8	.3
6	.3	.8	.6

ENGINEERING

Certification of High Efficiency Filters

High efficiency filters in use throughout the Laboratory must first be tested by the Plant and Equipment Division, and their efficiencies must be certified to fall within certain limits. To compute these limits an experiment was designed by the statisticians of the Mathematics Division and carried out by the personnel of the Plant and Equipment Division.

A split-plot experiment was performed with two whole plots (representing two concentrations of smoke blown through a filter) and five subplots (representing repeated tests of the filter). The tests were conducted by each of five technicians.

The standard error of a single test was computed under the assumption that the single test is performed by a technician chosen at random from the finite population of technicians participating in the experiment. From this standard error, a certification statement, quoting a 95% limit of error of $\pm 3.68 \times 10^{-3}\%$, was written.

HEALTH PHYSICS

Uptake of Strontium and Calcium

As an opening measure in studying the amounts of strontium and calcium taken up by shelled marine animals, an empirical study was undertaken in which snails were placed in environments of different strontium and calcium compositions. After a definite length of exposure, the amounts of the elements absorbed by the snails were chemically determined.

The experimental design which determined the Sr-Ca composition of the environments was a hexagonal design (with two center points) put down in the center of the region bounded by 0 and 10 ppm for strontium and by 0 and 200 ppm for calcium.

The data showed decided heterogeneity of variance for both strontium and calcium uptake. Weighted linear regression methods demonstrated planarity of the calcium response but decided curvature in the strontium response. Strontium uptake in environments of high calcium and high strontium was decidedly higher than would be expected by a planar predictor.

* * * * *

Algae were grown under simulated stream conditions to investigate the relationships between uptake and concentration of several elements.

Three linear regression models were applied to the data in an effort to describe the uptake of stable calcium or strontium by algae in terms of the concentration of these elements in the medium and the length of time in the medium. The following models were fitted to the data:

$$Y_i = a_{0i} + a_{1i} X_i + a_{2i} X_1 X_2 , \quad (1)$$

$$\ln Y_i = b_{oi} + b_{1i} \ln X_1 + b_{2i} \ln X_2 , \quad (2)$$

$$\ln Y_i = c_{0i} + c_{1i} \ln X_1 + c_{2i} \ln X_2 + c_{3i} \ln T , \quad (3)$$

where Y represents uptake by algae, X represents concentration in the medium, $i = 1$ for calcium, $i = 2$ for strontium, and T represents time.

The constants in models (1) and (2) were estimated by the method of least squares for each of ten intervals of time ranging from 1 through 840 hr. Equation (3) was applied to the combined data for all ten intervals.

Conferences with the investigators failed to produce a theoretical model, and models (1), (2), and (3) were constructed on empirical grounds. In addition to providing a means of summarizing the data, the models lead to a better understanding of the manner in which the variables are related. For example, the changes in estimates of the coefficients from one time interval to another and the separation of significant and nonsignificant terms aided in the interpretation. Each model was constructed using information based on the previous model, and since the deviations from model (3) are not random they are being studied in order to develop better models.

The models are consistent in the sense that they all indicate that calcium uptake is dependent on calcium concentration but generally independent of strontium concentration while strontium uptake is dependent on both calcium and strontium concentration.

Estimates of Radioactivity in White Oak Lake Bed

Last year's report[7] described the sampling plan devised to estimate the radioactivity in the White Oak Lake bed. During the current year the data gathered from that sample have been analyzed and the estimates calculated. The total amount of radioactivity in the top 24 in. of the bed is estimated at 1038 ± 88 curies of Ru^{106}, 704 ± 35 curies of Cs^{137}, 152 ± 9 curies of Co^{60}, 16.7 ± 3.3 curies of trivalent rare earths (excluding Y^{90}), and 14.6 ± 1.1 curies of Sr^{90}. About two-thirds of these amounts are found in the upper 6 in. of the bed soil.

Inflorescence of Local Sedges

Ecologists had collected data on the lengths of the flowering stems of two local sedges, *Carex frankii* and *Carex vulpinoidea*. The measurements were obtained from the plants as they grew naturally in seven distinct locations in the Oak Ridge area. The locations differed from each other in the constituency of the soil and the amount of radiation to which they had been exposed. The radiation dose and five measurable characteristics of the soil, pH, calcium, active phosphorus, exchangeable potassium, and organic matter, were proposed as contributors to the inflorescence of the sedges.

To screen for the contributing factors, the linear models

$$Y = \alpha + \sum_{i=1}^{k} \beta_i X_i ,$$

in which Y represents inflorescence, X_i is an amount of the ith contributing factor, and $k = 0$, 1, 2, 3, 4, 5, *or* 6, were proposed. Since the data were not orthogonal it was necessary to consider all of the 2^6 possible models to accomplish the screening. The model in which $k = 6$ was not fitted, because the resulting plane would pass through the seven averages and leave no means of assessing the adequacy of the equation.

The remaining 63 models were fitted and the best of the 63 was chosen for each of the sedges. For *Carex frankii*, pH, calcium, and radiation dose were jointly effective on inflorescence. Only radiation dose appeared to contribute to the inflorescence of *Carex vulpinoidea*.

[7] *Math. Div. Ann. Progr. Rept. Dec. 31, 1962*, ORNL-3423, p. 29.

METALS AND CERAMICS

Inspection of HFIR Fuel Plates

The advice of the statistician was sought on the problem of checking or verifying the results of nondestructive screening of HFIR fuel plates by a destructive chemical test. The fuel plates would be screened, using an x-ray technique, by the vendor of the plates. Then, presumably, a lot of approximately 500 plates would be accepted or rejected on the basis of an examination of a sample from the lot. The latter examination would involve the punching of disks from the plate (thus making the plate useless) and a chemical analysis of the disks.

Destructive testing of the screening plates was deemed inadvisable because too much of the lot would be destroyed. For example, if one were to correctly reject those lots containing 15 defective plates 95% of the time, a sampling plan with a rejection number of one defective plate would require a sample size of 100 plates. A destructive test of fuel plates is of questionable utility.

HFIR Fuel Assembly

Inner-Annulus Plate Cores. – Each of ten HFIR inner-annulus fuel plate cores was cut into thirds and a face of each cut was mounted for optical inspection of UO_2 depth. Analysis-of-variance techniques were used to decide that:

1. The UO_2 profile should be adjusted to add more UO_2 to the core.
2. There is approximately twice as much UO_2 depth variability within a core as there is among cores.
3. The variability of UO_2 depth within a core decreases with distance away from the thin edge.

Outer-Annulus Plate Cores. – The weights of 24 cores from each of 19 batches of cores for outer-annulus plates were analyzed to determine the average weight and weight variability of each batch. Analysis-of-variance calculations revealed that the batch average core weights varied from 80.334 to 80.590 g. The 95% level uncertainties on the batch averages varied from ±0.011 to ±0.037 g.

PHYSICS

Decay of Fluorine–21

The decay constant of F^{21} was estimated by a least-squares procedure for each of 17 experiments. A curve of the form $\ln N - \ln N_0 - kt$, where N is the number of atoms at time t, N_0 is the number of atoms at time 0, and k is the decay constant, was fitted to each of the 17 sets of data. The parameters k and $\ln N_0$, their uncertainties at the 95% level, and the standard deviation of $\ln N$ were estimated for each experiment.

REACTOR

Transport Characteristics of Suspensions

An attempt is being made to determine a satisfactory mathematical relationship between relative viscosity and concentration in a Newtonian suspension. Data were collected from the literature and fitted to ten different models by the method of nonlinear least squares. In no case was an adequate fit to the data obtained. Work continues on constructing mathematical models which describe the data.

Reproducibility of Critical-Heat-Flux Measurements

Many measurements of the boiling critical heat flux in each of four metal tubes had been collected by engineers of the Reactor Division. The engineers were interested in obtaining an estimate of the reproducibility of these measurements.

One tube was tested for eight days and the others for five days. The number of tests made per day varied from 2 to 13. Examination of the data revealed a negative trend in heat flux within a day's operations. The trend did not continue from one day to the next, but rather, the critical heat flux would jump back to a point near the original level at the start of the next day's testing. For a particular tube the within-day trend did not change from day to day.

It was postulated that Y_{ij}, the jth determination of critical heat flux on the ith day, could be represented by

$$Y_{ij} = \alpha_i + \beta X_{ij} + \epsilon_{ij} ,$$

in which α_i is the intercept peculiar to the ith day, β is the linear slope common to all days, X_{ij} is the jth test number for the ith day, and ϵ_{ij} is a random error.

With this model the variance of ϵ_{ij} was estimated by the residual mean square using least-squares regression theory. The residual mean squares for the four tubes provided the estimates of reproducibility desired.

UT-AEC AGRICULTURAL RESEARCH LABORATORY

The Effects of Radiation Dose and Humidity on Dry Weight of Rice Seedlings

Data collected from an experiment designed and performed by scientists of the UT-AEC Agricultural Research Laboratory were analyzed by the Statistics Group. These data furnished an excellent test of the use of a UCLA FORTRAN program (BIMD 14) in handling the analysis of data from complex experiments. BIMD 14, a general linear hypothesis program, was used to compute the analysis of variance for the experiment. This revealed real humidity and radiation dose effects and furnished estimates of variance useful for performing a weighted linear regression.

Another UCLA FORTRAN program (BIMD 31) was modified to accommodate the internal construction of weights to be used in linear regression problems. This program was used to estimate the coefficients of a two-dimensional cubic polynomial equation from the rice seedling data. Probability tests on the results of the regression analysis showed that although the weighting system was successful, the cubic model was not adequate to describe the results of the experiment.

Statistical Programming

BEHAVIOR OF INTERSTITIAL ATOMS IN Nb-Zr ALLOYS

Scientists in the Metals and Ceramics Division have been studying the behavior of interstitial atoms in Nb-Zr alloys by the use of internal friction. Their theory postulates the model

$$Y = \frac{B_1 B_2 \exp (B_3/X)}{1 + B_1 + [B_2 \exp (B_3/X)]^2} ,$$

in which Y represents a logarithmic decrement and X represents temperature in degrees centigrade. A program was written to estimate the parameters B_1, B_2, and B_3 by weighted least squares.

Because of the way in which B_2 and B_3 enter the model, the sum-of-squares hypersurface is rather unusual. Initial estimates of the parameters, as supplied by considerations exterior to the data, were not sufficiently close to the minimum of the hypersurface to accomplish convergence using a Gauss-Newton iterative technique.

An auxiliary program was written to display the sum-of-squares hypersurface in grid form. This enables the statistician to visually examine the hypersurface to better estimate the position of the minimum. In all cases to date the minimum was found in a long banana-shaped "valley." On one of the long sides of the valley the sums of squares increased gradually, while on the opposite side the sums of squares increased quite abruptly. This discovery, together with the discovery of a relative minimum in another location, is believed to explain the difficulty with convergence that was experienced earlier.

PROGRAM WBC

Program WBC is designed to process data from the Health Physics Division whole body counter. The data are taken from a 200-channel RIDL analyzer and a 512-channel Nuclear Data analyzer in the form of punched paper tape. From this form, the data are transferred to magnetic tape on the CDC 160-A and are merged with data (punched on cards from *in vivo* count data sheets) on the CDC 1604-A. WBC then processes individual spectra according to code and stores the original spectra, coded information, net spectra, and output information on magnetic tape for further use.

The code will strip K^{40} and Cs^{137} bands from a net spectrum and will calculate various quantities such as the sums, in counts per minute and in kilograms, over the low energy channels, and their estimated standard deviations.

ADDITIONAL OUTPUT FOR THE GENERALIZED LEAST SQUARES PROGRAM

In order to meet the demands for graphic representation of observed responses and of the estimated fit of their function, a FORTRAN subroutine SCALE has been written; this subroutine automatically labels the axes of a graph in such a fashion that reading between the labeled intervals is quite simple. Subroutine SCALE, given the minimum and the maximum value of a vector of an array, calculates a scale factor, an increment value, and a minimum axis value. The subroutine is designed for a 10-in. axis with 1-in. intervals which have an increment value of one, two, four, or five times an integral power of ten. The minimum value on the axis is a product of an integer and the increment value. Responses are distributed over one-half or more of the axis length.

SCALE has been incorporated into M. H. Lietzke's Generalized Least Squares program in such a way that either a linear or a semilogarithmic

graph may be prepared on the Calcomp plotter for each set of responses for which estimates of the parameters of the stated function are obtained. Both the responses and the estimated curve appear on the graph, the curve being plotted only between smallest and largest values observed for the controlled variable.[1] The subroutine has the capability for plotting curves from as many as six successive experiments on one graph.

Other additions to the output are the estimate of the variance of fit and the intermediate estimates of the parameters after each iteration in the least-squares solution.

CALCULATION OF STATISTICS DESCRIBING FREQUENCY DISTRIBUTIONS

The need for additional information characterizing coated particles led to the reprogramming and generalizing of an earlier version of a computer code. The new program calculates statistics which are helpful in describing frequency distributions. Such statistics include the mean, standard deviation, standard error of the mean, normality statistics (for skewness, kurtosis, and Geary's ratio), upper and lower confidence limits for the mean, upper and lower confidence limits for the standard deviation, and upper and lower tolerance limits.

The program will handle as many as six variables per problem. As options, linear relationships may be obtained between any two of the variables. Included, for each linear relation evaluated, are the slope, standard error of the slope, intercept, standard error of the intercept, variance, and coefficient of determination. In addition, a graph of the points and of the linear fit is plotted on the Calcomp plotter. This is the same kind of linear plot programmed as additional output for the Generalized Least Squares program described above. Although the program was written for describing distributions of coated particles, it is completely general and may be used with data in similar form from any source.

[1]For a special set of applications a program deck has been altered to include zero on the controlled-variable axis and to extrapolate each curve to the zero value.

OAK RIDGE LINEAR REGRESSION PROGRAM

Although there are many regression programs existing, there is a need for a program which will give sufficient analysis for a thorough statistical interpretation of data. In the past, programs were oriented toward the regression portion with only limited amounts of analysis. Further calculations were computed on a hand calculator, provided enough information was available from the program. To free the statistician from this chore and to enable him to give a more thorough analysis, the present general linear regression program was proposed. The planners, aware that voluminous data would be analyzed, have striven for flexibility and simplicity in preparing a method of transfer of data from experimenter to machine. The ALGOL language seemed to be the most suitable for this purpose.

The user indicates, as input, the number of replicates, treatments, and independent variables. In addition, he specifies a sentinel which may be any floating point number. The sentinel is used to separate one sample from another (a sample may contain one or more observations). The sentinels are punched after the last observation of each sample and after the last sample of each replicate of every treatment. Data are read, one word at a time, by the ALGOL *read* procedure. Observations are stored in a one-dimensional array. Whenever a sentinel is read, counters are incremented and arrays are set up; these are used to find the location of observations when referred to later in the program. A *real* procedure, Y, called by $Y(i, j, l, s)$, will give the value of the sth observation of the lth sample of the jth replicate of the ith treatment. An *integer* procedure, n, called by $n(i, j, l)$, produces the number of observations in the lth sample, jth replicate, and ith treatment. A table of the sums of weights and a table of the weighted sums of observations are printed for the total experiment, provided that each replicate contains the same number of samples per treatment; if not, each replicate is treated as a separate experiment, with output tables for each. If an experiment contains proportionate subclass numbers, a table for analysis of variance is printed; if proportionality restrictions are not met, each replicate is treated as a separate experiment and an analysis-of-variance table is provided for each replicate. The analysis-of-variance table contains rows labeled Total, Mean,

Replications, Treatments, Interaction, Sampling Error, and Error. The table contains two columns of F ratios, one for an experiment in which replications are a random effect and the other for experiments in which replicates are nonrandom.

That part of the program described above is complete and is being used routinely. Work continues on the other portions, which will provide the unified linear regression solution.

UCLA BIMD PROGRAMS

A series of programs was acquired from the University of California at Los Angeles to do the commonly requested types of statistical analysis. The 36 programs can be separated into several overlapping groups: Regression, Multivariate Analysis, Analysis of Variance and Covariance, Time Series Analysis, and Tabulating, Screening, and Plotting.

The programs have all been compiled and executed on the IBM 7090 under version III of FORTRAN II with the IBSYS monitor. The most frequently used programs have been converted for use on the CDC 1604-A.

BIOMATHEMATICAL MODELS

Subroutines to M. H. Lietzke's Generalized Least Squares program for the CDC 1604-A were written for the following nonlinear biomathematical models (the model numbers are shown in boldface type):

1: $y_i = 1 - (1 - e^{-kx_i})^n$,

1a: $y_i = k_2[1 - (1 - e^{-k_1 x_i})^n]$,

2: $y_i = e^{-k_2 x_i}[1 - (1 - e^{-k_1 x_i})^n]$,

3: $y_i = \alpha[1 - (1 - e^{-k_1 x_i})^n] + (1 - \alpha)e^{-k_2 x_i}$,

4: $y_i = e^{-k_2 x_i}[1 - (1 - e^{-k_1 x_i})^2]^n$,

5: $y_i = n(1 - e^{-k_1 x_i})^2$,

5b: $y_i = n(1 - e^{-k_1 x_i})^2 + k_2$,

7: $y_i = n\{1 - e^{-k_2 x_i}[1 - (1 - e^{-k_1 x_i})^2]\}$,

7a: $y_i = n\{1 - e^{-k_2 x_i}[1 - (1 - e^{-k_1 x_i})^2]\} + k_3$,

8: $y_i = (1 - k_1 x_i)e^{-k_2 x_i}$,

11: $y_i = 2p_{i1}^2(1 - p_{i1})[1 - (1 - p_{i3})^2] + p_{i1}^3[1 - (1 - p_{i3})^4]$,

where

$$p_{i1} = 1 - (1 - e^{-kx_i})^n ,$$

$$p_{i3} = -(1 - e^{-kx_i/2})^n .$$

TRAINING COURSES

A two-week lecture series by L. L. Bumgarner and Manuel Feliciano was held in July–August 1963. This series was designed to introduce the ALGOL language and the Oak Ridge ALGOL Compiler for the CDC 1604-A. Approximately 65 members of the Laboratory staff attended these lectures.

Seven two-week lecture series by Nancy B. Alexander, intended to give small audiences a working knowledge of FORTRAN 62 for the CDC 1604-A, were offered during 1963. 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 approximately 265 persons.

LECTURES AND PAPERS

Cavin, D. K., "Concurrent I/O Processing on a Small Computer," Mid-Southeastern Chapter of the Association for Computing Machinery, Huntsville, Alabama, December 6, 1963.

Downing, A. C., "A Method for Handling Mixed Boundary Conditions in Elliptic Problems with Curved Boundaries," Mid-Southeastern Chapter of the Association for Computing Machinery, Huntsville, Alabama, December 6, 1963.

Emmett, Margaret B. (with S. K. Penny and D. K. Trubey), "Radiation Shielding Information Center Information Retrieval System," American Documentation Institute, 26th Annual Meeting, Chicago, October 1963.

Feliciano, Manuel, Jr., "The Input-Output Problem in ALGOL," USAEC Computer Meeting, Argonne National Laboratory, Argonne, Illinois, May 3, 1963.

Feliciano, Manuel, Jr., "Input-Output Adjunct to ALGOL," Southeastern Regional Meeting of the Association for Computing Machinery, Atlanta, Georgia, September 21, 1963.

Gardiner, D. A., "Some Applications of Statistics at a Modern Research Laboratory," Clemson College, Clemson, South Carolina, February 1963; University of Oklahoma, Norman, February 1963; Oklahoma State University, Stillwater, February 1963; Georgia Institute of Technology, Atlanta, November 1963; Virginia Polytechnic Institute, Blacksburg, November 1963.

Gardiner, D. A., "Experiences with Nonlinear Estimation," North Carolina State College, Raleigh, December 1963.

Gosslee, D. G., "Some Applications of Statistics at a Modern Research Laboratory," Division of Biostatistics, Tulane University School of Medicine, New Orleans, Louisiana, February 1963; Department of Mathematics, Stephen F. Austin State College, Nacogdoches, Texas, February 1963; Graduate Institute of Technology, University of Arkansas, Little Rock, February 1963.

Harkrider, M. T. (with R. H. Ritchie), "Low Energy End of the Secondary Electron Cascade in Metals," Health Physics Society Annual Meeting, New York, June 1963.

Householder, A. S., "Localization of the Characteristic Roots of Matrices," University of Wisconsin, Madison, October 1963.

Kastenbaum, M. A., "Some Experiences with Fitting Nonlinear Models to Biological Data," University of Florida, Gainesville, March 1963; Florida State University, Tallahassee, March 1963; Radiobiological Research Unit, Harwell, England, September 1963; Hebrew University, Jerusalem, Israel, September 1963.

Kastenbaum, M. A., "Experimental Designs for Three-Dimensional Bioassays," University of Copenhagen, Copenhagen, September 1963.

Mader, Mary J. (with J. F. Agnew and J. L. Fowler), "Phase Shift Analysis of Differential Scattering of Neutrons from 0 Spin Nuclei," Tennessee Academy of Science, Chattanooga, November 29, 1963.

Nestor, C. W., Jr., "Direct Search Solution of Transcendental Equations," Mid-Southeastern Chapter of the Association for Computing Machinery, Chattanooga, Tennessee, March 15, 1963.

Parham, J. E., "Use of a Medium Scale Digital Computer for Biomedical Data: The IBM 1401 DPS," Oak Ridge Institute of Nuclear Studies, Oak Ridge, Tennessee, March 21, 1963.

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