MASTER

Mathematics Division

Annual
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Period Ending December 31, 1971

OAK RIDGE NATIONAL LABORATORY

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**MATHEMATICS DIVISION
ANNUAL PROGRESS REPORT
for Period Ending December 31, 1971**

H. P. Carter, Director
D. A. Gardiner, Assistant Director

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**OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
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Mathematical Research

MULTIPLE PRECISION ARITHMETIC PACKAGE¹

D. E. Arnurius V. A. Singletary

The four basic arithmetical operations of the package^{2,3} have been altered to yield "chopped" approximations instead of "rounded" ones. This direction was dictated to a degree by timing considerations and also by the discovery of a rather large number of special cases which had been overlooked in the original programs.

The package has been expanded to include subroutines for approximating these special functions: sine, cosine, logarithm, exponential, and square root. With the exception of square root, the user may supply a perturbation bound for the argument of the special functions. When this is done, the number of digits in the approximation closely reflects either the obtainable significance or the number of digits requested by the user.

MATRICES PERMUTATIONALLY SIMILAR TO DIRECT SUMS

J. A. Carpenter

Let $A_n^p(r) = (a_{ij})_{n \times n}$ with a_{ij} arbitrary for $|i - j| = 0, p, 2p, \dots, rp$, $r \leq [(n - 1)/p]$ and $a_{ij} = 0$ otherwise; that is, $A_n^p(r)$ consists of arbitrary elements in its diagonal and in the $2r$ equispaced parallels to the diagonal, symmetrically placed about the diagonal a distance p apart.

It is shown that if q is the least positive integer for which $n + q$ is divisible by p , there exists a permutation P for which $PAP^T = B_n^p(r)$, where $B_n^p(r)$ consists of the direct sum of p submatrices, $p - q$ of which are of order $m + 1$ and q of which are of order m , where $m = (n + q - p)/p$, and the transforming matrix $P = (p_{ij})$ is given by

$$p_{ij} = \begin{cases} 1 & j = \left(i - 1 - \sum_{s=1}^{k-1} m_s\right)p + k \\ 0 & \text{otherwise} \end{cases}$$

1. Work jointly sponsored by the Research Section and the Computing Applications Department of the Mathematics Division and by the Reactor Division.

2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, pp. 45-46.

3. D. E. Arnurius and V. A. Singletary, *A Base 16⁷ Arithmetic Package for the IBM 360 Computers with Sine, Cosine, Logarithm, Exponential, and Square Root*, ORNL-TM-3657 (to be published).

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where m_k is the k th part of the partition of n into $p - q$ parts of size $m + 1$ and q parts of size m listed in descending order; that is,

$$m_k = \begin{cases} m + 1 & k \leq p - q \\ m & k > p - q \end{cases}$$

In the case $r = 1$, $A_n^p(1)$ consists of an arbitrary diagonal, an arbitrary p th superdiagonal, and an arbitrary p th subdiagonal; $B_n^p(1)$ is the direct sum of $p - q$ tridiagonal submatrices of order $m + 1$ and q submatrices, which are tridiagonal for $m > 1$, diagonal if $m = 1$.

Special cases of the above are considered for which analytical expressions for inverses, characteristic values, and other properties can be obtained by these and related means.

A CONTACT PROBLEM IN VISCOELASTICITY

S. J. Chang

Because of the elastic-viscoelastic correspondence principle discovered by Lee, a large class of viscoelastic problems can be treated by their similar elastic problems. Hence it is interesting to seek their solutions. The contact problems are those which cannot be covered by the correspondence principle. They provide both the physical reality and the methodological interest in viscoelasticity. We have solved a dynamic contact problem of finite contact region.⁴ The problem is formulated as the generalized Wiener-Hopf equation and then reduced to a system of coupled integral equations. The coupling terms can be understood as the interaction of two half-plane viscoelastic wave problems. Previously only the static problems were treated by Lee, Hunter, and Morland through different methods.

PATH-INDEPENDENT INTEGRAL IN FINITE ELASTICITY⁵

S. J. Chang

The path-independent integral of Rice provides some interesting applications to the fracture of solids; for example, obtaining the stress intensity factor, estimation of the strain concentration along a rounded notch, and even use as a fracture criterion in inelastic solids. The theory, however, is restricted to the small strain assumption, which seems to be unrealistic. It is natural to ask whether the integral can be generalized to the finite strain condition so that either the integral can meet the finite strain case in elastic-plastic solids or can be applied to rubber elasticity. We have succeeded in so generalizing it.⁵ Incidentally, the path-independent integral concept was successfully used to provide an analytical basis⁶ for the equivalent energy method⁷ which was developed in the Reactor Division.

4. Paper was presented to the Department of Engineering Mechanics seminar, University of Tennessee, November 1971, and will be published.

5. S. J. Chang, "Path-Independent Integral for Rupture of Perfectly Elastic Materials," *Z. Angew. Math. Phys. (ZAMP)* (in press).

6. Report in preparation.

7. F. J. Witt, "The Equivalent Energy Method," paper No. 12, Fifth Annual Information Meeting, HSST Program, March 1971 and Fourth National Symposium on Fracture Mechanics, Pittsburgh, Pa., August 1970.

STOCHASTIC PARTICLE TRANSPORT THEORY

R. R. Coveyou

A theory of particle transport processes, treating these processes in consistent fashion as stochastic processes, is under development. The basic idea of this work is the construction of a model for such processes in which the observed behavior of the particle transport system under study is considered to be a *single realization*, among the ensemble of all possible realizations of the underlying stochastic process.

Certain conceptual difficulties of current expositions of the fundamentals of transport theory seem to be rooted in imprecise ideas concerning the application of probability theory to physical problems. During the examination of these questions, several interesting questions arose which are of some interest separately. These are reported in the following paragraphs.

Entropy of Finite Probability Spaces

The entropy of finite probability spaces is frequently identified with the mean number of bits of information needed to select a random member of this space. This identification is not exact, although the entropy of the distribution is a lower limit for the information content (with the above definition). An algorithm has been developed for the determination, in principle, of the exact information content of each finite probability space with rational probabilities. In the course of this work, two different algorithms were developed for the enumeration of the set of all partitions of integers.

Enumeration of Integer Partitions

An integer partition is a finite ordered set of positive integers $n_1 \geq n_2 \geq \dots \geq n_K$. We call K the number of parts and $n = n_1 + \dots + n_K$ the number of members of the partition. We can regard $n_1/n, \dots, n_K/n$ as the probabilities in a finite probability space with rational probabilities; there are other important interpretations. Methods for the systematic enumeration of such partitions may be of interest. In each case below, let $\pi(n)$ denote the integer partition associated with the integer n .

First method. Let $\pi(1)$ denote the "empty partition" of zero. Let $n = p_1^{\epsilon_1} \dots p_q^{\epsilon_q}$ be the factorization of n into prime power factors; $2 = p_1 < 3 = p_2 < p_3 < \dots$. We associate with n the partition $\pi(n)$ (of $N = \epsilon_1 + 2\epsilon_2 + \dots + q\epsilon_q$ into $K = \epsilon_1 + \epsilon_2 + \dots + \epsilon_q$ parts):

$$(q, \dots, q, q-1, \dots, q-1, \dots, 1, \dots, 1),$$

with each j appearing ϵ_j times. Thus $\pi(720) = \pi(2^4 \cdot 3^2 \cdot 5) = (3, 2, 2, 1, 1, 1, 1)$.

Second method. Here, denote the empty partition by $\pi(0)$.

Suppose

$$\pi(j) = (m_1, \dots, m_K).$$

Then:

$$\pi(2j) = (m_1 + 1, \dots, m_K + 1)$$

and

$$\pi(2j+1) = (m_1, \dots, m_K, 1).$$

Thus

$$\pi(1) = (1), \pi(2) = (2), \pi(3) = (1, 1), \pi(4) = (3), \text{ etc.}$$

It is not hard to see that, with either method, each integer partition acquires one and only one label. In any application, it is desirable that more complex partitions have larger labels; either method assures this.

Totally Finite Sets

We assume that each member of each set is itself a set. We may then define a totally finite set (recursively) as a finite set, each member of which is totally finite. Thus the empty set is totally finite. Although the set of all totally finite sets is not totally finite, or even finite, it is countable and can be enumerated (usefully) as follows. Let $S(n)$ denote the n th totally finite set, with $S(0)$ the empty set, and ascribe to the totally finite set with members $\{S(n_1), \dots, S(n_K)\}$ the label $S(n)$;

$$n = \sum_{j=1}^K 2^{n_j}.$$

POLYHEDRAL APPROXIMATIONS TO INITIAL-VALUE SETS OF OSCILLATION AND NONOSCILLATION

J. M. Dolan

Let

$$L(y) = p_n y^{(n)} + p_{n-1} y^{(n-1)} + \dots + p_0 y,$$

where $p_i \in C[a, \infty)$, $y \in C^{(n)}[a, \infty)$, and a is real, denote the classical n th-order linear differential operator.

A solution of the equation

$$L(y) = f, \quad f \in C[a, \infty) \tag{1}$$

is said to be oscillatory if and only if it has infinitely many zeros on $[a, \infty)$; otherwise, it is said to be nonoscillatory. Let $\mathcal{N}$ and $\mathcal{O}$ denote, respectively, the set of solutions of Eq. (1) that are nonoscillatory and oscillatory. For $x \in \mathbb{R}^n$, let x_i denote the i th component of the vector x , $i = 0, \dots, n-1$, and for $t_0 \geq a$, define

$$\begin{cases} \mathcal{N}_{t_0} = \{x \in \mathbb{R}^n; y^{(i)}(t_0) = x_i, \quad i = 0, \dots, n-1, y \in \mathcal{N}\}; \\ \mathcal{O}_{t_0} = \{x \in \mathbb{R}^n; y^{(i)}(t_0) = x_i, \quad i = 0, 1, \dots, n-1, y \in \mathcal{O}\}. \end{cases} \tag{2}$$

Polyhedral approximations to at least one of the sets in (2) have been given, depending on the oscillatory behavior of the companion homogeneous equation

$$L(y) = 0.$$

ATOMIC MASS ADJUSTMENT⁸

N. B. Gove Ruth B. Hofstra A. H. Wapstra⁹ K. Bos⁹

We reported on this project last year.¹⁰ During the current year, results obtained with the program were published.¹¹ These results consist of a new list of atomic masses and binding energies, decay and reaction Q values, and graphs of separation energies. The mass-to-energy conversion coefficient δ can be treated as a variable. The adjusted value for δ agrees with the value obtained from fundamental constants.

We improved the input data management routine and many other aspects of the program. We wrote a routine to calculate Q values for heavy-ion reactions.

INVARIANTS OF FINITE GROUPS

G. K. Haeuslein

We have continued our efforts to compute invariant rational functions of finite groups of linear transformations which were described in the last annual report.¹² This work leads to a study of integral group representations that is still in progress.

NUMERICAL ALGEBRA

A. S. Householder¹³

This heading will be taken to include the numerical treatment of equations, linear and nonlinear. The two papers on the Padé table and on multigradients have both appeared.^{14,15} The new identities established in the first of these have led to a new and very simple proof of the Koenig-Hadamard theorem, the fundamental theorem that proves the convergence of the sequences produced by the qd algorithm for solving a nonlinear algebraic or transcendental equation. This is being written up and will be published in a volume dedicated to Cornelius Lanczos. Not yet written is a further seemingly new set of identities relating entries in the Padé table and the residuals, that is, the differences between the entries and the power series being represented, and these bring out more directly the relation between the qd algorithm and that of Sebastião e Silva.

KWIC INDEX FOR NUMERICAL ALGEBRA

A. S. Householder¹³

The KWIC index is now in three volumes,¹⁶⁻¹⁸ two for matrices and linear equations and one for nonlinear equations. Many of the foreign language titles were not translated in time for inclusion in the first

8. Partially supported by the Nuclear Data Project.

9. Instituut voor Kernfysisch Onderzoek, Amsterdam, The Netherlands.

10. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 63.

11. A. H. Wapstra and N. B. Gove, "The 1971 Atomic Mass Evaluations," *Nucl. Data Tables* 9, 267 (1971).

12. G. K. Haeuslein, "On the Invariants of Finite Groups Having an Abelian Normal Subgroup of Prime Index," *J. London Math. Soc.* 3, 355-60 (1971).

13. Consultant.

14. A. S. Householder, "The Padé Table, the Frobenius Identities, and the qd Algorithm," *Linear Algebra and Its Applications* 4, 161-74 (1971).

15. A. S. Householder, "Multigradients and the Zeros of Transcendental Functions," *Linear Algebra and Its Applications* 4, 175-82 (1971).

16. A. S. Householder, *KWIC Index for Matrices in Numerical Analysis: Volume I. Primary Authors A-J*, ORNL-4418, vol. I (September 1969).

17. A. S. Householder, *KWIC Index for Matrices in Numerical Analysis: Volume II. Primary Authors K-Z*, ORNL-4418, vol. II (June 1970).

18. A. S. Householder, *KWIC Index for the Numerical Treatment of Nonlinear Equations*, ORNL-4595 (November 1970).

two volumes. However, these are now all translated, and several hundred new titles have become available. It is now intended to put out a single comprehensive volume including the new with the old titles for both areas, and further updated by giving references to more recent reviews.

APPLICATION OF SEVERAL FORMAL SYNTAX METHODS TO A LANGUAGE IMPLEMENTATION PROBLEM

R. P. Leinius

A study of several formal syntax-directed parsing methods is in progress, in order to determine which is most appropriate and/or efficient as a basis for the definition and implementation of a small programming language.¹⁹ The language has been formally defined, and code generators are currently being written, using a mixed strategy precedence parsing algorithm. When this phase has been completed, we will attempt the same implementation using another linear time parsing scheme, most likely based on a restricted LR(k)²⁰ algorithm. Error detection and recovery procedures, based on the parsing algorithm and on the syntax, will then be developed and evaluated.

POSITIVE INTEGRAL OPERATORS

P. Nelson

The critical sets²¹ associated with a positive integral operator have been successfully characterized. The characterization is too lengthy to be given here,²² but the underlying theory is essentially a generalization of the ideas underlying the normal form of a nonnegative matrix. The corresponding generalization of the concept of directed graph is currently being studied.

MODELS OF NUCLEAR REACTOR ECONOMICS

P. Nelson G. Young²³

The results described in the preceding annual report²⁴ were further generalized to include the situation in which either or both reactor types could be a net user of fuel.²⁵

APPLICATIONS OF THE METHOD OF INVARIANT IMBEDDING

P. Nelson D. E. Arnurius
D. W. Altom Carla A. Giles
V. A. Singletary

This is a continuation from the 1970 annual report. A successful implementation was made of the technique for numerical solution of partial differential equations by hybrid computer.²⁶ Studies are continuing regarding the application to a large boundary-value problem arising in structural mechanics.

19. W. B. Malthouse, *GRIND, a Desk Calculator Language System*, M.S. thesis, University of Tennessee (in progress).

20. D. E. Knuth, "On the Translation of Languages from Left to Right," *Inform. Contr.* 8 (October 1965).

21. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 1.

22. P. Nelson "The Structure of a Positive Linear Integral Operator," submitted to *J. London Math. Soc.*

23. Consultant.

24. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 1-2.

25. P. Nelson and G. Young, "Optimal Strategies in Reactor System Economics," *Nucl. Sci. Eng.* 46, 140-47 (1971).

26. P. Nelson and D. W. Altom, "Hybrid Solution of Partial Differential Equations by Application of Invariant Imbedding to the Serial Method," to appear in *Simulation*.

CONVERGENCE OF THE DISCRETE ORDINATES METHOD

P. Nelson

The basic approach of Anselone²⁷ and of Nestell²⁸ was extended to give convergence for any subcritical slab, including inhomogeneous slabs and quite general classes of scattering laws and quadrature rules.²⁹

27. P. M. Anselone, "Convergence of Chandrasekhar's Method for Inhomogeneous Transfer Problems," *J. Math. Mech.* **10**, 537-46 (1961).

28. M. K. Nestell, *The Convergence of the Discrete Ordinates Method for Integral Equations of Anisotropic Radiative Transfer*, Tech. Rep. No. 23, Mathematics Department, Oregon State University, Corvallis, 1965.

29. P. Nelson, *Convergence of the Discrete Ordinates Method for Anisotropically Scattering Multiplying Particles in a Subcritical Slab*, ORNL-TM-3553 (September 1971).

Computing Applications

INTRODUCTION

A. A. Brooks

Two trends in Computing Applications have been noticeable during the last year: (1) a significant increase (involving about 20 people) in the area of information processing in support of research projects and (2) an increase in work load which has brought the percentage of available time billed out to an unprecedented high of about 92% and has required the addition of several staff members. A great deal of the information processing work is being done in conjunction with the development of an integrated software system named ORCHIS, and abstracts of this work are so indicated in the table of contents.

CHEMICAL TECHNOLOGY DIVISION

Heat Transfer Analysis of the Proposed National Radioactive Waste Repository

W. D. Turner R. D. Cheverton¹ J. Smith² W. R. Wade²

We continued the analyses of the thermal effects on the proposed National Radioactive Waste Repository and its geological environment.³ This year the analyses have considered the repository in greater detail and have utilized updated data on the thermal properties and the stratigraphy. Studies were conducted to determine the sensitivity of the temperatures due to perturbations and variations in the parameters, some of which are: (1) stratigraphy, (2) room content, (3) thermal conductivity, (4) room and pillar dimensions, (5) transient thermal power of the waste, (6) age of the waste, and (7) mine loading sequence.^{4,5}

Currently, parametric studies are being made to provide preliminary information with which to "minimize" waste burial costs. Variables in this analysis consist of the initial power and age of the waste at burial, the waste container dimensions, the burial pattern of the waste containers, and the room and pillar dimensions in the mine.

The heat transfer code HEATING3⁶ was used to calculate the transient temperature distributions for the one- and two-dimensional models and some of the three-dimensional models. However, the computing

1. Chemical Technology Division.

2. Consultant, University of Tennessee.

3. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 18, 19.

4. R. D. Cheverton and W. D. Turner, *Thermal Analysis of National Radioactive Waste Repository: Brief Summary of Results Obtained through April 1971*, ORNL-TM-3426 (June 1971).

5. R. D. Cheverton and W. D. Turner, *Thermal Analysis of the National Radioactive Waste Repository: Progress through June 1971*, ORNL-4726 (December 1971).

6. W. D. Turner and M. Siman-Tov, *HEATING3 - an IBM 360 Heat Conduction Program*, ORNL-TM-3208 (February 1971).

time on many of the three-dimensional models was so long that the use of HEATING3 was not practical. Thus, a general three-dimensional heat transfer code was developed based on Douglas's algorithm.⁷ Presently, problems solved by this code must be described in Cartesian coordinates. The thermal conductivities may be both position- and temperature-dependent, while the heat generation rates and boundary temperatures may be both position- and time-dependent. In addition, the boundary conditions can include forced convection and specified heat fluxes. This code yielded a saving in computing time of more than an order of magnitude over that of the original HEATING code and was several times faster than Levy's modification to the classical explicit method which is available in HEATING3.

Sponsor: Chemical Technology Division

R. D. Cheverton

Design of a Neutron Radiography Facility

J. R. Knight V. A. DeCarlo¹

The DOT⁸ discrete ordinates transport code was used to determine the feasibility of using computer codes in the design of a proposed neutron radiography facility. The object of the study was to develop a design that maximized the thermal neutron flux and minimized the gamma radiation at the imaging plane.

Coupled neutron-gamma cross sections with 22 neutron groups and 18 gamma groups were used. Neutron fluxes and gamma-ray dose rates were determined for various positions along the imaging plane. The calculations showed that the design being considered was satisfactory in neutron collimation, neutron flux, and gamma-ray dose rate values. It was concluded that the computer calculations were useful for testing conceptual designs, but optimization of various parameters could probably be best achieved in an actual neutron radiography facility.

Sponsor: Chemical Technology Division

V. A. DeCarlo

Nuclear Safety Evaluation of the LMFBR Fuel Element Shipping Cask

J. R. Knight L. B. Shappert¹

The KENO⁹ Monte Carlo criticality code was used to evaluate the nuclear safety of the cask designed for the shipment of spent LMFBR fuel elements. The cross sections for materials in the core and blanket regions of the fuel elements were obtained from the XSDRN¹⁰ libraries and were collapsed to 16 groups. Cross sections for the remaining materials in the cask were obtained from the Hansen-Roach¹¹ 16-group library.

In order to consider the most reactive fuel loading, the fuel elements were described as fresh (with no fission products). The generalized geometry option of KENO was used to represent the arrangement of the various materials in the cask. This allowed the shape of the fuel elements to be described in sufficient detail

7. J. Douglas, Jr., "Alternating Direction Methods for Three Space Variables," *Numer. Math.* 4, 41-63 (1962).

8. F. R. Mynatt et al., *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (August 1969).

9. G. E. Whitesides and N. F. Cross, *KENO - a Multigroup Monte Carlo Criticality Program*, CTC-5 (September 1969).

10. N. M. Greene and C. W. Craven, *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

11. G. E. Hansen and W. H. Roach, *Six and Sixteen Group Cross Sections for Fast and Intermediate Assemblies*, LAMS-2543 (December 1961).

to minimize geometrical errors in the calculations. The results of these calculations indicate that the cask is safe when loaded as described in the calculations.

Sponsor: Chemical Technology Division

L. B. Shappert

CHEMISTRY DIVISION

Heat Capacity of Lead Fluoride

C. W. Nestor, Jr. R. A. Gilbert¹²

Cubic lead fluoride undergoes a phase transition near a temperature of 440°C. We have found that by assuming that the heat capacity is of the form

$$C_p(t) = ae^{-\beta t} + b(1 - e^{-\beta t}) + Ae^{-\alpha_1(t-t_c)} \quad (t \leq t_c)$$

$$= ae^{-\beta t} + b(1 - e^{-\beta t}) + Ae^{-\alpha_2(t-t_c)} \quad (t > t_c),$$

where t is the temperature in degrees C, t_c is the transition temperature in degrees C, and a, b, β, A, α_1 , and α_2 are constants, we can fit the measured enthalpies of PbF_2 over the temperature range 0 to 828°C. We used ORDEAL¹³ to fit the expression

$$\Delta H(t) = \frac{a}{\beta}(1 - e^{-\beta t}) + \frac{b}{\beta}[\beta t - (1 - e^{-\beta t})] + \frac{A}{\alpha_1}[e^{-\alpha_1(t-t_c)} - e^{-\alpha_1 t_c}] \quad (t \leq t_c)$$

$$= \frac{a}{\beta}(1 - e^{-\beta t}) + \frac{b}{\beta}[\beta t - (1 - e^{-\beta t})] + \frac{A}{\alpha_1}(1 - e^{-\alpha_1 t_c}) + \frac{A}{\alpha_2}[1 - e^{-\alpha_2(t-t_c)}] \quad (t > t_c)$$

using the nonlinear least-squares procedure. With the values for the constants from the fit, we calculated the heat capacity and the entropy

$$S(t) = \int_0^t \frac{C_p(t')}{t' + T_0} dt'$$

$$= (a - b)e^{\beta T_0} [E_1(\beta T_0) - E_1(\beta T)] + b \ln(T/T_0) + Ae^{-\alpha_1 T_c} [Ei(\alpha_1 T) - Ei(\alpha_1 T_0)] \quad (t \leq t_c)$$

$$= (a - b)e^{\beta T_0} [E_1(\beta T_0) - E_1(\beta T)] + b \ln(T/T_0) + Ae^{-\alpha_1 T_c} [Ei(\alpha_1 T_c) - Ei(\alpha_1 T_0)]$$

$$+ Ae^{\alpha_2 T_c} [E_1(\alpha_2 T_c) - E_1(\alpha_2 T)] \quad (t > t_c)$$

12. Chemistry Division.

13. M. Feliciano, C. W. Nestor, Jr., N. B. Gove, and T. D. Calton, *Oak Ridge Data Evaluation and Analysis Language*, ORNL-4506 (March 1970).

Fig. 1. Calculated and measured enthalpies of lead fluoride.

where $T_0 = 273.15^\circ\text{K}$, T is the absolute temperature in degrees K, and $T_c = t_c + T_0$. The exponential integrals are¹⁴

$$E_1(x) = \int_x^\infty \frac{e^{-t} dt}{t}$$

and

$$\text{Ei}(x) = \int_{-\infty}^x \frac{e^t dt}{t};$$

the bar through the integral sign denotes the Cauchy principal value. A plot of enthalpy as a function of temperature is shown in Fig. 1, with the experimental values indicated as discrete points.

Sponsor: Chemistry Division

R. A. Gilbert

14. M. Abramowitz and I. E. Stegun (eds.), p. 228 in *Handbook of Mathematical Functions*, National Bureau of Standards, 1964.

CIVIL DEFENSE RESEARCH PROJECT

Urban Growth Patterns

Norma J. Buhl Ruth B. Hofstra W. B. Malthouse N. B. Gove Peggy G. Fowler

We continue to provide computer support for research involving the 1970 census data. First Count census summary tapes are now available for all states. Study areas include population change related to interstate highway construction, migration from state of birth, and population changes since 1940. We made several thousand graphs on 35-mm film from data on county population changes by age, sex, and race between 1950 and 1960 sent by the University of Georgia. We wrote a computer program to select desired data from the Social Security LEED (Longitudinal-Employer-Employee Data). We wrote programs to process one of the Atlanta Office of Business Economics' files for analysis with the SADS program.

Sponsor: Civil Defense Research Project

Migration Studies

Peggy G. Fowler

Analysis programs were written for the SADS¹⁵ (Statistical Analysis of Data Subsets) program for studies on the migration of people into and out of Atlanta, Georgia. Similar programs will be written for migration studies of other cities in the United States.

Sponsor: Civil Defense Research Project

K. P. Nelson

Migration and Fertility Tables

F. D. Hammerling Neal Ritchey

Several programs were written, using census data, to produce tables of migration patterns for women of childbearing age. These tables were used to study the effects of migration upon fertility.

Sponsor: Civil Defense Research Project

Neal Ritchey

Net Migration Rate Graphs

Ruth B. Hofstra

We have completed work on the net migration rate graphs for the Urban Growth Patterns Project.¹⁶ Graphs were made for every county in the United States, using the Cathode Ray Tube Calcomp plotter. The principal plotting program used was the ORGRAPH system.^{17,18} One graph was made for each county of population below 50,000, showing the Age-Sex Net Migration Rate, 1950-1960. There were 2433 in this category, with seven counties having a maximum rate greater than 500%. There were 1920 counties with population more than 50,000. For these counties, graphs were made relating Age-Sex-Color as well as

15. A. A. Brooks and A. Hume, *The SADS Program - Statistical Analysis of Data Subsets*, CTC-19 (October 1969).

16. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 29, 59.

17. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 9.

18. N. B. Gove et al., *Preliminary Report on the ORNL Graphics Package, ORGRAPH*.

Age-Sex and Age-Color for 1950-1960 Net Migration Rate. Twenty graphs in this group showed a maximum above 500%.

It is planned to develop a consistent series of estimates for counties from 1940 to 1970, along with a scheme for grouping the counties in the South into the most useful analytical categories. Natural increase of black and white populations in Southern counties is being related to net migration in these studies. Some discussions of the project have been given at sociological meetings, showing the graph films.¹⁹

Sponsor: Civil Defense Research Project

Graphical Displays

D. W. Altom J. V. Wilson²⁰

The graphical display capabilities reported in the 1970 annual report²¹ have been expanded to permit: (1) graphs of the outline of the United States overlaid with various types of data and (2) graphs of population data bases within regional areas of the United States. The new display capabilities may be used to verify the accuracy of data bases and to determine suitable locations for antiballistic missile batteries and their associated radar sites.

Sponsor: Civil Defense Research Project

C. M. Haaland

Analysis of Shelter-Taking Time

M. T. Heath

For the purpose of this study it was assumed that if all persons leave for shelter simultaneously upon warning, then their various walking speeds are such that the arrival density of persons to shelter is parabolic between the fastest and slowest arrivals. However, simultaneous departure is unrealistic since some persons leave very soon after warning, others react more slowly, and there are always a few stragglers. To simulate this behavior it was assumed that the departures follow a gamma density function. It can be shown that the resulting arrival curve is the convolution of these two curves (parabolic and gamma). The computation of this convolution was carried out both by performing the integration directly in closed form and by using the Fast Fourier Transform algorithm. The resulting computer program was applied to detailed block-by-block population and shelter location data for the city of Detroit in order to confirm the validity of previous programs which use coarser data and a simpler movement algorithm.

Sponsor: Civil Defense Research Project

C. M. Haaland

Intercept Geometry

M. T. Heath

In order to study the feasibility of various simple guidance systems on projectiles used as interceptors, a program was written to solve the equations of motion for a reentry vehicle and an interceptor, given the

19. Gladys Bowles, *Measuring Components of Change in the Growth of Counties and Cities*, Southern Regional Demographic Group, Oak Ridge, Oct. 4, 1971.

20. Civil Defense Research Project.

21. *Math. Div. Annu. Prog. Rep. Dec. 31, 1970*, ORNL-4661, p. 11.

appropriate initial conditions. The reentry trajectory included the forces of gravity and atmospheric drag, while the interceptor was assumed to have constant velocity. The primary quantities of interest were the miss distance and the crossing angle. Computer plots of the trajectories aided greatly in interpreting the results.

Sponsor: Civil Defense Research Project

C. M. Haaland

Optimum Distribution of Interceptors to Protect U.S. Cities

M. T. Heath

Following an analysis by Eugene P. Wigner, a computer program was written to calculate the distribution of antiballistic missiles which minimizes the maximum number of fatalities which an attacker can cause, given fixed enemy capability and defense resources. The attack is nationwide, and for simplicity the attack is assumed to be time independent and the attacker is assumed to have perfect aiming and full knowledge of the defense posture. The SRI 5-km grid population data base was adapted for use with a square-root damage law for fatality calculations.

Sponsor: Civil Defense Research Project

C. M. Haaland

Analysis of Active-Passive Defense Mixes

M. T. Heath

The computer programs previously described²² have been used extensively in the analysis of cost effectiveness of various mixtures of active defense via interceptors and passive defense via blast shelters. The programs have been improved and modified to simulate a submarine-launched multiple warhead attack on an entire "defense island" (i.e., a cluster of nearby cities sharing a common radar system).

Sponsor: Civil Defense Research Project

C. M. Haaland

DIRECTOR'S DIVISION AND ENVIRONMENTAL INFORMATION SYSTEMS OFFICE

Computer Program for the Computation of Ionic Self-Diffusion Coefficients from Experimental Measurements

R. E. Funderlic

The estimation of ionic self-diffusion coefficients from experimental data taken with small spheres initially containing radioactive tracer suspended in a finite, well-stirred bath depends on fitting the data to the solution of the radial diffusion equation under the appropriate boundary conditions. The isotopic redistribution effected by diffusion is described by the time dependence of the fractional attainment of the final equilibrium distribution. The related equations²³ were solved by variants of the linear fractional

22. *Math. Div. Annu. Prog. Rep. Dec. 31, 1970*, ORNL-4661, p. 11.

23. G. E. Boyd and B. A. Soldano, "Self-Diffusion of Cations in and through Sulfonated Polystyrene Cation Exchange Polymers," *J. Amer. Chem. Soc.* 75, 6091-99 (1953).

iteration. Of some numerical analysis interest was the calculation of a sequence of zeros of a function which has poles at multiples of π . An iterative method based on fitting functions of the type $(x - a)'(x - n\pi)$ was found to be quite safe and efficient.

Sponsor: Director's Division

G. E. Boyd

Numerical Evaluation of an Indefinite Integral

P. R. Coleman

An indefinite integral of the form $F(x) = \int_a^x f(y) dy$ appears in the application of thermodynamic theory to the prediction of equilibrium constants for ion exchange reactions. Since f is an unknown function of the variable y , an empirical fit is often made to experimental data for some chosen functional form. Frequently, however, no simple form for $f(y)$ can be found which fits the data with requisite accuracy. Recourse then must be made to numerical quadrature using the table of experimental data. This integration was carried out using Simpson's rule. Values of $F(x)$ for arbitrarily chosen x values were then computed using Lagrangian interpolation.

Sponsor: Director's Division

G. E. Boyd

Environmental Information System

D. W. Altom Carla A. Giles
A. A. Brooks A. F. Joseph
Peggy G. Fowler V. A. Singletary
D. L. Wilson

A comprehensive project support system for bibliographic information is in the process of being developed.

The major accomplishment of Phase I is a system that provides for a smooth and orderly flow of information from input into the CRBE system to retrieval via the CRLLOOK program or computer output for publication via the various indexing programs. Included in this process for information flow are methods, programs, and techniques to (1) edit the information in the external format; (2) list files for initial proofreading; (3) transform other bibliographic data formats to the external format; (4) handle data from outside sources on cards, computer magnetic tape, or MTST magnetic tape; (5) transfer data from CRBE files to computer magnetic tape or the data cell for temporary or backup storage; (6) translate information from the external format to the generalized internal format and place it on data cell or magnetic tape; (7) search information in a variety of files in either an on-line conversational mode with Teletypes or IBM 2741 terminals or a background batch mode; (8) search subsets of the retrieved data and provide listing at a terminal or at a high-speed printer; (9) provide KWIC (key word in context) indices and KWOC (key word out of context) indices, for example, author or key word indices for publications, use in editing key words, titles, authors, and producing a thesaurus; (10) modify, correct, add, or delete information or complete records in the internal format; (11) assist the book ordering system in their work by providing among other things a duplicate checking procedure; and (12) provide for SDI services from the bulk data bases using the University of Georgia Text Search Programs.

Sponsor: Director's Division, Environmental Information Systems Office

PUBLISH – a Program for Page Composition from ADSEP Data Bases²⁴

A. A. Brooks F. D. Hammerling

A computer program, which, using ADSEP data bases, produces two-column pages for photoreduction and publication, has been written. The reports are produced in two formats, (1) a three-level hierarchical structure of the subject material and (2) a linear unordered structure. Any arbitrary identified text fields can be selected from the data base for publishing with arbitrary subtitles. The lowest level hierarchy title is placed in the page body, and the higher levels are posted at the page top with page number and lead entry number. The data base can be presorted on arbitrary fields prior to publication and must be sorted for the hierarchical structured report. The parameters to control the page format are input parameters. Page and column skills are controlled.

Sponsor: Directors Division, Environmental Information Systems Office

G. Ulrikson

The ORLOOK Program

V. A. Singletary A. F. Joseph

The ORLOOK program²⁵ is an integral part of Phase I of the project information retrieval system being developed for the Environmental Information System and has been modified to execute interactively on the IBM 360/75 computer with the user at a remote terminal. A special FORTRAN callable package has been implemented to accomplish the telecommunications input-output required by the ORLOOK codes. ORLOOK interprets a conversational-like command language that enables the user to request text searches through data base files and to display results either at his terminal or on the system printer. Text items are found by sequential scans of selected fields of each logical record or each complete record, and each find is recorded in a re-searchable random access answer file. ORLOOK utilizes a general internal data format²⁶ that is self-described by a table which is part of the file, thus allowing a variety of files to be implemented. This variety is indicated in the following data bases that are currently in use:

1. *Mercury* – at present this includes 540 references with abstracts and key words concerned with all aspects of mercury in the environment.
2. *IBP Abstract Journal* – 227 items with abstracts and some key words give descriptions of internal reports and data generated by the International Biological Program (IBP).
3. *Ecological Sciences Information Center* – 3397 selected references with some abstracts and key words on ecology and radioecology (2 files).
4. *Molten Salt Reactor Information File* – 322 references, abstracts, and key words of papers relating to Molten Salt Reactors Program.
5. *IBP 1971 Proposals* – 95 abstracts and key words of research proposals for the Deciduous Forest Biome of IBP.
6. *ORNL Non-AEC-Funded Research Projects (work for others)* – 13 items concerned with work done for others at Oak Ridge National Laboratory (ORNL).

24. F. D. Hammerling and A. A. Brooks, *PUBLISH – a Program for the Composition of Pages from ADSEP Data Bases*, in progress.

25. Math. Div. Annu. Prog. Rep. Dec. 31, 1970, ORNL-4661, p. 98.

26. A. A. Brooks, *ADSEP – an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

7. *Solid Waste Data Base* – 2147 references with abstracts and key words concerned with solid wastes as an environmental problem.
8. *Environmental Mutagen Information Center* – 3695 references concerned with mutagenicity and teratogenicity of chemicals.
9. *Materials Resources and Recycling* – 201 references with abstracts and key words on solid waste management, recycling, and air and water pollution.
10. *Regional Modeling* – 614 references, abstracts, and key words on land use and planning.
11. *Energy Data Base, ORNL-NSF Environmental Program* – 100 references, abstracts, and key words on production, consumption of electrical power, and the impact on the environment.
12. *Regional Modeling (2)* – 410 references with abstracts and key words.
13. *IBP 1971 Proposal Citations* – 80 references.

Sponsor: Director's Division, Environmental Information Systems Office

Indexing for ADSEP Data Sets

D. L. Wilson Ruth Slusher

A KWIC²⁷ Index can be obtained from bibliographic data sets which are stored in the ADSEP²⁶ format. The ADSEP data set is prepared for input to the KWIC program by a conversion program which can arrange for the index to be given on any field.

The conversion program allows the user to choose to be indexed either one or two fields from any of the fields in the ADSEP identifier table.

Sponsors: Director's Division, Environmental Information Systems Office

Terminal Input and Output

A. F. Joseph Carla A. Giles

We have made extensive modifications and additions to an Assembler language subroutine, acquired from the Systems group, which will perform telecommunication operations on Teletypes, IBM-2741 terminals, and other compatible models. The subroutine package may be called from FORTRAN or Assembler language to input and output data to an IBM 360 program via a terminal, card reader, or printer. The routine uses BTAM for all terminal operations and QSAM for card reader and printer. A report is in the process of being published.

Sponsor: Director's Division, Environmental Information Systems Office

University of Georgia Text Search Program

A. F. Joseph Carla A. Giles

A series of programs which comprise the University of Georgia Text Search System have been implemented on the IBM 360/75. This system will retrieve bibliographic information from 12 data bases

27. G. K. Haeuslein and Ann S. Klein, *The Oak Ridge National Laboratory KWIC Index*, ORNL-4536 (May 1970).

through a batch-mode-search technique. Profiles are created and maintained on-line through the use of a Teletype or an IBM-2741 terminal. The most important modification to the system has been to the profile creation procedure, which has been changed to operate on the above-mentioned terminals instead of a CRT IBM-2260. In addition, we have found it necessary to debug some of the PL/I programs which convert the data base format to a standardized search format.

Sponsor: Director's Division, Environmental Information Systems Office

Book Ordering

D. W. Altom D. L. Wilson A. F. Joseph

We designed and implemented a procedure to order books through the Central Research Library. This entailed (1) defining the input format for the book orders (2) developing the routines to do the actual processing, (3) producing order forms on the high-speed printer, and (4) maintaining a file of all books ordered.

The procedure includes an attempt at duplicate checking by comparing the titles of all books ready for order against the titles of all books previously ordered. If the title of some book ready for order is identical to the title of some book already ordered, the book awaiting order is not ordered. However, since identical titles do not necessarily imply identical books, the procedure can order books without checking for duplicates. This feature is particularly useful in ordering a book that in a previous run was mistakenly labeled a duplicate of some ordered book.

Sponsor: Director's Division, Environmental Information Systems Office

G. U. Ulrikson

B. L. McGill

ECOLOGICAL SCIENCES DIVISION

ADSEP²⁶ Data Bases

F. D. Hammerling A. A. Brooks

1. An ADSEP data base was prepared which contains weather data for the years 1955-70. The data were taken at five sites: X-10, K-25, Townsite, Y-12, and Tower Shielding Facility. The data base contains information, in hourly increments, such as temperature, wind direction, wind velocity, dew-point temperature, solar radiation, precipitation, and temperature gradient.

2. An ADSEP data base was prepared which contains TVA forest plot data for 1960, 1965, and 1970. The data consist of state, county, and plot information plus information about individual trees in a given plot. The tree data consist of items such as azimuth, species, and distance, which serve to identify the tree, diameter, height, total cull, rotten cull, tree status code (live, dead, cut, etc.), tree grade, DBH, injury, and crown class.

Both of these data bases required a considerable amount of editing and reformatting before the ADSEP program could be used to process them.

Sponsor: Ecological Sciences Division

Richard Sayrs

John Hett

Nancy Sollins

Modifications to ADSEP²⁸

A. A. Brooks Peggy G. Fowler

The ADSEP program has been modified to process character string input. The ability to make partial corrections to character string fields has also been added to the program.²⁸ Other request commands have been added to increase the ease and flexibility for updating data sets.²⁹

The new features of the program have been used to create bibliographic data sets with the generalized internal format that can be used by ORLOOK, SADS, and KWIC.

Sponsor: Ecological Sciences Division

RESAP³⁰ Modification

F. D. Hammerling

The RESAP program was modified to accept magnetic tape data produced by a PDP-8 computer where only every tenth channel number was digitized. The magnetic tape data also eliminated the paper tape to magnetic tape conversion and the editing program. The version which processes paper tape data is still available.

Sponsor: Ecological Sciences Division

N. A. Griffith

Acquisition, Storage, Retrieval, and Display of a Geographically Oriented Data Base for the Eastern Deciduous Biome

R. L. Stephenson T. C. Tucker

We are developing techniques and computer programs for the data base required by the Biome and Regional Synthesis Group for their study of the eastern U.S. deciduous biome. These data are similar to and are available on the same kind of predominant source document (printed maps) as much of the data for the ORNL-NSF Environmental Program's Regional Modeling Group. Therefore, we are working in conjunction with personnel of that project. All results to this point have applications common to both groups and are reported in the section of this report covering the ORNL-NSF Environmental Program.

Sponsor: Ecological Sciences Division

F. G. Goff

An Ecosystem Eigenvalue Sensitivity Program

R. E. Funderlic

A preliminary computer program has been written which calculates the partial derivatives of the eigenvalue of a matrix with respect to changes in the matrix elements. In a linear compartmental model of an ecosystem, these derivatives reflect the sensitivity of the stability or recovery time of the system to changes in its transfer coefficients. All such derivatives have been calculated for the 66 matrices which

28. A. A. Brooks, *ADSEP Text Input*, ORNL-CF-71-9-3.

29. A. A. Brooks and P. G. Fowler, *Errors and Addenda to ADSEP*.

30. *Math. Div. Annu. Prog. Rep. Dec. 31, 1970* ORNL-4661, p. 15.

appear in a recent report.³¹ Investigation is under way to find trends among these which would be helpful in understanding the stability of ecosystems.

Sponsor: Ecological Sciences Division

R. V. O'Neill

Sensitivity Analysis of Ecosystem Parameters

R. E. Funderlic M. T. Heath

The kinetics of a linear compartmental system may be expressed as a system of differential equations $\dot{x} = Ax$, where $A = (a_{jk})$ is the matrix of transfer coefficients and x is the vector of concentrations in the compartments. With a conservation of mass assumption, the matrix A has nonnegative off-diagonal elements and zero column sums. Such systems are of increasing importance in ecology.

Ecological Sciences personnel have given a simple 9×9 linear compartmental model of the Aleutian ecosystem.³² The vectors $\partial x(\infty)/\partial a_{jk}$ are helpful in gaining insight into why the Aleut population has evolved such an intimate dependence on the marine subsystem. For this model the matrix A is irreducible, and therefore $Ax(\infty) = \dot{x}(\infty) = 0$ has only one solution, $x(\infty)$, up to a scalar multiple.³³ Thus the normalization $\sum x_i(\infty) = 1$ determines $x(\infty)$ uniquely.

Small changes in the matrix A do not change the rank = 8 of A since the sum of the row vectors is the zero vector. Thus $x(\infty)$ is a continuous and rational function of the elements of A . This proves the existence of $\partial x(\infty)/\partial a_{jk}$. Therefore,

$$\partial [Ax(\infty)]/\partial a_{jk} = A[\partial x(\infty)/\partial a_{jk}] + x_k(\infty)(e_j - e_k),$$

where all the components of the vector e_i are 0 except the i th, which is 1. Thus $z \equiv \partial x(\infty)/\partial a_{jk}$ satisfies

$$Az = x_k(\infty)(e_k - e_j). \quad (1)$$

The solutions of (1) are of the form $z + cx(\infty)$, where z is any particular solution of (1) and c is any scalar. A multiple of the vector $\partial x(\infty)/\partial a_{jk}$ may be determined from (1) and $\sum \partial x_i(\infty)/\partial a_{jk} = 0$.

With respect to the Aleut model, calculations based on the above derivation show that land plants are about 300 times more sensitive to a change in uptake of atmospheric carbon than marine animals are to changes in uptake of surface water carbon.³² This would tend to indicate that the marine subsystem is a more reliable food source and might explain the dependence of the population on it.

Sponsor: Ecological Sciences Division

R. V. O'Neill

Nonlinear Parameter Estimation

M. T. Heath

This problem arose from an experimental study performed by ORAU Medical Division on the effects of DDT and other contaminants on thyroid activity in animals. Iodine retention is taken as a measure of thyroid activity and a two-compartment model used to describe the elimination process. The data consist of

31. R. V. O'Neill, *Examples of Ecological Transfer Matrices*, ORNL-IBP-71-3 (June 1971).

32. J. M. Hett and R. V. O'Neill, *System Analysis of the Aleut Ecosystem*, IBP-71-16 (1971).

33. R. E. Funderlic and M. T. Heath, *Linear Compartmental Analysis of Ecosystems*, ORNL-IBP-71-4 (August 1971).

readings of percent dose retained taken at approximately one-day intervals after initial injection. A computer program has been written to fit a sum of two exponentials to these data points in the least-squares sense, giving the resulting half-times and initial contents. Simplicity and storage optimization were emphasized in the programming, since the program is written for an IBM 1800 computer with very limited core storage. The method used is the Gauss-Newton with the Cholesky decomposition for the linearized subproblem and one iteration of parabolic search for the one-dimensional minimization. Since double precision is not available on this computer, numerical stability is a potential problem, and improvements in this area are planned. Currently the program requires initial estimates for the parameters, which are obtained graphically. Making the program self-starting by means of an automated peeling procedure is also under consideration.

Sponsor: Ecological Sciences Division

R. V. O'Neill

Infiltration of Water into Soils

M. Reeves III E. E. Miller³⁴

A very important process involved in watershed modeling is the division of water between runoff and infiltration occurring at the soil surface during a rainfall. Solution of the soil-moisture flow equation to model such a process is not feasible at present for the space and time scales involved in a typical watershed analysis. The objective of this research is to examine an approximation due to Raats.³⁵ The idea here is that the infiltration for an arbitrary rainfall event may be obtained from the characteristic cumulative infiltration for maximum seepage.

Using an iterative Crank-Nicolson algorithm similar to that used by Whisler and Klute,³⁶ we solve the soil-moisture flow equation both for maximum seepage from the surface and for a given rainfall event. The Raats approximation is then compared with the latter result. Hysteresis and a crust are included in the analysis.

Two soils,³⁷ Rideau Clay Loam and Caribon Silt Loam, four crusts, and four rainfall events are included in the analysis. For the cases run to date, the Raats approximation is good to less than about 15%. This error would appear to be acceptable in view of other comparable errors involved in the modeling of a watershed.

Sponsor: Ecological Sciences Division

Watershed Modeling

M. Reeves III C. W. Nestor T. C. Tucker

The Stanford Watershed Model³⁸ has been used quite extensively to simulate water movement through a watershed. Processes such as precipitation, interflow, overland flow, evapotranspiration, soil-water movement, ground-water movement, and channel flow are considered. Given a stream flow hydrograph and the corresponding precipitation records, parameters of the model may be adjusted so that the simulated

34. Departments of Soils and Physics, University of Wisconsin, Madison, Wis.

35. Private communication from P. A. C. Raats to E. E. Miller.

36. F. D. Whisler and A. Klute, *Soil Sci. Soc. Amer. Proc.* 29, 489 (1965).

37. G. C. Topp, *Water Resour. Res.* 7, 914 (1971).

38. N. H. Crawford and R. K. Linsley, *Digital Simulation in Hydrology: Stanford Watershed Model IV*, Stanford University Dept. of Civil Eng. Tech. Rept. No. 39.

hydrograph fits the experimental hydrograph. One then has a model which may be used to determine the stream flow for any other rainfall event.

If the character of the watershed is changed significantly by, say, land development or reforestation, then the model is no longer predictive. Also, biomass estimates are not made. We wish to alleviate these difficulties by describing the soil-water-plant system in more detail.

We also wish to consider topographical effects through the distributed parameter approach. Such effects are hidden in the lumped-parameter approach of the Stanford Watershed Model but could be important for certain changes in the watershed. Our input data will include land use, soil type, and mean slope distributed on a square grid. Such data are now being accumulated by the ORNL-NSF Environmental Project.

We envision a nonlinear subsystem of first-order ordinary differential equations coupled together to depict the internal flows within an element whose upper surface is one square of the grid mentioned above. These subsystems would then be coupled together by the lateral flows between volumes. By using the ORNL IBM 360/91 and by carefully considering the mathematical form of the couplings, we hope to avoid the excessive execution times reported by Dunn³⁹ for a similar model.

Since the work is at a very early stage of development, there are no results to report at this time.

Sponsor: Ecological Sciences Division

Stand Water Model

J. B. Mankin R. A. Goldstein⁴⁰

A model has been developed that simulates, on a day-to-day basis, atmosphere-plant-soil moisture relations. The model is being used to study the relative effects on the moisture relations of a forest ecosystem due to perturbations of the environment (such as yearly distributions of insolation and precipitation) and perturbations of forest characteristics (such as canopy albedo and moisture retention capacity of soil). The model is designed to operate in conjunction with stand energy and nitrogen models. The combined models will be used to study the relative effects on a forest ecosystem of perturbations of forest environment and characteristics.

The model applies a water balance to a homogeneous stand of vegetation. A combined energy-balance-aerodynamic approach is used to derive an equation for evapotranspiration. The evapotranspiration is a function of r_x , a resistance to vapor transfer which is characteristic of the surface from which evapotranspiration takes place. This resistance is a function of Ψ_x , the water potential of the surface. This conception is analogous to the relationship between stomatal resistance and leaf water potential. A mass balance is applied to the water flowing through soil and plant. The flow of water within and between soil and plant is a function of soil conductivity, soil water potential, and root characteristics for each soil level and Ψ_x . Soil conductivity and soil water potential are functions of volumetric soil water content.

Setting water-flow to the evapotranspiration surface equal to vapor flow away from the surface, Ψ_x , r_x , and evapotranspiration are calculated. Ψ_x is an important variable in regulating plant production and growth when the three models mentioned previously are combined. In addition to evapotranspiration, the water model traces daily volumetric water content of the different soil layers and runoff.

Sponsor: Ecological Sciences Division

R. A. Goldstein

39. D. E. Dunn, *An Experiment in Finite Difference Modeling*, Montana State University, 1970.

40. Ecological Sciences Division.

A Terrestrial Ecosystem Energy Model

J. B. Mankin R. A. Goldstein⁴⁰
H. H. Shugar⁴⁰ R. V. O'Neill⁴⁰

Efforts have been initiated by a team of investigators to formulate a mechanistic model of energy dynamics in a terrestrial ecosystem. The model is a compartment model described by a system of nonlinear ordinary differential equations. The transfer between each compartment is considered to be a function of recipient and donor variables and of environmental parameters such as solar radiation, temperature, moisture, etc. For present purposes, the system has been divided into vegetation, consumer, and decomposer submodels.

The vegetation submodel considers overstory, understory, and herbaceous subsystems. Each subsystem is subdivided into leaves, bole, roots, and storage compartments. Bole includes all aboveground biomass that is neither leaves nor labile storage. The forest is assumed to have a closed canopy, and vegetation development is simulated on a day-to-day basis. Photosynthesis is a function of solar radiation, water availability, temperature, and physiological time. Growth is a function of energy stored and past history as well as temperature, available water, and physiological time. Water availability is determined by the stand water mode¹.

The consumer submodel deals with individual groups of terrestrial consumers. Energy consumed is considered the basic input to the population, and excretion, respiration, and predatory and nonpredatory mortality are considered as losses. Multiple food supplies, as well as multiple predators, can be simulated for individual consumer groups. Each input and loss process can be modified by behavioral, physiological, and reproductive mechanisms. In its present implementation, the consumer module considers canopy herbivores, predators, and sap suckers, insectivorous birds, small mammals, and vertebrate predators as state variables.

The decomposer submodel operates to decompose an input of materials produced by the other two submodels of the model. Bacteria and fungi are considered an integral part of the litter and soil organic variables. Losses from the organic pools are controlled by explicit time functions expressing temperature-moisture responses expected in microbial processes. Macrobiotic compartments are expressed by a pair of differential equations: one for the energy pool, the second for the number of individuals. The macrobiotic components process fresh litter to a different state (old litter), with the associated effects of speeding decomposition.

The completed model should serve as a point of discussion for summarizing our current understanding of the mechanisms operating in the terrestrial ecosystem. Simplifications and elaborations can be made to improve the model for particular applications. By attempting to simulate the total system, the model may prove useful for testing preliminary hypotheses about ecosystem dynamics and for critically examining new experimental designs.

Sponsor: Ecological Sciences Division

R. A. Goldstein
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The Modeling of Energy Transfer in a Forest Canopy

J. B. Mankin, Jr. C. E. Murphy⁴¹ K. R. Knoerr⁴¹

In order to understand and predict the growth of vegetation, a thorough knowledge of the microenvironment in which plant growth occurs is necessary. Although fluctuations in the water balance

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frequently dominate the microenvironment, its basic characteristics are determined by the incident solar radiation. Solar energy provides the establishment of a satisfactory thermal environment for proper physiological functioning and a proper light environment for photosynthesis.

The difference between the incoming and outgoing radiation fluxes represents the rate at which energy is being absorbed by the plant and soil surfaces, and this energy is dissipated as sensible heat, latent heat, and in metabolic processes. Since the metabolic energy normally represents a small fraction of the total energy exchange, most energy transfer between community surfaces and the atmosphere is in the net exchange of sensible and latent heat. Both of these exchanges are due primarily to turbulent eddy movement in the lower atmosphere.

Consider a mature forest stand which is sufficiently flat, homogeneous, and of sufficient horizontal extent to be considered as a one-dimensional heat exchanger. The primary heat exchange surfaces are the soil (or litter) surface and the leaves, because of their relatively large surface area. Since the microenvironment is seldom in a steady-state condition, it is desired to determine the non-steady-state solution for the system of equations describing this process.

If $z = h$ is the height of the top of the canopy and $z = 0$ is the soil (or litter) surface, the process is described by the following system of equations:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(D \frac{\partial T}{\partial z} \right) + H, \quad (1)$$

$$\frac{\partial q}{\partial t} = \frac{\partial}{\partial z} \left(D \frac{\partial q}{\partial z} \right) + W, \quad (2)$$

where t and z are the time and space variables, respectively, T is the air temperature, q is the air specific humidity, D is the diffusivity, and H and W are source terms which account for sensible and latent heat transfer from the leaves and soil surfaces.

$$\tau_i \frac{dT_{l_i}}{dt} = \alpha_i (q_{e_i} - q_i) + \beta_i (T_{l_i} - T_i) + S_i + R_i, \quad (3)$$

where the subscript i indicates the i th layer, T_{l_i} is the leaf temperature, S_i is the solar radiation, R_i is the long-wave radiation, and τ_i , α_i , and β_i are the simplified coefficients of the heat balance equation,

$$S_i = (a - r - t) S_h [e^{-\rho F_{i+1}} - \exp(-F_i)], \quad (4)$$

where S_h is the short-wave radiation at the top of the canopy, F_i is an exponent dependent upon the absorbing area of the leaves, leaf angle, and solar attitude, and a , r , and t are the absorptivity, reflectivity, and transmissivity, respectively, of the leaves,

$$R_i = \sum_j G_{ij} (T_{l_j}^4 - T_{l_i}^4), \quad (5)$$

where G_{ij} is a factor representing the fraction of energy radiated from layer j which is absorbed by layer i ,

$$\begin{aligned} D &= A_D (z - d) / \phi, & z > h, \\ &= D_h \exp[B_D (z - h)], & h > z > 0, \end{aligned} \quad (6)$$

where D_h is the diffusivity at the top of the canopy and ϕ is a thermal stability correction factor,

$$\begin{aligned} u &= A_u \left[\ln \left(\frac{z-d}{z_0} \right) + \Psi \right], & z \geq h, \\ &= u_h \exp[B_u(z-h)], & h > z > 0, \end{aligned} \quad (7)$$

where u is the wind speed, u_h is the wind speed at the top of the canopy, and Ψ is a thermal stability correction factor,

$$\begin{aligned} \phi &= f \left(T, \frac{\partial T}{\partial z}, \frac{\partial u}{\partial z} \right), \\ \Psi &= q \left(T, \frac{\partial T}{\partial z}, \frac{\partial u}{\partial z} \right). \end{aligned} \quad (8)$$

If the system of equations (1) through (8) can be solved, the temperature and humidity profiles throughout the canopy can be computed.

Equations (1) and (2) are solved using the Crank-Nicolson algorithm by incrementing the time variable by an amount Δt . Equation (3) is solved during the time increment Δt by a Runge-Kutta algorithm. The diffusivity is dependent upon the correction factor ϕ , which is dependent upon the wind speed gradient, which is dependent on the correction factor Ψ , which is dependent upon the wind speed gradient. Therefore, Eqs. (6), (7), and (8) have to be solved simultaneously using an iterative procedure. Equation (5) is solved by summing the radiant energy transfer between the various canopy layers. Since the leaves absorb, reflect, and transmit solar energy, Eq. (4) must be solved iteratively for successive canopy layers until all the direct solar radiation is accounted for. A modification of this method is used for the diffuse radiation by considering the radiation source to be distributed over several solar attitudes. The diffuse

Fig. 2. Initial temperature profiles.

Fig. 3. Temperature profile at 25 min.

radiation absorbed by each layer can be computed iteratively by summing the contributions from the various radiation sources. These calculations must be performed for each succeeding time increment.

These equations have been implemented in a computer program. Starting with the initial temperature profiles shown in Fig. 2, Fig. 3 shows the temperature profile after 25 min. The conditions under which this sample calculation is made are an incident direct radiation of $0.7 \text{ cal cm}^{-2} \text{ min}^{-1}$, an incident diffuse radiation of $0.07 \text{ cal cm}^{-2} \text{ min}^{-1}$, and a wind speed of 250 cm sec at the top of the canopy.

Sponsor: Ecological Sciences Division

R. V. O'Neill

Steady-State Photosynthesis Model

J. B. Markin R. A. Goldstein⁴⁰

We are currently developing a steady-state leaf photosynthesis model, which applies energy, carbon, and water balances to a leaf. For specified environmental conditions and general physiological and morphological characteristics of the leaf and plant to which the leaf is attached the model calculates Ψ_L , leaf water potential; T_L , leaf temperature; and C_L , carbon dioxide concentration at the carboxylation sites. From the above variables, the model calculates rates of net photosynthesis and transpiration.

The energy balance stipulates that the rate of energy absorption by the leaf of solar plus long-wave radiation equals the rate of energy emission by the leaf through the processes of radiation, transpiration, and convection:

$$aS + 2\epsilon R = 2\epsilon\sigma T_L^4 + L_V \frac{\rho_{VL} - \rho_{VA}}{r'_A + r'_S} + 2\rho_A C_P \frac{T_L - T_A}{r_A}, \quad (1)$$

where a is the fraction of solar radiation absorbed by the leaf, S is the intensity of solar radiation, ϵ is the

emissivity of the leaf, R is the intensity of long-wave radiation, σ is the Stefan-Boltzmann constant, T_L is the leaf temperature, $\lambda_v = L_v(T_L)$ is the latent heat of vaporization, $\rho_{VL} = \rho_{VL}(T_L)$ is the saturation water vapor density at the mesophyll surface, ρ_{VA} is the water vapor density of the atmosphere, r'_A is the boundary layer resistance to flow of water vapor, $r'_S = r'_S(C_L, \Psi_L)$ is the stomatal resistance to flow of water vapor, ρ_A is the density of the air, C_p is the specific heat of the air at constant pressure, and r_A is the boundary layer resistance to diffusion of heat. The processes that take place on both surfaces of the leaf are multiplied by 2. The leaves in which we are interested only have stomata on the abaxial surface.

The carbon balance stipulates that the rate of diffusion of carbon to the carboxylation sites is equal to the net rate of photosynthesis:

$$\frac{C_A - C_L}{r''_A + r''_S + r''_M} = \frac{1}{(1/\epsilon_1 aS) + (1/\epsilon_2 C_L)} f(T_L), \quad (2)$$

where C_A is the carbon dioxide concentration of the atmosphere, C_L is the carbon dioxide concentration at the carboxylation sites, r''_A is the boundary layer resistance to diffusion of CO_2 , $r''_S = r''_S(C_L, \Psi_L)$ is the stomatal resistance to diffusion of CO_2 , r''_M is the mesophyll resistance to diffusion of CO_2 , ϵ_1 is the maximum efficiency of utilization of absorbed solar radiation in photosynthesis, ϵ_2 is the maximum efficiency of utilization of CO_2 in photosynthesis, and $f = f(T_L)$ is the function giving the effect of leaf temperature on net rate of photosynthesis.

The water balance stipulates that the rate at which water vapor is leaving the plant equals the rate at which water is flowing from the soil to the leaves:

$$\frac{\rho_{VL} - \rho_{VA}}{r'_A + r'_S} = \frac{\Psi_{SO} - \Psi_L}{\alpha r''_{SO} + r''_P}, \quad (3)$$

where Ψ_{SO} is the soil water potential, Ψ_L is the leaf water potential, α is the ratio of transpiration area of plant to effective water-conducting area between roots and soil, r''_{SO} is the resistance to movement of water between roots and soil, and r''_P is the resistance of plant to movement of water.

The water balance differs from the energy and carbon balances in two major respects. Most often, it takes only on the order of minutes for a leaf to come into equilibrium with its environment in terms of carbon and energy, while it takes on the order of hours to reach a steady state in terms of water transport through the plant. While, conceptually, it is perfectly acceptable to isolate a single leaf and impose a carbon and energy balance, water uptake by the plant from the roots will be dependent on the transpiration of the entire plant canopy. The environment and physiological properties of the leaves throughout the canopy are in most instances not uniform. Hence, the water balance appears to be a grosser approximation, but it is considered adequate for the objective of estimating relative effects of environmental and plant parameters on photosynthesis in order to identify the major variables and mechanisms. However, plant-water relations is an area requiring considerably more intensive research.

The model has been applied to a hypothetical plant whose descriptive parameters have been found scattered throughout the literature. We are presently in the process of replacing many of these with others based on experiments performed by investigators in the Ecological Sciences Division. This model is being used to identify the parameters most affecting plant growth and determine the conditions under which they are most sensitive. It is recognized that some relevant factors, such as the effect of trace nutrients, have not been included; however, ways to include these are under consideration.

HEALTH PHYSICS DIVISION

A Modification of INREM

W. D. Turner R. E. Funderlic

INREM is a computer code written by W. D. Turner⁴² to estimate the cumulative dose-equivalent to body organs resulting from a continuous intake of radionuclides. Under restrictive conditions this code was modified to allow for a more general dose rate in the form of sums of exponentials.

Sponsor: Health Physics Division

P. S. Rohwer

Plutonium Body Burden Estimation

L. W. Gilley

A computer program was written which systematically analyzes the "goodness of fit" of the functions reported previously⁴³ to experimental data for various parameter values. The program divides the curve into specified segments and computes various measures of goodness of fit for each segment.

Also, a number of modifications were made to the programs reported previously.

Sponsor: Health Physics Division

W. Snyder

Microcurie-Days Residence in Man Due to Radionuclide Intake

G. G. Warner C. C. Webster W. S. Snyder⁴⁴

A code has been developed which uses as input the intake of radionuclides into the human body by inhalation, ingestion, or injection into the blood to calculate the dose in microcuries delivered to the blood and the microcurie-days residence in those organs of the body directly involved in the passage of the material from point of intake to point of elimination. The code is capable of taking as input any radionuclide in a decay chain and any combination with successive members of that chain. It then calculates the dose to the blood and microcurie-days residence in specific organs for all successive nuclides in the decay chain due to any combination of the methods of intake.

The output is given as total dose and microcurie-days residence of each specific nuclide for the blood and all organs of the body associated with transit through the body. Space is provided for several additional organs. The output is tabulated by nuclide for unit input of each method of intake indicated on the input data cards. In addition, the program calculates the total dose to the blood and microcurie-days residence to the specific organs for any combination of radionuclides intake and gives a tabulated output.

Sponsor: Health Physics Division

W. S. Snyder

42. W. D. Turner, S. V. Kaye, and P. S. Rohwer, *EXREM and INREM Computer Codes for Estimating Radiation Doses to Populations from Construction of a Sea-Level Canal with Nuclear Explosives*, K-25 report K-1752 (1968).

43. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 20.

44. Health Physics Division.

Beta Dose

G. G. Warner W. S. Snyder⁴⁴

We have written a computer code which calculates dose at a point or dose on a line in tissue from a source of beta particles in a stainless-steel-shielded right circular cylinder of $^{90}\text{SrSiO}_3$ beads in an aluminum matrix. Two formulations were used: one by Loevinger⁴⁵ and another by Berger.⁴⁶

Sponsor: Health Physics Division

Effective Energy

G. G. Warner W. S. Snyder⁴⁴ L. T. Dillman⁴⁷

Near completion is a computer code, SPEFEN, which calculates specific effective energies, that is, total energy absorbed in a region per gram of the region, for four kinds of radiation. The code will be used to determine effective energies for many radionuclides in 22 source organs to 31 target organs in reference man. The radiations are photon (gamma ray, x ray, and annihilation), beta and electron, alpha, and recoil. Neutron radiation is to be added when a model for its behavior is determined. Input for these computations includes radiation energies and yields from decay schemes and specific absorbed fractions. Fractions for the photon radiations were obtained from production runs of ALGAM⁴⁸ with a knowledge of the masses of the target organs. Fractions for beta and electron radiations were based on complete absorption in the organ of origin except for the pulmonary and tracheal-bronchial regions of the lungs where complete absorption is assumed if the range of the beta-like particle is less than the average thickness of the bronchial tree. If the range is greater than that, the dose is averaged over the lung.⁴⁹ Also excepted from the general rule is the specific absorbed fraction of beta-like energies in bone and bone marrow. All the radionuclides that deposit largely in bone deposit initially on the bone surface. While some remain there, others tend to diffuse throughout the bone. A model for this imprecise behavior has been developed from data of Spiers.⁵⁰ For alpha radiation, complete absorption of energy in the organ of origin is assumed. Specific absorbed fraction for recoil radiation is the same as for alpha radiation, but the recoil energy is $(\text{alpha energy} \times 4)/(\text{mass of isotope} - 4)$.

Sponsor: Health Physics Division

Dose from Gamma-Ray Sources

G. G. Warner W. S. Snyder⁴⁴

We used ALGAM⁴⁸ to estimate gamma and x-ray dose to reference man's internal organs from sources of ^{99m}Tc in the contents of the lower large intestine, the contents of the upper large intestine, the liver, the

45. R. Loevinger et al., *Radiation Dosimetry*, eds. Gerald J. Hine and Gordon L. Brownell, chap. 16, pp. 694-754, Academic, New York, 1958.

46. Martin J. Berger, "Distribution of Absorbed Dose around Point Sources of Electrons and Beta Particles in Water and Other Media," MIRD Pamphlet No. 7, suppl. No. 5, *J. Nucl. Med.* (March 1971).

47. Consultant, Ohio Wesleyan University.

48. G. G. Warner and A. M. Craig, Jr., *ALGAM, a Computer Program for Estimating Internal Dose from Gamma Ray Sources in a Man Phantom*, ORNL-TM-2250 (June 1968).

49. W. S. Snyder et al., "Estimation of Dose Due to Inhalation," preliminary draft for revision of *ICRP Publication No. 2* by Committee 2 on Internal Exposure of the ICRP, Sept. 22, 1971.

50. F. W. Spiers, *Radioisotopes in the Human Body*, Academic, New York, 1968.

lungs, and the thyroid. We also conducted depth-dose studies in reference man from monoenergetic external sources which gave a collimated beam of photons incident on the front, on the back, and on the left side of the trunk.⁵¹ We compiled and executed an amended version of ALGAM whereby the dimensions of the phantom and its internality are reduced by a similitude, making it possible to study doses in variable-age phantoms, namely, a newborn, a 1-year-old, a 5-year-old, a 10-year-old, and a 15-year-old.⁵² Data were gathered for 12 monoenergetic sources in the contents of the stomach.

We wrote, compiled, and executed a computer code to calculate the continuous photon dose to the bladder from a radioactive emitter in its contents by the following formulation:

$$D(E_i, i, I_j) = \frac{3.2 \times 10^9 a_i f_i}{\lambda_i} \int_{T_{j-1}}^{T_j} e^{-\lambda_i t} (e^{-\lambda_i T_{j-1}} - e^{-\lambda_i T_j}) \times \left\{ A e^{-\lambda(V_0 \delta_i^1 + R_i(t - T_{j-1}))} + B e^{-\mu(V_0 \delta_i^1 + R_i(t - T_{j-1}))} \right\} dt,$$

where E_i is energy of photon of radionuclide, f_i is yield of photon of radionuclide, I is time interval during bladder filling ($T_j - T_{j-1}$), R is rate of bladder filling, V_0 is initial volume contents of bladder, δ_i^1 is Kroneker's delta function, a_i and λ_i are biological half-life parameters, λ_i is a radiological half-life parameter, and A , B , λ , and μ are parameters from a two-exponential formula which represents the discrete dose to bladder wall as a function of volume of contents.⁵³ A , B , λ , and μ were available for 12 photon energies, so $D(E_i, i, I_j)$'s were computed for "neighboring" energies and $D(E_i, i, I_j)$ was obtained through interpolation.

We continued to conduct studies of depth-dose estimates and dose estimates to reference man from cloud sources of photons.^{54,55} We wrote yet another code to study the photon exposure (rads/day)/(μCi per gram of air) in the thickness of the skin for the following nuclides: ^{83m}Kr , ^{85m}Kr , ^{85}Kr , ^{87}Kr , ^{88}Rb , ^{131m}Xe , ^{133}Xe , ^{135m}Xe , ^{137}Xe , and ^{138}Cs . Dose to skin is averaged over a thickness 0 to 0.2 cm. Input to this code consists of energy of photon from decay scheme, rads/photon from version of ALGAM, and photon flux spectra in cloud, both mentioned earlier.⁵⁴ We compiled and executed a Monte Carlo code which provided flux calculations for photons impinging on a semi-infinite slab of tissue with a cosine angular distribution of incidence.

Sponsor: Health Physics Division

Calculations of the Effect of Shields on Neutron Dose Rate from the DOSAR Reactor

J. R. Knight J. W. Poston⁴⁴ T. D. Jones⁴⁴

The DOT⁵⁶ two-dimensional discrete-ordinates transport code has been used to calculate the effects of Lucite and steel shields on the neutron dose rate from the DOSAR reactor. The cross sections used were

51. J. A. Auxier et al., "Dosimetry for Human Exposures and Radiobiology," *Health Phys. Div. Annu. Progr. Rep.* July 31, 1971, ORNL-4720, pp. 85-90.

52. W. S. Snyder and Mary J. Cook, "Preliminary Indications of the Age Variation of the Specific Absorbed Fraction for Photons," *Health Phys. Div. Annu. Progr. Rep.* July 31, 1971, ORNL-4720, pp. 116-18.

53. G. G. Warner, W. S. Snyder, and Mary R. Ford, "Estimation of Dose and Dose Commitment to Bladder Wall from a Radionuclide Present in Urine," *Health Phys. Div. Annu. Progr. Rep.* July 31, 1970, ORNL-4584, pp. 205-8.

54. *Math. Div. Annu. Progr. Rep.* Dec. 31, 1976, ORNL-4661, p. 19.

55. L. Thomas Dillman, "Absorbed Dose for Immersion in a Radioactive Cloud," *Health Physics Society Annual Meeting*, July 11-15, 1971, New York, N.Y.

56. F. R. Mynatt et al., *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (August 1969).

obtained from the nuclear data libraries⁵⁷ available and collapsed to 34 groups using the XSDRN⁵⁸ code. Two calculations were made for each shielding configuration in an effort to minimize "ray effects."⁵⁹ The first calculation was done with 30 discrete angles, and the second, starting with fluxes generated by the first calculation, was done for 328 angles. Neutron dose rates at various positions around the reactor were obtained from the neutron fluxes generated by the latter calculations.

Sponsor: Health Physics Division

J. W. Poston

**Microscopic Cross Sections for Production of O^- , NO_2^- , and N_2O^- from Cs^0
Bombardment of O_2 , NO_2 , and N_2O Respectively**

V. E. Anderson H. C. Schweinler⁴⁴ R. N. Compton⁴⁴

A new unfolding technique was used to obtain microscopic production cross sections from ion counts from collisions of cesium with oxygen, nitrogen dioxide, and nitrous oxide. This defines the thresholds for ion production, which is of great interest to physicists.

Sponsor: Health Physics Division

R. N. Compton
H. C. Schweinler

Photon Diffusion Studies

V. E. Anderson C. E. Klotz⁴⁴

A Monte Carlo program to study the behavior of a trapped photon in a given homogeneous medium was written for slab and cylindrical geometries. The number of absorptions and remissions necessary to travel a given distance was calculated. Production runs were made for many combinations of input parameters, and the results were in agreement with previous established results.

Sponsor: Health Physics Division

C. E. Klotz

Swarm-Determined Electron Attachment Cross Sections as a Function of Electron Energy

V. E. Anderson L. G. Christophorou⁴⁴ D. L. McCorkle⁴⁴

By utilizing a new unfolding technique, the electron attachment cross section as a function of electron energy can be determined from high-pressure swarm experiments alone. The results, for a number of molecules, agree favorably well with those obtained using quasi-monoenergetic electron beams. The success of this method enhances the potential of the electron swarm method in electron attachment studies.

Sponsor: Health Physics Division

L. G. Christophorou

57. J. L. Lucius et al., *The INDEX System: An Index of Nuclear Data Libraries Available at ORNL*, ORNL-TM-3334 (March 1971).

58. N. M. Greene and C. W. Craven, *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

59. K. D. Lathrop, "Ray Effects in Discrete Ordinates Equations," *Nucl. Sci. Eng.* 32 (1968).

Environmental Impact of Atmospheric Releases

M. Reeves III Peggy G. Fowler Chris S. Day

In an ORNL-TM report⁶⁰ we have presented a description of the mathematical model and the computer code which we have developed for atmospheric transport of short-lived radioactive nuclides. Currently this code is being used to determine population doses due to submersion, air inhalation, and ground contamination. Calculations completed to date are for the reactors Arkansas, Oconee (Units 1, 2, and 3), Vermont Yankee, Indian Point (Units 1 and 2), and Palisades.

Sponsor: Health Physics Division

K. E. Cowser

INSTRUMENTATION AND CONTROLS DIVISION

ECAP: Electronic Circuit Analysis Program

C. W. Nestor, Jr. C. C. Webster

This code⁶¹ was adapted to the ORNL IBM 360 and has been used to evaluate complex electronic circuitry using miniature components prior to assembling the circuit. A circuit was built with components of the sizes used in a sample problem, and the measured values at specific points in the circuitry agreed with the output of the computer program.

Sponsor: Instrumentation and Controls Division

J. T. DeLorenzo

PAL Assembler

D. L. Wilson J. M. Jansen⁶²

A disk resident FORTRAN program PALFTN has been written and is available for use on the ORNL IBM/360 computer system to assemble programs written in PAL-III and PAL-D languages for a PDP-8 series computer. The PAL source program must be input on 80-column punched cards, one statement per card. The output from the Assembler consists of: a program assembly listing, several informative program tables which have proved to be of great benefit for work involving large PDP-8 programs, and a seven-track magnetic tape containing the formatted information for punching a paper tape of the program. With the magnetic tape as input, a service program can be run on an auxiliary device to produce an eight-level paper tape in the PDP-8 series binary format, which may be loaded into the PDP-8 computer with a PDP-8 series BINARY LOADER (DEC-08-LBAA-PM).

The Assembler is based on an earlier version, written in FORTRAN-63 by W. R. Busing and modified by S. P. King, and includes features provided by the 360 assembly language version programmed by S. P. King.

A users' manual is being prepared and is to be published soon.

Sponsor: Instrumentation and Controls Division

60. M. Reeves III, P. G. Fowler, and K. E. Cowser, *A Code for Routine Atmospheric Releases of Short-Lived Radioactive Nuclides*, ORNL-TM-3613 (in preparation).

61. G. R. Hogsett, *ECAP/360-E Electronic Circuit Analysis Program for the IBM System/360 Data Processing System*, IBM Document 360D-16.4.001 (August 1966).

62. Instrumentation and Controls Division.

Revisions to TASK, a Code for Time-Dependent Reactor Calculations

O. W. Hermann A. R. Buhl⁶³

Significant modifications to the TASK code⁶³ are being developed for the purpose of making the program easier to use. The original version^{64,65} was written for computations involving space, energy, and angular dependent fast reactor kinetics. A transfer and scattering matrix technique is used to solve one-dimensional time-dependent multigroup discrete-ordinate equations, including effects of delayed neutrons. Solutions are obtained to provide a more direct means for interpretation of kinetic experiments in the LMFBR Subcritical Measurement Program. Anisotropic spatially distributed sources and anisotropic scattering can be accommodated. The solutions are found using a method which does not require an iterative technique.

The code was "flexibly dimensioned" in the current revision. The versatile "Free Form FIDO" input routines, developed for the ANISN code, were utilized to greatly improve the ease of data preparation. The output is also being revised to show concisely the problem definition, the tables of cross sections and other input data, and the tables of final results. The code also allows the optional output of various intermediate results.

Sponsor: Instrumentation and Controls Division

A. R. Buhl

The Response of the FFTF Ex-Vessel Detectors to Large ^{252}Cf Sources

A. R. Buhl⁶² R. L. Childs

The response of the Fast Flux Test Facility (FFTF) ex-vessel detector to large ^{252}Cf sources was evaluated to determine the feasibility of eliminating the in-vessel low-level flux monitor (LLFM) from the FFTF design. The LLFM consists of three in-vessel assemblies each of which contains a movable cooled fission counter. The elimination of the LLFM is desirable because of mechanical complexities, the extreme fission counter environment, and mechanical interference of the LLFM with other systems in the FFTF.

Two-dimensional transport theory calculations were made to determine the response of the ex-vessel detector to a ^{252}Cf source located at the center of the core and then to three sources in the seventh reflector row. These calculations were made in R - θ geometry, using 50 energy groups, 30 angles, and a P_3 expansion of the scattering cross sections. Reflector source locations proved unsatisfactory because the large direct source contribution to the ex-vessel detector masked the core information.

The effect of placing fresh core-zone 1 fuel in the three in-vessel stored fuel baskets was calculated for the inherent core source and the inherent core source plus 25 mg of ^{252}Cf at the core midplane and axis. These calculations were made at a subcriticality of 25 dollars. The effect of small reactivity changes was evaluated by repeating several of the calculations at 30 dollars subcritical.

The major uncertainties in this evaluation are the effects of stored fuel and, hence, the amount of ^{252}Cf required. Without stored fuel, the calculations (and, in principle, the measurements) are straightforward. However, when fuel is stored in the three baskets, the amount and isotopic content must

63. Acronym for Transfer and Scattering Matrix Method in Reactor Kinetics.

64. A. R. Buhl and J. C. Robinson, "Application of Transport Theory Kinetics to the Interpretation of Experimental Neutron Noise Spectra in Large Fast Reactors," *Trans. Amer. Nucl. Soc.* 14, 857 (1971).

65. H. L. Dodds, Jr., *A New Computational Method for Space-Energy-Angular Dependent Reactor Kinetics*. ORNL-TM-3136 (1971).

be known precisely to determine the fraction of the detector response that is core information (signal) and the fraction that is due to the stored fuel (noise).

Sponsor: Instrumentation and Controls Division's LMFBR Program

A. R. Buhl

ISOTOPES DIVISION

Revisions to the ISOCRUNCH Code

J. R. Knight

The ISOCRUNCH⁶⁶ code for calculating the amount of given isotopes in a decay chain produced by a known neutron flux and exposure time has been revised. The computer code, which was originally written for the IBM-7090, was updated to run on the IBM System 360 model 75 or 91. Other changes allow the calculation of the disintegration rate per unit mass of any isotope in the chain. The new ISOCRUNCH code has been used to predict yields, verify experimental results, and to find optimum exposure times for the production of various isotopes.

Sponsor: Isotopes Division

J. J. Pinajian

Electron Scattering from Hydrogen

M. Reeves III G. D. Alton⁶⁷ P. R. Coleman

Low-energy ($E \sim 1$ rydberg) elastic scattering of electrons from hydrogen is being analyzed in a manner quite similar to that of an earlier report.⁶⁸ Couplings to nonelastic channels are included through a nonlocal potential obtained from the Feshbach⁶⁹ formalism. The resulting mathematical model is an integrodifferential Schroedinger equation. Computer codes,⁷⁰ developed at Oak Ridge to integrate such an equation, are being used to calculate the scattering.

Sponsor: Isotopes Division

MATHEMATICS DIVISION

Text Entry into Computers

Arline H. Culkowski A. M. Legg⁷¹
N. B. Gove Carolyn P. Walker
D. W. Cardwell⁷¹ W. B. Gardner⁷²
Janice B. Ellison

We are making a study of the capabilities and operating procedures of systems available to ORNL for entering, editing, and printing documents through the IBM/360. The systems investigated are the MT/ST

66. C. W. Friend and J. R. Knight, *ISOCRUNCH - Modifications to the CRUNCH Program for the IBM-7090*, ORNL-3689 (January 1965).

67. Isotopes Division.

68. M. Reeves III, doctoral dissertation, University of Tennessee (unpublished).

69. H. Feshbach, *Ann. Phys.* 19, 287 (1967).

70. M. Reeves III and L. W. Owen, *J. Comp. Phys.* 4, 572 (1969).

71. Reactor Division.

72. International Business Machines Corporation.

(Magnetic Tape Selectric Typewriter), ATS (Administrative Terminal System), CRBE (Conversational Remote Batch Entry), and NOVAR. All four involve IBM Selectric Typewriters and can conveniently handle upper- and lower-case characters.

ORNL-TM-3600, *A Study of Four Methods of Entering Text into Computers*, was written to describe these modes and to list some of the conclusions reached.

We gave several demonstrations of ATS to interested personnel and have started using ATS for some reports where ease of editing is required.

Sponsor: Mathematics Division

ORCHIS – Oak Ridge Computerized Hierarchical Information System⁷³

A. A. Brooks

The coordination of several parts of the Mathematics Division information work into a single system has proceeded satisfactorily. Whereas in January of 1971 we had only a single program (SADS) operating from the now standard ADSEP record format, we now have the following programs operating from or interfaced to the standard format – SADS, ORLOOK, KWIC, TRACE, PUBLISH. In addition work is proceeding on the interfacing to the RECON and UGATS programs, which will complete the interfacing with the essential elements of the system. The regional modeling data base will incorporate a direct-access version of the standard format.

In January 1971, there was one active ADSEP data base at ORNL, and there are now about 40 such data bases containing both bibliographic and research data.

A complete bibliography is contained in the referenced progress report. The interfacing and development have been supported by various users, particularly the Director's Division, EISO, IEPIC, and ESIC.

Sponsor: Mathematics Division

ADSEP Data Set Access

A. A. Brooks D. L. Wilson

A multiple-entry FORTRAN subroutine, ADBASE,⁷⁴ was written to access data sets constructed by ADSEP.⁷⁵ The subprogram uses several of the ADSEP routines to retrieve the data set records. The identifier table stored in the first record of the data set is utilized to access any field defined in this table. A new identification table can be supplied in order to redefine the structure. In addition to access by names, access by the index of the name can be used in an equivalent manner to minimize the identifier table searching.

Sponsor: Mathematics Division

73. A. A. Brooks, *ORCHIS – a Mathematics Division Project*, ORNL-CF-71-12-29 (Dec. 20, 1971).

74. A. A. Brooks and D. L. Wilson, *ADBASE – a Subprogram to Access ADSEP Data Sets*, ORNL-CF-71-9-21 (Sept. 20, 1971).

75. A. A. Brooks, *ADSEP – an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

Paper Tape Conversion

P. R. Coleman

Work is beginning on a project to convert all existing paper tape programs from the CDC 160-A computer to the PDP-10 computer. This is being done in order to release the CDC 160-A.

Sponsor: Mathematics Division

Converting Single-Precision Programs to Double Precision

P. R. Coleman

A PL/I program, DOUBLE, has been written to convert most FORTRAN programs to double precision. It performs such tasks as changing specification statements, library function calls, and literal constants. A programmer making such changes might overlook necessary changes as well as spend a great deal of time — especially on large programs. DOUBLE can also translate BCD characters to EBCDIC representation. One feature it does not have is the ability to reorder COMMON blocks.

Sponsor: Mathematics Division

Ill-Conditioned Linear Systems

M. T. Heath

The motivation for this study was the solution of linear integral equations, the discretization of which often leads to a very poorly conditioned system of linear algebraic equations. Direct solution of such a system by standard matrix routines usually gives a completely meaningless answer having wild oscillations, especially if the observation vector is subject to error. Several methods for combating this problem and arriving at a meaningful answer were investigated, particularly when the "true" solution is known, perhaps for physical reasons, to have some additional property such as smoothness or nonnegativity. Among the methods tried were damped least squares, truncated singular value expansion, dynamic programming, linear programming, and iterative methods. For comparison purposes a computer program was written which employs each of these methods successively to the same linear system. While no clear superiority was apparent for any method, the best approach in practice seems to be to try several and look for consistency in the results.

Sponsor: Mathematics Division

Angular Momentum Coupling Coefficients

M. R. Patterson J. A. Carpenter

Implementation and evaluation of a new set of routines by Ford and Braley⁷⁶ to compute the Clebsch-Gordan, Racah, and 9-j coefficients and the reduced rotational matrices were undertaken. The Racah coefficient routine has been compared with those of Tamura⁷⁷ and Wills,⁷⁸ which were made

76. W. F. Ford and R. C. Braley, *FORTRAN IV Subroutines for Coupling Coefficients and Matrix Elements in the Quantum Mechanical Theory of Angular Momentum*, NASA TN D-6173 (February 1971).

77. T. Tamura, *FORTRAN Programs for the Clebsch-Gordan and Racah Coefficients and the 9-j Symbols*, ORNL-3877 (February 1966).

78. J. G. Wills, *Numerical Evaluation of Clebsch-Gordan and Racah Coefficients*, ORNL-TM-1949 (August 1967).

available by C. W. Nestor, Jr. The Ford-Braley routine for the Racah coefficient appears to be about 10% faster than that of Tamura and almost twice as fast as that of Wills. The Ford-Braley and Tamura routines for the $9-j$ coefficient appear to be about equal in speed; however, a special entry in the Ford-Braley routine for the particular case having spins $s_1 = \frac{1}{2} = s_2$ reduces the time required by about 40%. Accuracy of the Ford-Braley routine for the Clebsch-Gordan coefficient is better than that of Tamura and comparable with that of Wills, but no timing runs have yet been done. Further evaluation of these routines continues.

Sponsor: Mathematics Division

Retraining Program

J. S. Crowell R. K. Gryder R. P. Leinius R. D. McCulloch Delores Paulk

One of the laboratory efforts to lessen the impact, for some of the personnel involved, of the reductions in force scheduled at the end of fiscal 1971 was a retraining course in problem solving using the computer. Eighteen technical people scheduled for termination were chosen to attend the class.

Classes were scheduled full time, 8 hr per day, for ten weeks, from April 19th through June 25th. Each class consisted of approximately 4 hr of lectures and 4 hr of problem solving using the computer.

The course curriculum consisted of one week of basic computer concepts, five weeks of PL/I, and two weeks of FORTRAN. The remaining two weeks were used to discuss special topics such as sorting techniques, data base management, numerical techniques, etc. Since hands-on experience is necessary in computer problem solving, some 20 exercises which required machine solution were assigned to the students. The problems ranged in difficulty from trivial (early in the exposition of the problem-solving language) to very difficult (after the students had been exposed to the complete language). Problems were assigned not only to exercise the students in language constructs but also to familiarize them with computer I/O hardware, disks, tapes, and data cell drives.

There was some member attrition as the class progressed. Some members received offers of employment from outside ORNL. Some quit the class so they could concentrate their efforts in interviewing to secure employment. Twelve students completed the full training session. Four of these students received job offers from the Mathematics Division. The majority of the remainder of the class was offered employment within ORNL.

The members of the class were asked to comment on the class after completion of their work. All members indicated that the main goal of increasing their problem-solving ability had been achieved.

Sponsor: Mathematics Division

METALS AND CERAMICS DIVISION

Impedance of Coils Encircled By or Encircling Multiple Coaxial Cylindrical Conductors

C. W. Nestor, Jr. C. V. Dodd¹⁹

We have written two computer programs in BASIC to compute the normalized impedance of a cylindrical coil in the presence of multiple coaxial cylindrical conductors. These programs run without modification on either the PDP-10 time-sharing computer or the IBM 360/75.

For the special case of two conductors inside a coil⁸⁰, we obtained satisfactory numerical agreement with the results of a prior calculation;⁸⁰ however, for the case of two conductors outside the coil, both the program for two conductors only and the program for multiple conductors produced results on the PDP-10 which differed significantly from the results of the two-conductor program on a GE-430. When we ran the multiple-conductor program on the 360/75, we obtained results in agreement with those of the two-conductor program on the GE-430. We found that this discrepancy was due to buildup of round-off error in the calculation of the modified Bessel function $K_0(x)$ and $K_1(x)$ of real argument. In both the two-conductor and the multiple-conductor programs, we had used a series expansion for the Bessel functions for real arguments less than 8; for arguments larger than about 4, however, there is considerable loss of significant figures, since the terms of the series start out positive and then turn negative. We therefore replaced the series expansion for arguments larger than 4 with expressions obtained from Gauss-Hermite quadrature applied to integral representations of the Bessel functions:^{81,82}

$$K_0(x) = \int_0^\infty e^{-x \cosh t} dt \cong 2e^{-x} \sum_{i=1}^3 \frac{w_i}{(u_i^2 + 2x)^{1/2}},$$

$$K_1(x) = \int_0^\infty e^{-x \cosh t} \cosh t dt \cong \frac{2e^{-x}}{x} \sum_{i=1}^3 \frac{w_i(u_i^2 + x)}{(u_i^2 + 2x)^{1/2}},$$

where u_i and w_i are, respectively, the abscissas and weights for six-point Gauss-Hermite quadrature.⁸¹ We found that these expressions give at least six-figure accuracy for arguments larger than 4. This change produced results on the PDP-10 which differed only in the sixth significant figure from results obtained on the GE-430; this is probably unavoidable, due to the difference in word length of the two machines.

Synthetic Metals and Ceramics Division

C. V. Dodd

Electromagnetic Measurement of Liquid Level

C. C. Lu⁸³ C. V. Dodd⁷⁹

The computer-based studies of electromagnetic induction and the mathematical models that have been developed^{84,85} have applicability beyond the field of nondestructive testing. For example, a project for the development of a liquid-level monitor using electromagnetic induction techniques is being supported by the Chemical Technology Division. The problem is to measure (at elevated temperatures) the relative level of liquid bismuth, a poor electrical conductor, surrounding an electromagnetic probe that is encased in a molybdenum tube, a good electrical conductor. The measurement of the low-conductivity medium surrounding the high-conductivity tube is much more difficult than if the circumstances were reversed, for example, with liquid sodium surrounding steel.

As a part of this study, we have made calculations to determine optimum conditions for maximum sensitivity to a level change and minimum drift due to temperature. In our preliminary calculations we used a two-conductor model consisting of a bifilar coil inside a molybdenum tube, with either liquid bismuth or air outside. These calculations showed how the magnitude and phase of the signal in the secondary coil

80. W. A. Simpson et al., *Computer Programs for Some Eddy-Current Problems* - 1970, ORNL-TM-3295 (June 1971).

81. M. Abramowitz and I. E. Stegun, *Handbook of Mathematical Functions*, National Bureau of Standards Applied Mathematics Series, No. 55, Department of Commerce, Washington (1964), pp. 376 and 924.

82. We first change the variable of integration by the substitution $u^2 = x \cosh t - x$.

83. Now at University of Miami, Coral Gables, Fla.

84. C. V. Dodd et al., *Some Eddy-Current Problems and Their Integral Solutions*, ORNL-4384 (April 1969).

85. W. A. Simpson et al., *Computer Programs for Some Eddy-Current Problems* - 1970, ORNL-TM-3295 (June 1971).

varied as tube size, wall thickness, and operating frequency were changed. We determined that we should get an adequate phase shift in the sinusoidal electromagnetic signal (about 11° from no bismuth to all bismuth) using a 0.30-in.-thick molybdenum tube with a diameter of 0.785 in.

Using a more accurate three-conductor model, which included the effects of an outer molybdenum container, we found that the phase shift could be measured at any frequency between 20 kHz and 34 kHz with approximately the same sensitivity. The maximum change in magnitude of the secondary voltage was about 30% at a frequency of 8 to 12 kHz.

Once maximum sensitivity had been achieved, we began to minimize the drifts produced by the large temperature variation from 600 to 700°C. This caused a calculated thermal expansion of the molybdenum tube of about 0.05%. The calculated phase shift for this expansion is less than 0.01° . The calculated change in the resistivity of liquid bismuth is from 145.7 to 151.3 $\mu\Omega\text{-cm}$ and for the molybdenum is 17.0 to 21.0 $\mu\Omega\text{-cm}$. While this change in properties produces a large phase shift over most of the frequency range, there is a minimum change of about 0.1° at 25.2 kHz for no bismuth and at 30.2 kHz for all bismuth; thus there should be a minimum near 27.7 kHz for the system half full of bismuth.

Another big variation is the dc resistance of the primary and secondary coils, which increases from 69.4 Ω to 79.2 Ω over the 600 to 700°C temperature range. However, by matching the impedance of the primary circuit and the secondary circuit with cable capacitance, we were able to essentially eliminate this effect.

Experimental measurements at room temperature, using Inconel disks to simulate liquid bismuth, gave a phase shift change with level at 10 kHz of 0.6° per inch, compared to the calculated value of 0.525° per inch.

Sponsor: Metals and Ceramics Division

C. V. Dodd

An Accounting Program

J. A. Carpenter

We have written a FORTRAN program to generate three accounting reports for each monthly reporting period and the same reports cumulatively for each reporting period of the fiscal year up to and including the present reporting period. The program utilizes a two-level sort that is executed internally.

Sponsor: Metals and Ceramics Division

Roy G. Cardwell, Jr.

Analysis and Processing of Creep-Rupture Data

Ruth B. Hofstra

We have modified and improved some of the data management programs previously written for the processing of creep-rupture data.⁸⁶ This is part of the CADCAPS system.⁸⁷ The same programs are being applied for irradiated and unirradiated conditions, for tensile data, and for several different alloys.⁸⁸

We have also completed work on one of the plotting programs originally written by E. M. Thomas.⁸⁷

Sponsor: Metals and Ceramics Division

H. E. McCoy

J. C. Feltner

86. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, p. 28.

87. R. T. King, E. M. Thomas, and H. E. McCoy, *The Computer - an Aid for Analyzing and Processing Creep-Rupture Data, I. Metals*, November 1969, pp. 62-68.

88. H. E. McCoy and R. E. Gehlbach, *J. Nucl. Metals* 40, 151-65 (1971); H. E. McCoy and D. A. Canonico, *Weld. J. Res. (Suppl.)* pp. 1-8 (1969); H. E. McCoy and R. E. Gehlbach, *Nucl. Technol.* 11, 45-60 (1971).

NEUTRON PHYSICS DIVISION

Monte Carlo Calculations of the Response Functions for Bonner Ball Neutron Detectors⁸⁹

Margaret B. Emmett

Adjoint MORSE calculations were performed to verify the response functions of Bonner ball neutron detectors. Bare, 3-in., and 6-in. Bonner balls were considered. These calculations utilized 123 group cross sections with 30 groups of thermal upscatter. The response function shapes are in good agreement, and the normalizations are within 10% of previously reported results.

Sponsor: Neutron Physics Division

C. E. Burgart

Application of DOT-MORSE Coupling to the Analysis of Three-Dimensional SNAP Shielding Problems^{90,91}E. A. Straker⁹² R. L. Childs Margaret B. Emmett

Many radiation transport problems can best be solved by using both discrete ordinates and Monte Carlo techniques with a coupling between the two techniques occurring at a geometry interface. A general discussion of two possible coupling schemes is given. The calculation of the reactor radiation scattered from a docked service and command module is used as an example of coupling discrete-ordinates (DOT) and Monte Carlo (MORSE) calculations.

Sponsor: Neutron Physics Division

E. A. Straker

INTRIGUE-II-C

Margaret B. Emmett

The plotting package INTRIGUE-II, which was previously reported,⁹³⁻⁹⁵ has been modified in order to allow use of the CRT plotter as well as the pen-and-ink plotter. All subroutines have the same calling sequences as in INTRIGUE-II. The subroutines accomplish the necessary computations and prepare a magnetic tape for use by the CRT. In addition to the CRT option, two changes have been made to the package: the use of scale factors for labeling of linear plots and the addition of subroutine SUBVAL for inserting a value in a subtitle. A report is in preparation and should be published soon.

Sponsor: Neutron Physics Division

E. A. Straker⁹⁶

89. Report to be published.

90. Abstract of ORNL-TM-3365 (April 1971).

91. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705, p. 59.

92. Present address: Science Applications, Inc., Huntsville, Ala.

93. M. B. Emmett, "INTRIGUE-II, an IBM-360 Subroutine Package for Making Linear, Logarithmic and Semilogarithmic Graphs using the CALCOMP Plotter," ORNL-4664 (1971).

94. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705, p. 54.95. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 44-45.

96. Present address: Science Applications Inc., Huntsville, Ala.

MORSEC, a Revised Cross-Section Module for the MORSE Multigroup Monte Carlo Code⁹⁷⁻⁹⁹

E. A. Straker¹⁰⁰ Margaret B. Emmett

The cross-section module for the MORSE neutron and gamma-ray Monte Carlo transport code has been revised to treat upscattering, point total, scattering, and fission cross sections and to output a processed cross-section tape for use on subsequent problems. Several other minor changes in the logic have also been made to improve the overall capabilities of the code.

Sponsor: Neutron Physics Division

E. A. Straker

Collision Site Plotting Routines and Collision Density Fluence Estimates for the MORSE Monte Carlo Code¹⁰¹⁻¹⁰³

E. A. Straker¹⁰⁰ Margaret B. Emmett

Routines for use with the Monte Carlo transport code MORSE have been written to provide collision site plots, that is, plots of the locations of collisions occurring during the random walk process. The plots can be made either on the on-line printer or, through a collision tape, on a pen-and-ink or cathode-ray plotter. The user must decide what type of events and over what spatial range the collisions are to be plotted. Also, an output routine has been added to take advantage of the collision counter information in MORSE in providing a region-averaged estimate of the fluence. Printer plots of the resulting energy spectra for both neutrons and gamma rays are part of the output. This output may be obtained for both forward and adjoint calculations. These routines can also be utilized in other Monte Carlo codes.

Sponsor: Neutron Physics Division

E. A. Straker

Modification of PLOTFB for DNA Phase I Data Testing Program

J. E. White R. Q. Wright

The PLOTFB¹⁰⁴⁻¹⁰⁶ program has been extended and improved for the Defense Nuclear Agency (DNA) Phase I data testing program. Plots of nuclides in ENDF/B format that are of interest to DNA are needed to assist various reviewers in making comparisons with the ENDF/B data files. The primary aim of the present work was to plot quantities more directly related to experimental results. As a consequence, the following features have been incorporated in the program:

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- 97. Abstract of ORNL-4716 (August 1971).
 - 98. This work partially funded by Defense Atomic Support Agency under Subtask PE08001.
 - 99. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705, p. 55.
 - 100. Present address: Science Applications, Inc., Huntsville, Ala.
 - 101. Abstract of ORNL-TM-3585 (October 1971).
 - 102. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705, p. 56.
 - 103. This work partially funded by Defense Nuclear Agency under Subtask PE08001.
 - 104. H. C. Honeck, *Description of the ENDF/B Processing Codes and Retrieval Subroutines*, BNL-13582 (ENDF-110) (Rev. Sept. 1970).
 - 105. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4461, p. 60.
 - 106. R. Q. Wright and J. L. Lucius, "PLOTFB, a Plotting Program for ENDF/B Data," this report

1. The differential cross section is now plotted in ENDF/B files 4, 5, 14, and 15. The units used are millibarns per steradian and millibarns per kilo-electron volt.
2. The reaction Q value has been added to the heading in file 3.
3. An identification number is now associated with each plot.
4. The simple fission spectrum ($LF = 7$) has been included in the file 5 routines.
5. Tick marks are made on all axes.
6. For logarithmic plots of matrices containing zeros, the number of decades required is minimized to best represent the nonzero elements. (The previous version arbitrarily replaced the zeros with 10^{-10} .)
7. A modification number is used to distinguish between different versions of the same ENDF/B evaluation.

In addition to its normal role, the modified version of PLOTFB has proven to be a very useful tool in spotlighting inconsistencies in the neutron energy representation for threshold reactions in files 4 and 5.

Sponsor: Neutron Physics Division

R. W. Roussin

Neutron-Energy-Dependent Capture Gamma-Ray Yields in Tantalum and Tungsten¹⁰⁷

K. J. Yost¹⁰⁸ J. E. White C. Y. Fu¹⁰⁹ W. E. Ford III

Gamma-ray yields as a function of neutron energy for tantalum and tungsten have been calculated with the cascade code DUCAL. The results are presented in a format that would facilitate use in coupled neutron-gamma-ray transport calculations. In the case of tungsten, pronounced variations in the capture yield spectra were noticed above 3.0 MeV. On the other hand, only slight variations in the yield spectra were evident for tantalum. The results have been compared with integral gamma-ray yield measurements, and the agreement is favorable.

Sponsor: Neutron Physics Division

C. E. Clifford

Preparation of Data Sets in ENDF Format for Na, Mg, Cl, and K for Use in Shielding Calculations^{110,111}

R. W. Roussin¹¹² S. K. Penney V. A. Singletary J. B. Wright¹¹²

Neutron interaction and gamma-ray production cross sections for sodium, magnesium, potassium, and chlorine, which were originally evaluated by Drake et al., have been placed in the currently approved ENDF/B formats. This involved a format change for the neutron files and two format changes for the

107. Abstract of ORNL-TM-3436 (June 1971).

108. Now with Department of Nuclear Engineering, Purdue University, Lafayette, Ind.

109. Neutron Physics Division.

110. This work partially supported by Defense Atomic Support Agency under Subtask PE055.

111. Abstract of ORNL-TM-3429 (ENDF-151) (May 1971).

112. Radiation Shielding Information Center, Neutron Physics Division.

gamma-ray production files. Gamma-ray interaction cross sections were then added to the neutron interaction and gamma-ray production data to obtain a reasonably complete set of data for use in shielding calculations.

Sponsor: Neutron Physics Division

R. W. Roussin

**Penetration into a Missile Silo of Neutrons and Secondary Gamma Rays Produced
by Point Isotropic Neutron Sources^{1 13}**

Margaret B. Emmett	W. W. Engle, Jr. ^{1 14}
F. R. Mynatt ^{1 14}	J. V. Pace III
E. A. Straker ^{1 15}	L. R. Williams ^{1 14}

The radiation fields produced in a missile silo by low-altitude point isotropic neutron sources have been calculated for two weapons source spectra and three thicknesses of the silo concrete cover (40, 50, and 60 in.). The purpose of the calculations was twofold: to predict the radiation-induced displacement and ionization in the silicon components of electronic systems in the silos and to illustrate possible techniques for coupling Monte Carlo and discrete-ordinates transport methods to obtain the most efficient solution to this type of problem. Both time-integrated and time-dependent results were obtained, the latter to determine silicon response rates. The time-dependent calculations were performed in three successive steps corresponding to the radiation transport through air over ground, through the silo cover, and within the silo proper. The first and second steps were performed in slab geometry with the MORSE Monte Carlo code^{1 16} and the TDA^{1 17} (Time Dependent ANISN) discrete-ordinates code, respectively, and the third step was done in cylindrical geometry with MORSE; in each case the output from one code was used as the source term for the next. The time-integrated calculations were carried out in two steps, the first describing the transport through air over ground and the second describing the transport through the cover and down into the silo. Both steps were performed in cylindrical geometry with the DOT^{1 18} discrete-ordinates code. A few additional calculations were done with the ANISN^{1 19} discrete-ordinates code, which used the DOT air-transport results as the source for calculating the penetration through the silo cover in slab geometry. When integrated over time, the MORSE-TDA-MORSE results were in good agreement with the DOT-DOT and DOT-ANISN results at common detector points, indicating that the coupling techniques were successful.

Sponsor: Neutron Physics Division

F. R. Mynatt
E. A. Straker

113. From ORNL-TM-3599 (to be published) (classified).

114. Neutron Physics Division.

115. Presently with Scientific Applications, Inc., Huntsville, Ala.

116. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (1970).

117. W. W. Engle, Jr., and F. R. Mynatt, "One-Dimensional Time-Dependent Discrete Ordinates," *Trans. Amer. Nucl. Soc.* 12, 400 (1969).

118. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

119. W. W. Engle, Jr., *A User's Manual for ANISN - a One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693, Union Carbide Corp. (1967).

Plotting of ENDF/B Evaluated Neutron Cross Sections for General ORNL Use¹²⁰

Margaret B. Emmett R. Q. Wright S. K. Penny

Work continued on plotting the ENDF/B version II neutron cross sections and is now essentially complete. In addition to plots of version II data, plots of Penny-Kinney¹²¹ iron data were done.

Sponsor: Neutron Physics Division

E. A. Straker¹²²

A Calculation of Neutron-Energy-Dependent Capture Gamma-Ray Yield Spectra for Iron and Comparisons with Experiments^{123,124}

J. L. White C. Y. Fu¹²⁵ K. J. Yost¹²⁶

The spin-dependent gamma-ray cascade model DUCAL has been applied to calculate neutron-energy-dependent capture gamma-ray spectra in iron. There are significant variations in the capture gamma-ray yield spectra with neutron energy. The results have been compared with a series of integral gamma-ray yield measurements above 1 MeV, and the agreement found was reasonably good. The yield data are presented in a neutron energy format that would facilitate the preparation of the capture component of the secondary gamma-ray production cross sections in iron.

Sponsor: Neutron Physics Division

C. E. Clifford

Reevaluation of Neutron and Gamma-Ray Production Cross Sections of Natural Iron – DNA Material 4124 Mod 2 and ENDF/B Material 1124 Version III¹²⁷

S. K. Penny R. Q. Wright
W. E. Kinney¹²⁸ F. G. Perey¹²⁸
C. Y. Fu¹²⁹

The evaluation for natural iron cross sections which bore the MAT numbers 4124 and 1124 (not ENDF/B version II) were reported by Penny and Kinney.¹²⁹ The changes in the evaluation reported here are as follows:

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- 120. *Math Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 38–39.
 - 121. S. K. Penny and W. E. Kinney, "A Reevaluation of Natural Iron Neutron and Gamma-Ray Production Cross Sections – ENDF/B Material 1124," ORNL-4617 (1971).
 - 122. Present address: Science Applications, Inc., Huntsville, Ala.
 - 123. Abstract of ORNL-TM-3442 (August 1971).
 - 124. Submitted to *Nuclear Science and Engineering* for publication.
 - 125. University of Tennessee.
 - 126. Purdue University.
 - 127. This work was partially funded by the Defense Nuclear Agency under Subtask PC 102-04.
 - 128. Neutron Physics Division.
 - 129. S. K. Penny and W. E. Kinney, *A Reevaluation of Natural Iron Neutron and Gamma-Ray Production Cross Sections – ENDF/B Material 1124*, ORNL-4617 (ENDF-139) (1971).

1. resonance parameters were included for the neutron energy range 1 to 60 keV,^{130,131}
2. the direct-interaction component for exciting the first level in ^{56}Fe via inelastic scattering was decreased,
3. direct-interaction components for exciting other levels in ^{56}Fe via inelastic scattering were included, and the continuum secondary energy distributions for ^{56}Fe were changed to account for direct interaction,^{132,133}
4. the number of entries in the smooth cross-section file (file 3) was reduced, and the numbers of Legendre polynomial coefficients for the inelastic scattering angular distributions were reduced,
5. the secondary neutron energy distribution for the $(n,2n)$ reaction was changed,¹³⁴ and
6. the gamma-ray production files have been modified taking into account the data of Orphan and Hoot.¹³⁵

Sponsor: Neutron Physics Division

F. G. Perey

Preliminary Work on an Evaluation of Natural Calcium Neutron Cross Sections — ENDF/B Material 1152

S. K. Penny

Some preliminary work was performed in the area of model cross-section calculations to aid in the evaluation of neutron cross sections for natural calcium.

The upper limit of the section energy range was 15 MeV. Thus there were three important reactions for neutrons incident on ^{40}Ca , namely, (n,n') , $(n,p)^{40}\text{K}$, and $(n,\alpha)^{37}\text{Ar}$. The level structures, as determined experimentally for the three nuclei, were obtained from the Nuclear Data Group library. Parameters for level densities for excitation energies above the discrete levels were obtained from Gilbert and Cameron.¹³⁶

Optical-model parameters were chosen initially from standard sets. Searches were performed iteratively with the programs GENOA¹³⁷ and HELGA,¹³⁸ varying only the real and imaginary well depths. The differential elastic scattering data used as the basis for the searches were taken from a recent SCISRS¹³⁹ listing and from Perey and Kinney.¹⁴⁰

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130. J. S. Story, U.K.A.E.A., Winfrith, private communication (1970).
 131. R. W. Hockenbury et al., *Phys. Rev.* **178**, 1746 (1969).
 132. G. S. Mani, "Spin Assignments to Excited States of ^{56}Fe Using Inelastic Proton Scattering," Shuster Laboratory, Manchester University, England (1970).
 133. R. J. Peterson, *Ann. Phys.* **53**, 40 (1969).
 134. Suresh C. Mathur et al., *Phys. Rev.* **186**, 1038 (1969).
 135. V. J. Orphan and C. G. Hoot, *Gamma-Ray Production Cross Sections for Iron and Aluminum*, GULF-RT-A10743 (1971).
 136. A. Gilbert and A. G. W. Cameron, *Can. J. Phys.* **43**, 1446 (1965).
 137. F. G. Perey, ORNL, private communication.
 138. S. K. Penny, *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4661, p. 33.
 139. Experiment data file, National Neutron Cross Section Center.
 140. F. G. Perey and W. E. Kinney, *Calcium Neutron Elastic and Inelastic-Scattering Cross Sections from 4.0 to 8.5 MeV*, ORNL-4519 (1970).

Calculations were made with the code HELGA, and it was discovered that the (n,α) and (n,p) cross sections differed greatly from a previous evaluation.¹⁴¹ However, data taken by Dickens¹⁴² supported the calculations. It is now believed that the previous evaluation was incorrect. Calculations were also performed with JULIE¹⁴³ for the direct-interaction excitations.

Sponsor: Neutron Physics Division

F. G. Perey

Low-Energy Electron Transport with the Method of Discrete Ordinates¹⁴⁴

D. E. Bartine F. R. Mynatt¹⁴⁵
R. G. Alsmiller, Jr.¹⁴⁵ W. W. Engle, Jr.¹⁴⁵
J. Barish

Efforts have been in progress for some time to treat the transport of low-energy (≤ 10 MeV) electrons by the method of discrete ordinates.¹⁴⁶⁻¹⁴⁸ In principle, the discrete-ordinates transport code ANISN¹⁴⁹ may be used to simulate the transport of electrons by the simple expedient of introducing into the code the differential cross sections for electron-nucleus elastic collisions, electron-nucleus bremsstrahlung-producing collisions, and electron-atomic-electron collisions. In practice, these cross sections are quite different from those that occur in neutron transport, where the method of discrete ordinates has been used extensively, and it is not clear to what extent the method may be used to successfully transport electrons. Furthermore, some of the differential cross sections that are needed, particularly the cross section for electron-atomic-electron collisions, are not well established, and the extent to which this lack of information will prevent a successful application of the method is also not known.

In the work reported here, the differential cross sections for electron-nucleus elastic scattering and the electron-nucleus bremsstrahlung-producing collisions have been taken from standard sources,^{150,151} and the differential cross section for electron-electron collisions that result in large energy transfers is taken from the work of Moller.^{150,152} This Moller cross section applies to collisions between free electrons and presumably does not accurately describe electron-atomic-electron collisions that result in energy transfers of the order of the atomic binding energies. To describe electron-electron collisions involving small energy transfers, two methods have been used. In method 1 (ANISN with Moller cross section), which is due to

141. M. K. Drake, *Neutron and Gamma Ray Production Cross Sections for Sodium, Magnesium, Chlorine, Potassium, and Calcium - Part VI - Calcium*, NDL-TR-89-VI (AD 665364) (1967).

142. J. K. Dickens, ORNL, private communication.

143. R. H. Bassel, R. M. Drisko, and G. R. Satchler, *The Distorted Wave Theory of Direct-Nuclear Reactions. I: "Zero-Range" Formalism without Spin-Orbit Coupling, and the Code SALLY*, ORNL-3240 (1962).

144. For comparisons other than those given here, see D. E. Bartine et al., *Low-Energy Electron Transport with the Method of Discrete Ordinates*, ORNL-TM-3318 (Feb. 22, 1971); also presented at the National Symposium on Natural and Manmade Radiation in Space, Las Vegas, Nevada, March 1-5, 1971, and also submitted to *Nucl. Sci. Eng.*

145. Neutron Physics Division.

146. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 54.

147. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1970*, ORNL-4592, pp. 85, 86.

148. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705, pp. 95, 96.

149. W. W. Engle, Jr., *A Users Manual for ANISN*, K-1693 (1967).

150. C. D. Zerby and F. S. Keller, *Nucl. Sci. Eng.* 27, 190 (1967).

151. H. W. Koch and J. W. Motz, *Rev. Mod. Phys.* 31, 920 (1959).

152. C. Moller, *Ann. Physik* 14, 531 (1932).

Fig. 4. Transmitted electron current per unit energy from 1-MeV electrons normally incident on a 0.22-g/cm²-thick aluminum slab.

Spencer and Fano¹⁵³ the Moller cross section is assumed to be valid even for small energy transfers, and the lowest energy transfer that is allowed in an electron-electron collision is determined by the requirement that the energy loss per unit distance from all electron-electron collisions corresponds to the well-established total energy loss per unit distance.¹⁵⁴ In method 2 (ANISN with continuous slowing down), the effects of electron-electron collisions which result in small energy transfers are included in the transport equation by introducing a term which corresponds to a continuous slowing down of the electrons being transported. The stopping power that is used in the continuous slowing-down term is obtained by subtracting the energy loss per unit distance due to large-energy-transfer collisions from the well-established total energy loss per unit distance.¹⁵⁴ In the calculations reported below, the continuous slowing down in ANISN was used to describe all electron-electron collisions that result in an energy loss of $<10I$, where I is the average ionization potential of aluminum and is equal to 163 eV.

In Fig. 4 the transmitted currents per unit energy calculated with ANISN using both methods 1 and 2 above are compared with the measured¹⁵⁵ transmitted current per unit energy for 1-MeV electrons normally incident on a 0.22-g/cm²-thick aluminum slab. Also shown in the figure are the calculated results

153. L. V. Spencer and U. Fano, *Phys. Rev.* 93, 1172 (1954).

154. M. J. Berger and S. M. Seltzer, *Tables of Energy Losses and Ranges of Electrons and Positrons*, NASA-SP-3012 (1964).

155. D. H. Rester, *Comparisons of Experimental and Calculated Electron Transmission and Bremsstrahlung Spectra for Electron Energies below 3.0 MeV*, Ling-Temco-Vought, Inc., report No. 0-71100/OK-6 (1973).

of Rester and Derrickson¹⁵⁶ obtained with the Monte Carlo code ETRAN of Berger and Seltzer.¹⁵⁷ The two different ANISN calculations are in excellent agreement with each other and are in good agreement with the Monte Carlo calculations. All of the calculations, however, are lower than the experimental data over much of the energy range shown in the figure.

Sponsor: Neutron Physics Division's Radiation Shielding Program for the National Aeronautics and Space Administration R. G. Alsmiller, Jr.

HIC and Analysis Codes, for Determining Nuclear Reactions Using a Heavy-Ion Cascade Collision Model

O. W. Hermann T. A. Gabriel¹⁵⁸ R. T. Santoro¹⁵⁸ H. W. Bertini¹⁵⁸

The Neutron Physics Division is developing a heavy-ion collision model from which heavy-ion reactions with nuclei (e.g., oxygen on copper) may be computed. This model will be an extension of the computational methods used over the past several years to obtain results of low- and medium-energy bombardment with nucleons and charged pions on nuclei, in accordance with the intranuclear cascade model.^{159,160} The new project requires major additions and changes in the present versions of the MECC code,¹⁶¹ the EVAP code, and the MECCAN code. Also, new analysis codes are to be written.

Assistance from the Mathematics Division was enlisted to supplement the prior and current work on the project. Some test routines have been written to verify changes to MECC and for future checks of the code computations as the final version of the HIC code is developed. Revisions to MECCAN are being made for an initial analysis and checking the new computations. Other analysis codes are also in the process of being developed. Representative test data have been constructed to enable analysis codes to be executed before the HIC code is finished.

The computations conducted in this project have a somewhat "pioneer-type" nature, and comparable experimental data are lacking. Objectives of particular interest are the studies of the dosimetry of heavy ions in space applications and the effects of heavy-ion beams in cancer research.

Sponsor: Neutron Physics Division R. G. Alsmiller, Jr.

Calculations Relating to the Design of Asymmetric 4π Shields for Space Reactors

W. W. Engle, Jr.¹⁵⁸ R. L. Childs F. R. Mynatt¹⁵⁸

The one-dimensional shielding code ASOP¹⁶² was used to determine material thickness used in asymmetric 4π shields for space power reactors. The object of the study was to determine the

156. D. H. Rester and J. H. Derrickson, *J. Appl. Phys.* 42, 714 (1971).

157. M. J. Berger and S. M. Seltzer, *ETRAN, Monte Carlo Code System for Electron and Photon Transport through Extended Media*, National Bureau of Standards reports NBS-9836 (1968) and NBS-9837 (1968).

158. Neutron Physics Division.

159. H. W. Bertini, *Phys. Rev.* 131, 1801 (1963).

160. H. W. Bertini, *Phys. Rev.* 182, 1711 (1969).

161. H. W. Bertini, M. P. Guthrie, and O. W. Hermann, *Instructions for the Operation of Codes Associated with MECC-3, a Preliminary Version of an Intranuclear-Cascade Calculation for Nuclear Reactions*, OPNL-4564 (1971).

162. W. W. Engle, Jr., *A User's Manual For ASOP*, CTC-INF-941 (1969).

minimum-weight shield subject to a given set of dose constraints. Since the problem is really multidimensional, the two-dimensional discrete-ordinates program DOT¹⁵³ was used to check the design and to evaluate the approximations required to perform the one-dimensional calculations. The DOT calculations were also used as a guide in shaping the shield and can be considered a first step in two-dimensional shield optimization.

Sponsor: Neutron Physics Division

F. R. Mynatt

Eyges-Dublin-Shape

J. Barish R. G. Alsmiller, Jr.¹⁵⁸

Reported previously in the 1970 annual report,¹⁶⁴ work is continuing on the transport of high-energy muons through various materials. Calculations¹⁶⁵ differ now from those previously reported in that, in addition to the angular scattering of muons due to Coulomb elastic collisions, an estimate of the angular scattering of the muons due to bremsstrahlung production, pair production, and nonelastic nuclear collisions is included. In addition, the case of laminated shields is considered.

Sponsor: Neutron Physics Division (Project: Muon Transport)

R. G. Alsmiller, Jr.

*The Space Shielding Handbook*¹⁶⁶

J. Barish R. T. Santoro¹⁶⁷
R. G. Alsmiller, Jr.¹⁶⁷ H. C. Claiborne¹⁶⁸

Preparation of *The Space Shielding Handbook*, which will summarize the available information on the shielding of manned space vehicles against protons and alpha particles in space, is continuing. The handbook is primarily intended for nonexperts and is expected to be most useful to mission planners, who must decide with little effort whether a radiation hazard is likely to exist during a specific mission. It will also serve as a useful starting point for obtaining more adequate information about the shielding required when a radiation hazard is thought to exist on a specific mission.

The calculational model that is being used is that of a 300-cm-ID spherical shell shield of a specified material and thickness with a 30-cm-diam tissue sphere at the center. This configuration simulates only very approximately a manned space vehicle, but it does serve to illustrate many of the significant features in spacecraft shield design.

163. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

164. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661 (1971).

165. R. G. Alsmiller, Jr., F. S. Alsmiller, J. Barish, and Y. Shima, *Muon Transport and the Shielding of High-Energy (<500 GeV) Proton Accelerators*, ORNL-TM-3353 (April 1971); also, *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705 (October 1971); also presented at the International Congress on Protection against Accelerator and Space Radiation, CERN, Geneva, Apr. 26-30, 1971.

166. Work funded by the National Aeronautics and Space Administration under Orders W-12792 and H-38280A.

167. Neutron Physics Division.

168. Chemical Technology Division Advanced Planning Group - ORNL.

In addition to the handbook, the Transport of Alpha and Proton Primaries Code, TRAPP, is being documented. TRAPP gives the absorbed dose and dose equivalent at the center of the tissue sphere for incident proton and alpha particles as a function of varying spherical shell shield thickness.

Sponsor: Neutron Physics Division (Project: *The Space Shielding Handbook*)

R. G. Alsmiller, Jr.

Shielding against Neutrons in the Energy Range 15 to 75 MeV

J. Barish R. G. Alsmiller, Jr.¹⁶⁷ R. W. Roussin¹⁶⁷

Coupled neutron and gamma-ray transport calculations have been performed¹⁶⁹ for monoenergetic neutrons normally incident on an infinite slab shield of concrete with 5.5% water content by weight. The transport of gamma rays produced by interactions of neutrons with energy greater than 15 MeV was ignored. For the 50- and 75-MeV incident neutron energies, the gamma-ray dose equivalent was found to be no more than 5% of the total dose equivalent. For the 15- and 25-MeV incident neutron energies, the gamma-ray dose equivalent dominates at greater depths into the slab. A conservative estimate of the effect of including gamma rays produced in interaction by neutrons of energies greater than 15 MeV indicates that the calculated total dose equivalent would increase by less than 2%.

Sponsor: Neutron Physics Division (Project: High Energy Shielding)

R. W. Roussin

Galactic Cosmic Ray Transport Calculations in the Earth's Atmosphere

J. Barish Kay C. Chandler T. W. Armstrong¹⁶⁷ R. G. Alsmiller, Jr.¹⁶⁷

Work is in progress to compute the neutron flux in the earth's atmosphere due to galactic cosmic ray bombardment using the transport codes HETC¹⁷⁰ and ANISN.¹⁷¹ The calculational method will provide the neutron flux spectrum from thermal energies to ~100 GeV as a function of the depth in the atmosphere. Primary purposes of the calculations are to compare the calculated neutron spectra with the balloon-flight measurements of Zobel et al.¹⁷² and to evaluate the importance of the decay of albedo neutrons as a proton source for the Van Allen belt.

Sponsor: Neutron Physics Division (Project: Air-Ground Calculations)

T. W. Armstrong

Monte Carlo Calculation of High-Energy Nucleon-Meson Cascades

Kay C. Chandler T. W. Armstrong¹⁷³

Development of the high-energy transport code HETC,¹⁷⁴ a Monte Carlo code for treating the nucleon-meson cascade induced in matter by high-energy (up to several hundred GeV) nucleons and

169. R. W. Roussin, R. G. Alsmiller, Jr., and J. Barish, "Shielding against Neutrons in the Energy Range 15 to 75 MeV," *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705 (October 1971); also to be published as an ORNL-TM.

170. K. C. Chandler and T. W. Armstrong, *Operating Instructions for the High Energy Nucleon Transport Code, HETC*, ORNL-4744 (in press).

171. W. W. Engle, Jr., *A User's Manual for ANISN, a One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693, CTC (1967).

172. W. Zobel et al., *Neutron Spectral Measurements in the Upper Atmosphere*, paper presented at National Symposium on Natural and Manmade Radiation in Space, Las Vegas, Nev., March 1-5, 1971.

173. Neutron Physics Division.

174. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 62.

charged pions, has continued, and an operation's manual for the code has been written.¹⁷⁵ Several subroutines for analyzing the data generated by HETC and the medium-energy transport code NMTC¹⁷⁶ have also been written.¹⁷⁷

HETC has been used to study a variety of problems related to cosmic ray bombardment of the moon,^{178,179} astronaut dosimetry for solar flare bombardment,¹⁸⁰ and the application of negative pions in cancer radiotherapy.¹⁸¹

Sponsor: Neutron Physics Division

Calculated Low- and High-Altitude Neutron and Gamma-Ray Dose Distributions Due to the HENRE Neutron Source¹⁸²

J. V. Pace III E. A. Straker¹⁸³ C. E. Burgart¹⁷³

Calculations have been performed to obtain the neutron and gamma-ray tissue dose¹⁸⁴ distributions at low and high altitudes due to the 14-MeV anisotropic HENRE (High Energy Neutron Reactions Experiment)¹⁸⁵ neutron source. The DOT¹⁸⁶ two-dimensional discrete-ordinates code was utilized. Source heights of 54 and 1125 ft and detector heights of 3.28 and 1000 ft with ranges out to 3000 ft were considered. A comparison of an isotropic source (with the HENRE energy distribution) at a height of 1125 ft with the HENRE source revealed that the effects of the anisotropic source disappeared at a slant range of approximately 500 m. Neutron and gamma-ray doses using air and ground cross sections from earlier transport calculations¹⁸⁷ were in good agreement with experimental data. Neutron doses using the nitrogen cross sections evaluated by Young¹⁸⁸ were within 10% of the previous result; however, gamma-ray doses were everywhere a factor of 1.5 to 2 lower than those obtained previously. This discrepancy is causing continued investigation and hopefully will be resolved at a later date.

Sponsor: Neutron Physics Division

C. E. Burgart

175. K. C. Chandler and T. W. Armstrong, *Operating Instructions for the High Energy Transport Code, HETC*, ORNL-4744 (in press).

176. W. A. Coleman and T. W. Armstrong, *Nucl. Sci. Eng.* 43, 353-54 (1971).

177. T. W. Armstrong and K. C. Chandler, *Analysis Subroutines for the Nucleon-Meson Transport Code, NMTC*, ORNL-4736 (1971).

178. T. W. Armstrong and R. G. Alsmiller, Jr., "Calculation of Cosmogenic Radionuclides in the Moon and Comparison with Apollo Measurements," *Geochim. Cosmochim. Acta* 2, 1729-45 (1971).

179. T. W. Armstrong, "Calculation of the Lunar Photon Albedo from Galactic and Solar Proton Bombardment," *J. Geophys. Res.* (in press).

180. T. W. Armstrong, "Calculation of the Dose, Radionuclide Production, and Delayed Photon Leakage Due to Solar-Proton Bombardment of Tissue with Potential Application to Astronaut Dosimetry," *Health Phys.* (in press).

181. T. W. Armstrong, R. G. Alsmiller, Jr., and K. C. Chandler, *Calculation of Depth-Dose Distribution Produced in Tissue by Negative Pions*, paper presented at the American Nuclear Society Winter Meeting, Miami Beach, Fla., Oct. 17-21, 1971.

182. To be published.

183. Presently with Scientific Applications, Inc., Huntsville, Ala.

184. E. A. Straker and M. L. Gritzner, *Neutron and Secondary Gamma-Ray Transport in Infinite Homogeneous Air*, ORNL-4464 (1969).

185. A. E. Fritzsche, N. E. Lorimer, and Z. G. Burzon, *Measured High-Altitude Neutron and Gamma Dose Distributions Due to a 14-MeV Neutron Source*, EGG-183-1438 (1969); and *Measured Low-Altitude Neutron and Gamma Dose Distributions Due to a 14-MeV Neutron Source*, EGG-182-1449 (1969).

186. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

187. E. A. Straker, *Time-Dependent Neutron and Secondary Gamma-Ray Transport in an Air-over-Ground Geometry Vol. II. Tabulated Data*, ORNL-4289 (1968).

188. P. G. Young and D. C. Foster, Jr., *An Evaluation of the Neutron and Secondary Gamma-Ray Production Cross-Sections for Nitrogen*, LA-4725 (to be published).

Identification of Radiation Streaming Paths in the Minuteman Silo

T. J. Hoffman C. E. Burgart¹⁷³ J. V. Pace III

The initial approach to the problem of radiation streaming for the Minuteman silo will consist of a time-independent study of the transport through the bearing plate-T-box area. A four-step procedure is planned:

1. Discrete-ordinates calculation of the radiation environment exterior to the silo. Present plans call for an air-over-ground DOT¹⁸⁹ calculation with an unclassified thermonuclear source at an altitude of 1000 ft and possible ground ranges of 500, 1000, 1500, and 2000 ft. The angular flux at these distances will be examined to determine whether restart cases with higher quadrature are necessary.

2. Monte Carlo calculation through the isolated bearing-plate-T-box assembly. The source in this MORSE¹⁹⁰ calculation will be selected from and normalized to the exterior environment obtained in the above DOT calculation. The intent is to obtain the angular fluxes at the inner surface of the silo launcher.

3. DOT calculation through the front part of the bearing-plate region between the lid and the T-box assembly with a refined quadrature to obtain a high degree of angular resolution along the streaming paths. This will be used as a verification for the above MORSE calculation.

4. Adjoint Monte Carlo calculation from points of interest within the silo to the inner surface of the launcher. Calculations for several detector positions and responses will be performed and coupled with the above bearing-plate-T-box assembly calculation.

It is hoped that through this initial phase the important streaming paths and weak areas in the silo will be determined. Subsequent to this, time-dependent studies will be undertaken.

Sponsor: Neutron Physics Division

C. E. Burgart

A Comparison of One-Dimensional Air-Ground with Two-Dimensional Air-Ground Discrete-Ordinates Calculations

J. V. Pace III F. R. Mynatt¹⁹¹

In order to study radiation transport in an air-over-ground geometry, two-dimensional and sometimes three-dimensional codes are required. In this investigation, a study is being made to determine whether one-dimensional or two-dimensional air-ground calculations should be used for the source definition for an underground shelter. The method employed will be to compare an ANISN¹⁹² air calculation coupled to an ANISN concrete calculation with a DOT¹⁹³ air-ground calculation coupled to an ANISN concrete calculation. As a first step, an ANISN air and a DOT air-air calculation were made, and a comparison of the angular distribution at a preselected position revealed good agreement. The next step will be to couple the ANISN air to an ANISN concrete calculation, followed by a DOT air-ground coupled to an ANISN concrete calculation. A possible follow-up to this technique will be a coupled TDA¹⁹⁴ air to a TDA concrete

189. F. R. Mynatt et al., *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

190. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4589 (1970).

191. Neutron Physics Division.

192. W. W. Engle, *A User's Manual for ANISN*, K-1693 (March 1967).

193. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

194. W. W. Engle and F. R. Mynatt, "One-Dimensional Time Dependent Discrete Ordinates," *Trans. Amer. Nucl. Soc.* 12, 400 (1969).

calculation compared with a coupled MORSE¹⁹⁵ air-ground to a TDA concrete calculation. If one-dimensional calculations can be substituted for two-dimensional calculations for air-ground cases, then a substantial saving in computer time can be realized.

Sponsor: Neutron Physics Division

F. R. Mynatt

Development of Shield Optimization Techniques

R. L. Childs

The one-dimensional shield optimization code ASOP¹⁹⁶ has been used extensively in the design of space reactor shields. The outstanding advantage of this code is that it incorporates ANISN¹⁹⁷ transport calculations directly into the optimization procedure. A disadvantage of the ASOP method is that a relatively large number of transport calculations are required. Also, the method is difficult to apply to two-dimensional problems.

Another approach to the shield optimization problem is to use perturbation theory. A small change in layer thickness can be approximated by a small change in the density of the layer. If the change in density is not large enough to substantially distort the flux, the change in dose rate can be calculated if both the forward flux and the adjoint flux are known. With this technique, the dose-weight derivatives, which ASOP calculates from several forward transport calculations, can be calculated from one forward and one adjoint calculation.

A one-dimensional shield optimization code, SHAPE, which utilizes the perturbation theory method, is presently under development. Preliminary calculations indicate that the new method obtains essentially the same results as ASOP with significantly less computation. For shields with six layers, as is now common, the new code has proven to be at least five times faster than ASOP.

Future plans include an investigation of the application of perturbation theory to two-dimensional shield optimization. Two-dimensional shield optimization is a very difficult problem for a number of reasons. Instead of one dose constraint, a two-dimensional problem usually has a number of constraints for detectors in different positions. Also, the amount of computation and data storage required is much greater for two-dimensional problems than for similar one-dimensional problems.

Sponsor: Neutron Physics Division

F. R. Mynatt

Optimization of a Shield for a Nuclear Electric Space Power Plant

W. W. Engle, Jr.¹⁹¹ R. L. Childs F. R. Mynatt¹⁹¹

Computations were made using the ASOP¹⁹⁶ shield optimization code and the DOT¹⁹³ radiation transport code to determine the minimum-weight shield for a small fast reactor designed for a space nuclear electric power plant.

The reactor, cylindrical in shape, is fueled with uranium nitride and cooled by potassium circulating through a matrix of stainless steel heat pipes embedded in the core; the design power is 450 kW(t). The surrounding shield is typically asymmetric, having the overall shape of a truncated 90° cone whose thick-

195. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (1970).

196. W. W. Engle, Jr., *A User's Manual for ASOP*, CTC-INF-941 (1969).

197. W. W. Engle, Jr., *A User's Manual for ANISN, a One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693, CTC (1967).

base is positioned between one end of the reactor and the crew compartment. The heat pipes emerge from the opposite end of the reactor, penetrating through the apex of the shield. The dose constraints are 3 millirems/hr at all 100-ft radii falling within the shadow cast by the base of the cone and 300 millirems/hr at all other 100-ft radii. The optimized shield consists of alternate layers of tungsten and lithium hydride, the thick bottom section extending out to a radius of 112 cm and the tapered side decreasing to a radius of 89 cm. The top heat-pipe shield region consists of a 59-cm-thick inner layer of a stainless steel-B₄C mixture and a 30.5-cm-thick layer of a BeO-B₄C mixture. The total shield weight is 25,589 lb. A partially optimized shield having a 45° cone angle and a higher dose constraint for positions outside the cone shadow (100 rems/hr) has a total weight of 14,708 lb. These shield weights include an allocation of 3.5 vol % of stainless steel structure in the LiH regions.

Sponsor: Neutron Physics Division

F. R. Mynatt

Perturbation Approach to Radiation Transport Sensitivity Studies

D. E. Bartine F. R. Mynatt¹⁹¹

A program has been written to estimate the effect of cross-section uncertainties on one-dimensional transport calculations by linear perturbation methods. The forward and adjoint angular fluxes for the unperturbed case are used together with the perturbed cross-section expansion coefficients to determine the change in activity produced by the perturbation for each position in the cross-section matrix. Results are stated as percent change in activity per percent change in cross section. The activity change is also calculated as a function of energy group and Legendre expansion moment. Perturbation effects due to changes in cross-section sets describing only part of the system (specific reactions and/or elements) can be determined as well as perturbation effects for the entire system. Activity changes resulting from cross-section perturbations may also be determined separately for neutron and gamma responses.

Preliminary results have been obtained for the effect of a 1% cross-section perturbation on the tissue dose resulting from a fission neutron source in air and show good agreement with results obtained in the perturbed forward case. The effective range of the linear perturbation approach is being investigated. Future applications will include infinite air problems for various sources and ranges and shielding calculations in other media.

Sponsor: Neutron Physics Division (Project: Radiation Shielding Programs
for the Defense Nuclear Agency)

F. R. Mynatt

Calculation of the Perturbation Caused by Neutron Interactions with Structural Material on Measured Values of ²³³U, ²³⁵U, and ²³⁹Pu Fission Cross Sections for the Neutron Energy Range 5 to 500 keV

D. E. Bartine J. V. Pace III F. R. Mynatt¹⁹⁸

Calculations were made to determine the effect of aluminum structural materials in certain fission chambers on the measured fission cross section. A ²³⁹Pu, a ²³⁵U, and two ²³³U chambers with differing amounts of aluminum were considered. This work was intended to obtain aluminum correction factors for the four chambers and to provide a check on the relative effects of aluminum in the two ²³³U chambers as measured by R. Gwin.¹⁹⁸

198. Neutron Physics Division.

Point cross sections were obtained from the ENDF/B files and multigrouped, then reduced to a 64 broad-group set by the one-dimensional discrete-ordinates code ANISN.¹⁹⁹ P_3S_8 adjoint calculations were made on each fission chamber with and without aluminum present, using the two-dimensional discrete-ordinates code DOT.²⁰⁰ Since the fission cross sections were input as the source for the adjoint calculations, the resulting adjoint angular flux at the surface of the fission chamber represents the probability that an incident neutron with a given energy, traveling in a given direction, will cause a fission within the chamber. This adjoint boundary flux was multiplied by a normalized flat (equal number per kilo-electron volt) incident neutron flux spectrum and integrated over the surface on which the experimental neutron beam was incident and the most forward angle in the S_8 quadrature to obtain the fission rate as a function of incident energy. An aluminum correction factor was then obtained for each group by dividing the fission rate without aluminum by the fission rate with aluminum.

The calculations indicated that the presence of aluminum in these fission chambers caused an increase in the fission rate. This increase ranged from less than 1% up to 6% depending on the energy of the incident neutron. It was observed that the magnitude of the correction varied directly with the aluminum elastic cross section, which describes an energy loss and an angular deflection. Since the fission cross sections investigated here were relatively constant in energy compared with the aluminum elastic cross section, this establishes that the prime effect of the aluminum was to cause the neutrons to "see" more fuel, thereby increasing the fission rate. Correction factors obtained from these calculations were in excellent agreement with those inferred from the cross-section measurements recorded by the two ^{235}U fission chambers.

Sponsor: Neutron Physics Division

R. Gwin

Analysis of Neutron and Gamma-Ray Transport Using the O6R and OGRE Codes

E. A. Straker²⁰¹ G. W. Morrison

Concrete is an important shielding material that is utilized in reactor shields, bunkers, and missile silos. The accuracy of the calculation of the effectiveness of a shield depends on the cross sections utilized in the calculation and in the adequacy of the transport code. To provide an experimental bench mark, measurements of the time-dependent energy spectrum of neutrons and secondary gamma rays emerging from slabs of various thicknesses were made at Gulf Radiation Technology. The analysis of this experiment may be used to judge the adequacy of cross sections employed and/or the adequacy of the transport codes as applied to the calculational model of the experiment.

The neutron and secondary gamma-ray cross sections employed in the calculations were provided by Young.²⁰² These cross sections for H, O, Ca, Si, and Al were in the ENDF/B format. Codes were written to process for the O6R Monte Carlo²⁰³ code those parts of the ENDF/B format that had previously not been treated. The resulting cross sections in variable supergroup format were utilized in the latest version of the O6R Monte Carlo neutron transport code. (Neutron cross sections for only the major constituents of the

199. W. W. Engle, Jr., *A User's Manual for ANISN, a One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693, CTC (1967).

200. F. R. Mynatt, *A User's Manual for DOT, a Two-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1694 (to be published).

201. Science Applications, Inc., Huntsville, Ala.; formerly with ORNL Neutron Physics Division.

202. P. Young, "Cross-Section Compilation and Evaluation for Analysis of Concrete Shields," special session on Radiation Penetration through Concrete Shields at ANS Winter Meeting, Oct. 17, 1971.

203. C. L. Thompson and E. A. Straker, *O6R-ACTIFK, Monte Carlo Neutron Transport Code*, ORNL-CF-69-8-36 (1969).

Fig. 5. Time-dependent count rate for neutrons for concrete thicknesses of 40.64 cm. Dashed line shows results of calculations.

concrete were used.) The secondary gamma-ray production was treated by a neutron-to-gamma-ray "multigroup matrix." Time-dependent count rates and energy spectra in given time intervals were calculated for comparison with experimental results. Secondary gamma-ray sources were calculated by the O6R code and transmitted to the OGRE²⁰⁴ code for transport and analysis. Figure 5 shows the comparison between the experimental spectra and the calculated spectra.

Sponsor: Neutron Physics Division

204. D. K. Trubey and J. R. Stockton, *OGRE - General-Purpose Monte Carlo Gamma-Ray Transport Code System*, ORNL-3305 (1969).

O6R Calculations of Nitrogen and Iron LRL Pulsed Sphere Experiments

R. W. Roussin²⁰⁵ E. A. Straker²⁰¹ G. W. Morrison

O6R²⁰³ Monte Carlo calculations were made of the time-dependent count rate vs time for neutrons leaking from spherical media pulsed at their center with a nominal 15-MeV neutron source and compared with LRL pulsed sphere measurements.²⁰⁶⁻²⁰⁸ The source anisotropy, energy-angle correlation, pulse width, and detector energy response and time resolution were considered in the calculations. The cross-section processing package for O6R was revised to treat the tabulated energy distributions which are used to represent secondary neutrons from $(n, 2n)$ and continuum inelastic scattering.

Figure 6 compares results for a 55.9-cm-radius nitrogen sphere using ENDF/B²⁰⁹ version I data with results using ENDF/B version II data. Version II data included the $(n, 2n)$ continuum. Figure 6 illustrates that the version II data provide better agreement between calculated and experimental results.

Sponsor: Neutron Physics Division

UKE – a Computer Program for Translating Neutron Cross-Section Data from the UKAEA Nuclear Data Library to the Evaluated Nuclear Data File

R. Q. Wright

The UKE^{210,211} program has been extensively revised to conform with the ENDF/B²¹² version II format. The translation of some of the United Kingdom Atomic Energy Authority Nuclear Data Library²¹³⁻²¹⁴ secondary energy distributions was revised. The translation of 91 materials in the UK library to the ENDF/B version II format was completed. Of particular interest at ORNL were the ^6Li and ^7Li cross sections because these materials were not available in the officially released ENDF/B-II library.

Sponsor: Neutron Physics Division

R. W. Roussin

Cross-Section Sensitivity Studies

S. N. Cramer F. G. Perey²¹⁵ R. W. Roussin²¹⁵

The calculations of the LRL pulsed sphere experiments²¹⁶ have been extended to sensitivity studies of the cross-section data in an effort to determine which specific areas of the data are important in the final

205. Radiation Shielding Information Center.

206. L. F. Hansen et al., "Time Spectra from Spheres Pulsed with 14 MeV Neutrons," *Nucl. Sci. Eng.* 35, 227-39 (1969).

207. L. F. Hansen et al., "Predictions for Neutron Transport in Air, Based on Integral Measurements in Nitrogen and Oxygen at 14 MeV," *Nucl. Sci. Eng.* 40, 262-82 (1970).

208. L. F. Hansen et al., "The Transport of 14 MeV Neutrons in Iron," *Proc. Third Conf. Neutron Cross Sections and Technology* (to be published).

209. M. K. Drake (ed.), *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, BNL-50274 (ENDF-102) (1970).

210. R. Q. Wright, S. N. Cramer, and D. C. Irving, *UKE – a Computer Program for Translating Neutron Cross Section Data from the UKAEA Nuclear Data Library to the Evaluated Nuclear Data File Format*, ORNL-TM-2880 (March 1970).

211. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL 4661, p. 58.

212. H. C. Honeck, *ENDF/B – Specifications for an Evaluated Nuclear Data File for Reactor Applications*, BNL-50066 (May 1966) (revised by S. Pearlstein, Brookhaven National Laboratory, July 1967).

213. K. Parker, *The Aldermaston Nuclear Data Library As of May 1963*, AWE-O-70/63 (May 1963).

214. K. Parker, *The Format and Conventions of the UKAEA Nuclear Data Library*, unpublished (June 1965).

215. Neutron Physics Division.

216. R. W. Roussin et al., "O6R Calculations of Nitrogen and Iron LRL Pulsed Sphere Experiments," *Trans. Amer. Nucl. Soc.* 14(2), 925-26 (1971).

Fig. 6. 55.9-cm-radius nitrogen sphere - measured count rate vs time compared with O6R calculation using ENDF/B MAT = 1012 and DASA MAT = 4133, MOD = 1 cross sections.

results. Primary attention has been given the iron data, where the calculations have the poorest agreement with experiment. Other experiments to be investigated include the nitrogen, oxygen, and water spheres.

The O6R Monte Carlo code²⁰³ is being used in these studies due to its applicability in isolating specific aspects of the neutron transport and collision processes. In this manner the results at various times can be analyzed with respect to (1) reaction type, (2) secondary energy distribution, (3) reaction energy, and (4) number of collisions. The MORSE Monte Carlo code²¹⁷ has been used to a lesser degree in order to verify the results. These two codes process basic cross sections in entirely different methods; however, the calculated time-dependent count rates compare favorably in all cases.

Calculations on the iron spheres indicate that the results at all times are highly sensitive to the source spectrum (14 MeV) and the secondary energy distribution of nonelastic reactions at these energies. This information is useful to the cross-section evaluators in deciding if any changes in the data should be made.

Sponsor: Neutron Physics Division

Preanalysis of ORELA Cross-Section Testing Experiments

S. N. Cramer G. L. Morgan²¹⁵

Several ORELA experiments are planned on various materials such as C, Fe, and Al so that calculations of these experiments can be performed to test the existing cross-section sets. Also, measurements of inelastic scattering cross sections will be performed. A preanalysis of the carbon experiment has been performed using the MORSE code²¹⁷ in an effort to optimize the sample size and detector locations in the experiment.

The MORSE results have enabled the experimenter to design hollow cylindrical samples yielding acceptable counting rates. If there are too many counts per ORELA burst, the detection equipment becomes saturated, and if there are too few counts the counting time is too long.

The MORSE calculation uses last flight statistical estimation to point detectors in compiling results. The detector responses are, however, given as counts per neutron incident on a finite detector, and an effective area was included in the point detector response functions. These calculations were compared with ones using finite detectors and boundary crossing estimation with the experimental response functions. The agreement in the two methods enabled the use of the more efficient statistical estimation in all subsequent runs.

For inelastic scattering cross-section measurements, thin samples must be used so that there is little multiple scattering, and it is desirable to have a high inelastic scattering counting rate without saturating the detection equipment with the elastic scattering rate. In an effort to optimize the counting rate ratio, calculations were run with the detectors placed such that elastically scattering neutrons reaching them would have scattered at the minima of the angular distribution. The inelastic scattering is assumed to be isotropic.

Sponsor: Neutron Physics Division

217. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (1970).

Calculated Neutron and Secondary Gamma-Ray Leakage from the Army Pulse Radiation Facility Reactor

W. E. Ford III Jackie S. Gillen

The neutron and secondary gamma-ray leakage from the Army Pulse Radiation Facility Reactor (APRFR) is being calculated for the bare reactor and for the reactor surrounded with a vertical B₄C shroud. The APRFR is an unreflected and unmoderated nuclear reactor designed to produce large fast-neutron and gamma-radiation doses. At this time the calculations are approximately 70% complete.

Sponsor: Neutron Physics Division

The POPOP4 Library of Neutron-Induced Secondary Gamma-Ray Yield and Cross-Section Data²¹⁸

W. E. Ford III Jackie S. Gillen

As a part of the continuous program of updating the POPOP4 library, 20 data sets were added, two were voided, and three existing data sets were modified. Included among the data sets added to the library were (*n*, *γ*) yield data for Be, C, Fe, Cr, Ni, Nb, Mo, Sn, Ta, Pt, Bi, and ²³⁸U, inelastic yield data for C and Nb, and total secondary gamma-ray production cross-section data for Nb and ²³⁸U. These data were distributed through the Radiation Shielding Information Center.

Sponsor: Neutron Physics Division

MSC, a Program to Evaluate Multiple-Scattering Corrections in Thick Samples

N. M. Greene R. B. Perez²¹⁵ G. de Saussure²¹⁵ L. M. Petrie

During the past year, the MSC²¹⁹ program has been incorporated into a resonance parameter adjustment scheme. Results, though preliminary, support the feasibility of the approach. However, certain anomalies have been observed which suggest the inadequacy of the usual method for representing angular cross sections in the *S_n* method.

The "multitable" approach specifies the differential cross section for a group-to-group transfer through an ordinary Legendre expansion of the form

$$\sigma(g \rightarrow g', \mu) = \sum_{l=0}^N \frac{(2l+1)}{2} \sigma_l(g \rightarrow g') P_l(\mu),$$

where $\sigma(g \rightarrow g', \mu)$ is the differential scattering cross section for a transfer from group *g* to *g'* through an angle whose cosine is μ in the lab system, $\sigma_l(g \rightarrow g')$ are the terms normally called "transfer coefficients," and $P_l(\mu)$ is the *l*th Legendre polynomial evaluated at μ .

This approach is adequate if the differential cross sections are smoothly varying functions. However, in certain energy ranges, resonance widths are such that MSC must take such small energy group widths as to

218. W. E. Ford III, *The POPOP4 Library of Neutron-Induced Secondary Gamma-Ray Yield and Cross Section Data*, CTC-42 (1970).

219. N. M. Greene et al., *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 35.

cause the differential cross sections to appear as "spikes" about a "preferential" scattering direction. This is clearly a difficult condition to represent with a low-order Legendre fit. (High-order fits are ruled out by significance problems which occur when the higher-order transfer coefficients are evaluated by the MSC analytical approach.) Craven²²⁰ has developed and tested a more direct method for representing group-to-group transfers which does not suffer from the same restrictions. Future work will attempt to incorporate these techniques into MSC.

Sponsor: Neutron Physics Division

CMODE and MERGE, GAM II Satellite Programs

J. L. Lucius

GAM II²²¹ Cross Section Libraries at ORNL have traditionally resided on a single reel of magnetic tape in the binary mode acceptable only by IBM 360 computers. However, the use of the SUPERTOG²²² code to generate GAM II Cross Section Libraries from ENDF/B²²³ data has created an interest in the ORNL GAM II Libraries by installations who do not use IBM 360 computing equipment. The codes CMODE and MERGE have been written to facilitate the distribution and use of ORNL GAM II Libraries.

CMODE copies the data for selected nuclides from a binary tape onto one or more BCD tapes and also performs the reverse process by compressing the data from several BCD tapes onto a single reel of binary tape.

MERGE generates a new library consisting of nuclides selected from two existing libraries.

Sponsor: Neutron Physics Division, Radiation Shielding Information Center

PLOTFB, a Plotting Program for ENDF/B Data

R. Q. Wright J. L. Lucius

The PLOTFB^{224,225} program has been extended and improved. The program now processes the photon production data (ENDF/B files 12-16), and the plotting of ENDF/B file 5 (secondary energy distributions) has been implemented. A modified version of the program, PLOTFC, utilizes the Calcomp (rather than the CRT) plotter. Both the PLOTFB and PLOTFC programs have been made available on the NUCLIB disk pack.

Sponsor: Neutron Physics Division

R. W. Roussin

220. C. W. Craven, Jr., *Inscattering Approximations in Discrete Variable Transport Theory*, unpublished Ph.D. dissertation, University of Tennessee, 1965.

221. G. D. Joanou and J. S. Dudek, *GAM II, a 3_3 Code for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants*, GA-4265 (1963).

222. R. Q. Wright et al., *SUPERTOG: A Program to Generate Fine Group Constants and Pn Scattering Matrices from ENDF/B*, ORNL-TM-2679 (1969).

223. H. C. Honeck, *ENDF/B - Specifications for an Evaluated Nuclear Data File for Reactor Applications*, BNL-50066 (1966). Revised by S. Pearlstein, Brookhaven National Laboratory, July 1967.

224. H. C. Honeck, *Description of the ENDF/B Processing Codes and Retrieval Subroutines*, ENDF-110, BNL-13582 (September 1967; revised September 1970).

225. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 60.

Multigroup Cross-Section Processing Code Development (AMPX)

N. M. Greene W. E. Ford

J. L. Lucius J. E. White

R. Q. Wright

A system of interfaced computer codes called AMPX is being developed to automate the process of obtaining multigroup coupled neutron-gamma cross sections for discrete-ordinates codes and for the Monte Carlo code MORSE. Basic cross-section data are obtained from ENDF/B libraries, and all operations required to generate and collapse multigroup cross-section sets are carried out in the same system. AMPX consists in part of computer codes originally designed to operate independently. The incorporation of these codes into the system has been accomplished with minimum degradation of their independence, permitting the execution of any one process, all processes, or any meaningful combination of processes.

AMPX is flexibly dimensioned; neutron group structures, gamma group structures, expansion orders to represent anisotropic processes are all arbitrary and limited only by available computer core and budget. The basic processes provided will (1) generate multigroup neutron cross sections; (2) generate multigroup gamma cross sections; (3) generate gamma yields for gamma-producing neutron interactions; (4) combine neutron cross sections, gamma cross sections, and gamma yields into final "coupled sets"; (5) perform one-dimensional transport calculations for neutrons and gammas and, on option, collapse the cross sections to a broad-group structure, using the one-dimensional results as weighting functions; (6) plot cross sections, neutron fluxes, gamma fluxes, etc., on option to facilitate the "evaluation" of a particular multigroup set of data; (7) update and maintain multigroup neutron cross sections, gamma cross sections, and gamma yields on libraries in such a manner as to make it not only easy to combine new data with previously processed data but also to do it in a single pass on the computer; and (8) output multigroup cross sections in convenient formats for other codes.

The programs which will perform the tasks described above have been selected and are being reworked to fit into the AMPX system. These are

1. XLACS²²⁶ — an ORNL program that generates fine-group neutron cross sections in both the fast and thermal energy ranges from ENDF/B data,
2. MUG²²⁷ (SMUG)²²⁸ — an ORNL program that generates fine-group gamma-ray cross sections from ENDF/E data,
3. LAPHANO²²⁹ (LAPHNGAS) — a Los Alamos program that generates photon production matrices in multigroup form from ENDF/B data,
4. XSDRN²³⁰ (NITAWL, XSDKNPM) — an ORNL program that performs resonance calculations, generates one-dimensional weighting spectra, and weights fine-group cross sections to make broad-group libraries for several other codes.

Figure 7 is a skeletal description of AMPX showing the module arrangement.

226. N. M. Greene et al., *XLACS: A Program to Produce Fine Group Averaged Neutron Cross Sections from ENDF/B* (to be published).

227. J. R. Knight and F. R. Mynatt, *MUG: A Program for Generating Multigroup Photon Cross Sections*, CTC-17 (1970).

228. Names of AMPX parts derived from a code name are shown in parentheses.

229. D. J. Dudziak, R. E. Seamen, and D. V. Susco, *LAPHANO: A P₀ Multigroup Photon Production Matrix and Source Code for ENDF*, LA-4750-MS (ENDF-156) (Los Alamos Scientific Laboratory) (1971).

230. N. M. Greene and C. W. Craven, Jr., *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (1969).

Fig. 7. AMPX flow chart.

The "driver" program which couples the AMPX modules has been written and partially checked using dummy routines for the calculational modules.

Tentative input specifications have been made. The original input "specs" were used except in certain cases for which redundant input data would have been required to retain them.

General formats for the various multigroup libraries which can be constructed have been devised. The same format now applies to an all-neutron, an all-gamma, or a coupled neutron-gamma library. The new format is broad enough to include most foreseen modifications and generalizations which will be added, such as a general representation of anisotropy for any process.

SMUG. MUG has undergone considerable revamping to create its AMPX counterpart SMUG. The new program is five to ten times faster than the older one. It is now flexibly dimensioned and has been used to

run problems which because of time and dimensional limitations could not have been run before (e.g., a 180-group P_5 set was produced in 15 min on the IBM 360/90). Future work will (1) change its input to a FIDO-type format, (2) add a form-factor processing capability, (3) check the adequacy of the present means of arriving at the transfer matrices, and (4) cause the program to write and update multigroup gamma libraries in the new AMPX format.

LAPHNGAS. As received, LAPHANO was programmed for the CDC-6600. The program has been implemented on the IBM 360 and is currently being tested with a series of sample problems. The code also has been flexibly dimensioned and modified to accept FIDO-type input. Future work is needed to put the data in the correct form for other modules in AMPX.

XLACS. XLACS is operational but will need work to (1) do $(1/\sigma_T E)$ weighting and (2) revise the neutron library format.

NITAWL, XSDRNPM. XSDRN has been split apart into NITAWL and XSDRNPM. Except for minor problems, both pieces appear operational. Work is needed mainly to make the code read and work with the new AMPX library tapes.

CHOX. No work has been done on this part, which will serve to couple the various libraries into master AMPX libraries. This step should produce no great difficulty once the others produce their respective libraries.

Sponsor: Neutron Physics Division's Cross Section Code
Development Program for the Defense Nuclear Agency

C. E. Clifford
F. R. Mynatt

The POPOP4 Library and Codes for Preparing Secondary Gamma-Ray Production Cross Sections²³¹

W. E. Ford III

The POPOP4²³² code for converting secondary gamma-ray yield data to multigroup secondary gamma-ray production cross sections and the POPOP4 library of secondary gamma-ray yield data²³³ are described. Recent results in the "testing" of uranium and iron data sets from the POPOP4 library are given.^{234,235} The data sets were tested by comparing calculated secondary gamma-ray pulse-height spectra with spectra measured at the ORNL TSR-II reactor.

Sponsor: Neutron Physics Division

Calculated Perturbations in Threshold Foil Measurements Due to Neutron Interactions in B_4C Shells²³⁶

W. E. Ford III Jackie S. Gillen

Calculations were made to determine expected perturbation effects to the measured neutron flux in B_4C -shielded threshold foils resulting from neutron interactions in the B_4C . Results indicated that there is a

231. Abstract of paper presented at the National Symposium on Natural and Manmade Radiation in Space, Las Vegas, Nev., Mar. 1-5, 1971; also abstract of ORNL-TM-3367 (1971).

232. W. E. Ford III and D. H. Wallace, *POPOP4 - a Code for Converting Gamma-Ray Spectra to Secondary Gamma-Ray Production Cross Sections*, CTC-12 (1969).

233. W. E. Ford III, *The POPOP4 Library of Neutron-Induced Secondary Gamma-Ray and Cross-Section Data*, CTC-42 (1970).

234. W. E. Ford III and J. S. Gillen, *The Testing of ^{238}U Secondary Gamma-Ray Production Data Sets from the POPOP4 Library*, ORNL-TM-3482 (in press).

235. J. E. White, C. Y. Fu, and K. J. Yost, *A Calculation of Neutron Energy-Dependent Capture Gamma-Ray Yield Spectra for Iron and Comparisons with Experiments*, ORNL-TM-3442 (Aug. 30, 1971).

236. Abstract of ORNL-TM-3519 (1971).

significant increase in the measured flux below the source energy of monoenergetic neutron beams due to scattering.

The activities in a series of threshold foils encased within a B_4C shell were calculated for exposure of the shell to monoenergetic 13.57- and 1.01-MeV neutron beams incident at 0° with respect to the shell axis. Calculations were also made to determine if there would be a significant change in the measured threshold foil activities if the detector were inadvertently positioned "upside down" (beam incident at 180°) during an experiment. The difference between the 0° and 180° activities was not sufficient to distinguish which end of the detector was oriented toward the beam.

Sponsor: Neutron Physics Division

The Testing of ^{238}U Secondary Gamma-Ray Production Data Sets from the POPOP4 Library²³⁷

W. E. Ford III Jackie S. Gillen

The ^{238}U nonfission capture, fission capture, and inelastic-scattering data sets included in the POPOP4 library of neutron-induced secondary gamma-ray yield and cross-section data were tested for use in the preparation of ^{238}U secondary gamma-ray production cross sections (SGRPXS's). The data sets were tested over various neutron energy ranges by comparing calculated secondary gamma-ray pulse-height spectra with previously measured spectra²³⁸ resulting from the exposure of a 30-mil-thick depleted uranium foil to bare, thermal, and Cd-, ^{10}B -, ($Cd-^{10}B$)-, and ($Cd-1.377^{10}B$)-filtered neutron beams from the ORNL TSR-II reactor. ^{235}U fission capture and inelastic scattering data sets 925801 and 925301, respectively, were found to be suitable for use in the preparation of ^{238}U SGRPXS's. ^{238}U nonfission capture data sets 928109, 928112, and 928113 and the total SGRPXS data set 928901 are adequate for use in shielding calculations when used over the neutron and gamma-ray energy ranges for which the data are defined.

Sponsor: Neutron Physics Division

Neutron Cross Section Evaluation

G. S. McNeilly F. G. Perey²³⁹

Essentially any application of neutron physics — reactor shielding or core design, weapons development, weapons effects, etc. — requires an accurate determination of the important neutron cross sections involved in the investigation. Typically, experimental data do not exist for many neutron reaction channels with high cross sections, and available experimental efforts often contain conflicting results. It is the task of the neutron cross-section evaluator to determine the most exact representation of existing experimental data and to calculate unknown cross sections using appropriate nuclear models.

As part of a larger effort involving numerous nuclides and investigators, current research is concerned with the understanding of the total neutron cross sections of ^{40}Ca and ^{12}C . Recent measurements by Cierjacks et al. at Karlsruhe²⁴⁰ and Schwartz et al. at the National Bureau of Standards²⁴⁰ contain

237. Abstract of ORNL-TM-3482 (in press); also abstract of paper presented at the American Nuclear Society Winter Meeting, Miami, Fla., Oct. 17–21, 1971.

238. The measured spectra were obtained by the TSR-II staff under the direction of F. J. Muckenthaler (Neutron Physics Division).

239. Neutron Physics Division.

240. Private communication.

significant disagreements. Experiments at ORELA, currently being analyzed, may help determine the total cross sections more accurately.

Sponsor: Neutron Physics Division

F. G. Perez

NUCLEAR DATA PROJECT

Level Scheme Plotting Program

T. J. Tyrrell C. C. Webster M. Feliciano

The program as it existed when described in the last annual report²⁴¹ has been modified to include improvements in the plotting routine. The program has been modified with the addition of subroutines giving the capability of drawing multiple scales and drawing gamma-ray transition lines across two or more scales and two or more scale breaks to the proper energy level value. The program can now be used with either the pen-and-ink CALCOMP plotter or the CRT plotter to draw a multiple ladder diagram with multiple scales.

Sponsor: Nuclear Data Project

D. Horen

Isotope Reference Retrieval Program

F. D. Hammerling

An isotope reference retrieval program has been written which allows the user to retrieve references associated with a given mass number from a master file on which the references are identified and sorted by a unique key number only. The user may also retrieve only the references that were entered after a specified date, which permits an updated list without duplication. The references retrieved, along with mass number, chemical symbol, atomic number, and key number, are printed in order of increasing atomic number. Since a method already existed for creating a file which contains the mass number, chemical symbol, and the associated key number, a program was written to reformat and append the atomic number, neutron number, and the date the record was entered into the data set. This program will also update, edit, and sort the file in the appropriate order. By the use of this file, the retrieval program selects all of the key numbers after a specified date for given mass numbers. These key numbers are then sorted and the corresponding references retrieved from the master file. Both the update and retrieval programs are coded in PL/I. The desired order of output was accomplished by an INDEXED data set.

Sponsor: Nuclear Data Project

D. J. Horen

D. C. West

OPERATIONS DIVISION

Interpolation of the HFIR Reactor Power Density

M. R. Patterson F. D. Hammerling P. R. Coleman

Cylindrical symmetry of the HFIR reactor indicates that periodicity in the azimuthal angle θ must be introduced in interpolation of power density data. These data are available only at unequally spaced values

241. Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4661, p. 63.

of θ because of the location of access ports, and only a small number of azimuthal angles are available, caution. Application of the fast Fourier transform of Cooley and Tukey was not possible because of the unequal intervals at which the data are available. No standard numerical technique was available to Fourier analyze unequally spaced data.

Thus, a method was developed to compute these Fourier coefficients.²⁴² This method applies the well-established numerical techniques of linear algebra to extract the Fourier coefficients. By solving an overdetermined set of equations, experimental error which is unavoidably present in the data can be treated in the least-squares sense.

Dependence of the data on the radial and vertical coordinates is treated by spline interpolation. Using this interpolation package, the power density was integrated over the volume of the reactor with a Romberg integration scheme for several test cases. From these results, a normalized power density can be interpolated at arbitrary points in the reactor. Extensive application of this code awaits availability of the detailed experimental data.

Sponsor: Operations Division

F. B. K. Kam

ORNL-NSF ENVIRONMENTAL PROGRAM

An Electricity Supply-Demand Prediction System

T. J. Tyrrell L. D. Chapman²⁴³

During our first full year of investigation²⁴⁴ we have examined 36 econometric models of residential, commercial, and industrial demand for electricity for 49 states and 10 FPC regional areas. These models are equations for kilowatt-hour demand as a function of population, per capita income, the price of electricity, and competitive fuel prices. The equations are, in general, quite accurate and have logical and significant coefficients.

Our results indicate electricity price elasticities significantly higher than previous demand studies²⁴⁵ and complementary to at least one current cross-sectional demand study.²⁴⁶

The principal shortcomings are autocorrelation and intercorrelation, traditionally associated with time-series data. We are currently investigating an appropriate lag model as a possible solution.

The preliminary results of our study, including an initial test of our models on a hypothetical problem (an SO₂ emissions tax), were reported at the annual AAAS convention.²⁴⁷

Sponsor: ORNL-NSF Environmental Program, Energy Group

R. S. Carlsmith

Economic Regional Modeling Program

R. J. Olsen²⁴⁸ G. W. Westley

As part of a general export-base model for the East Tennessee Development District (ETDD), work has been directed to the development of an economic submodel. The primary function of the economic

242. M. R. Patterson and F. D. Hammerling, *Fourier Analysis of Unequally Spaced Data*, ORNL-TM-3547 (September 1971).

243. Cornell University.

244. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 16.

245. F. M. Fisher and C. Kaysen, *A Study in Econometrics: The Demand for Electricity in the United States*, North-Holland Publishing Co., Amsterdam, 1962.

246. J. W. Wilson, "Residential Demand for Electricity," *Quart. Rev. Econ. Bus.*, spring 1971.

247. L. D. Chapman, T. J. Tyrrell, and T. Mount, "Electricity and the Environment: Economic Aspects of Interdisciplinary Problem-Solving," presented at annual AAAS convention, Dec. 26, 1970, Philadelphia.

248. Consultant to the NSF Regional Modeling Program.

submodel is to derive (forecast) labor supply quantities from known population data. There are, of course, exogenous variables such as past labor participation rates, past unemployment rates, and past migration rates that are used in the forecasting procedure. The procedure is basically to generate the population at a time step by modifying the population at the previous time step with respect to births, deaths, aging, and net migrations. The procedure generates labor participation rates that are used to calculate a forecasted labor supply. Eventually, the economic submodel will be combined with a procedure for forecasting labor demand to provide the export-base model for the region. The procedure to date is quite general and is applicable with obvious adjustments to other regions than ETDD. The regression analysis capability used to derive the statistical relationships is to be released soon.²⁴⁹

Sponsor: ORNL-NSF Environmental Program

C. W. Craven

Analysis and Display of Topographic Data

T. C. Tucker

The topography of a region has a great influence on the use of the land in that region. The shape of the earth's surface at any location may affect not only the suitability of that location for a particular use but also the suitability of relatively distant land areas for other uses. For example, if a mountain valley is shaped so that frequent heavy rainfalls cause very high runoff rates, the flood danger downstream from that valley affects land use near the stream. Although we know what to expect in most watersheds today, we must know what will happen if the upstream valley is changed by strip mining, for example. We are developing a program to determine the topographic characteristics required by hydrologic models²⁵⁰ from elevation data.

We have also written subprograms to aid in visualizing the topography of a region. The first of these is a contouring subroutine, CR3CON, designed for a cathode ray tube plotter. This subroutine has the capability of operating with data in either rectangular or triangular grids.

While contour plots are useful, they do not give an immediate impression of shape. We have written subroutine SHADED to make a map with shaded relief. In this technique, uniform illumination is assumed to come from the upper left, or northwest, at an angle of 45° from horizontal. Gray level shading is calculated based upon the angles between the incident radiation and the normal to the surface and between the normal and the position of the observer. Figure 8 is the result of combining the CR3CON and SHADED subroutines. For this case, the elevation data²⁵¹ consisted of a 101 by 101 square array. There are ten gray levels and a 400 by 400 raster in the shaded relief. The width of the contour lines increases with elevation in a five-element cycle. Approximately 16 sec of IBM 360/91 time were required for shading and 2 sec for contouring.

An even better impression of the topography of an area can be obtained from a perspective drawing. We wrote subroutine PERSPX to generate perspective line drawings from elevation data. Using the same data as in Fig. 8, we produced Fig. 9 in about 3 sec of 360/91 time. Also derived, but not shown, is an array indicating the visibility of each data point in the perspective of Fig. 9. An important characteristic of PERSPX is that the execution time is virtually independent of the number of ridge lines. As a result, PERSPX operates from at least six to over 40 times faster than another perspective plotting algorithm.²⁵²

249. G. W. Westley, *SIMPLE - a Flexible Multivariate Regression Program*, ORNL-NSF-EP report to be issued.

250. See Reeves, Nestor, and Tucker, Ecological Sciences Division section of this report.

251. Elevation data have been furnished by Mr. Dean Edson, Research Division, United States Geological Survey, Washington, D.C.

252. M. A. Lintner, *PROJ Algorithm and Computer Programs for the Hidden Line Problem for Single Valued Surfaces*, Idaho Nuclear Corp., IN-1342 (December 1969).

ORNL-DWG 72-1713

Fig. 8. A contour plot with shaded relief produced by CR3CON and SHADED from an elevation array of 101×101 points. The width of contour lines increases with elevation in a five-element cycle.

ORNL-DWG 72-1714

Fig. 9. A perspective drawing produced by PERSPX from the same data used in Fig. 8. The near corner of this drawing corresponds to the lower left corner of Fig. 8.

We plan to combine the features of SHADED and PERSPX in a subroutine to give a shaded perspective.

Sponsor: ORNL-NSF Environmental Program

C. W. Craven, Jr.

Acquisition and Display of a Geographically Oriented Data Base for Regional Modeling

T. C. Tucker D. L. Wilson R. L. Stephenson A. H. Voelker²⁵³

We are developing techniques and computer programs for the geographically oriented portion of the data base of a regional modeling computer simulation. These data are similar to, and have the same kind of predominant source document (printed maps) as, much of the data for the study of the eastern deciduous biome undertaken by the Biome and Regional Synthesis Group of the Ecological Sciences Division. Therefore, we are working in conjunction with personnel of that project. All results to this point have applications common to both groups.

The acquisition portion of this problem requires digitization of the information contained on printed maps in pictorial form. We have chosen to represent the earth's surface by a set of "cells," subregions of the region being studied. The problem then is to assign values or codes to each cell to represent the characteristics of that cell. This is done by visual reading of the map and manual recording of the data or by photographing the map and using a line scanner to form a digital pattern on magnetic tape.

For the visual-manual technique, we have developed computer programs which draw maps of the cells in various projections and scales, using the CALCOMP plotters. These cell maps are then used as overlays when reading the source maps. These overlays are produced in less time and at less expense than were those formerly produced by draftsmen.

The Hough-Powell line scanner at the University of Pennsylvania employs a PDP-9 computer to produce digital magnetic tape from photographs of various maps. One program we have written is used to produce the reference grids and fiducial marks used in the photographs. We have written other programs to read the data tapes received from the University of Pennsylvania, to separate the digital data into map coordinate and gray levels and write a modified data tape, and to interpret the modified data and make the proper cell assignments.

To facilitate visual verification of the data base, we have written programs to plot the output of the line scanner as a reconstructed map and to draw maps from the information contained in the cell system.

Although the cells could be free-form, we believe that simulation algorithms will operate more efficiently if the cells are identical rectangles in an orthogonal coordinate system. Although the plane rectangular coordinate systems of some map projections have been used for similar projects elsewhere, we have concluded²⁵⁴ that geographical coordinates, latitude and longitude, are better for our purposes. This is so because no single plane rectangular coordinate system can represent the large areas which we are, or anticipate, studying, and the use of multiple systems, or zones, creates difficulties at the boundary between zones.

Because the source maps available and output maps desired are in various map projections, we are developing a set of subprograms which will perform the necessary conversions. These subprograms are being written with a standard nomenclature and calling sequence. This facilitates the writing of general programs which can operate with specific map projections. For example, we have written a subprogram which will produce a graticule, a system of latitude and longitude lines, in the Albers equal area, the Lambert

253. Director's Division

254. ORNL-CF-71-10-29.

conformal, or the polyconic projection, merely by naming the desired projection in the calling sequence. This subprogram is being extended to the Universal Transverse Mercator (UTM) and other map projections.

We are currently studying a number of other cartographic problems. One of these is the development of an algorithm for assignment of distinctive colors to adjacent areas on a map. Another involves conversion of data from one system of cells to another. Still another is finding and implementing an efficient method for storing and displaying geographic and political boundaries. For example, a line segment may be part of a state line, a county line, a city limit, and more. If a map containing all of these political entities is to be drawn, the relative merits of drawing this line segment only once must be weighed against the simplicity of programming which would result from drawing each entity independently.

Sponsor: ORNL-NSF Environmental Program

C. W. Craven, Jr.

ISA – Intrinsic Suitability Analysis

R. C. Durfee

We have begun a study to determine if certain statistical analysis techniques can be used with geographical data to gain a basic insight and understanding of the area in question. A test site of 10,000 acres in the Brandywine area of Pennsylvania was chosen for study since a good deal of data was readily available. A total of 47 variables had been measured for each of 10,000 cells in the area. The data involved land-use data, geology data, soils data, aspect data, and topography. We used both factor analysis and cluster analysis in analyzing the data to find underlying relationships (1) among the 47 variables and (2) among the 10,000 cells they were measured on. A factor analysis of the 47 variables resulted in 11 different factors which described the area. The first three factors, which were the most important (explained 65% of the variance), were (1) growing capability of the land, (2) flood hazard areas, and (3) residential areas. In order to see these 11 factors on the ground, we calculated factor scores for all 10,000 cells on each factor and then displayed these scores as if they were elevation data.

The cluster analysis was used to analyze one-fourth of the cells to see if meaningful clusters of these cells could be formed. The initial analysis revealed 7 to 12 different clusters, some of which were rather large. In order to identify each cluster it was necessary to calculate cluster profiles for each cluster. From these profiles we were able to see what distinguished one cluster from another. For example, one cluster represented a residential area which had been built on a flat limestone valley on poor bedrock, while another cluster represented an area of granodiorite rock covered by forest on steep stony slopes. Another cluster was made up of commercial businesses built near several streams on a flat limestone valley with poor soil drainage.

The next step in the process, which we have not done yet, is to determine which clusters are intrinsically suited for a given use and which are not. To do this we will calculate cluster scores for each cluster from their profiles, weighted perhaps to reflect the importance of one variable over another relative to the specified use. The scores will then be ranked so that the highest score represents the best cluster and the lowest is the worst. Thus if a user were wishing to locate a new factory in the area, these analyses could tell him which area was intrinsically suited for it, in terms of the variables used and the weights applied to each.

Sponsor: ORNL-NSF Environmental Program

C. W. Craven, Jr.

A Simple FORTRAN Preprocessor

R. C. Durfee

Two new features have been added to the FORTRAN language through the use of a precompilation job step. The first feature allows one or more sets of prespecified FORTRAN statements to be inserted anywhere within a FORTRAN program through the use of an INCLUDE statement. Thus the programmer has available, in a limited sense, the use of FORTRAN macros. The second feature allows any array to be variably dimensioned prior to compilation. The actual array limits are specified by the user and then inserted automatically into the COMMON or DIMENSION statements, as required. Through the use of both features, the programmer can, for example, define his variably dimensioned COMMON arrays just once and then INCLUDE them whenever necessary within later subroutines. These editing features are done by a PL/I program, FORTMAC, in the precompilation job step. A report is in preparation.

Sponsor: ORNL-NSF Environmental Program

C. W. Craven, Jr.

ORRMIS - Oak Ridge Regional Modeling Information System

R. C. Durfee

We have begun the development of an information system, ORRMIS, for the Regional Modeling Group at ORNL. The work has been divided into three phases:

1. phase 1 - development of a generalized direct-access storage-retrieval system,
2. phase 2 - development and use of a generalized record structure to support complex hierarchical data structures,
3. phase 3 - development of a user-oriented question-answer language to communicate with the information system.

The implementation of phase 1 is currently under way. We have decided to use the ADSEP Generalized Record Format²⁵⁵ in phase 2. Phase 3 has been thought about briefly, but no basic design exists yet. It is planned that the system will be used either as a stand-alone retrieval system or as an information supervisor for simulation models. The file structure is hierarchical in nature, with three levels currently supported. Thus the user may have multiple data sets within one data base and multiple data bases within the information system. The data sets may be chained together in such a way that a history of past generations may be kept. The records within each data set are accessed randomly, and their length is dynamically variable. The system has been designed so that it may be tailored at SYSGEN time or execute time to fit the user's needs (memory requirements, number of data sets, amount of table swapping, etc.).

Sponsor: ORNL-NSF Environmental Program, Regional Modeling Group

C. W. Craven, Jr.

1970 Census Data

Ruth B. Hofstra R. C. Durfee

The First Count File A and File B Census Tapes were used to obtain data relative to the East Tennessee Development District, consisting of 16 counties in the Knoxville area. A program MOD-3²⁵⁶ was used to

255. A. A. Smoks, Jr., *Adoption of Generalized Record Format*, CF-71-1-9, Oak Ridge National Laboratory (Jan. 8, 1971).

256. Programs from DUALabs, Suite 916, 1411 Jefferson Davis Highway, Arlington, Va.

obtain the listings. Much use is made of the program DDLIST²⁵⁶ to list out the Data Descriptor Codes and their meanings.

A new tape was prepared for users interested in the East Tennessee Development District. The Enumeration District totals for all the census data items, 409 in all, were written with the identifying data descriptors on a new reference data tape. This may be used for any purpose such as graphs or statistical programs. A printout was also prepared of this information for reference and checking.

Sponsor: ORNL-NSF Environmental Program, Regional Modeling

C. R. Meyers

PHYSICS DIVISION

PDP-9 Computer

G. W. Chandler

We wrote two major programs to handle future experiments for high-energy physics. One program is a General Utility program written to run on a PDP-9 interfaced with a multichannel analyzer. It calculates averages and standard deviations and writes the raw data on magnetic tape.

The other program uses a CRT display that is interfaced with a PDP-9 computer. The program collects data, displays it, and writes the raw data on DEC tape.

Sponsor: Physics Division, Fission Group

H. Schmitt

Relativistic Hartree-Fock-Slater Calculations

C. W. Nestor, Jr. T. C. Tucker T. A. Carlson²⁵⁷ F. E. Obenshain²⁵⁸

We have modified the program²⁵⁹ for the calculation of electron densities to provide either punched-card or graphical output (either pen-and-ink or microfilm) of the electron densities for selected subshells as well as for the atom as a whole. Sample plots are shown in Figs. 10 and 11.

We have used the modification of the Hartree-Fock-Slater program described previously²⁵⁹ to compute electron densities inside the nuclear volume for several isotopes of interest in Mössbauer studies.

Sponsor: Physics Division

T. A. Carlson
F. E. Obenshain

Calculation of the K X-Ray Intensities for Elements from $Z = 92$ to 126

C. C. Lu²⁶⁰ F. B. Malik²⁶¹ T. A. Carlson²⁵²

We have made calculations of the radiative transition rates for filling a K -shell vacancy from electrons in the L , M , N , O , and P shells for each element from $Z = 92$ to 126. With the help of these results and the previously calculated x-ray energies,²⁶² one may use x ray spectra arising from K vacancies of the heavy

257. Chemistry Division.

258. Physics Division.

259. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 69.

260. Now at University of Miami, Coral Gables, Fla.

261. Consultant from Indiana University, Bloomington, Ind.

262. T. A. Carlson et al., *Nucl. Phys. A* 135, 57 (1969).

FORM NO. 62-2-70.00

BY 607400 0713 ON

PL 02 11-02-71

EX. 0017 - 1.50

Fig. 10. Total electron density in a free gold atom.

FORM NO. 62-2-70.00

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EX. 0017 - 1.50

Fig. 11. Electron density in the 6s_{1/2} subshell in a free gold atom.

and superheavy elements as an unambiguous means for identifying these elements. The calculations are relativistic and use relativistic Hartree-Fock-Slater wave functions.²⁶³

We have compared our results with those of the calculations of Scofield²⁶⁴ and Bhalla²⁶⁵ and with recent experimental results²⁶⁶ for $Z = 92$ to 99. In both cases the agreement is good.

Sponsor: Physics Division

T. A. Carlson

Renormalized Finite-Nuclear Brueckner Theory

M. R. Patterson R. L. Becker²⁵⁸

The exclusion of occupied states to satisfy the Pauli principle yields so-called Pauli-corrected two-body nuclear t -matrix elements which are computed from realistic nuclear potentials. In the work previously reported²⁶⁷ the Pauli corrections were done using perturbation theory. This code has been modified to do these corrections more exactly by solving a matrix equation involving a set of t -matrix elements partitioned by parity, isospin, and total angular momentum. The results of the more exact calculation were strikingly similar to those obtained from perturbation theory; however, the code is now more general and allows for level shifts of unoccupied (particle) states. Fractional occupation probabilities were computed for the lower particle states and indicated about 1% occupancy.

The Hartree-Fock (HF) coefficients obtained by K. T. R. Davies²⁶⁸ for ^{16}O were used to superimpose single-oscillator two-body matrix elements, thus transforming the t -matrix elements to an HF space. Despite the fact that these spherical HF states are almost purely single-oscillator states, significant differences were observed in the matrix elements in the two representations. This effect is expected to be exaggerated for deformed nuclei and has spurred interest in performing deformed HF calculations.

Consequently a collaboration²⁶⁹ with R. C. Braley and W. F. Ford of NASA Lewis Research Center was begun in which ORNL furnishes the realistic t -matrix elements for deformed HF calculations. The NASA Lewis code is, however, restricted to nuclei containing an even number of nucleons. Interest in separation energies²⁷⁰ of the most weakly bound nucleon makes it desirable to do HF calculations for odd- A nuclei near closed shells, and such a code is presently being written locally.

Sponsor: Physics Division

Spiral Reader

R. D. McCulloch

Work is continuing on program development to support the Spiral Reader, a computer-controlled semiautomatic device to digitize information from bubble chamber photographs.

263. C. C. Lu et al., *At. Data* 3, 1 (1971).

264. J. H. Scofield, *Phys. Rev.* 179, 9 (1969).

265. H. R. Rosner and C. P. Bhalla, *Z. Phys.* 231, 347 (1970); C. P. Bhalla, *J. Phys.* B3, 916 (1970).

266. P. F. Dittner and C. E. Bemis, *Bull. Amer. Phys. Soc.* [II] 16, 617 (1971).

267. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 67-68.

268. R. L. Becker, K. T. R. Davies, and M. R. Patterson, *Renormalized Brueckner-Hartree-Fock Calculations of ^4He and ^{16}O with Center-of-Mass Corrections*, ORNL-4659, pp. 26-28.

269. R. C. Braley et al., "Deformed Brueckner-Hartree-Fock Calculations for Light Nuclei," *Bull. Amer. Phys. Soc.* 16, 1165 (1971).

270. R. L. Becker and M. R. Patterson, "Analogue of Koopman's Theorem on Separation Energies in the Renormalized Brueckner-Hartree-Fock Theory," *Bull. Amer. Phys. Soc.* 16, 1165 (1971); *Nucl. Phys.* (in press).

The pattern recognition and filtering program, POOH, written at LRL and rewritten at SLAC for the IBM 360/91, is now operational for the Spiral Reader at ORNL. Successful track finding and matching is accomplished in 80% of the events in a gamma exposure of the 82-in. SLAC bubble chamber filled with deuterium and in 75% of the events in π^+ exposure of the 80-in. BNL chamber filled with deuterium. Data have successfully passed through the entire processing system, which includes data logging with the Spiral Reader, filtering and track matching, spatial reconstruction, and kinematic fitting.

Test events have been measured on a conventional measuring machine and also the Spiral Reader and yield the same physics.

Sponsor: Physics Division

H. O. Cohn

REACTOR DIVISION

Use of MORSE for Calculation of Reaction Rates for a Standard Model for Comparison of Neutronics Codes

Margaret B. Emmett D. Steiner²⁷¹ S. K. Penny

We used the MORSE²⁷² Monte Carlo code and the associated SAMBO²⁷³ analysis package to calculate reaction rates in regions of ^6Li , ^7Li , and niobium and energy-dependent fluence in three media: niobium, carbon, and a mixture of ^6Li , ^7Li , and niobium. The source was isotropic, consisting of 14-MeV neutrons distributed uniformly throughout a central cylinder of 150 cm radius. The cylindrical geometry package was altered slightly to make it capable of handling a large number of media and region boundaries. Two sets of 100-group neutron cross sections were used. The results of these calculations are being compared with results from other computer programs such as ANISN in an effort to resolve a conflict between previously reported results of reaction rate calculations by having as the only variable the method of calculation. In other words, a standard blanket model was used in all these calculations.

Sponsor: Reactor Division.

D. Steiner

Finite-Element Programs for the Reactor Division

J. S. Crowell Peggy G. Fowler

Extensions and revisions have been made to the programs SAFE-3D and SAFE-CRACK.²⁷⁴ A version of SAFE-3D was submitted to the Argonne Code Center.

An evaluation study has begun on preliminary versions of two elastic-plastic-creep finite-element programs being developed for ORNL and the LMFBR industry by outside subcontractors. One of these programs, CREEP-PLAST, applies to plane and axisymmetric structures; the other program, EPACA, treats arbitrary three-dimensional thick-shell structures. It is hoped that the experience gained from this early study will help enable rapid implementation of the final versions of the programs.

Sponsor: Reactor Division

J. M. Corum

271. Reactor Division.

272. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (1970).

273. V. R. Cain, *SAMBO, a Collision Analysis Package for Monte Carlo Codes*, ORNL-CF-70-9-1 (Sept. 1, 1970).

274. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 75.

Finite-Element Analysis of Piping Elbows

J. S. Crowell

The finite-element analysis program SHELL,²⁷⁵ originally written at the University of California (Berkeley), has been rewritten and tested. The program is suitable for the static analysis of thin shells of arbitrary geometry. The program is being used to obtain analytical results for comparison with experimental data collected from four machined-elbow models.²⁷⁶ These models are designed and instrumented to study the effects of controlled geometry variations (ovaling and wall thinning) in piping elbows. Extensions to the program will enable parametric studies of machined-elbow models to be easily conducted.

Sponsor: Reactor Division

S. E. Moore

Documentation of a Cost Effectiveness Procedure for Desalination Projects

R. A. Carter²⁷⁷ G. W. Westley W. G. Fort²⁷⁸ J. V. Wilson S. Moore²⁷⁸

The effort over the past several years²⁷⁹ toward developing a procedure for estimating the cost effective indices for various desalting development proposals has been partially documented in report form.^{280,281} The report consists of six volumes, of which two will be issued in the near future. The remaining four volumes will be released at a later date.

Sponsor: Reactor Division (OSW Contract)

I. Spiewak

Mass Transfer to Circulating Bubbles

C. W. Nestor, Jr. T. S. Kress²⁸²

The concentration of a material in a fluid field surrounding a spherical bubble can be described by the parabolic partial differential equation

$$\frac{\partial \theta_*}{\partial t_*} = \alpha \left(\frac{\partial^2 \theta_*}{\partial r_*^2} + \frac{2}{r_*} \frac{\partial \theta_*}{\partial r_*} \right), \quad (1)$$

where

$$\theta_* = \theta / \theta_0,$$

θ = concentration,

θ_0 = bulk fluid concentration,

275. C. P. Johnson and P. G. Smith, *A Computer Program for the Analysis of Thin Shells*, report No. 69-5, University of California, Department of Civil Engineering (January 1969).

276. *Program Plan for the ORNL Piping Program*, pp. 4.2.1, 4.2.2.

277. Computing Technology Center.

278. Oak Ridge Gaseous Diffusion Plant.

279. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 73.

280. R. A. Carter and G. W. Westley, *Computer Code for OSW Program Analysis, Part I: ECON 21: A FORTRAN Code for the Calculation of Cost Effectiveness Index and Accumulated Benefits Evaluations to Improvements of Desalination Processes*, ORNL-TM-3535.

281. W. G. Fort et al., *Computer Code for OSW Program Analysis, Part II: Program Listing for Code ECON 21*, ORNL-TM-3535.

282. Reactor Division.

$$r_* = r/d,$$

r = distance from center of bubble,

d = bubble diameter,

$$t_* = tV/d,$$

t = time,

V = bulk fluid velocity,

α = normalized diffusivity.

We assume that the diffusivity α is the sum of a constant contribution from the molecular diffusivity and a varying contribution from the eddy diffusivity, which we assume to be a function of the Reynolds number and Schmidt number characteristic of the bulk fluid and of distance from the bubble interface.

At the initial contact between the fluid and the bubble, we assume that there is no material inside the bubble and that the fluid concentration is uniform. We also assume that the normalized concentration just inside the bubble remains zero and that the slope of the concentration vanishes at an outer normalized radius given by

$$r_{*e} = \frac{1}{2} \left(1 + \frac{Q_L}{0.73Q_G} \right)^{1/3},$$

where Q_L and Q_G are the flow rates of liquid and gas respectively. Our boundary conditions are then:

$$\theta_* \left(\frac{1}{2}, t \right) = 0, \quad (2)$$

$$\left. \frac{\partial \theta_*}{\partial r_*} \right|_{r_* = r_{*e}} = 0, \quad (3)$$

and the initial condition is

$$\theta_*(r_*, 0) = 1. \quad (4)$$

We define an average normalized concentration in the fluid as

$$\bar{\theta}_*(t) = \int_{1/2}^{r_{*e}} r_*^2 \theta_* dr_* / \int_{1/2}^{r_{*e}} r_*^2 dr_*; \quad (5)$$

and the Sherwood number is

$$N_{Sh}(t) = \frac{\partial \theta_*/\partial r_*|_{r_* = 1/2}}{\bar{\theta}_*(t)}, \quad (6)$$

and a time-averaged Sherwood number

$$\bar{N}_{Sh} = \frac{1}{T} \int_0^T N_{Sh}(t) dt. \quad (7)$$

We wrote a computer program to calculate approximate solutions of Eq. (1) using the Crank-Nicholson method²⁸³ and to compute the Sherwood number and the time-averaged Sherwood number. With the initial condition as stated in Eq. (4), the Sherwood number is infinite at the initial contact of the bubble with the fluid; however, we were able to show that the Sherwood number is very nearly of the form

$$Sh(t) \cong Sh_{\infty} + Bt^{-1/2} e^{-ct}. \quad (8)$$

To do the integration required in Eq. (7), we developed a quadrature formula assuming that the Sherwood number can be represented over two adjacent time steps by an expression of the form

$$f(t) = t^{-1/2} (a + bt^{1/2} + ct^2),$$

so that

$$\int_{t_j}^{t_{j+2}} f(\tau) d\tau = w_j f(t_j) + w_{j+1} f(t_{j+1}) + w_{j+2} f(t_{j+2})$$

with weights

$$w_j = t_j^{1/2}(t_{j+2}^{1/2} - t_j^{1/2}) \left(t_{j+1}^{1/2} - \frac{1}{3}t_{j+2}^{1/2} - \frac{2}{3}t_j^{1/2} \right) / (t_{j+1}^{1/2} - t_j^{1/2}),$$

$$w_{j+1} = t_{j+1}^{1/2}(t_{j+2}^{1/2} - t_j^{1/2})^3 / 3(t_{j+1}^{1/2} - t_j^{1/2})(t_{j+2}^{1/2} - t_{j+1}^{1/2}),$$

$$w_{j+2} = t_{j+2}^{1/2}(t_{j+2}^{1/2} - t_j^{1/2}) \left(\frac{2}{3}t_{j+2}^{1/2} - t_{j+1}^{1/2} + \frac{1}{3}t_j^{1/2} \right) / (t_{j+2}^{1/2} - t_{j+1}^{1/2}).$$

With $t_1 = 0$, integration over the first two time steps requires a special formula, which can be derived from the assumption that $t^{1/2} f(t)$ is parabolic in $t^{1/2}$ for $0 \leq t \leq t_4$.

We estimated values for Sh_{∞} in Eq. (8) by using Wynn's²⁸⁴ epsilon algorithm with values for the Sherwood number from the last ten time steps in a calculation. We found that for fixed bubble diameter and Schmidt number, Sh_{∞} was not a function of Reynolds number, in agreement with analytical results obtained assuming a constant diffusivity. The constant c in Eq. (8) decreased with increasing Reynolds number, also in agreement with the analytical results.

Sponsor: Reactor Division

T. S. Kress

283. J. Crank and P. Nicholson, "A Practical Method for Numerical Evaluation of Solutions of Partial Differential Equations of the Heat-Conduction Type," *Proc. Cambridge Phil. Soc.* 43, 50 (1947).

284. H. C. Thacher, Jr., "Algorithm 215," *Comm. Ass. Comput. Mech.* 6, 662 (1963).

Gas Behavior in Molten-Salt Reactors

T. C. Tucker L. W. Gilley H. A. McLain²⁸⁵

We revised and expanded the program²⁸⁵ to describe the behavior of inert gas bubbles in the circulating salt loop of a molten-salt reactor. Both mass transfer correlations and salt loop configurations were changed, as we had anticipated.

We are now writing a program for the calculation of xenon and tritium concentrations throughout the reactor.

Sponsor: Reactor Division

Fission Product Diffusion Code

C. C. Webster

The diffusion code FIPER-Q developed by GGA had been adapted to ORNL's IBM 360 computer. It has been used to simulate experimental runs wherein cesium (representing volatile fission products) diffused through the wall of a graphite cylinder. Many possible parameters and equipment dimensions were used to evaluate the best choice of parameters and dimensions to use for the experiments which simulated the diffusion of radioactive cesium through the graphite walls of gas-cooled reactor fuel assemblies.

Sponsor: Reactor Division

M. D. Silverman

Energy Suppression and Fission Product Transport in Pressure-Suppression Pools

C. C. Webster L. E. Stanford²⁸⁶

A final report (ORNL-TM-3448) was prepared which describes experimental work performed, when in the Operations Division, to evaluate the dissipation of energy (in the form of steam) into a pool of water in the event of a double-ended pipe rupture with a BWR power reactor. The computer code ORDEAL was used to determine a mathematical relationship showing the effect of bulk water temperature on the length of steam jet in water.

The ability of the water in the pool to retain the fission product iodine was investigated within the capabilities of the experimental equipment. The data from the experimental program were not sufficient for complete mathematical modeling of the results as observed.

Sponsor: Reactor Division

T. H. Row

Analytical Model of a Tube-in-Tube Molten-Salt-Heated Supercritical Steam Generator

D. E. Arnurius J. A. Carpenter R. E. Helms²⁸⁷

We have written a computer program to determine the heat transfer and the temperature profiles for a tube-in-tube steam generator section.²⁸⁷ The program evaluates an analytical model based on known heat

285. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 86.

286. Now with Tennessee Valley Authority.

287. D. E. Arnurius and R. E. Helms, *Analytical Model of a Tube-in-Tube, Molten Salt Heated, Supercritical Steam Generator*, ORNL-TM-3673 (to be published).

transfer correlations supplied by personnel of the Molten Salt Reactor Project. In the generator, fresh water/steam flows in the inner cylinder in one direction and salt flows in the annulus countercurrent to the steam flow. The boundary conditions are given as (1) the inlet fresh water temperature, (2) the outlet salt temperature, and (3) the inlet fresh water pressure.

Approximate temperature profiles for the water, the salt, and the inside wall of the inner tube are obtained at discrete points along the axis of the section.

The steam properties required in the heat transfer correlations are obtained with the subroutine package STEAM.²⁸⁸

Sponsor: Reactor Division (Molten Salt Reactor Project)

R. E. Helms

The Molten-Salt Reactor Information System

Ruth B. Hofstra J. A. Carpenter

An up-to-date and accessible file of abstracts of documents dealing with all aspects of molten-salt reactor technology is being assembled and maintained at Oak Ridge National Laboratory.²⁸⁹ The MSR Information System is to include any kind of document that is made available to the public.

We have helped in developing this information system by processing the references.

The MSRIS references have been arranged in order of accession number, and an update correction procedure has been developed. Publication printouts were made of the whole file, with key-word index, personal author index, and category index.²⁹⁰ The file has been converted to the ADSEP format and may be used with ORLOOK as well as other programs.

Sponsor: Reactor Division

D. W. Cardwell

SCID Code, for Conversion of Flux from CITATION to Source for DOT

O. W. Hermann J. D. Jenkins²⁹¹

The SCID code^{292,293} was designed to convert the final flux computed by the CITATION code²⁹⁴ to a source flux for use in the DOT code.²⁹⁵ In general, SCID starts with the *M*-group-flux tape generated, at specified mesh points, by diffusion theory and constructs a fixed source flux at a desired boundary within the mesh; the new source flux is incorporated into a reconstructed mesh and also is restructured to fit a finer *N*-group-flux required in the transport calculation. The SCID code contains about 600 FORTRAN statements and executes in less than 500K on the IBM/360 computer.

288. D. W. Altom, *Steam Properties*, ORNL-CF-69-6-52 (June 26, 1969).

289. P. N. Haubenreich and D. W. Cardwell, *The Molten-Salt Reactor Information System*, ORNL-TM- (partially completed draft).

290. D. W. Cardwell and P. N. Haubenreich, *Indexed Abstracts of Selected References on Molten-Salt Reactor Technology*, ORNL-TM-3595 (in press).

291. Reactor Division.

292. Acronym for Source Flux Produced from CITATION for Input to DOT.

293. J. D. Jenkins and O. W. Hermann, *A Code for Converting Flux Computed by CITATION Code to Source Flux for Direct Use in DOT Code* (to be published).

294. T. B. Fowler and D. R. Vondy, *Nuclear Reactor Core Analysis Code: CITATION*, ORNL-TM-2496 (1969).

295. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

The code performs three primary functions: (1) it determines the source flux in terms of the CITATION group structure, (2) it restructures the flux into groups desired in the execution of DOT, and (3) it provides punched cards for the distributed fixed source array for use in DOT.

The CITATION-SCID-DOT procedure was found applicable to power distribution determinations within an experimental capsule in the reflector of the ORR reactor. This method should greatly enhance studies of this type.

Sponsor: Reactor Division

J. D. Jenkins

Use of Thermal-Neutron Scattering Law in Monte Carlo Calculations

G. W. Morrison L. M. Petrie R. S. Carismuth^{2,9,1}

A new technique for sampling from the double-differential cross section at thermal energies has been implemented in Monte Carlo calculations of thermal-neutron spectra in various materials. This technique minimizes the required computer storage and is quite fast for picking the scattered neutron energy and scattering angle. Unlike other thermal kernels, which approximate the chemical binding effects of the moderator molecules, this technique uses scattering law data for the moderator materials that depend only on the structure and dynamics of the scatterer.

For a single scattering species, Egelstaff^{2,9,6} has shown that the double-differential cross section is related to the scattering law by the relation

$$d^2\sigma(E_f, \Omega|E_i)/(d\Omega dE_f) = [\sigma_b/(4\pi kT)] (E_f/E_i)^{1/2} [\exp(-\beta/2)] \times S(\alpha, \beta), \quad (1)$$

where E_i and E_f are the initial and final neutron energies for scattering into an element of solid angle $d\Omega$ through an angle θ , T is the absolute temperature, k is Boltzmann's constant, and $S(\alpha, \beta)$ is the scattering law for the particular scatterer, expressed in terms of the dimensionless quantities α and β , where

α = dimensionless momentum exchange

$$= E_i + E_f - 2\mu(E_i E_f)^{1/2}/(AkT), \quad (2)$$

β = dimensionless energy exchange

$$= E_f - E_i/(kT), \quad (3)$$

and σ_b is the bound-atom cross section, which is related to the free-atom cross section, σ_f , by the relation

$$\sigma_b = [(A + 1)^2/A^2] \sigma_f, \quad (4)$$

A being the ratio of the scatterer mass to the mass of the neutron.

For sampling in the Monte Carlo code, it is necessary to integrate Eq. (1) over E_f and Ω to form the conditional distribution functions. Because of numerical instabilities in integrating Eq. (1) over E and Ω space, it is advantageous to transform to α and β space. This gives

$$d^2\sigma(\alpha, \beta|E_i)/(d\alpha d\beta) = [A\sigma_b kT/(4E_i)] [\exp(-\beta/2)] S(\alpha, \beta). \quad (5)$$

Fig. 12. Infinite-medium neutron spectrum in borated carbon.

In principle, sampling Eq. (5) for α and β is straightforward. At each energy, E_i , an integration over α and β must be performed. However, this results in extremely large data tables, which must be stored in the computer memory during the calculation. Bischoff²⁹⁷ has attempted to solve this problem by precomputing some of the integrals and calculating the remainder at execution time. This often results in long running times.

In this work, generalized Gaussian quadrature²⁹⁸ was used to integrate Eq. (5). This type of integration results in finding a discrete distribution, ω_i , having its first $2n$ moments identical to those of the original distribution. That is, given $\omega(x)$, $a \leq x \leq b$, such that $\omega(x) \geq 0$, then determine $\{x_i, \omega_i\}$ for $i = 1, n$ such that

$$\int_a^b f(x) \omega(x) dx = \sum_{i=1}^n f(x_i) \cdot \omega_i$$

holds for all $f(x)$, where $f(x)$ is a polynomial of degree $2n - 1$ or less.

The sampling scheme then follows by replacing the continuous conditional distributions $f(\beta|E)$ and $f(\alpha|\beta, E)$ with the discrete distributions $\omega(\beta_i, E)$ and $\chi(\alpha_j|\beta_i, E)$. Standard Monte Carlo sampling techniques may then be used to pick β_i and α_j . The scattered energy E_f and cosine of the scattering angle μ are then determined by use of Eqs. (2) and (3).

The above procedure has been implemented in a Monte Carlo neutron transport code. Figure 12 shows the Monte Carlo calculated thermal spectra obtained with the $S(\alpha, \beta)$ data for a mass 12 free gas and the results of a numerical integration of the transfer probability matrix for the infinite medium fluence.²⁹⁹

297. F. A. Bischoff, unpublished Ph.D. thesis, Rensselaer Polytechnic Institute, Troy, N.Y., 1969.

298. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (September 1970).

299. M. E. Tsargaris, *AGS - 7090 Computer Program for the Calculation of Average Group Cross Sections*, ORNL-TM-512 (February 1963).

The close agreement between the Monte Carlo and the analytic results demonstrates the adequacy of replacing a continuous distribution function by the discrete set of energy and momentum changes. Similar agreement has also been observed in the comparison of experimental data³⁰⁰ in finite geometries with calculations using this technique.

Sponsor: Reactor Division

Updating of the GAM-II and 100-Group XSDRN Cross-Section Libraries

R. Q. Wright

Ten materials in the ENDF/B³⁰¹ version III (preliminary) library have been processed by SUPERTOG,³⁰² and the GAM-II³⁰³ and XSDRN³⁰⁴ libraries have been updated. Materials with resonance parameters appear on these libraries in two forms, once as an infinite dilution nuclide and also as a resonance nuclide requiring an additional resonance calculation.

Transmission of data from ENDF/B to GAM-II and XSDRN has been described previously.³⁰⁵

Since the ENDF/B version III data are preliminary and not officially released by CSEWG,³⁰⁶ the complete processing of ENDF/B-III data will be delayed until the data are officially released.

Sponsor: Reactor Division

J. D. Jenkins

Monte Carlo Analysis of the Exact Geometric Mockup of ZPR-III Assembly 48³⁰⁷

S. N. Cramer

The ZPR-III Assembly 48 has been described in full geometric detail in a series of Monte Carlo eigenvalue calculations using the ESP code.³⁰⁸ An array version of the generalized geometry package and the many "fine group" energy structure of this code combine to allow a direct application of the "fictitious scattering" transport model to this calculation. Use of this model provides rapid evaluation of the neutron trajectories across the many thin plates of the assembly core. However, the explicit description of each plate type creates difficulty in establishing the correct weighting functions in the resonance energy cross-section calculations. For this reason, special attention has been given to the unresolved resonance cross-section evaluation for ²³⁹Pu and ²³⁸U. This geometric and cross-section detail, together with the modified ENDF/B II data, gives a value of $k_{\text{eff}} = 0.997 \pm 0.005$ for the assembly.

Sponsor: Reactor Division

300. J. R. Beyster et al., *Experimental and Theoretical Neutron Spectra*, GA-5319 (May 1964).

301. H. C. Honeck, *ENDF/B - Specifications for an Evaluated Nuclear Data File for Reactor Applications*, BNL-50066 (ENDF-102) (May 1966) (revised July 1967).

302. R. Q. Wright et al., *SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B*, ORNL-TM-2679 (1969).

303. G. D. Jounou and J. S. Dudek, *GAM-II: A B_3 Code for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants*, GA-4265 (1963).

304. N. M. Greene and C. W. Craven, Jr., *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

305. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 77.

306. Cross Section Evaluation Working Group of the National Neutron Cross Section Center at Brookhaven National Laboratory.

307. Abstract of ORNL-TM-3596.

308. S. N. Cramer et al., *ESP - a General Monte Carlo Reactor Analysis Code*, ORNL-TM-3164 (to be published).

ESP – a General Monte Carlo Reactor Analysis Code

S. N. Cramer G. W. Morrison J. L. Lucius

Development and application of the ESP code³⁰⁹ has continued with respect to:

1. analysis of the ZPR-III Assembly 48 and heterogeneity effects of various models of the reactor drawers using the fictitious scattering model and array geometry,^{309,310}
2. inclusion of the thermal-neutron scattering kernel [ENDF/B $S(\alpha, \beta)$ data] based on the work described in refs. 311 and 312,
3. modification of the code to handle ENDF/B version II and III data and all secondary energy distributions,
4. creation of an option to input energy-dependent resonance cross-section weighting functions for those cases where the automatic calculation of these functions by the code is not sufficient,
5. creation of an option to treat multiplying media with external sources present.

Sponsor: Reactor Division

M. L. Tobias

Monte Carlo Analysis of Heterogeneity Effects in ZPR-III Assembly 48

S. N. Cramer M. L. Tobias³¹³

Heterogeneity effects in ZPR-III Assembly 48 have been investigated with respect to three mockups of a standard core drawer – one-, two-, and three-dimensional models. These calculations were performed using the fictitious scattering and array geometry version of the ESP code.^{309,310} This work was done as a support study for more extensive diffusion and discrete-ordinate calculations on heterogeneity effects in fast reactors.³¹⁴ A summary of the Monte Carlo work appears in ref. 314.

Sponsor: Reactor Division

Reactor Division Cooperative Code Development – Implementation of the FUMBLE Code

G. W. Cunningham D. R. Vondy³¹⁵

In order to better understand the problems of computer code exchange between installations, the code FUMBLE³¹⁵ was obtained from General Electric. This code was written for the GE-635 computer. Several problem areas arose when the code was first compiled:

309. S. N. Cramer and M. L. Tobias, *Monte Carlo Analysis of Heterogeneity Effects in ZPR-III Assembly 48* (this report).

310. S. N. Cramer, *Monte Carlo Analysis of the Exact Geometric Mockup of ZPR-III Assembly 48*, ORNL-TM-3596 (October 1971).

311. G. W. Morrison, L. M. Petrie, and R. S. Carlsmith, "Use of Thermal-Neutron Scattering Law in Monte Carlo Calculations," *Trans. Amer. Nucl. Soc.* 14(2), 827 (October 1971).

312. L. M. Petrie and G. W. Morrison, "Calculations of Several ²³⁸U Thermal Systems by Monte Carlo Using ENDF/B Material 103," *Trans. Amer. Nucl. Soc.* 14(2), 827–28 (October 1971).

313. Reactor Division.

314. E. M. Page et al., *Comparison and Analysis of Methods for Determining Heterogeneity Effects in Fast Critical Assemblies and Reactors*, APDA-269 (June 1971).

315. P. Greebler and C. L. Cowan, *FUMBLE: An Approach to Fast Power Reactor Fuel Management and Burnup Calculations*, GEAP-13599 (November 1970).

1. The maximum number of arguments in a CALL statement exceeded 196.
2. The maximum number of arguments in unique parameter lists in an entire program exceeded 1024.
3. DATA statements contained implied DO's.
4. Data initialization with octal constants.
5. EQUIVALENCE statements involving arrays did not indicate a subscript.

These problems were easily removed with the exception of the octal constants. The input routines were written for semi-free form input [the first 20 columns on a card were fixed format, and the last 60 columns were variable format on the basis of a 36-bit (six-character) word]. After careful study of the programming, it was found that, with relatively few changes, the routines could be converted to our 32-bit (four-character) word.

Additional problem areas arose when trying to execute the program. These included:

1. Data arrays were not initialized (they assumed zero at the start).
2. Literal data were stored six characters per word.
3. An array passed through a subroutine to another was not dimensioned in the intermediate subroutine.
4. The value of a DO variable was tested after completing the range of the DO statement in several places.
5. The sample data provided did not match the sample output.

The code has been implemented on the IBM 360 but would not, in its present form, be usable on the originator's GE-635.

Sponsor: Reactor Division

CITATION Code Development

G. W. Cunningham T. B. Fowler³¹³ D. R. Vondy³¹³

The development effort on CITATION³¹⁶ has been continuing in several areas. These include:

1. The diffusion-theory treatment was extended to cover triangular geometry in both two and three dimensions.
2. Both 90 and 180° rotational symmetry have been implemented in slab geometry. These rotational symmetry conditions are special in that the derivative of the flux is not zero but rather there is coupling between boundary points which are not adjacent.
3. The criticality search procedure was extended to allow searches on physical dimensions using the indirect-search technique. The technique permits region thicknesses in any or all directions to change — some increasing and others decreasing.
4. Capability to move control rods on a prescribed schedule during depletion has been implemented.
5. Provision has been made to generate few-group zone macroscopic cross sections for later input to the code.
6. The use of microscopic cross sections has been extended to treat the (n,2n) reaction differently and to account for cross-section dependence on the local nuclide concentration.

316. T. B. Fowler, D. R. Vondy, and G. W. Cunningham, *Nuclear Reactor Core Analysis Code: CITATION*, ORNL-TM-2496, Rev. 2 (July 1971).

7. The auxiliary cross-section processing code has now been incorporated directly into CITATION to allow cross-section input from cards and modification of data at run time.

8. Considerable effort has gone into changing the code so as to make it more easily adaptable to users on other types of computers.

9. The fuel management has been extended to iterate on each cycle to obtain some desired end-of-cycle condition, for example, k -effective or exposure time. Also, the capability to establish quasi equilibrium has been added.

Sponsor: Reactor Division

CASDAR Program

G. W. Cunningham J. D. Jenkins³¹³

The CASDAR (Cross Section and Spectrum Direct Access Retrieval) program is being written to gather one-dimensional cross sections [absorption, fission, (n , α), etc.] and spectra (or flux) from various sources, put them in a standard form, and store them in direct access files for later recovery. The user will then be able to call upon selected data and perform various operations (calculate, plot, edit, punch, update, or replace). The program is still in its infancy and currently will not perform all the operations indicated.

Sponsor: Reactor Division

Cell-in-a-Cell Resolved Resonance Treatments

N. M. Greene J. L. Lucius
G. W. Ragan³¹³ O. L. Smith³¹³
W. R. Cobb, Jr.³¹⁷

Several methods³¹⁸⁻³²⁰ have been used for calculating effective resonance integrals for the situation where very tiny fuel grains (or plates) are bundled along with moderating material into so-called fuel elements. Most of these methods use analytic approaches for calculating the term denoted "grain shielding factor" used to "cell average" cross sections that are used in rigorous resonance calculations of the actual reactor. In the reactor system the fuel elements are homogenized.

A method has been developed within the framework of the XSDRN³²¹ program for performing a calculation of this type using the Nordheim³²² integral treatment for both the "grain shielding factor" calculation and for the final "rod" calculation. The self-shielding required on the cross sections for the second case has been automated so that the entire calculation is done in one pass. A significant modification to the original Nordheim treatment was made to allow both a "lump" and a "moderator" flux to be determined.

Present work involves setting up and running involved test cases to check the method.

Sponsor: Reactor Division

317. Formerly with Reactor Division; presently with Nuclear Fuel Services, Inc., Gaithersburg, Md.

318. P. Walte, *Evaluation of Grain Shielding Factors for HTGR Coated Fuel Particles*, GAMD-10134 (May 1970).

319. M. W. Dyos and G. C. Pomraning, *Nucl. Sci. Eng.* 25, 8 (1966).

320. R. K. Lane, L. W. Nordheim, and J. B. Sampson, *Nucl. Sci. Eng.* 14, 390 (1962).

321. N. M. Greene and C. W. Craven, Jr., *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

322. L. W. Nordheim, "The Theory of Resonance Absorption," in *Symp. Appl. Math.* XI (1961).

SOLID STATE DIVISION

A Computer System for Controlling an Autocorrelation Neutron Time-of-Flight Spectrometer

Sandra H. Merriman

Further additions and refinements have been made to the library of programs which controls a TOF spectrometer used for neutron inelastic scattering research.³²³

We mentioned in an earlier report³²³ that this spectrometer utilizes a magnetic pulser which modulates the incoming neutron beam intensity in a pseudorandom way. We have completed a program which calculates the TOF spectrum as the cross-correlation of this modulating signal and the detector output. A background program displays all or part of the spectrum, allowing the experimenter to make decisions on further progress of the experiment. Another program allows him to add or average chosen spectra and to make statistical analyses of them. Since further classification, reduction, and inspection of the TOF data are limited by the confines of the PDP 15/30, we have written an IBM 360 program to perform these functions.

Sponsor: Solid State Division

H. A. Mook

Computer Control and Data Acquisition Routines for a Neutron Time-of-Flight Spectrometer

L. W. Gilley

Work has been completed³²⁴ on routines to control experimental apparatus and collect data in scan mode for a neutron time-of-flight spectrometer reported on previously.³²⁵ Various experimental parameters such as detector location, pulsing crystal orientation, sample orientation, etc., can be varied by Teletype command input or under computer control. Data are collected in scan (field survey) mode and printed out on the Teletype.

Sponsor: Solid State Division

H. A. Mook

THERMONUCLEAR DIVISION

RCONTR - Contour Plotting Program

P. R. Coleman

A contour plotting program for unequal mesh spacing has been written to utilize the ORGRAPH package.³²⁶ It was adapted from a similar routine³²⁷ written at Lawrence Livermore Laboratory. An attractive feature is its simple calling sequence.

Sponsor: Thermonuclear Division

Glen Haste

323. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 90.

324. L. W. Gilley, *Setup and Control Routines for a Pulsed Neutron Time-of-Flight Spectrometer*, ORNL-TM-3683 (January 1972).

325. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 90.

326. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 29.

327. Fred Fritsch, *Contour Plotting Routines*, CIC report N2.3-003, Lawrence Livermore Laboratory, Livermore, Calif. (May 25, 1966).

Polarization Effect on Autoionization Rates of H_2

M. R. Patterson F. R. Coleman A. Russek³²⁸

Energy correction terms for the hydrogen molecular ion H_2^+ have been computed using the exact electronic states of Bates, Ledsham, and Stewart³²⁹ by a combination of Legendre-Gauss, Laguerre-Gauss, and Newton-Cotes numerical integrations. These terms were incorporated as polarization-effect correction terms to autoionization rates of H_2^+ previously computed³³⁰ and are being used in ion source studies by C. F. Barnett.

Sponsor: Thermonuclear Division

C. F. Barnett

Complex Exponential Integral

Gregory S. McNeilly

The complex exponential integral

$$E_1(z) = \int_z^\infty (e^{-t}/t) dt, \quad |\arg z| < \pi,$$

is evaluated for complex z with either a series expansion, continued fraction, or asymptotic expansion.³³¹ The appropriate choice used by the program EXPINT is determined by the value of z . The program can be generalized in a straightforward manner to the case $F_n(z)$.

Sponsor: Thermonuclear Division

Charged Particle Trajectories

R. H. Fowler J. F. Clarke³³²

A computer code is being developed to calculate ion orbits in a Tokamak environment by numerical integration of the guiding center equations of motion.

Sponsor: Thermonuclear Division

J. F. Clarke

Fast Ion and Plasma Ion Distributions in Tokamak Plasmas

R. H. Fowler J. F. Clarke³³² Julius Smith³³³

The kinetic equation³³⁴ has been solved numerically to investigate the effect of the electric field on the slowing down of fast ions in Tokamak plasmas. The computer code calculates the fast ion velocity

328. Consultant to Thermonuclear Division, University of Connecticut, Storrs, Conn.

329. M. R. Patterson and R. L. Becker, *Non-Adiabaticity Corrections to the Born-Oppenheimer Approximation with Calculations for Mesic and Electronic Hydrogen Molecular Ions*, ORNL-TM-1850 (August 1967).

330. A. Russek, M. R. Patterson, and R. L. Becker, "Auto-ionization in Molecular Systems," *Phys. Rev.* 167, 17-25 (1968).

331. Milton Abramowitz and Irene A. Stegun, p. 227 in *Handbook of Mathematical Functions*, U.S. Government Printing Office, Washington, D.C., 1965.

332. Thermonuclear Division.

333. Consultant, University of Tennessee.

334. B. A. Trubnikov, *Rev. Plasma Phys.* 1, 105 (1965).

distribution for plasmas with unequal ion and electron temperatures. The situations which have been investigated are as follows: (1) the case of injection heating with neutral beams of 30, 50, and 100 keV; (2) the case of energetic (200 keV) tritium injected into a deuterium plasma; and (3) the case of 3.5-MeV alpha particles produced from fusion reactions slowing down in the plasma. These cases have been studied for a range of electric fields and plasma temperatures. The results³³⁵ indicate that with reasonable electric fields the fast ion distribution is significantly altered and the mean density, current, kinetic energy, and, where applicable, fusion reaction rate are increased.

The calculations of the fast ion distribution have been modified in order to treat the plasma ion distribution. The deviation from a Maxwellian distribution for a nonisothermal plasma is taken into account for the unperturbed distribution ($\mathcal{E} = 0$). The effect of the electric field on the plasma ion distribution is being investigated.

These calculations are in support of the ORMAK experiments being conducted by the Thermonuclear Division.

Sponsor: Thermonuclear Division

J. F. Clarke

INTERDIVISIONAL PROJECTS

CENTERS: A Computer Program to Determine the Distribution of Populations in Several Arbitrary Central Circular Regions Given the Locations of the Centroids of Population Districts

A. A. Brooks P. R. Coleman

A program has been written to determine the distribution of populations about several arbitrary central circular regions given the locations of the centroids of population districts. It produces summary tables of population and housing units for arbitrary annuli and sectors. The population lying in multiple central regions is also tallied. It also produces a file of centroids and their direction and bearing from the arbitrary locations of central sites. It also furnishes a list of centroids sorted by site, annulus, and sector.

Using the Census Medlist tapes (1970), the program has been used to study reactor siting and other siting problems.

Sponsor: Mathematics Division and Directors Division

Information Retrieval for Tree-Structured Data

P. R. Coleman

A program has been completed^{336,337} to extract the "family tree" of a node from a general directed graph. Data can also be associated with each node in the graph and thus can be retrieved along with the tree.

³³⁵. A preliminary account of this work has been given by J. F. Clarke and R. H. Fowler, *Bull. Amer. Phys. Soc.* 16, 1261 (1971).

³³⁶. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 107.

³³⁷. P. R. Coleman, *TRACE - an Information Retrieval Program for Tree-Structured Data*, ORNL-4709 (October 1971).

Work is now in progress to link the capabilities of this program with an ADSEP – Automated Data Set Edit Program^{338,339} -- data base.

Sponsors: Y-12 Metallurgical Development Department and
ORNL Mathematics Division

Trygve Myhre

Perspective Plotting and Contour Plotting

Peggy G. Fowler J. S. Crowell

A program has been written to produce three-dimensional perspective plots of finite-element shell surfaces viewed from any point in space. The program will also produce plots of contour values on the surfaces.

Two contour-plot programs, HOLES³⁴⁰ and CNTUR, have been used as building blocks to aid in writing plotting programs for displaying neutron density in a reactor, stresses arising from finite-element analyses, and temperatures calculated in two- and three-dimensional heat transfer analyses of the National Radioactive Waste Repository.

Sponsors: Reactor Division
Chemical Technology Division

S. E. Moore
J. P. Sanders
R. D. Cheverton

DEXTR³⁴¹ Data Reduction Programs

O. W. Russ, Jr.

Programs for SolGel-2 and -3 and UN-3 fuel capsule experiments in the ORR were further expanded to include fuel capsules UN-4, -5, and -6. The reduced data were optionally punched into cards or written on magnetic tape for input to statistical analysis programs³⁴² or printed and Calcomp-plotted. Programs were completed for ORTC-4, a high-temperature thermocouple test in the ORR, covering two reactor startup and shutdown cycles. The reduced data were printed and Calcomp-plotted on optionally variable time scales for short or long time periods of interest. Programming was begun for the MINT-1 fuel capsule experiment in the ORR to investigate fuel-cladding mechanical interaction under irradiation. Reduced data will be printed and punched into cards daily, and major parameters vs irradiation time will be Calcomp-plotted monthly.

Programs for the HTGR HRB-2 fuel capsule experiment in the HFIR were completed for printing and Calcomp-plotting of the reduced data. Additional programming will be required for the HRB-3 experiment when it is installed in the HFIR.

Programs for the MSRP FCL-1 experiment in Building 9201-3 at Y-12 were completed, and new programming for FCL-2 for printing and Calcomp-plotting of temperatures throughout the loop was completed and added to the daily computer run. Programs for the LMFBR Failed Fuel Mockup (FFM)

338. A. A. Brooks, *ADSEP, an Automated Data Set Edit Program*, CTC-34 (May 1 1970).

339. *Math. Div. Annu. Prog. Rep. Dec. 31, 1970*, ORNL-4661, pp. 99-100.

340. G. W. Westley and J. A. Watts, *The Computing Technology Center Numerical Analysis Library*, CTC-39, pp. 448-62 (Oct. 6, 1970).

341. *Math. Div. Annu. Prog. Rep. Dec. 31, 1970*, ORNL-4661, p. 21; *Instrumentation and Controls Division Annual Progress Reports, 1965 through 1971*.

342. Written by Claudia S. Lever and F. L. Miller, Jr., of the Mathematical Statistics Department of the Mathematics Division.

experiment in Building 9201-3 at Y-12 were completed to print and optionally punch the reduced data and to CRT-plot temperatures at 2-in. intervals along the heated test section and pressure drop vs flows at various test conditions. Additional programming will be required for a larger, more fully instrumented tube bundle currently being installed.

Sponsors: Reactor Division

P. A. Gnad
W. R. Huntley
B. H. Montgomery
L. F. Parsly
R. L. Senn
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Metals and Ceramics Division

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Instrumentation and Controls Division

R. M. Burnett
R. F. Hyland
R. L. Shepard

Use of MT/ST Tapes for Data Input

Ruth B. Hofstra

Programs are available to process Magnetic Tape Selectric Typewriter (MT/ST) tapes for data input to the computer.

Text that was originally typed on an MT/ST produces a magnetic tape. This tape is converted to a computer magnetic tape by a Digidata converter. Various other conversions are made, including use of a modification of a program RSICMTST written originally by the Computing Technology Center for the Radiation Shielding Information Center.

Conversion was done on information files to an external format which can be used as input to the program ADSEP.³⁴³ In this way information files are produced in an internal format which is compatible with other information processing computer programs. This conversion was done for a number of projects.

Sponsors: Reactor Division
Ecology Division

D. W. Cardwell
N. F. Sollins

SUPERTO, a Multigroup Neutron Cross-Section Generator

R. Q. Wright

SUPERTO-II. A revision of SUPERTO,^{344,345} designated as SUPERTO-III, has recently been completed. SUPERTO-III will process ENDF/B³⁴⁶ version II and version III data.

343. A. A. Brooks, *ADSEP, an Automated Data Set Editing Program*, CXC-34 (May 1970).

344. R. Q. Wright et al., *SUPERTO: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B*, ORNL-TM-2679 (1969).

345. Math Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4661, p. 94.

346. H. C. Honeck, *ENDF/B-Specifications for an Evaluated Nuclear Data File for Reactor Applications*, BNL-50066 (May 1966) (revised by S. Pearlstein, Brookhaven National Laboratory, July 1967).

Changes in the calculation model for SUPERTOG-III are:

1. Smooth cross sections: SUPERTOG now processes the $(n,2n)\alpha$ reaction if data are given in ENDF/B file 3. These results are used to generate contributions to the $(n,2n)$ scattering matrix as well as being included in the total cross section.
2. Resonance cross section: The resolved resonance treatment has been changed to allow an integration mesh of 100 points per resonance with a maximum of 2400 mesh points per group. The procedure for averaging the elastic scattering cross section in the resolved resonance region was also improved. Some minor changes to the unresolved resonance treatment were made.
3. Elastic scattering matrices: A new treatment³⁴⁷ for the within-group scattering which applies in the energy range for which elastic scattering is isotropic has been added to the code.
4. Inelastic and $(n,2n)$ matrices: The $(n,2n)\alpha$ reaction is now processed if data are given on the ENDF/B tape. SUPERTOG now processes LF = 5 (general evaporation spectrum) data for secondary energy distributions.

SUPERTOG-III is on production status and has been used to process a number of cases.

Implementation of SUPERTOG-II on Control Data Computers. SUPERTOG-II was implemented on a CDC-6400 computer at Kaman Nuclear Corporation, Colorado Springs, Colorado, by ORNL and Kaman Nuclear staff members. This effort was sponsored by the Radiation Shielding Information Center, which distributes versions of SUPERTOG operational on both IBM and CDC computing equipment.

SUPERTOG Verification. During the past year, considerable effort has been expended in verifying the results obtained from the SUPERTOG code. Detailed comparisons with the results obtained from the ETOX³⁴⁸ code have been conducted for three important nuclides: ^{235}U , ^{238}U , and ^{239}Pu . In general, the results are in good agreement; however, a discrepancy in the ^{239}Pu comparison for the energy range 1 to 10 eV is being investigated. Documentation of this study is in preparation.

Sponsors: Neutron Physics Division and Reactor Division

The Maintenance of EDITOR: An ENDF/B Processing Code

J. E. White S. K. Penny

The ENDF/B processing code EDITOR^{349,350} has been improved and updated in accordance with the revised ENDF/B formats and procedures.^{351,352} Most of the modifications were made to improve the edit portion and to make the code operational on the CDC machines. EDITOR will now print the literal information used to identify the ENDF/B file and reaction type on each page. This feature is especially useful when editing very large arrays. In addition, some of the quantities previously represented by FORTRAN variables have been replaced by more familiar physics terms. For example, consider the case where multiplicities are given in file 12, section 102. The variables ES and EG(I) have been changed to LEVEL ENERGY and PHOTON ENERGY respectively.

347. R. A. Grimesey, W. Serrano, and R. A. Dannels, *Nucl. Sci. Eng.* 41, 140 (July 1970).

348. R. E. Schenter et al., *ETOX - a Code to Calculate Group Constants for Nuclear Reactor Calculations*, BNWL-100? (May 1969).

349. C. L. Thompson et al., *EDITOR, a Processing Code for ENDF/B Format Data*, ORNL-TM-3266 (ENDF-142) (February 1971)

350. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 93.

351. M. K. Drake, *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, BNL-50274 (T-601) (ENDF-102, vol. I) (October 1970).

352. D. J. Dudziak, *ENDF/B Formats and Procedures for Photon Production and Interaction Data*, LA-4549 (ENDF-102, vol. II) (October 1970).

Table 1. Changes in Hollerith data string

Section	From	To
Neutron interaction and photon production files		
4	INELASTIC	(N,N*) TOTAL
51-90	(N,N*) MT-40	(N,N*) LEVEL
91	(N,N*) MT-40	(N,N*) CONT
Photon interaction files		
501	TOTAL	TOTAL PHOTON
502	ELASTIC	COHERFNT
504	INELASTIC	INCOHERENT
516	PAIR PROD	PAIR PRD TOT

Table 1 summarizes the changes that have been made to the Hollerith information used to identify the ENDF/B reaction types in the BLOCK DATA statement.

EDITOR will now process the following ENDF/B formats:

1. the revised formats for radioactive decay data (MT = 453), fission product yield data (MT = 454), and delayed neutron data (MT = 455),
2. Reich-Moore and Adler-Adler resolved resonance parameters,
3. the new formats³⁵³ for the average number of prompt neutrons per fission and the LR flag.

The above-mentioned extensions have not affected the core size required to execute the program.

Sponsor: Oak Ridge Cross Section Steering Committee (Reactor and Neutron Physics Divisions)

The INDEX Data System: An Index of Nuclear Data Libraries³⁵⁴ Available at ORNL

J. L. Lucius R. Q. Wright J. D. Jenkins³⁵⁵

The contents of several of the basic neutron data libraries in production use at ORNL have been compiled into a data library index. The information has been entered into the computer in a form accessible to a search and manipulation program. A description of the computer program, INDEX, a brief description of the libraries, and an index of the contents of each are given.

Sponsor: Oak Ridge Cross Section Steering Committee (Neutron Physics and Reactor Divisions)

CHECKER Modification

R. Q. Wright J. L. Lucius

A new version of the CHECKER³⁵⁶ program was obtained from the National Neutron Cross Section Center, Brookhaven National Laboratory, and is now operational on ORNL computers. The purpose of

353. S. Pearlstein, minutes of the Cross Section Evaluation Working Group, May 19-20, 1971.

354. Abstract of ORNL-TM-3334.

355. Reactor Division.

356. H. C. Honeck, *Description of the ENDF/B Processing Codes and Retrieval Subroutines*, ENDF-110, BNL-13582 (September 1967) (revised September 1970).

CHECKER is to check the data on an ENDF/B³⁵⁷ BCD card-image tape. CHECKER has been used to process the ENDF/B-III preliminary tapes.

Sponsor: ORNL Cross Section Steering Committee (Neutron Physics and Reactor Divisions)

NATIONAL LEAD COMPANY OF OHIO

Criticality Evaluation of M-101 Shipping Containers

J. R. Knight

Criticality calculations on the M-101 shipping containers³⁵⁸ filled with 10% enriched $\text{UO}_2(\text{NO}_3)_2$ and packed in vermiculite-filled 55-gal drums were performed using the KENO³⁵⁹ criticality code. An array of 770 units stacked in an approximately cubical configuration was evaluated. The results of the calculations show that the array is safe and that variations in the density of the vermiculite packing have no significant effect on the criticality of the system. This indicates that accidental loss of vermiculite should not give rise to any criticality problems.

Sponsor: National Lead Company of Ohio

D. Dunaway

ORGDP

Spectral Analysis and Digital Filtering of Compressor Data

M. R. Patterson F. D. Hammerling

Sets of compressor data which were digitized at equal time increments have been Fourier transformed to frequency space using the fast Fourier transform.³⁶⁰ Study of the amplitude in frequency space (the spectrum) revealed a small number of very dominant frequencies, which were identified with various blade harmonics. A digital band-pass filter³⁶¹ was then applied in frequency space to isolate a given dominant frequency, and the result was transformed back to time space. The contribution of this one mode to the original input data could then be accurately assessed. Further development of this code was entrusted to ORGDP.

Sponsor: ORGDP

R. E. Ziegler

357. H. C. Honeck, *ENDF/B Specifications for an Evaluated Nuclear Data File for Reactor Applications*, BNL-50066 (ENDF-102) (May 1966) (revised July 1967).

358. G. R. Handley et al., *Evaluation of the M-101 and M-102 Shipping Containers in Vermiculite-Filled 55-Gallon Drums*, Y-DD-19 (1968).

359. G. E. Whitesides and N. F. Cross, *KENO - a Multigroup Monte Carlo Criticality Program*, CTC-5 (September 1969).

360. J. W. Cooley and J. W. Tukey, "An Algorithm for the Machine Calculation of Complex Fourier Series," *Math. Comp.* 19, 297-301 (1965).

361. M. R. Patterson, E. C. Long, and F. L. Miller, Jr., *Digital Filtering and Spectral Comparison Using the Fast Fourier Transform*, CTC-44 (1970).

Vibration Analysis

M. R. Patterson C. V. Smith, Jr.³⁶² M. Feliciano

The results of the Oak Ridge analysis of floor vibrations in buildings K-31 and K-33 have been reported previously.^{363,364} During the last year the AEC decided to obtain an independent check of the calculations for K-33. Contracts for this purpose were let to Catalytic Corporation of Philadelphia, Pennsylvania, and Conrad Associates of Van Nuys, California. Liaison with these contractors was provided at two phases of their study. Initially, the definition of the problem was worked out at joint meetings. After several months, the report then submitted by Conrad Associates was reviewed in conjunction with C. T. McLoughlin of ORGDP. The report was found to be substantially in agreement with the local results, indicating that vibrational stresses are small compared with static stresses.

Sponsor: ORGDP

D. S. Pesche

PORTSMOUTH GASEOUS DIFFUSION PLANT

Portsmouth Criticality Safety Analysis

Nancy F. Cross R. J. Hinton J. R. Knight J. L. Feuerbacher³⁶⁵

A wide variety of safety calculations were performed using the KENO code. However, most of the work concerned the following problems.

1. Investigate the safety aspects of storing 5, 10, and 37.5% enriched oxide in 6- and 9-in. cylinders. Determine the maximum safe array size, and determine the effect of various reflectors.
2. Determine the criticality safety of proposed storage arrays for 2½-ton cylinders containing 5% enriched UF₆ and a 14-ton cylinder containing 4½% enriched UF₆.
3. Study the effect of varying the boron and fuel content in 8- and 12-in. cylinders containing UO₂F₂. Also, verify the safety of using various reflector materials.
4. Investigate the effect of internal interspersed moderation in 8- and 12-in. cylinders of UF₆ and UO₂F₂ as well as the effect of sprinklers external to the storage arrays. Various water densities were used, and optimum interspersed moderation was determined.
5. Determine the effect of various water and concrete reflectors on 7 X 7 X 7 arrays of 8-in. shipping containers of UF₆ at various enrichments with varying interspersed moderation.

Sponsor: Portsmouth Gaseous Diffusion Plant

J. L. Feuerbacher

TVA

XLUX, a Version of XLACS

J. L. Lucius N. M. Greene R. Q. Wright

XLACS,³⁶⁶ described in last year's annual report, calculates multigroup neutron cross sections from ENDF/B data for use by the XSDRN³⁶⁷ code. XLUX is a version of XLACS designed to provide

362. Consultant, Georgia Institute of Technology, Atlanta, Ga.

363. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 104.

364. M. R. Patterson et al., *Vibration Analysis of a Floor Structure*, CTC-30 (June 1970).

365. Portsmouth Gaseous Diffusion Plant.

366. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 95.

367. N. M. Greene and C. W. Craven, Jr., *XSDRN, a Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

multigroup cross sections for the LASER³⁶⁸ code. The development of XLUX required a major modification of the XLACS resonance treatments. Modifications of the XLACS inelastic scattering, elastic scattering, and thermal treatments were also required. New programming was generated to create and update cross-section libraries in the MUFT³⁶⁹ and THERMOS³⁷⁰ formats which are used by the LASER code.

The development of XLUX is complete, and the code is currently undergoing validity tests by the Tennessee Valley Authority.

Sponsor: Nuclear Engineering Branch, Tennessee Valley Authority.
Chattanooga, Tennessee

USAEC

RECON

N. B. Gove	R. E. Plemens	W. B. Malthouse	Arline H. Culkowski
C. E. Hammons	A. F. Joseph	G. K. Haeslein	A. A. Brooks
F. D. Hammerling (and many others)			

RECON (REmote CONsole) is an information retrieval program for interactive retrospective searching of large bibliographic files. The AEC version of RECON was developed by Lockheed and installed on the IBM 360/75 computer in December 1970. Operation began in January 1971 with five terminals (LBL-Berkeley, DTIE-Oak Ridge, Bettis-Pittsburgh, ORNL-X-10, and AECW-Germantown). A sixth terminal, NSIC-Y-12, was added in March.

RECON has a high degree of user acceptance, due in part to the simple, though effective, command language. Some results can be obtained with only a little knowledge of the thesaurus or indexing scheme. Also, spelling requirements are minimal. For example, it is not necessary to know an author's initials to retrieve his publications.

Several thousand RECON searches have been performed on bibliographic data and key words from 2½ years of *Nuclear Science Abstracts*.

Downtime has been high, about 50%, due to many causes, chief of which is trouble with the dedicated phone line.

RECON uses inverted files to reduce search time. Programs to help prepare these files were provided by Lockheed. Some initial difficulty was encountered in using the programs to add new material to the inverted files. Two update operations were performed at Lockheed. A modified update procedure was written and tested at ORNL in August.

By special arrangement, RECON was shown at the Atoms for Peace Conference in Geneva, September 6-16. A special hookup, involving a satellite, microwave stations, and phone systems of several countries, was set up to link the ORNL computer with the exhibit hall in Geneva. The hookup worked remarkably well, with less than one day total malfunction time during the conference.

368. C. G. Poncet, *LASER - a Depletion Program for Lattice Calculations Based on MUFT and THERMOS*. WCAP-6073 (1966).

369. H. Bohl, Jr., E. M. Gelbard, and G. M. Ryan, *MUFT-4 Fast Neutron Spectrum Code for the IBM-704*. WAPD-TM-72 (1957).

370. H. C. Honeck, *THERMOS - a Thermalization Transport Theory Code for Reactor Lattice Calculations*. BNL-5826 (1961).

At ORNL, special operating procedures were set up for the Geneva run. An unusually high level of backup procedures were tested. A complete set of spare data cells and disk packs were created with identical files. A mini-RECON which does not require the data cell drive was created. All files on disks and cells were dumped to tape, and restore operations were tested. The systems group checked out RECON performance on both the 360/75 and the 360/91 computers. Finally, we were prepared for failure of even the card reader, by putting a copy of the RECON card deck on disk.

Several independent reports indicate that the Geneva demonstration of RECON was well received.

We wrote a program to convert Chem Condensates files into a format suitable for RECON. We put a sample file on the data cell for use as one of the RECON files.

We are planning some improvements in the RECON software. For one thing, we hope to make the program run faster and still use less core and disk space. For another, we plan to reduce the number of false drops by using the "split" information which is given with each key word. We have written several routines display information on the cathode ray tube screen.

Sponsor: U.S. Atomic Energy Commission, Division of Technical Information

Reactor Fuel Costs

R. L. Stephenson J. D. McDowell N. B. Gove R. A. Brogli³⁷¹

GACUST is a computer program written by Gulf General Atomic Corporation to compute the cost of fuel for various types of reactor operation and various interest rates and prices. We modified this program to run interactively, to ask questions and display results on a CRT screen. The user may choose English, French, or German and is asked a series of questions to define the reactor type, size, costs of fuel processing, reprocessing, and interest rates. The user answers as many questions as he wishes; the program chooses reasonable values for the rest, calculates the various costs for five years, and writes a table in the specified language. We made this program available to the participants of the Atoms for Peace Conference in Geneva via the RECON hookup. Certain types of communication line failure caused the program to terminate. The exact cause and cure for this are still unknown. At present, there are no plans to continue this project.

Sponsor: U.S. Atomic Energy Commission, Division of Technical Information

The Addition of Radiation and Natural Convection as Boundary Conditions to the Transient Heat Transfer Code ORTHAT

R. C. Durfee

We have added two types of boundary conditions to the Transient Heat Transfer Code ORTHAT.³⁷² They are radiation and natural convection. Thus the heat transfer coefficient at the boundary is made up of three parts, forced convection, natural convection, and radiation, as shown in the equation below:

$$h_T = E\sigma(T_b + T_{ext})(T_b^2 + T_{ext}^2) + h_c + h_n \left| \frac{T_b - T_{ext}}{T_c} \right|^{h_e};$$

371. Gulf General Atomic.

372. R. C. Durfee and C. W. Nestor, Jr., *ORTHIS, ORTHAT - Two Computer Programs for Solving Two-Dimensional Steady-State and Transient Heat Conduction Problems*, ORNL-TM-3324 (July 1971).

h_T is the total heat transfer coefficient; E is the emissivity of the surface material; σ is the Stefan-Boltzmann constant; T_b is the boundary temperature; T_{ext} is the external temperature; h_c is the heat transfer coefficient for forced convection; h_n and h_e are the coefficient and exponent, respectively, for the term simulating natural convection; and T_c is a temperature difference of 1°F.

Sponsor: U.S. Atomic Energy Commission, Division of Materials Licensing

R. H. Odegaarden

Monte Carlo Criticality and Shielding Analysis of an Irradiated Fuel Shipping Cask

G. W. Morrison E. A. Straker³⁷³ J. R. Knight

A series of Monte Carlo neutron and gamma-ray transport calculations has been performed to validate the design specifications of the GE-IF 300³⁷⁴ irradiated fuel shipping cask. The cask geometry was described by the general geometry program GEOM, which allowed an exact representation of the shipping cask.

The Monte Carlo calculations were performed using the MORSE³⁷⁵ multigroup neutron and gamma-ray transport code. A coupled set of neutron and gamma-ray P_3 expanded cross sections were used.

Sponsor: U.S. Atomic Energy Commission, Division of Materials Licensing

Atmospheric Turbulence Partial Differential Equations

P. R. Coleman

Work has continued on the model to describe turbulence and diffusion in the atmospheric boundary layer over urban areas.³⁷⁶ It is hoped that this model will tell more about the distributions of temperature, wind speed, and turbulent energy in this layer.

Progress is now being made toward transfer of this project to a new employee of the sponsor.

Sponsor: Atmospheric Turbulence Diffusion Laboratory, NOAA

S. R. Hanna

U.S. ARMY, ABERDEEN PROVING GROUND

The Adjoint Difference Method and Its Application to Deep-Penetration Radiation Transport³⁷⁷

T. J. Hoffman J. C. Robinson³⁷⁸ P. N. Stevens³⁷⁹

An important radiation transport problem is that of determining an effect of interest in a geometrically complex object (vehicle) far removed from the radiation source. The direct solution to this problem

373. Science Applications, Inc., Huntsville, Ala.

374. *Design and Analysis Report, IF 300 Shipping Cask*, Reactor Fuels and Reprocessing Department, General Electric Co., San Jose, Calif.

375. E. A. Straker et al., *The MORSE Code, a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (September 1970).

376. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 106.

377. Abstract of NEUT 0150-2 by T. J. Hoffman, J. C. Robinson, and P. N. Stevens (November 1971).

378. The University of Tennessee.

379. Oregon State University.

involves a deep-penetration Monte Carlo calculation. Calculations of this type are always costly and often impossible.

To deal with this problem, the adjoint difference method was developed. This method decomposes the original problem into two independent calculations:

1. a geometrically simple (one- or two-dimensional) deep-penetration calculation that is independent of the vehicle,
2. a localized three-dimensional calculation that is independent of the radiation source.

The first calculation is suitable to deterministic methods of solution, such as discrete ordinates. The second, by nature of the geometry, must be solved by Monte Carlo techniques; however, this is not a deep-penetration calculation. Therefore, the dual complexity of geometry and statistics inherent in a deep-penetration Monte Carlo calculation is avoided.

Since the above calculations are independent, only the coupling of these calculations depends on the relative position and orientation of the source and vehicle. With this property, a great deal of information can be obtained from a single Monte Carlo calculation.

The method was examined through application to several problems. All results were compared with those obtained from presently acceptable methods of problem solution. In all cases, the adjoint difference method was shown to be an efficient, versatile method of calculation.

Sponsor: Department of the Army, Aberdeen Proving Ground, Md.

U.S. ARMY MISSILE COMMAND

Monte Carlo Calculations for Triggering a Chemical Laser with a Neutron Pulse

G. W. Morrison

A series of Monte Carlo neutron transport calculations has been performed in a feasibility study of triggering a chemical laser with a pulse of neutrons. The chemical laser studied was the hydrogen-fluorine laser with the reactions:

A cylindrical cell was used in the calculations with a mixture of UF_6 gas (93% enriched) and H_2 gas. Because the UF_6 and H_2 react only at elevated temperatures, a triggering mechanism is necessary to start the reaction. A neutron pulse incident on the laser cell was selected as a possible starting mechanism. The incident neutrons release fluorine atoms for reaction (1) to occur by causing fissions in the uranium. It is also expected that additional fluorine atoms will be released by the collisions of the fission products with the UF_6 molecules.

The Monte Carlo calculations were performed with several sets of system parameters, such as the gas density, size of the cell, and uranium enrichment, to maximize the fission rate. Neutron spectra from a LINAC, a fast-burst reactor, and a Van de Graaff accelerator source were used. The fast-burst reactor spectra gave the largest fission rate. As a result of the Monte Carlo calculations, an experimental effort has been undertaken by Reactor Chemistry Division personnel to construct several laser cells for irradiation by a fast-burst reactor. This will provide an experimental check on the calculations.

Additional calculations are also being performed to evaluate future cell designs.

Sponsor: Physical Sciences Laboratory of the U.S. Army Missile Command,
Huntsville, Alabama

Y-12 PLANT

Electron Microprobe Spectral Analysis Routines

L. W. Gilky

A program has been written to qualitatively identify all elements having a $K\alpha_1$, La_1 , or Ma_1 x-ray peak corresponding to a peak in the given experimental spectrum.

A program is under development to determine the percent of each element from atomic number 22 through 29 present in a microprobe spectrum of special alloy samples. Except for impurities, the alloys consist of two or more of the specified elements. The percentage content is determined by comparison of the integrated peak counts for the highest-energy $K\beta_1$ peak in the mixed spectrum with the integrated peak counts in the corresponding peak of a known standard spectrum of the pure element; then, using this percent and the standard spectrum, counts corresponding to this element are stripped from the mixed spectrum, exposing the next lower $K\beta_1$ peak. The process is repeated until the percentages of all elements present have been determined.

Sponsor: Y-12

D. R. Davidson

Heat Transfer and Stress Analysis

M. R. Patterson Mark Reeves III J. S. Crowell Peggy G. Fowler

Numerically computed temperature distributions resulting from convective boundary conditions³⁸⁰ have been used to furnish the thermal loading to Wilson's finite-element stress code.³⁸¹ This code has been modified locally to allow a limited type of plastic flow, using an effective stress formulation. Consequently, if the yield stress is exceeded, a later return to an isothermal condition (no thermal loading) leaves a residual stress field in the material. The spatial distribution and magnitudes of these stresses are being computed for different geometries.

Sponsor: Y-12

L. T. Royer

Revisions to LCR-2 Code, for Determining Refined Crystal Lattice Parameters

O. W. Hermann A. L. Cooley³⁸²

Use of the LCR-2 code³⁸³ was continued during the year. This code has been proven excellent for refinement of lattice parameters of various materials analyzed from x-ray diffraction data. The hkl indices,

380. Math. Div. Annu. Prog. Rep. Dec. 31, 1970, ORNL-4661, p. 107.

381. E. L. Wilson, *A Digital Computer Program for the Finite Element Analysis of Solids with Nonlinear Material Properties*, Aerojet General Corp. Technical Memo 23 (July 1965).

382. Development Division, Y-12.

383. D. E. Williams, *LCR-2, a FORTRAN Lattice Constant Refinement Program*, Iowa State University, Ames Laboratory, IS-1052 (1964).

required as input to the code, must either be known or determined by other codes.³⁸⁴⁻³⁸⁶ The code applies the least-squares method to observed reflection angles and the hkl indices in determining the best values for the unknown parameters. The number of lattice constants found varies from 1 to 6, for cubic cells to triclinic systems, respectively. An additional parameter can also be found, which relates to the "drift correction" normally obtained only by graphical extrapolation. The code was modified with routines to give a somewhat crude plot, with the normal output printer showing the scatter of experimental data with respect to the linear plot of the Nelson-Riley extrapolation function.³⁸⁷ This has been helpful in analyzing the effects of data errors.

Other revisions were made to permit variations in the type of input data. Two-theta values, d spacings, or scale readings can be used. Also, several measurements of the same angle may be input.

The chief source of data used in executing the code was produced by the Laboratory Development Department.³⁸⁸

Sponsor: Development Division, Y-12

A. L. Coffey

A New Method of Indexing Orthorhombic Crystalline Systems

O. W. Hermann A. L. Coffey³⁸⁸

The INDOCX code^{384,389} was developed for indexing orthorhombic cell crystals from observed diffraction angles produced by x rays of known wavelength. This code was written to apply one of the most promising techniques found in our search for more satisfactory performance in methods of indexing x ray lines for lower-symmetry systems. It produced good results in almost all of the orthorhombic materials tested.

The method initially applied in the code follows that reported by Barabash and Devydov³⁹⁰ and earlier suggested by Neskuchaev.³⁹¹ Although their skillful procedure was very useful, it appeared that computer time might be too great in its more complete application and that it would not always index less precise data sufficiently. Also, it was found that these difficulties could be resolved more lucrably by first concentrating on finding a solution using only four reflections having low indices. Once this 3 by 4 "basic matrix" is determined, values of the three lattice constants are found. Then, a complete indexing of all lines is determined, excluding possibly a few. These are considered as a result from either too great an error or an impurity. The problems that were encountered and the method of resolving them are given in more detail elsewhere.³⁸⁴ Satisfactory crystal indexing was derived with the INDOCX code in more than a dozen test cases on materials for which results were already known. Test data applied were produced by the Laboratory Development Department of the Development Division at Y-12 and the National Bureau of Standards.

384. O. W. Hermann and A. L. Coffey, *A New Method for Indexing Orthorhombic Crystalline Systems Applied in the FORTRAN IV Code, INDOCX* (to be published).

385. C. R. Heiple, *A Computer Program for Indexing Crystals from Their X-Ray Powder Patterns*, The Dow Chemical Co., Rocky Flats Division, RFF-1292 (1969).

386. C. E. Hrkomb, *Determination of the Crystal System and Lattice Parameters of Previously Unreported Compounds*, Y-1687 (1969).

387. L. V. Azaroff and M. J. Buerger, *The Powder Method in X-Ray Crystallography*, pp. 219-45, McGraw-Hill, 1958.

388. Development Division, Y-12.

389. Acronym for Indexing Orthorhombic Crystals from X-Ray Diffraction Data.

390. I. P. Barabash and G. V. Devydov, "On the Indexing of Powder Patterns for Polycrystalline Materials of the Orthorhombic System," *Acta Cryst.* A24, 608 (1968).

391. V. Neskuchaev, *Zh. Tekh. Fiz.* 1, 105 (1931).

INDOCX contains about 1300 FORTRAN IV source statements and uses about 140K bytes of core. Cases were executed usually within 0.25 to 1 min CPU time on the IBM 360/91.

Sponsor: Development Division, Y-12

A. L. Coffey

Major Revisions to Diffraction Data Plot Code

O. W. Hermann W. E. Baucum³⁹² D. A. Carpenter³⁹³

A code for plotting neutron or x-ray diffraction patterns from experimental data was rewritten for use with the Calcomp plotter, and other new features were added. The INTRIGUE Plotting Package³⁹² was applied. The original code, developed earlier by the authors, required use of the EAI-430 Electroplotter. It also required the conversion of the paper tape input data to punched cards.

After the paper tape data are produced at the Y-12 Plant, the following procedure is used. The tape is fed through a Teletype at Y-12 to be stored in the core of the IBM 360/75 at ORNL by using the PTAPE program.³⁹³ The data are then brought into an active file of a CRBE terminal, and a class G disk plot job is executed. This method enhanced "turnaround" time considerably. Slight modifications to the error check routine in PTAPE may be feasible, in order to diminish difficulties that sometimes arise in reading paper tape.

Also, the additional "background suppress" feature was found to be unusually desirable in attempting to discover small peaks in the diffraction patterns. The background position is controlled to enable peaks to be shown, which were normally off scale with the required magnification applied.

Sponsor: Development Division, Y-12

W. E. Baucum

D. A. Carpenter

Spatial Correction for the Point Kinetic Theory of Rossi Alpha Calculations

J. R. Knight J. T. Mihalczo³⁹⁴

Several computer programs have been prepared for analyzing data used for interpretation of Rossi alpha measurements. One program was used for the analysis of experimental data obtained from uranium metal spheres. Other studies were made using output from ANISN³⁹⁵ neutron transport calculations as input to several other computer programs. Both the number of spatial intervals and the number of discrete angles in the quadrature set were varied to determine the effect of finite approximations on the results.

Sponsor: Critical Experiments Facility, Y-12

J. T. Mihalczo

The Use of Borosilicate Glass Raschig Rings in Fissile Systems

J. R. Knight D. W. Magnuson³⁹⁶

The ANISN³⁹⁵ and KENO³⁹⁶ criticality codes were used to do a nuclear safety evaluation of borosilicate glass Raschig rings in fissile solutions. The effects of variations in the solution concentration,

392. M. B. Emmett, *INTRIGUE-II: An IBM-360 Subroutine Package for Making Linear Logarithmic and Semi-logarithmic Graphs Using the Calcomp Plotter*, ORNL-4664 (1971).

393. R. P. Lelands, *CRBE Paper Tape Facilities*, memo to D. W. Cardwell (1971).

394. Critical Experiments Facility, Y-12.

395. W. W. Eagle, *A User's Manual for ANISN*, K-1693 (March 1967).

396. G. E. Whitton and N. F. Cross, *KENO - a Multigroup Monte Carlo Criticality Program*, CTC-5 (September 1969).

boron content of the glass, and Raschig ring dimensions were analyzed. The results of varying the orientation of the rings as packed in a given array were also studied. These calculations are needed to evaluate the usefulness of Raschig rings in assuring criticality safety in the storing and processing of fissile solutions.

Sponsor: Critical Experiments Facility, Y-12

D. W. Magnuson

The Reactivity Effects of Accidental Leakage of D_2O Tanks at the BSR Facility

J. R. Knight

The ANISN³⁹³ and KENO³⁹⁶ criticality codes have been used to determine the reactivity effects of leakage of D_2O from large tanks placed adjacent to the BSR core. Possible situations considered are the mixing of D_2O with the water moderator in the core and mixing of water with D_2O in the tanks, which act as reflectors for the core. The possibility of the formation of a layer structure of D_2O and water within the tank was also considered. Preliminary calculations indicate that any mixing or layering of D_2O with water does not lead to a more reactive configuration than the reactor operating without any leaks.

Sponsor: Critical Experiments Facility, Y-12

E. B. Johnson

Pipe Intersection Criticality Studies

G. E. Whitesides R. J. Hinton L. M. Petrie E. B. Johnson³⁹⁴

Using the KENO³⁹⁶ code, Monte Carlo criticality calculations were performed using data gathered from pipe intersection experiments done at the Y-12 Critical Facility. Two major configurations were considered: (1) an 11-in.-ID aluminum piece in the shape of a 29.26° lateral (Y-shaped) and (2) a Plexiglas cross which was successively boxed out to yield inside diameters of from 10.5 to 11.25 in. Both pieces were reflected by a thick blanket of water and were filled to various levels with a 5.06% enriched aqueous solution of uranyl fluoride (UO_2F_2). The KENO calculations utilized both the 16-group Hansen-Roach cross-section sets and the 123-group cross sections produced by the XSDRN³⁹⁷ code from ENDF data and covered solution concentrations ranging from 744.9 to 907.0 g U per liter. Agreement between the KENO results and experimental values was quite good for both cross-section sets, with only slight disparities at the higher concentrations.

Sponsor: Critical Experiments Facility, Y-12

E. B. Johnson

Monte Carlo Criticality Studies

Nancy F. Cross Chris S. Day R. J. Hinton J. T. Thomas³⁹⁴

A number of problems of interest to nuclear criticality safety in the storage of fissile materials was explored utilizing the KENO code with the Hansen-Roach neutron cross-section sets. Typical problems studied were:

1. The influence on the array reactivity when water at variable density is introduced into the void space of

397. N. M. Greene and C. W. Craven, Jr., *XSDRN, a Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

arrays simulating sprinkler systems in storage arrays has led to a relationship between peak reactivity and water density.

2. The effect of replacing a water reflector by Oak Ridge concrete was examined systematically and has led to a relationship between reactivity effect, concrete thickness, and mass of fissile material present in the storage cells.
3. Infinite planar arrays of fissile materials reflected by water were examined to determine the influence of the number of units in the z direction and the mass of fissile material per cell on the spacing required for criticality.
4. Currently in progress is a series of calculations designed to display the influence of reflected array shape on the criticality of water-reflected arrays.

Sponsor: Critical Experiments Facility, Y-12 Plant

J. T. Thomas

Point Cross Section Monte Carlo

L. M. Petrie, Jr.

A Monte Carlo program using point cross sections was reported on in a previous Mathematics Division annual progress report.³⁹⁸ Studies of several different methods of treating the unresolved resonance region were made. A method proposed by L. B. Levitt³⁹⁹ has been adopted. The method consists in allowing the cross section to assume a range of values at an energy instead of only one value. When the cross section is needed, it is selected randomly from the range of values based on the probabilities of the various values occurring. This method has been implemented and is now being tested.

The cross-section preparation code has been modified to generate the tables of cross sections and probabilities needed for the new unresolved resonance treatment. At the present time, it is being updated to accept ENDF/B⁴⁰⁰ version III data.

Sponsors: Criticality Safety Section, Radiation Safety Dept., Y-12
Critical Experiments Facility, Y-12

G. R. Handley
J. T. Thomas

A Difficulty in Computing the k_{eff} of the World⁴⁰¹

G. E. Whitesides

In the course of applying Monte Carlo programs in the solution of criticality safety problems, a difficulty in correctly computing certain types of systems has arisen. In view of the increasing use of Monte Carlo-type programs, it is important that some statement be made about the type of systems in which the difficulty is likely to be encountered, since when one attempts to compute the multiplication factor for such a system, the result will almost always yield a low, and hence, for criticality safety purposes, nonconservative, result. This can occur with no hint that the computed result is in error.

398. L. M. Petrie, Jr., *Monte Carlo Criticality Studies Using Point Cross Sections*, ORNL-4661, III (December 1970).

399. L. B. Levitt, "The Probability Table Method for Treating Unresolved Resonances in Monte Carlo Criticality Calculations," *Trans. Amer. Nucl. Soc.* 14(2), 648 (October 1971).

400. H. C. Honeck, *ENDF/B*, BNL-50066 (May 1966).

401. Summary of paper presented at the American Nuclear Society Meeting, Miami Beach, Fla., Oct. 17-21, 1971.

The extreme example, which defines a situation in which this difficulty can exist, is the " k_{eff} of the world" problem. That is, if one attempts to calculate the k_{eff} of the world using a Monte Carlo calculation, what k_{eff} would be computed assuming that there are several critical assemblies located around the world? The answer would likely be the k_{eff} of the world with no critical assemblies present. The cause of the erroneous result is the fact that the volume of fissile material in the world would be so large relative to the volume of fissile material in the critical assemblies that commonly used forms of sampling would almost never "see" the critical assemblies. Hence, this would not reflect their existence in the computed k_{eff} .

A more commonly encountered example in which a user of Monte Carlo programs might observe this difficulty is illustrated by a $9 \times 9 \times 9$ array of plutonium metal spheres with a radius of ~ 4 cm spaced on 60-cm centers. The array is reflected on all sides by a thick water reflector. The k_{eff} of this system is computed to be 0.93. If the sphere in the center unit of the array is replaced by a sphere of plutonium that is exactly critical as a bare unit and the calculation repeated in the standard fashion using the Monte Carlo method, the calculation will likely yield a k_{eff} of 0.93, reflecting the same difficulty encountered in the "world k_{eff} " problem.

The erroneous results for these types of problems are the result of the failure of the calculation to converge the source to the fundamental source mode. The difficulty can range from a problem which converges so slowly that the normal number of generations examined is insufficient to assure convergence to problems that perhaps will never converge.

The answer to the problem lies in being sure that source convergence is achieved. Most Monte Carlo programs start all neutrons initially with either a flat or a cosine distribution over the fissile material in the system. For the majority of problems this is adequate and maybe even exact. Unfortunately, the choice of a standard start procedure that is adequate for a system with a region of localized multiplication that is somewhat higher than the multiplication of the major portion of the volume of the system is difficult, if not impossible, to define. One difficulty, which should not be underestimated, is trying to determine if, and where, this situation exists. Because of this, it is not the intention of this paper to offer a solution to the general problem, but only to bring to the attention of the users of Monte Carlo programs the fact that the computed multiplication may be in error for such systems.

If the region of highest multiplication can be established, it appears to be adequate to ensure eventual source convergence to the fundamental mode by starting all neutrons in this region. If there is more than one such region, it may be necessary to run several cases varying the initial source in order to determine the initial conditions that will lead to a fundamental mode source distribution.

The Monte Carlo method has opened up the path to very precise evaluations of the criticality safety of almost any situation likely to be encountered. Its use, however, should be tempered by the realization that unless the correct fission distribution is achieved, the results will most likely be nonconservative.

Sponsor: Criticality Safety Section, Radiation Safety Dept., Y-12

Criticality Search Package for KENO

Nancy F. Cross L. M. Petrie, Jr. G. R. Handley⁴⁰²

A vastly improved array size search package has been incorporated into the KENO code. It alters the array size of a problem in the X, Y, or Z direction or any combination thereof. This is continued until the

402. Y-12 Radiation Safety Department, Criticality Safety.

desired value of k -effective has been achieved, the specified number of iterations has been executed, or the code determines that all possibilities have been exhausted.

The search package assumes k -effective varies linearly with the number of units in any direction and solves either a linear, quadratic, or cubic equation for the slope, depending on the manner in which the array is to be altered.

This type of search is useful in determining the maximum safe array size for an array of given fissile units.

The dimension search portion of the criticality search package has been extended to allow dimension searches on arrays containing more than one type of unit. This type of search package is especially useful in determining the maximum safe size of fissile units in a shipping or storage array or the minimum amount of absorber that must be placed about fissile units in order to meet specified criticality conditions.

Sponsor: Criticality Safety Section, Radiation Safety Dept., Y-12

G. R. Handley

Nuclear Safety Evaluation for the Storage and Shipment of Uranium Materials

J. R. Knight

Criticality calculations for determining the effect of the accidental activation of sprinkler systems on storage arrays⁴⁰³ were continued to include several additional storage configurations. Other criticality problems of interest to Y-12 operations that were studied include safety evaluation of various shipping containers and solution storage arrays. The criticality of metal parts submerged in uranium solutions was also investigated.

Sponsor: Technical Division, Y-12

G. R. Handley

403. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 110.

Systems Programming

OPERATING SYSTEMS ON THE IBM SYSTEM/360 COMPUTERS

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Summary of System History

The operation of the IBM 360/91 and IBM 360/75 computers was carried out using ORNL modified versions of the IBM-supplied operating system referred to as Multiprocessing with a Variable Number of Tasks (MVT). Release 17 of the IBM operating system was used for the first quarter of the year. At that time it was replaced by release 19.6. Release 2.3 of the Houston Automatic Spooling Program (HASP) was installed on both of the 360 computers early in the year. The use of HASP 2.3 provided a stable subsystem that allowed the transition from the release 17 system to the release 19.6 system to take place with a smaller effect on the user community than normally occurs with an operating system release change.

During the second quarter of the year, the remote computing systems on the 360/75 were converted to interface with the HASP system. Modifications to the HASP system and the Conversational Remote Batch Entry (CRBE) system enabled jobs that were submitted to the 360/75 to be handled by HASP rather than the regular IBM operating system. Terminal users of the CRBE system were also provided with some ability to interface with HASP in order to determine and modify the status of their jobs. The handling of the batch job input from the IBM 2780 terminal at Y-12 was also taken over by HASP. The reliability of the HASP Remote Terminal Access Method (RTAM) was at least an order of magnitude better than that of the standard IBM Remote Job Entry (RJE) program. The use of RJE was discontinued in order to alleviate the impact (including frequent system crashes) of remote processing on the entire operating system.

The use of the HASP system resulted in a saving of memory which was on the order of 100,000 bytes (100K). It would not have been possible to provide remote terminals on the 360/91 and still have 1536K of memory available without the implementation of the HASP system.

Release 3.0 of HASP was announced in February, but our implementation of this version of HASP was delayed until June in order to use the stabilized HASP 2.3 as the vehicle for the operating system release change. HASP 3.0 was installed on both 360 computers at the end of the second quarter. This version of HASP was a major revision of the original HASP facility which provides an efficient means for the handling of the large volumes of unit record input and output associated with large-scale computing. The new HASP had an overlay structure which further reduced its memory requirements, and HASP 3.0 provided all of the facilities to remote terminals that had been available to users of RJE. The facilities available to remote users, local users, and the system operators were more numerous and varied than had been available prior to HASP 3.0.

Two more generations of HASP 3.0 were carried out in August and in November in order to incorporate additional options into the HASP system.

A liaison with the user community and new systems developments has been maintained through attendance and participation at two meetings of SHARE Inc. (an IBM users' group of which ORNL is a member) and through attendance at an IBM HASP school and a seminar on HASP held by the Triangle Universities Computation Center. Exchanges of systems programming information and techniques with other installations has continued.¹

Shared Direct Access Devices

A major development during the year was the implementation of the hardware and the programming to allow the sharing of direct access devices between the 360/91 and the 360/75. The shared devices are two 2314 Direct Access Storage Facilities, four 2311 disk drives, and a 2321 Data Cell Drive. The only direct access devices which are not shared are two 2301 drums and a 2314 Direct Access Storage Facility on the 360/91 and four 2311 disk drives on the 360/75. The use of the sharing facility was begun during the second quarter of the year. An immediate benefit of the shared system was the ability to eliminate the need for one of the two duplicated disk packs which were used for storage of frequently used programs and data on each of the two computers. The single disk pack was left mounted on a drive that could be shared between the computers, so that the data on this pack were accessible from either computer. This also reduced the maintenance activity on this pack, since it was now only necessary to perform updates to a single pack. By the end of the second quarter, a second pack for the storage of frequently used programs and data was also mounted on a shared drive.

Switchable Devices

The IBM 2914 switching unit has the ability to selectively switch either a 1403 printer with a Universal Character Set (UCS) or all of the 360/75 remote communication lines or both between the 360/91 and the 360/75. This nondynamic switching may be done at the operator's convenience in order to allow the use of the UCS printer by either computer. The ability to switch the communication lines is normally used only to provide a backup facility to allow the support of the remote terminals and work stations normally operated on the 360/75 when the 360/75 is down for extended periods of time. All of the programs which normally provide remote communication on the 360/75 have been operated successfully on the 360/91. Such operation does reduce the amount of memory available for batch jobs on the 360/91 during this period.

Replacement of Semidynamic Dispatching

The function of the Semidynamic Dispatching (SDD) program² was taken over by the HASP 3.0 program (see HASP in this report) during the second quarter of the year. The SDD program had helped to improve the utilization of the computers by assigning a priority to each step of a job based on the average performance of all job steps of that type. The HASP 3.0 system actually measures the performance of each job step which is in execution and it can restructure the priority sequence of all job steps once per second based on the immediate past performance of that job step. The discontinuation of the SDD program reduces the number of modifications which must be made to each successive IBM-supplied operating system by the ORNL systems group.

1. Math. Div. Annu. Prog. Rep. Dec. 31, 1970, ORNL-4661, pp. 119-20.

2. Math. Div. Annu. Prog. Rep. Dec. 31, 1970, ORNL-4661, p. 115.

Controlled Memory Allocation

The function of the Controlled Memory Allocation (CMA) program² has been extended in order to further increase the extent to which both the fast and the slow memory of the IBM 360/75 computer can be utilized. The previous version of the CMA program used the name of the supervisor program which executed the users' program as a key to determine where in memory all of the job steps of the user's job should be placed for execution. The extension to the CMA program can provide for automatic placement of each individual job step of a job in the most advantageous memory location. In addition, the options which are available to the computer operator to specify where in memory some or all of the steps of a job should be placed have been increased.

With the extended features of the CMA program operating in the automatic mode, a job will compile partially or totally in fast memory. If, as is often the case, the job fails in this step, it can quickly be removed from the system at this point. If the job does compile successfully, it will be located in slow memory for the execution of the Input/Output limited link-edit step. The job may also fail during this step, in which case it can then be removed from the system. In any event, the fast memory is available at this time for other job steps to compile or execute programs.

If the job does successfully link-edit, it will then be executed in slow memory if it is a short-running job. If it is a longer-running job with small memory requirements, it will be executed totally in fast memory as soon as the memory becomes available. If it is a longer-running job with a large memory requirement, it will be executed mainly in slow memory with a portion of the program located in fast memory. However, in this case 270K of fast memory will be left, so that a compiler or a short executable program may be executed concurrently with the large job.

The automatic feature of the CMA program is designed for the peak hours of the day, when there are a large number of relatively short "debugging"-type jobs being submitted from remote locations. The computer operators have options which allow them to change the mode of operation of the CMA program during nonpeak hours so that all programs will run in fast memory. This allows full utilization of the fast memory at times when it is not necessary to reserve a portion of the fast memory for fast turnaround of the debugging jobs.

The implementation of the automatic feature of the CMA program during the fourth quarter of the year virtually eliminated the backlog of class A and class C jobs which had existed previously.

A new feature which has been included in the extensions to the CMA program is the Minimum Partition Cancel (MPC) facility. MPC allows the operator to cancel jobs which are waiting for an amount of memory which they will be unable to obtain in a reasonable length of time. This feature is being used in conjunction with the ORNL modification in HASP 3.0 which allows a job to be canceled and re-enqueued for later execution.

The extended features of the CMA program have also been useful on the IBM 360/91 computer even though all of the memory on this computer is of a single, high-speed type. In addition to the existing facility of the CMA program that can execute long-running jobs against the lower boundary of memory, the extended CMA program executes the compilers, link-editors, and other short-running job steps in the high portion of memory while the longer-running executable program steps are run in the low portion of memory. This tends to reduce memory fragmentation and increase the utilization of memory on the 360/91.

Scattered Nucleus

The scattered nucleus was developed at ORNL in order to provide additional fast memory for the execution of compilers and user programs on the IBM 360/75 computer. This made approximately 1.50K

of fast memory available. The system has been operated successfully with this amount of nucleus scattered into slow memory. A program to determine which components of the nucleus were used with the least frequency was written and run.

During the development of the program to scatter the nucleus, modifications were made to the Initial Program Load (IPL) program. These modifications provided the extremely useful fringe benefit of allowing the computer operator to initiate the IPL program from any of several direct access volumes rather than the system residence volume. Further, the operator now has the ability to designate the system residence volume, the volume from which the system nucleus is to be loaded, and in fact the name of any of several versions of the nucleus to be loaded. Dynamic modifications can also be made to the IPL program by the operator at the time the IPL program is loaded.

These facilities have a number of significant effects on the operation of the system. The ability to load alternate nuclei from any of several volumes allows development to be carried out on these alternate nuclei independent of the normal operation of the regular operating system. It had previously been necessary for the systems group to take over operation of the computer to perform the extensive modifications and subsequent restoration of those modifications in order to test a new nucleus. In addition, when IBM has the need to incorporate corrections to its operating system in the system nucleus, it is no longer necessary to provide for the extensive downtime for the computer in order to create, test, and restore.

Other Developments

The ORNL FORTRAN compiler has been reduced in size from 470K to 270K. This has not only allowed multiprocessing of jobs involving compilers on the 360/75 computer but also has allowed a higher degree of multiprocessing on the 360/91 computer.

The accounting program on both of the ORNL IBM computers has been expanded to consider additional information about the execution of the job which is used both for charging and for studies of the system operation.

The facility to allow the computer operators to start the execution of routine maintenance and service programs via a console command has been improved by the creation of the ROWRDR system task. This single task replaces a number of separate tasks which were once needed to start a variety of programs. Any of these programs may now be started by the execution of the ROWRDR with appropriate parameters.

Remote Computing

The remote computing facilities on the IBM 360 computers include both remote terminals and remote work stations. During this year the operation of all of the remote terminals has come under the control of the HASP system. The HASP system accepts jobs which are generated at remote work stations and submits them for execution on the central computer.

There has been an increase in the number of remote work stations which are connected to the 360 computers during this year. There are stations at the Naval Research Laboratory (IBM 2780 and IBM 360/20), Reactor Division (IBM 2780), Neutron Physics Division (Data 100), Harry Diamond Laboratory (IBM 1130), and Weapon Systems Analysis Office (IBM 2780), and the ORNL PDP-10.

Special modifications to both the central HASP system and the HASP remote work station program have been made in order to provide for the transmission of plotting data via HASP from the 360/91 to a magnetic tape on the IBM 360/29 computer at NRL. This activity has been continuing on an experimental basis during the third and fourth quarters of the year.

The interface between CRBE and HASP was established in May. This implementation provided for jobs submitted from CRBE to be run under control of HASP. Commands were provided in CRBE which permitted CRBE users to interrogate the HASP system in order to determine the status of their job. Output from the job could then be routed either to the remote CRBE terminal, to the central printer, or, via HASP commands, to a remote HASP work station printer geographically closer to the CRBE terminal than the central computer facility.

Culler-Fried System. The Culler-Fried System went into operation in August and has been used from both the terminal at the ORNL central computer and the terminal in the Thermonuclear Division at ORNL. The final version of the system as prepared by the University of California at Los Angeles was received in November, and generation is scheduled for early next year.

RECON. During the year the number of remote terminals serviced by the RECON system increased from 5 to 6. A large amount of effort was directed toward the preparation and maintenance of several special RECON systems which were used to provide a demonstration at the Fourth International Conference on the Peaceful Uses of Atomic Energy which was held in Geneva, Switzerland, during September.

Administrative Terminal System (ATS). The number of persons using ATS grew modestly in 1971.³ Facilities have been added to ATS which provide for the transfer of data to magnetic tape for storage as well as for the retrieval of data from magnetic tape. Provisions for output from ATS data files to punched cards and output to the high-speed printers at the central computer have also been provided.

Current Systems Projects

Scattered nucleus and relocated system. Monitoring is being carried out in order to determine how best to relocate components of the nucleus and other parts of the system in order to locate the most frequently used parts of the operating system in fast memory. While the facility to scatter the components of the nucleus between fast and slow memory, as described in this report, is now operational, it will be necessary to implement coding to relocate selected portions of the operating system other than the nucleus from slow memory into the fast memory made available by scattering some components of the nucleus.

Controlling System Queue Space (SQS) utilization and overflow. Each of the multiple tasks operating under the IBM operating system requires varying amounts of SQS. At present this requires the allocation of a wasteful amount of memory for SQS in order to prevent the entire operating system and all of the associated remote computing facilities of the system from being shut down without warning or potential for recovery due to the action of a single task.

Two projects are designed to attack this problem. Some means of monitoring the use of SQS is to be designed as well as a means of providing a warning when the limit of the existing SQS is being approached. In the event that the need to expand SQS does occur, the existing program will be changed to cause only a single job (which can be restarted) to be terminated, so that the expansion of SQS can be accomplished without disruption of the programs which support the remote computing operations.

Further extensions to Controlled Memory Allocation. Developments in Controlled Memory Allocation (CMA) include creation of controls over memory allocation for long-running jobs in order to prevent location of these jobs in memory locations which will fragment available memory. Modifications which will allow the operator to specify absolute memory locations for selected jobs as well as options for the operator to specify relocation of pending jobs prior to their execution are being considered.

3. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4661, p. 118.*

Data Set Monitoring. During 1970 a program was written which monitored the frequency with which data sets on direct access devices were used. The program is presently being generalized into a Supervisor Call program and will be extended to monitor the use of concatenated data sets and data sets which reside on the IBM 2321 Data Cell, which is, for most practical purposes, a nonstandard direct access device.

Conversational Remote Batch Entry System (CRBE)

R. P. Leinius J. D. McDowell

The ORNL CRBE system continued to provide access to the 360/75 for users at remote typewriter terminals. Although file manipulation and job submission remain as the primary functions of CRBE, a third application, data inquiry, has developed.

Programming to allow CRBE support of Teletype terminals was completed, and a facility for paper tape input from these terminals was provided.

A new feature of the system, the deallocation mode, has been used frequently; with this feature, control of a remote terminal may be automatically passed from CRBE to a user program executing on the 360/75, and then returned to CRBE when execution is completed.

A data set management facility was designed and programmed to enable CRBE to perform some of the system maintenance functions which are currently handled manually. This facility has been completed and will soon be put into general use.

Other programming improvements include support for correspondence-mode 2741 terminals, a desk calculator command, and creation of a backup system to be run on the 360/91 when necessary.

During the past year, new hardware has been acquired so that there are currently 7 phone lines for Teletype terminals and 13 for 2741 terminals.

Approximately 140 persons are enrolled as CRBE users; an average of 2300 terminal sessions are processed and 2000 jobs submitted each month.

A study of several new teleprocessing systems has been undertaken. The IBM Time Sharing Option (TSO) system has received the most attention; a preliminary version of TSO is currently undergoing extensive testing and evaluation.

Serial Communications Access Method (SCAM)

J. D. McDowell

A communications access method has been developed for use with the Computer Communications, Inc., CC-7012 data adapter/CC-30 communications station serial interface circuit (the RECON circuit). The access method is directly accessible to users of FORTRAN, COBOL, and BAL via calls to its function processor CAPER. In addition to providing a programmable means for entering or displaying data at the CC-30 communications stations by way of the 360 computer systems, it offers the ability to dynamically select from among the stations on the circuit those which require attention or those to which data are to be directed. Facilities are provided for dynamic monitoring and recording of communications equipment errors and for automatic or user-provided error recovery.

SCAM is currently being used to provide a base-line error monitoring and recording service for the RECON operation.

Disk Plotting Package

Linda P. Helton Delores Paulk J. G. Sullivan

A major deterrent to fast turnaround time on the IBM computers is the operator time consumed in the mounting and dismounting of magnetic tapes. One considerable use made of tapes was to produce output tape for plotting off-line on the Calcomp plotters. A package of subroutines was developed which were transparent to the user and put plot information from a user job on disk instead of tape. Then, at the operator's convenience, a special job is run which scans all the information put on disk and creates a magnetic tape (or tapes) which would represent several user plots collected together. The number of tapes used for plotting was reduced by a factor of 8 through widespread acceptance of this package.

Teleprocessing Study

G. K. Haeuslein

We conducted studies in teleprocessing using CCI cathode ray tube terminals on a common line. An experimental program was written which permitted each terminal (independently of the others) to activate the different features of the CCI control unit, such as, for example, generating flashing pictures and writing on arbitrary points of the screen. Further efforts will study the use of the terminals as input/output devices for "conversation mode" programs.

Immediate Analysis and Coordinating Computer⁴

C. E. Hammons

The Immediate Analysis and Coordinating Computer (IACC) was installed in April 1971. After the standard software and hardware were accepted, Digital Equipment Corporation employees began finalizing the special software packages which they had contracted to create. Most of the work remaining involved telecommunications software which was to interface to a variety of remote computers, four DEC graphics displays, and a remote job entry station. There were several communications languages implemented in the communications processor (PDP-15 computer) to service the variety of telecommunications links. Concurrent with this activity was the development by us of the communication link spooling packages. These packages were in stage I of production by the time the special software was in an acceptable state, December 9, 1971. The IACC began extended (final) acceptance test December 13, 1971.

PDP-10 Systems Programming

C. E. Hammons

SYSDPY. The DECsystem-10 (PDP-10) display-controlled system monitor program was modified to better support our operations. Instead of all jobs in the system being displayed, the operator has a choice of (1) all jobs monitored, (2) system jobs monitored, or (3) user jobs monitored. This eases system operation significantly.

FAILSAFE. The disk dump/restore program for DECsystem-10 (FAILSA) was modified to accommodate the unusually large number of disks that are on the IACC/DECsystem-10.

⁴ *Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4561, p. 120.*

PDP-15. A PDP-15 DECtape manipulating program, which was written to list ASCII files from a PDP-9 or PDP-15 computer on the DECsystem-10, was modified to handle PDP-15 or PDP-9 binary DECtape files. This was done to allow local data acquisition systems (PDP-15's) quicker data conversion for use on the 360 computers.

Communications between the IACC DECsystem-10 and Remote Stations

D. R. Winkler

The IACC DECsystem-10 is connected by telephone lines to an IBM (International Business Machines) 360 computer at the Computing Center, an SEL (Systems Engineering Laboratory) 840A computer at ORIC (Oak Ridge Isochronous Cyclotron), an SEL 810B at ORELA (Oak Ridge Electron Linear Accelerator), and an IBM 2780 remote job entry station at Y-12. The IBM 360 line, the SEL 810B line, and the SEL 840A line are high speed (5100 characters per second), while the IBM 2780 line is low speed (300 characters per second).

Each link has a unique DECsystem-10 queue and a job always residing in the DECsystem-10. The job is dormant until either line activity occurs or work is placed in its queue. The job becomes active to process the request.

IBMSPL is the job which controls the link to the IBM 360 computer. Its queue consists of files created by other jobs controlling remote links and by DECsystem-10 time-sharing users. The files consist of batch jobs to be submitted to the IBM 360 computer. **IBMSPL** creates a disk file to store output from the IBM 360 computer. This output is then forwarded to its true final destination, which may be any other remote station, the DECsystem-10 printer or punch, or any DECsystem-10 user's disk area.

Y12SPL is the job controlling the link to the IBM 2780 station. Its queue consists of files, generated by **IBMSPL**, to be printed or punched at the 2780 station. Card decks received from the 2780 station are stored in a disk file which is passed on by a queue entry to **IBMSPL**. Printing may be interrupted at the remote station to submit a job.

RICSPL is the job controlling the link to the SEL 840A computer. This job is functionally identical to **Y12SPL**; however character translation must be performed, as the link employs four of eight transmission code.

ORESPL controls the link to the SEL 810B computer. Raw data stored on the data acquisition disks at ORELA can be dumped across the link into a disk file at the DECsystem-10. The data can be dumped in a format suitable for immediate access by FORTRAN display programs. Jobs can be submitted to the DECsystem-10 batch controller and to the IBM 360 computer. Print files, 810B object files, and dumped files can be sent from the DECsystem-10 to the SEL 810B computer.

Time-Sharing Job Submission to the IBM 360 Computer

D. R. Winkler

SUBMIT is a program which enables the DECsystem-10 user to send jobs to the IBM 360 computer. An interactive dialogue enables the user to build the job stream from Teletype lines and/or data files.

Each job submission to the IBM 360 computer results in a response which shows the job is in the input queue. This response is placed in a file in the time-sharing user's disk area. **STATUS** searches for this file and, when found, types the file.

Preparing for ORNL Time Sharing

R. K. Gryder

Extensive efforts have been devoted to preparing the DECsystem-10 computer to service the time-sharing computing requirements of the Laboratory.

The three objectives of this work are (1) to develop and maintain a user-oriented time-sharing system capable of immediate response to requests, (2) to provide quick and competent technical assistance for users, and (3) to provide the greatest possible range of capabilities consistent with the above objectives.

Objective 1 has been pursued by modification of DEC software to provide more meaningful diagnostics and reduce likelihood of disastrous user errors, collection and adaptation of computer-aided tutorial programs, and implementation of a HELP command which supplies information to the user at his terminal.

Objective 2 has required study of the many facets of time sharing, both on the DEC 10 and commercial services. Techniques for communicating with other systems have been resolved, and idiosyncrasies of the DEC-10 have been identified. Timing comparisons with other computing equipment were made to enable development of guidelines for machine utilization.

Objective 3 has dictated collection and implementation of languages (BLISS, PAL, LISP, etc.) and libraries of programs. FORTRAN libraries available include the Scientific Subroutine Package, the CTC Numerical Analysis Library, and numerous interactive programs from DECUS (DEC Users Society). The BASIC library includes statistical, engineering, mathematical, and general utility programs, in addition to a generous supply of games.

Data Acquisition and Analysis Systems

Nancy A. Betz J. K. Dyer
J. G. Craven C. H. Perritt
C. L. Thompson

ORELA. Operation of the data acquisition system⁵ was improved through the use of new routines which allow the accelerator operator to ascertain which experiments are operating, to determine how much data has been collected by each experiment, and to continue data acquisition when it is stopped due to intermittent hardware malfunctions. Samples, at the experimenters' stations, can now be moved into and out of the neutron beam under program control due to improvements in the hardware and software. The maximum obtainable data rate was slightly increased, new options were added to the display routines, and new CRUNCH⁶ routines were written as needed. The PDP-9 interface was completed, and the corresponding software which handles channel-connected data acquisition computers was expanded to allow the PDP-9 to use the peripherals on data acquisition computer 2 (DAC-2) in the same manner as the PDP-4 and DAC-1 are using them.

The IACC⁷ and DAC-2's interface to it arrived at about the same time. Considerable effort was consumed in locating problems which prevented communications between the two systems to proceed smoothly. The purpose of the link is to allow rapid transmission of information between the data acquisition and data analysis facilities. It will permit an experimenter to obtain a more accurate check on the progress of his experiment. New software which uses the binary synchronous communication method

5. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, p. 36.

6. *Phys. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4513, p. 105.

7. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1970*, ORNL-4592, p. 27.

of data transmission was developed for DAC-2 in order to handle the telephone link between DAC-2 and the IACC. Although a few problems remain in both the hardware and software, considerable use has been made of this link. The ability to list PDP-10 programs on DAC-2's line printer has been invaluable in debugging software for the display stations.⁸ The routines currently enable either computer to use the peripherals located on the other computer. Use of the link will be expanded to allow DAC-2 to submit jobs to the PDP-10, to allow the data acquisition computer connected to DAC-2 to use the link to the IACC, and to allow use of the IBM 360/75, which is also connected to the IACC, from DAC-2 and its associated computers.

Much time was spent in checking out the hardware and graphics system software provided by Digital Equipment Corporation for the display stations. The software provided consists of five subsystems (PDP-10 graphics primitives, PDP-15 display file handler, interface handlers, line encoders, and PDP-15 graphics primitives) which enable a picture to be built at a display station from FORTRAN calls to the PDP-10 graphics primitives. Interaction with the picture is allowed via a light pen and function keys with the information being transmitted back to the PDP-10 for determination of the display user's request and action to fulfill it. The display stations will be the experimenters' main port of entry to the ORELA data analysis system, which will use the PDP-10, the IBM 360/75, DAC-2, and the display stations. Work on this system has barely begun. Although parts of the analysis system will be available for use about mid-1972, it will require about 1½ years to achieve normal operation.

Specifications for ORELA Phase IIIA have been written and let out on bid. It will be another data acquisition system similar to DAC-1, with a channel connect to DAC-2. Approval for Phase IIIB has been granted. Phase IIIB is a peripheral exchange controller which will replace DAC-2's duties of controlling the traffic among the computers and peripherals, thus enabling DAC-2 to acquire more data. Detailed specifications for this system will be written in early 1972.

Thermonuclear Division data acquisition computer system. The Thermonuclear Division is in the process of greatly expanding its data acquisition facilities in order to improve the efficiency and reliability of data taking and to extend the range of feasible studies.⁹ The main experiments to be serviced by the new equipment are (1) ORMAK, Oak Ridge Tokamak; (2) ELMO, which provides mirror-confined high-beta plasmas for basic studies; and (3) HBBT, High Beta Bumpy Torus. We have been involved in planning the system and writing the specifications for it. The completed system will consist of two data acquisition computers to service the above-mentioned experiments and a remote entry station (RES).

Each data acquisition computer will be interfaced to the RES via telephone lines. The RES will also be interfaced to the IACC system via telephone lines. It will be used to submit jobs to the computer at the Central Computing Facility, to list output from those jobs, and to transfer data between the data acquisition and Central Computing Facility. Although analysis of the data will be performed at the Central Computing Facility, an experimenter will often create and run his analysis programs via time-sharing Teletypes located at the Thermonuclear Division. He will also be able to send data back to the data acquisition computer.

The detailed specifications for the system are almost complete and will be placed out for bid in the first quarter of 1972.

8. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 122.

9. *Proposal for Computer Assisted Data Acquisition for ORNL Fusion Experiments*, ORNL-TM-3593 (October 1971).

Computer Services

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EQUIPMENT

The DEC Computer

During the first half of the year, a Digital Equipment Corporation PDP-10 computer system was installed at the ORNL Computing Center. The system is to function as the Immediate Analysis and Coordinating Computer¹ (IACC), which will provide for the immediate analysis requirements of ORELA Phase II and the coordinating computer requirements of the Mathematics Division.² The system is made up of one PDP-10 computer with a PDP-15 computer subsystem to handle all the communications requirements between the PDP-10 and the other remote facilities. Among these remote facilities are four interactive graphic terminals (a PDP-15 computer driving a display console), the data acquisition computers at ORELA, the IBM 360/75, Teletypes, and other remote job entry terminals.

Following preliminary acceptance of the hardware, further development and testing of the special software required were carried out for several months. When this task was completed and all was determined to be ready, an extended acceptance test of the entire computer system with remotes was begun on December 13, 1971, and extended past the end of this report period. At that time, there was every indication that the system would pass the acceptance test with no difficulty.

Figure 13 is a schematic diagram of the PDP-10 system showing the equipment component, as well as the links to remote stations which make up the entire network.

The IBM Computers

The IBM 360/75 and 360/91 computer systems have been described in earlier reports.³ During this report period, one IBM 2314-1 Direct Access Facility was procured via excess ADP equipment procedures and added to the 360/91 system in March 1971. In January 1971, the two remote links to the Naval Research Laboratory⁴ were finalized with the installation of one IBM 2701 Data Adapter on each IBM computer system. At this time, a 2701 was also installed on the 360/75 to enable communication with the anticipated PDP-10 computer. In February 1971, a two-channel switch was installed on the 2314-1 Direct

1. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1970*, ORNL-4592, p. 27.
2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 120-22.
3. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, pp. 55-57.
4. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 125.

Access Storage Facility already installed on the 360/75. This feature permits both the 360/75 and 360/91 to share (electronically) this storage device. In March 1971, additional features were installed on the 360/75 to permit more low-speed terminals (Teletype- IBM 2741's) to access the computer simultaneously. A total of 22 such lines are now available to users. In April 1971, a universal character set capability was installed on one of the printers (the one which is switchable between computers) to accommodate users with special print requirements (lower case, special symbols, etc.). Also in April, two-channel switches were installed which permitted both computers to share the IBM 2321 data cell and four IBM 2311 disk drives. This installation made it possible to run all remote terminal systems on either computer system, thus increasing

the reliability of the remote service considerably. In May 1971, a two-channel switch was installed on the 2314-1 Direct Access Storage Facility installed earlier during this year. Also installed in May were (1) another 2701 Data Adapter to permit remote linkage with the U.S. Army's Harry Diamond Laboratories and (2) an additional feature to an already-installed 2701 to permit linkage with the U.S. Navy's Weapons Systems Analysis Office.

All of the equipment installed during this period has resulted in a rather extensive and elaborate computer network with linkages to a variety of remote terminals ranging from other small computers to Teletypes. Several figures follow which describe the present equipment configuration at the ORNL Computing Center, as well as the rather elaborate network they form and the remote terminals they serve. Figure 14 depicts the three main computer systems at the ORNL Computing Center and shows the links between them and to other remote terminals. Some indication is given as to physical location in the three computer rooms. Figures 15 and 16 show the remote terminal services and linkages provided by the 360/75 and 360/91, respectively, while Fig. 17 shows, in more schematic form, the total network of computers and remote terminals.

ORNL DWG 71-13339

Fig. 15. Remote terminals to the IBM 360/75.

ORNL-DWG 71-13338R

Fig. 16. Remote terminals for the IBM 360/91.

Fig. 17. Computer links and remote terminal services — ORNL Computing Center.

The CDC Computers

The CDC 160-A continues to provide a variety of peripheral services (card-to-printer, card-to-tape, paper tape processing, etc.), although at a considerably reduced level. More and more of this type of function is being transferred to the newly installed PDP-10. Only the absence of a heavy-duty paper tape reader on the PDP-10 has prevented the complete transition of all peripheral work to the new machine. At the end of the report period, a new paper tape reader for the PDP-10 had been approved and procedures begun for its acquisition. When this device is installed and all paper tape work has been successfully transferred to the PDP-10, the CDC 160-A will be retired and disposed of through appropriate excess property procedures.

WORK LOAD AND PERFORMANCE

The following figures give some indication of equipment performance and utilization for the report period. Figures 18 and 19 show the hours in use and the hours of downtime for the IBM 360/91 and 360/75, respectively, with previous experience included for comparison purposes. Figures 20 and 21 show the use of the 360/91 and 360/75, respectively, by the various divisions during 1971, while Fig. 22 indicates the work load at the ORNL Computing Center as measured by the average number of jobs received per scheduled workday. Since the acceptance test period for the PDP-10 had not yet been finished at the end of this report period, data and graphs depicting its performance will not appear until the next report.

The IBM computer systems were operated for most of the report period under Release 19.6 of the IBM operating system as modified at ORNL. (See the section on Systems Programming for additional descriptions of the operating system and its modifications.) The addition of several remote lines and the capability of sharing files of storage between computers put additional demands on the system, but any difficulties were overcome locally, and smooth operation of the computer network has been the normal mode. Slightly over 200,000 jobs were processed during 1971 by both computers. This represents a large increase over last year and is attributed to the addition of several remote job entry terminals to the network, and to the increased use of the CRBE remote terminal system.

The Computing Center continues to operate on a scheduled basis 24 hr a day, Monday through Friday, with extra shifts (an average of three to four) on the weekends on an overtime basis. The Computer Services staff remained at about 45 people, the same level reported at the end of the last period.

Fig. 18. Hours in use and downtime for the IBM 360/91.

Fig. 19. Hours in use and downtime for the IBM 360/75.

Fig. 20. Divisional use of the IBM 360/91 in 1971.

Fig. 21. Divisional use of the IBM 360/75 in 1971.

Fig. 22. Work load at ORNL Computing Center.

Mathematical Statistics

INTRODUCTION

D. A. Gardiner

During the past two years, especially, the Oak Ridge National Laboratory has paid more than the usual amount of attention to interdisciplinary research. This was motivated for the most part, probably, by the Environment and Technology Assessment project undertaken for the Office of Interdisciplinary Research of the National Science Foundation. To some of the Laboratory personnel the concept may have appeared novel, especially since a survey was conducted within the Laboratory to obtain information about experience with and attitudes toward this "team" approach to solving important problems. To the practicing statistician, of course, there is nothing new or novel about interdisciplinary research. It is his life's work. His accomplishments are measured, in the main, by his contributions to the solution of someone else's problems.

This year, as in the past, the ORNL statisticians have contributed to the solutions of problems emanating from the other research divisions of ORNL. Their greatest efforts continue to be directed toward biological problems as a consequence of demand. Some of this is reported in the Applications section, following, along with accounts of some of the work performed at the request of other divisions and projects. The reader will not fail to note, also, that the accounts contained in the Research section are accounts of research suggested by problems from other disciplines.

Two ORAU Fellows were graduated from the Statistics Department in 1971, receiving their Ph.D. degrees from the University of Tennessee and Virginia Polytechnic Institute and State University. A total of ten statisticians now have written doctoral dissertations as ORAU Fellows with members of the Statistics Department.

STATISTICAL RESEARCH

Invariance and Minimization of Information in Sequential Tests

E. C. Anderson¹

A study² was made of information in sequential tests of simple hypotheses based on a sequence of observable random variables $X_1, X_2, X_3, \dots$. This extends the work of Tittle³ and Kork⁴ in this area.

1. ORAU Fellow.

2. E. C. Anderson, Ph.D. thesis, University of Tennessee, Knoxville, 1971.

3. R. L. Tittle, *Information Theory in Sequential Analysis*, ORNL-4208 (1968).

4. J. O. Kork, unpublished doctoral thesis, University of Tennessee, Knoxville, 1969.

Probability spaces originally developed by G. E. Albert are used along with the analytical representation of information obtained by Kork in any σ -algebra $\mathbb{C}$ that lies between the σ -algebra $\mathbb{C}$ generated by the stopping random variable N and the decision random variable Y .

Let (a_k, b_{ki}) be a sequential test of simple hypotheses. If $T_1, T_2, T_3, \dots$ is a sequence of sufficient and transitive statistics for a family of probability measures $\{P_l, l \in L\}$, then a sequential test (a_k^0, b_{ki}^0) based on the sequence $T_1, T_2, T_3, \dots$ can be constructed from the test (a_k, b_{ki}) such that $I(\mathbb{B}) = I(\mathbb{C}_t)$, where $\mathbb{C}_t$ is the σ -algebra generated by the terminal random vector (T_N, N, Y) . Conditions are obtained under which $I(\mathbb{B}_t) = I(\mathbb{C}_t)$ when the original test (a_k, b_{ki}) is based on the sequence $T_1, T_2, T_3, \dots$ and the condition of sufficiency is removed. The latter generalizes results obtained by Tittle.

A concept of minimum information is discussed which extends to the sequential case work begun by Kullback.⁵ It is shown that if a probability measure P_2 is fixed and constraints are placed on probability measures P_1 by a sequence of statistics $T_1, T_2, T_3, \dots$, then the minimum information of P_1 with respect to P_2 occurs when P_1 has the differential form

$$cP_1 = d\bar{P}_1^* = \frac{e^{rT_N}}{M_2(r)} dP_2.$$

Conditions under which the minimum information is obtained when P_1 and P_2 are constructed from a sequence of compatible density functions and the minimizing measure $\bar{P}_1^*$ has the same form are also considered.

An Algorithm for the Construction of "D-Optimal" Experimental Design

T. J. Mitchell

There has been considerable interest among statisticians in the problem of choosing an experimental design to satisfy a specific criterion. While it is usually more desirable in practice to choose a design that is good with respect to several criteria, without necessarily being optimal with respect to any one of them, the method of using a single criterion is an important way of constructing new designs.

I shall consider here the usual linear model $y = X\beta + \epsilon$, where y is an $n \times 1$ vector of observations, X is an $n \times k$ estimation matrix (of rank k) of constants, β is the $k \times 1$ vector of coefficients to be estimated, and ϵ is an $n \times 1$ vector of independently and identically distributed random variables, each having mean 0 and unknown variance σ^2 . The i th row of X is $f(x_i)'$, where x_i is the i th design point and the function f depends on the model. I shall denote the number of independent variables by p , so that x_i is a point in a p -dimensional region χ in which it is feasible to perform experiments.

The least-squares estimate of β is $\hat{\beta} = (X'X)^{-1} X'y$, and the covariance matrix of $\hat{\beta}$ is $(X'X)^{-1} \sigma^2$. At any point $x \in \chi$, the predicted (or estimated) value of the "true" response is $\hat{y}(x) = f(x)'\hat{\beta}$. If the model is correct, the expectation of $\hat{y}(x)$ is $\eta(x)$, the mean value of the response at the point x . The variance of $\hat{y}(x)$ is given by $v(x) = f(x)'(X'X)^{-1} f(x) \sigma^2$.

Several criteria have been advanced for the purpose of comparing designs and for constructing optimal designs. Probably the most popular is the maximization of $|X'X|$. One of the attractive features of this criterion is that designs which are optimal with respect to it are invariably "good" in other respects (e.g., low variances for the parameters, low correlations among parameters, low maximum $v(x)$ over χ). I shall

5. S. Kullback, *Information Theory and Statistics*, John Wiley and Sons, Inc., New York, 1959.

refer to designs that maximize $|X'X|$, given a specified linear model and a value of n , as " D -optimal" designs.

There has been some attention given to constructing D -optimal designs for specified n , but the problem is a very difficult one. Recently, attempts have been made to attack this problem using a computer. These algorithms are based, for the most part, on conventional constrained maximization techniques, with a few special wrinkles. The most frequently encountered difficulties are:

1. the large number of variables (np) that must be handled;
2. the complex nature of the objective function $|X'X|$, especially the existence of several local maxima.

Further difficulties arise if each independent variable is required to take one of a specified number of levels, as, for example, in a factorial type of experiment. This then becomes an integer programming problem.

Probably as a result of the computational difficulties, very few new designs in the literature owe their existence to the application of computer algorithms to the maximization of $|X'X|$. The purpose of this report is to describe a new algorithm which I have applied to this problem and to discuss the performance of this algorithm in some test cases.

A preliminary version of the algorithm has already been described in a previous report.⁶ Starting with a randomly chosen n -run design, the initial set of n runs is then improved by

1. adding an $(n + 1)$ st run, chosen so that the maximum possible increase in $|X'X|$ is achieved, then
2. removing (subtracting) that run in the resulting design which results in the minimum possible decrease in $|X'X|$.

These two steps are accomplished by first adding to the original design that point at which $v(x)$ is maximum, then subtracting from the resulting $(n + 1)$ -run design that point at which $v(x)$ is minimum. It can easily be shown that the resulting n -run design has $|X'X|$ greater than or equal to that of the original. Similarly, one could attempt to improve the original design by subtracting a point first and then adding a point.

This basic algorithm has recently been modified to permit the replacement of more than one point of the original design at each iteration. Rather than insisting that an $(n + 1)$ -point design be returned immediately to an n -point design through the subtraction of a point, I now permit the algorithm to make an "excursion" in which designs of various sizes are constructed (always by adding or subtracting a single point from the previous design in the excursion), eventually returning to an n -point design. If no improvement in the determinant is made, all the designs constructed on the excursion are ostracized by placing them in a set of "failure designs" called F . The set F is then used to guide the course of the next excursion, which always starts with the currently best n -point design. The choice of whether to begin an excursion with the addition or subtraction of a point is made randomly.

Letting D be the current design at any point during the course of an excursion, the rules for continuing the excursion are as follows:

1. If the number of points in D exceeds n , subtract a point if D is not in F , and add a point otherwise.
2. If the number of points in D is less than n , add a point if D is not in F , and subtract a point otherwise.

(To determine whether or not D is in F , only the determinant of $X'X$ is examined. This is not a foolproof method for testing the equivalence of designs, since two different designs may have the same $|X'X|$.)

6. Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4661, p. 130.

However, its use does not seem to impair the overall performance of the algorithm, and it takes only a fraction of the time that would be required by an exact test of equivalence.)

It is easy to see that, at the beginning, when the set F is empty, the algorithm simply adds and then subtracts (or subtracts and then adds) as it would in the initial, more restrictive version previously described. The rules are such that the excursion always proceeds in the direction of an n -point design, unless it comes to a design in F , which has already led to failure. Then it reverses direction, after adding to F those designs constructed during the excursion up to that point.

Each time an excursion improves the currently best n -point design (i.e., increases $|X'X|$) the set F is cleared, and a new start is made. Eventually, as it gets more and more difficult to do better, the excursions stray widely from the n -point level. To stop the algorithm, I have set limits on the minimum and maximum number of points permitted in a design constructed during an excursion. When the upper limit, for example, is encountered, that excursion is ended, and future excursions are restricted to designs with n or less points. (This restriction is, of course, lifted when an improved n -point design is found, in which case the algorithm starts anew.) If both limits are encountered before an improved n -point design can be found, the algorithm stops.

The choice of these upper and lower limits on permissible design size is made arbitrarily. I have found that excursions that wander far away from the n -point level take up a good deal of computer time and seldom result in an improvement of the currently best design. On the other hand, narrowly spaced limits are too restrictive. I usually set these limits at $n \pm 6$, having found this to be a reasonable compromise.

What does one do when, during the course of an excursion, designs are constructed in which the number of runs is less than the number of parameters to be estimated? For such designs $|X'X|$ is 0, no matter where the design points are located. To avoid this problem, I actually attempt to maximize $D^* = |X'X + \epsilon I|$, where ϵ is a small positive number, rather than $D = |X'X|$. Although I have not studied the consequences of this very carefully, it appears that the set of points that maximizes D^* also maximizes D . The advantage is that D^* is never 0.

This algorithm has been applied to the construction of designs for the first-order model: $y = \mu_0 + \beta_1 x_1 + \dots + \beta_p x_p$ over a cubic region of interest $-1 \leq x_i \leq 1, i = 1, 2, \dots, p$. For this model, it is known that D -optimal designs are such that each x_i must be -1 or 1 . One reason for considering this situation, first is that there are so many cases for which the optimum design is known, so the algorithm can be tested. In particular, if n is a multiple of 4, the optimal design is orthogonal (i.e., $X'X$ is a diagonal matrix).

Table 2. Ratio of successes to tries in test cases for first-order model

Numbers in parentheses refer to computer time in seconds per try on the IBM 360/91

p	$n = 8$	$n = 12$	$n = 16$	$n = 20$
2	10/10 ^a	10/10 ^a	10/10 ^a	10/10 ^a
3	10/10 ^a	10/10 ^a	10/10 ^a	10/10 ^a
4	9/10 ^b	10/10 ^b	8/10 ^a	7/10 ^a
5	5/10(4.2)	2/10 ^b	4/10 ^b	2/10 ^b
6	10/10(5.7)	2/10(6.0)	2/10(6.3)	1/10(7.0)
7	10/10(8.9)	1/10(12.5)	2/20(10.7)	1/20(9.8)
8		2/10(21.8)	0/20(23.5)	
9		1/10(50.1)		

^aComputer time for all these designs averaged 1.1 sec per try.

^bComputer time for all these designs averaged 2.3 sec per try.

To test the algorithm, therefore, I considered the cases given in Table 2. Since the algorithm is not guaranteed to find a global optimum, I gave it ten different "tries" in each case. (In three of the more difficult cases, 20 tries were made.) The entries in the table indicate the ratio of successes (optimal designs) to tries and also, in parentheses, the average amount of computer time per try on the IBM 360/91. The object of these test cases is to demonstrate the feasibility of the algorithm and to identify its limitations. These results will be used as a guide in applying the algorithm to the construction of new designs, corresponding to values of n not considered in Table 2.

An earlier version of this algorithm has already been used to construct some new two-level designs, for both first-order and second-order models. The goal now is to apply the most recent version of the algorithm, which has been discussed here, to the development of a comprehensive catalog of D -optimal designs. The algorithm is also expected to be useful in constructing designs for special cases, in which either the model or the set of permissible experimental points differs from the standard situation.

Fixed-Precision Estimation of the Binomial Parameter θ ⁷

T. A. DeRouen⁸ T. J. Mitchell

We have recently considered various methods of estimating the parameter θ in the binomial distribution, where the probability of obtaining x "successes" in n trials is $\binom{n}{x} \theta^x (1 - \theta)^{n-x}$. The usual estimator of θ is the maximum likelihood estimator $\hat{\theta} = x/n$, which has great intuitive appeal. A well-established alternative approach to the estimation of θ is to define formally a "loss function" which quantifies the "badness" of the estimate $\hat{\theta}(x)$ used when a particular experimental result (x) is observed. This loss function is largely arbitrary and should depend on the use that is to be made of the estimator. The "risk" is defined to be the loss averaged over all possible experimental results (i.e., over all values of x) and is a function of θ . For every proposed method of estimating θ , a risk function can be calculated, and any two methods may be compared by comparing their risk functions. There are, however, two critical decisions involved, namely (1) the choice of an appropriate loss function and (2) the choice of a criterion by which risk functions can be ranked. The "optimality" of an estimator is, of course, highly dependent on these choices.

In this research, we have considered the estimation of θ for the following loss function:

$$L(\hat{\theta}(x), \theta) = \begin{cases} 0 & \text{if } |\hat{\theta}(x) - \theta| \leq \Delta/2 \\ 1 & \text{otherwise,} \end{cases} \quad (1)$$

where Δ , which is between 0 and 1, is chosen to express the desired precision of the estimation. Under this loss function, the estimate $\hat{\theta}(x)$ is considered "right" if $\hat{\theta}(x)$ is sufficiently close to θ and "wrong" otherwise. The risk function is then simply the probability that the estimate $\hat{\theta}(x)$ is "wrong."

We have restricted our attention to the class of SBP estimators (i.e., those estimators which can be derived as Bayes estimators for a symmetric beta prior). (We refer to such estimators as "Bayes-suggested" estimators.) The risk functions within this class of estimators have been compared by two criteria:

C_1 : minimization of the maximum risk over θ , and

7. This research is based on part of T. A. DeRouen's doctoral dissertation completed June 1971 at Virginia Polytechnic Institute. Dr. DeRouen's research was supported by an Oak Ridge Associated Universities Graduate Fellowship at Oak Ridge National Laboratory.

8. Now at Tulane University Medical School.

C_2 : Minimization of the maximum integrated risk over θ , where the maximum is taken over the class of weighting functions used in the integration. This class of weighting functions is again the class of symmetric beta densities.

(Results for a third criterion were also obtained,⁹ but there is some doubt as to their interpretation and usefulness.)

It is easily shown that, for a given symmetric beta prior, defined by

$$\xi(\theta) = \frac{\theta^a (1 - \theta)^a}{B(a + 1, a + 1)}, \quad a > -1, \quad (2)$$

where B is the beta function, the posterior density of θ , given the observation x , also is beta:

$$\xi(\theta|x) = \frac{\theta^{a+x} (1 - \theta)^{a+n-x}}{B(a+x+1, a+n-x+1)}. \quad (3)$$

The Bayes estimator of θ for the assumed loss function (1) can then be shown to be the midpoint of the interval of width Δ that includes the maximum posterior probability. For each value of a in (2) there is a particular set of estimates $\hat{\theta}(x)$; it remains to choose the value of a that is optimal with respect to criteria C_1 and C_2 .

This was done numerically for the 21 combinations of the following values of n and Δ for which $\Delta \geq 1/(n+1)$:

$$\Delta = 0.05, 0.10, 0.15,$$

$$n = 9, 16, 25, 36, 49, 64, 81, 100.$$

(For $\Delta < 1/(n+1)$, the maximum risk is always 1 no matter what method of estimation is used, so we did not consider such cases.)

For all 21 cases studied, it was found that the value $a = 0$ in (2) yields the optimal estimator with respect to both criteria C_1 and C_2 . These results, which cover a fairly wide range of values for n and Δ , lead us to conjecture that for a general n and Δ , the uniform prior (i.e., $a = 0$) gives Bayes estimates that are optimal with respect to our two criteria.

The maximum risks (i.e., the probability that the estimate is "wrong") corresponding to this optimal estimator are given in Table 3 for the various combinations of n and Δ . One peculiarity in the behavior of

9. T. A. DeRouen and T. J. Mitchell, *Bayes-Suggested Solutions in Binomial Estimation*, ORNL-4700 (1971).

Table 3. Maximum risks corresponding to optimal SBP estimator ($a = 0$)

Δ	$n = 9$	$n = 16$	$n = 25$	$n = 36$	$n = 49$	$n = 64$	$n = 81$	$n = 100$
0.05			0.84	0.87	0.78	0.71	0.66	0.62
0.10		0.80	0.69	0.62	0.57	0.45	0.38	0.32
0.15	0.75	0.62	0.55	0.41	0.32	0.26	0.18	0.13

the maximum risk is that it does not decrease uniformly as n increases. Plotted as a function of n , the maximum risk was observed to experience a series of sharp declines or "drops" at values of n that are multiples of $1/\Delta$. At these values of n the maximum risk does decrease with increasing n . Between "drops," however the maximum risk increases somewhat with increasing n . This strange behavior is also shared by the usual maximum likelihood estimator, $\hat{\theta}(x) = x/n$, under the loss function (1).

Although this research was concerned mainly with fixed-precision estimation of the binomial parameter θ , the set of estimates $\hat{\theta}(x)$, $x = 0, \dots, n$, immediately gives a set of fixed-width confidence intervals for θ . The interval corresponding to the outcome x is simply $[\hat{\theta}(x) - \Delta/2, \hat{\theta}(x) + \Delta/2]$, and the confidence $C(\theta)$ is simply $1 - R(\hat{\theta}, \theta)$, where $R(\hat{\theta}, \theta)$ is the risk function.

We have compared the intervals derived from the optimal Bayes-suggested estimates described above with those given in the literature by Naddeo.¹⁰ Naddeo suggests using the maximum likelihood estimate, x/n , as the midpoint of the interval. This leads to the interval

$$x/n - \Delta/2 \leq \theta \leq x/n + \Delta/2,$$

where Δ is the fixed interval width. In order to determine the value of n necessary to make $\min_{\theta} C(\theta)$ sufficiently large, Naddeo gave the following approximation:

$$\bar{n} \Delta^2 \cong z_{\alpha/2}^2, \quad (4)$$

where $z_{\alpha/2}$ is defined as the point that leaves probability $\alpha/2$ in the right-hand tail of the standard Gaussian density and $\bar{n}$ is the minimum n necessary to ensure that

$$Pr\{x/n - \Delta/2 \leq \theta \leq x/n + \Delta/2\} \geq 1 - \alpha.$$

For 95% confidence, therefore, $\alpha = 0.05$ and $z_{0.025} = 1.96$, so the sample size n should be approximately $4/\Delta^2$.

A comparison of the two sets of interval estimates and a study of the accuracy of the approximate relationship (4) in predicting the minimum confidence level for Naddeo's set of intervals estimates were conducted simultaneously. The exact minimum confidence level was plotted as a function of n for both sets of estimates, along with the predicted minimum confidence level for Naddeo's estimates, $1 - \alpha$, where α is determined by (4).

In no case was the minimum confidence greater for Naddeo's intervals than for the Bayes-suggested intervals based on the uniform prior. Moreover, when $\alpha = 0$ in (2) (i.e., the beta prior is simply the uniform density) the posterior density, $\xi(\theta|x)$ in (3), is proportional to the likelihood function, $p(x|\theta)$. Thus the Bayes-suggested fixed-width confidence intervals based on the uniform prior are such that every value of θ in an interval has a greater likelihood than every point outside the interval. Naddeo's intervals do not have this property, since they are centered on the maximum values of the likelihood functions, which are not generally symmetric. However, the advantage of using the optimal Bayes-suggested intervals instead of Naddeo's intervals did not, in most cases, appear to be worth the extra effort involved.

The degree of inaccuracy of the approximation (4) for the minimum confidence level for Naddeo's estimates was also investigated. Unfortunately, Naddeo's approximation overestimates the minimum confidence for given n . Equivalently, if (4) is to be used to select n to achieve a specified confidence, the

10. A. Naddeo, *Rev. Int. Statist. Inst.* 36, 313-18 (1969).

value of n obtained is too small. A rule of thumb for correcting this error can be formulated by letting n_j be the smallest integer greater than or equal to J/Δ , $J = 1, 2, 3, \dots$. For a specified confidence $1 - \alpha$, use (4) to find $\bar{n}$. Then let the sample size n be the smallest n_j which is greater than or equal to $\bar{n}$. An added advantage of choosing n in this way is that the minimum confidence for Naddeo's intervals then appears to be very close to that of the "optimal" Bayes-suggested ($\alpha = 0$) intervals, which are difficult to construct without the aid of a computer.

Notwithstanding all this research we should remark that fixed-width confidence intervals for fixed sample sizes are appropriate only in very special situations, and the experimenter should be convinced that they are actually what he wants before he abandons the conventional confidence interval approach.

Estimation of a Linear Combination of Binomial Probabilities^{1 1}

T. A. DeRouen^{1 2} T. J. Mitchell

Let $\{X_i\}$ $i = 1, 2, \dots, k$, be independent random variables, each having a binomial distribution:

$$\text{Prob}[X_i = x] = f_i(x|\theta_i) = \binom{n_i}{x} \theta_i^x (1 - \theta_i)^{n_i - x}, \quad x = 1, 2, \dots, n_i.$$

Let γ be an arbitrary linear combination of the binomial probabilities θ_i , that is,

$$\gamma = \gamma(\theta) = \sum_{i=1}^k \alpha_i \theta_i = \alpha' \theta,$$

where $\alpha' = (\alpha_1, \alpha_2, \dots, \alpha_k)$ is a vector of specified constants and $\theta' = (\theta_1, \theta_2, \dots, \theta_k)$. Estimation of γ is the problem considered in this research. This problem arises, for example, in the estimation of main effects and interactions in factorial experiments with binomial responses.

We shall measure the accuracy of the estimator $\hat{\gamma}(x)$, where x' is the vector of observations $(x_1, x_2, \dots, x_k)$, by the quadratic loss function:

$$L(\hat{\gamma}(x), \gamma(\theta)) = [\hat{\gamma}(x) - \gamma(\theta)]^2.$$

The risk associated with the estimator $\hat{\gamma}$ is, as usual, the expectation of the loss:

$$r(\hat{\gamma}, \theta) = E_{(x|\theta)} [L(\hat{\gamma}(x), \gamma(\theta))] = \sum_x L(\hat{\gamma}(x), \gamma(\theta)) f(x|\theta),$$

where

$$f(x|\theta) = \prod_{i=1}^k f_i(x_i|\theta_i).$$

11. This research is based on part of T. A. DeRouen's doctoral dissertation completed June 1971 at Virginia Polytechnic Institute. Dr. DeRouen's research was supported by an Oak Ridge Associated Universities Graduate Fellowship at Oak Ridge National Laboratory.

12. Now at Tulane University Medical School.

The evaluation of an estimator is usually made by considering some measure of the overall performance of its risk function. The measure of performance used here is an average risk:

$$R(\hat{\gamma}, \tau) = \int_{\Theta} r(\hat{\gamma}, \theta) \tau(\theta) d\theta, \quad \Theta = \{\theta | 0 \leq \theta_i \leq 1, \quad i = 1, 2, \dots, k\},$$

where τ may be thought of as a weighting function to be used in integrating the risk function, or, from a Bayesian point of view, as a prior probability density on Θ .

Given a set D of estimators from which to choose $\hat{\gamma}$ and a set T of weighting functions (priors) with which to integrate the risk functions, consider the following definitions of optimality for estimators:

1. $\hat{\gamma}^* \in D$ is (D, T) -minimax if

$$\sup_{\tau \in T} R(\hat{\gamma}^*, \tau) \leq \sup_{\tau \in T} R(\hat{\gamma}, \tau), \quad \hat{\gamma} \in D. \quad (1)$$

2. $\hat{\gamma}^* \in D$ is $(D, \cdot)$ -minimax if (1) holds when T is the set of all possible weighting functions.
3. $\hat{\gamma}^* \in D$ is $(\cdot, T)$ -minimax if (1) holds and D is the set of all estimators. This is what Blum and Rosenblatt¹³ call the T -minimax estimator.
Note that if T consists of a single weighting function (prior), then the $(\cdot, T)$ -minimax estimator is the Bayes estimator for that prior.
4. $\hat{\gamma}^* \in D$ is $(\cdot, \cdot)$ -minimax if (1) holds when T is the set of all possible weighting functions and D is the set of all possible estimators. This corresponds to the usual minimax estimator.

The approach we used was to restrict consideration initially to the class of Bayes estimators derived from beta priors and then to determine whether this class contains an estimator that is optimal with respect to the chosen criterion.

The following results were obtained:

1. Let T be the class of all priors on θ which can be expressed as the product of independent priors on θ_i , each with specified mean μ_i . Then the $(\cdot, T)$ -minimax estimator of γ may be written $\hat{\gamma}^* = \sum \alpha_i \hat{\theta}_i^*$, where $\hat{\theta}_i^*$ is a weighted average of the specified prior mean μ_i and the maximum likelihood estimate (x_i/n_i) of θ_i . The weights are proportional to 1 and $\sqrt{n_i}$ respectively. This intuitively appealing result should have application to situations in which the experimenter is unwilling to specify the prior densities $\tau_i(\theta_i)$ but agrees to provide a prior guess of each θ_i . In practice, one would probably take these guesses as the prior means $\mu_1, \mu_2, \dots, \mu_k$.
2. Suppose all sample sizes are the same ($n_1 = n_2 = \dots = n_k$) and $\gamma = \sum \alpha_i \theta_i$ is such that all the $|\alpha_i|$ are equal. Then the estimate $\hat{\gamma} = \sum \alpha_i (x_i + C) (n_i + 2C)^{-1}$, where $C = (n/4k)^{1/2}$, is $(\cdot, \cdot)$ -minimax.
3. Let $\gamma = \theta_1 - \theta_2$, and let D be the class of Bayes estimators derived from independent symmetric beta priors on θ_1 and θ_2 ; that is, the estimator $\hat{\gamma}$ is of the form:

$$\hat{\gamma} = (x_1 + c_1) (n_1 + 2c_1)^{-1} - (x_2 + c_2) (n_2 + 2c_2)^{-1}; \quad c_1, c_2 \geq 0.$$

13. J. R. Blum and J. Rosenblatt, *Ann. Math. Statist.* 38, 1671-78 (1967).

Then the $(D, \cdot)$ -minimax estimator of γ is determined by choosing c_1 and c_2 to satisfy simultaneously the two equations:

$$c_1 (n_1 + 2c_1)^3 n_1^{-2} = c_2 (n_2 + 2c_2)^3 n_2^{-2},$$

$$4c_1^2 n_1^{-1} + 4c_2^2 n_2^{-1} = 1.$$

Although these equations do not provide a closed-form solution, they can easily be solved numerically for specified values of n_1 and n_2 . Values of c_1 and c_2 for various combinations of n_1 and n_2 have been tabulated¹⁴ together with maximum risk. A comparison of these maximum risks with those corresponding to the usual estimator $\hat{\gamma} = x_1 n_1^{-1} - x_2 n_2^{-1}$ shows not much difference as long as the sample sizes are approximately the same. If the sizes are heavily unbalanced, however, the maximum risk of the $(D, \cdot)$ -minimax estimator is considerably less than that of the usual estimator. It should be noted, however, that this "superiority" of the $(D, \cdot)$ -minimax estimator depends on the appropriateness of the squared error loss function as well as acceptance of the minimax approach for comparing estimators.

Air Quality Indices

J. J. Beauchamp F. L. Miller, Jr. W. D. Shults¹⁵

The Environmental Indices Team of the ORNL-NSF Environmental Program has been looking into the development of air quality or air pollution indices. A number of ways for combining measured information into a single number that reflects the overall state of the air quality within a given area have been proposed and investigated. It has been assumed that for each pollutant a standard has been set, that is, a concentration level which the pollutant should not exceed or at least exceed only a small portion of the time. It has also been assumed that the observed concentrations follow a log normal distribution, which implies that the distribution of the logarithms of the concentrations for each pollutant may be described by the two parameters: (1) the mean and (2) the variance of this distribution.

During the investigation of air quality indices, various weighting factors for each pollutant have been considered. These weighting factors represent an attempt to place a measure of importance on each of the observed pollutants. For example, if the prevailing level of a pollutant is high in a given city, then it is believed that this pollutant is more important there than it might be in another city where the prevailing level of the pollutant is normally low. In addition, it was thought that these weighting factors should take into account the normal fluctuations in the pollutant level. Since a desirable range for the individual pollutant index would be between 0 and 1, each individual pollutant index value was set equal to the estimated probability of the observed pollutant concentration being less than or equal to its observed value.

By using the above-mentioned considerations and assumptions the two following air quality indices have been proposed:

$$I_1(t) = \sum_{i=1}^{k(t)} w_i p_i(t)/k(t) \quad (1)$$

14. T. A. DeRouen and T. J. Mitchell, *Bayes-Suggested Solutions in Binomial Estimation*, ORNL-4700 (1971).

15. Analytical Chemistry Division and Environmental Indices Team.

and

$$I_2(t) = \left\{ \prod_{i=1}^{k(t)} p_i^{w'_i(t)} \right\}^{1/k(t)}, \quad (2)$$

where

t = particular time of observation;

$k(t)$ = number of pollutants observed at time t ;

$w_i = \sigma_i / (S_i - \mu_i)$ = weight of the i th pollutant, where it is assumed that $S_i > \mu_i$;

$w'_i = \min_j (w_j) / w_i$;

σ_i = standard deviation of the distribution of the logarithm of the observed concentrations for the i th pollutant;

μ_i = mean or average value of the distribution of the logarithm of the observed concentrations for the i th pollutant;

S_i = logarithm of the standard value for the i th pollutant; and

p_i = estimated probability that the concentration of the i th pollutant is less than or equal to its observed value under the log normal assumption.

The values of μ_i and σ_i may be set at fixed values, or they may be estimated from existing sets of data.

In Figs. 23–26, plots are shown for the two indices given in Eqs. (1) and (2) using 1968 CAMP data¹⁶ of 24-hr average concentrations for the two cities of Philadelphia and Denver. In this application the following four pollutants were observed: (1) carbon monoxide, (2) nitrogen dioxide, (3) sulfur dioxide, and (4) oxidants. A computer program was written to estimate the quantities needed in Eqs. (1) and (2) under the log normal assumption and to calculate the values of I_1 and I_2 for each day of the year 1968. For the times when no observations were taken on a particular pollutant, the indices were evaluated by using only the observed pollutants. The legend in Figs. 23–26 indicates how many pollutants were observed each day. Whenever there were no observations for any of the pollutants, both indices were set equal to zero. Computer programs have been written to test whether the distributions of the observed pollutant concentrations follow the normal or log normal distribution.

From an investigation of the plots of these proposed indices the following properties were noted:

1. The range of the index I_1 depends upon the number of observed pollutants and their respective weights.
2. It is possible that some high concentrations could be averaged down, which would yield an index that gives no indication that a bad situation exists.
3. The range of the I_2 index is always between 0 and 1.
4. If the observed pollutant concentrations are independent random variables and the weights, w_i , are equal, then

$$\{I_2(t)\}^{k(t)} = \prod_{i=1}^{k(t)} p_i(t),$$

16. National Air Pollution Control Administration Air Quality Data, *Camp Daily Average Values 1968*, Durham, N.C. (November 1969).

ORNL-DWG 72-2C28

Fig. 23. Values of $I_1(t)$ during 1968 for Philadelphia.

ORNL-DWG 72-2C29

Fig. 24. Values of $I_2(t)$ during 1968 for Philadelphia.

ORNL-DWG 72-2030

Fig. 25. Values of $I_1(t)$ during 1968 for Denver.

ORNL-DWG 72-2031

Fig. 26. Values of $I_2(t)$ during 1968 for Denver.

which represents the estimated joint probability that the pollutant concentration levels are less than or equal to their observed values.

Research work is continuing in the development and investigation of meaningful air quality indices, and these indices will be applied to existing sets of data.

Log Normal Regression

J. J. Beauchamp Norma C. Hull J. S. Olson¹⁷

Consider the random variable z and an independent nonrandom variable x such that

$$y = \ln z \quad (1)$$

has a normal distribution with mean

$$E(y) = \beta_0 + \beta_1 x \quad (2)$$

and variance σ^2 ; in other words, z has a log normal distribution. From a sample of n observations on z it is desired to find unbiased estimates of the mean and variance of the distribution of z . By following an approach similar to the one used by Finney¹⁸ and by using some of the properties of the log normal distribution, the following unbiased estimator of $E(z)$ is found:

$$[\exp(\hat{\beta}_0 + \hat{\beta}_1 w)] \psi(\hat{\sigma}^2/2), \quad (3)$$

where (i) $\hat{\beta}_0$ and $\hat{\beta}_1$ are the least-squares estimates of β_0 and β_1 , respectively, from a regression of y on x ; (ii) w is a particular value of the independent variable x ; (iii) $\hat{\sigma}^2$ is the residual mean square from the regression analysis of y on x ; and (iv) ψ is given by

$$\psi(t) = 1 + (1 - \phi/n)t + \frac{(n-2)(1 - \phi/n)^2}{n} \frac{t^2}{2!} + \frac{(n-2)^2(1 - \phi/n)^3}{n(n+2)} \frac{t^3}{3!} + \dots, \quad (4)$$

with

$$\phi = \frac{\left[\sum_{i=1}^n (x_i - w)^2 \right]}{\left[\sum_{i=1}^n (x_i - \bar{x})^2 \right]}. \quad (5)$$

Since $\psi(\hat{\sigma}^2/2)$ may converge slowly for the form given in Eq. (4), $\psi(t)$ is expanded in increasing powers of t to give

$$\psi(t) = e^t \left\{ 1 - \frac{t(\phi + t)}{n} + \frac{t^2 [t^2 + (16/3 + 2\phi)t + \phi^2 + 4\phi]}{2n^2} \right\} \quad (6)$$

17. Ecological Sciences Division.

18. D. J. Finney, *J. Roy. Statist. Soc. Suppl.* 7, 155-61 (1941).

through terms of order $1/n^2$. By using a similar procedure an unbiased estimator of $\text{Var}(z)$ through terms of order $1/n^2$ is given by

$$[\exp(2\hat{\beta}_0 + 2\hat{\beta}_1 w + \hat{\sigma}^2)] \left\{ e^{\hat{\sigma}^2} \left[1 - \frac{2\hat{\sigma}^2(\phi + 2\hat{\sigma}^2)}{n} + \frac{2(\hat{\sigma}^2)^2 [4(\hat{\sigma}^2)^2 + 2(16/3 + 2\phi)\hat{\sigma}^2 + \phi^2 + 4\phi]}{n^2} \right] \right. \\ \left. - \left[1 - \frac{\hat{\sigma}^2}{n} (\hat{\sigma}^2 + 2\phi) + \frac{(\hat{\sigma}^2)^2 [(\hat{\sigma}^2)^2 + (16/3 + 4\phi)\hat{\sigma}^2 + 4\phi^2 + 8\phi]}{2n^2} \right] \right\}. \quad (7)$$

In order to calculate the variance of the unbiased estimator given in expression (3) for $E(z)$, let

$$a_1(\hat{y}, \hat{\sigma}^2) = e^{\hat{\beta}_0 + \hat{\beta}_1 w} \psi\left(\frac{\hat{\sigma}^2}{2}\right). \quad (8)$$

Since the estimator given in Eq. (8) involves the product of two functions which are independent of each other, it follows that

$$\text{Var}(a_1(\hat{y}, \hat{\sigma}^2)) = \text{Var}(e^{\hat{\beta}_0 + \hat{\beta}_1 w}) \text{Var}\left(\psi\left(\frac{\hat{\sigma}^2}{2}\right)\right) + E^2(e^{\hat{\beta}_0 + \hat{\beta}_1 w}) \text{Var}\left(\psi\left(\frac{\hat{\sigma}^2}{2}\right)\right) \\ + E\left(\psi\left(\frac{\hat{\sigma}^2}{2}\right)\right) \text{Var}(e^{\hat{\beta}_0 + \hat{\beta}_1 w}). \quad (9)$$

After a determination of the different expressions in Eq. (9) and substituting them into this equation, it may be shown that

$$\text{Var}(a_1(\hat{y}, \hat{\sigma}^2)) = \left(\frac{c^2\phi}{n} + \frac{\sigma^4}{2n}\right) \exp[2(\beta_0 + \beta_1 w) + \sigma^2] \quad (10)$$

to terms of order $1/n$.

In many biological and ecological problems it is assumed that a dependent variable, Y , is a power function of an independent variable, X , of the form αX^β , for example, the regression of weight or mass of tree parts, like bole, branches without leaves, and leaves, on tree diameter. It is known that such data are appropriately treated with the logarithm of mass as a linear function of the logarithm of tree diameter, height, or a combined function. Numerous analyses which are appropriately treated with the logarithmic transformation of regression variates could be refined by using the above-derived unbiased estimators. A computer program, described in the Statistical Programs section of this report, has been written to calculate the necessary expressions needed to perform a log normal regression analysis on a set of observed data.

On Gini's Index of Diversity

V. R. R. Uppuluri

Suppose we have a population which is classified into k distinct categories. There are several measures proposed in determining the "diversity" in the population. Some of these measures are in terms of the probabilities $\pi_1, \pi_2, \dots, \pi_k$ associated with the categories. Among these, the only measure which was

derived in an axiomatic way is the entropy function,¹⁹

$$\sum_{i=1}^k \pi_i \log \pi_i .$$

Gini's index of diversity,

$$\sum_{i=1}^k \pi_i (1 - \pi_i) ,$$

is derived in an axiomatic approach, and some of its properties are studied.

Extension of Griffiths' Inequalities to Gaussian "Spin" Configuration Models

V. R. R. Uppuluri J. M. Dolan

The Ising model²⁰ was set up to investigate the behavior of substances when molecules possess a magnetic moment. The Ising model in its simplest form is a linear chain of n "sites"; each site has a spin σ_i taking values $+1$ and -1 with equal probability $1/2$. Let $\sigma^T = (\sigma_1, \sigma_2, \dots, \sigma_n)$ denote a typical spin configuration out of the set of 2^n possible configurations. In the classical Ising model of a ferromagnet, let $J_0 (\geq 0)$ denote the interaction between the nearest neighbors on the lattice. This model has been studied extensively by Onsager,²¹ Newell and Montroll,²² and Griffiths²³ among others. The *Hamiltonian* of the system is a real-valued function with the 2^n spin configurations as the domain and is defined by

$$H_\sigma = -J_0 \sum_{1 \leq i < j \leq n} \sigma_i \sigma_j , \quad (1)$$

where σ_i denotes the i th component of the vector σ .

The *partition function* Z is defined by

$$Z = \frac{1}{2^n} \sum_{\sigma} \exp(-\beta H_\sigma) , \quad (2)$$

where $\beta = 1/kT$, k being Boltzmann's constant and T the (absolute) temperature.

The *Gibbs probability* on the space of configurations is defined by

$$P(\sigma) = Z^{-1} \exp(-\beta H_\sigma) . \quad (3)$$

The expected value of a random variable X on this probability space is called the *thermal average* and is

19. D. K. Faddejev, *Usp. Mat. Nauk* 11, 227-31 (1956).

20. E. Ising, *Z. Phys.* 31, 253-58 (1925).

21. L. Onsager, *Phys. Rev.* 65, 117-49 (1944).

22. G. Newell and E. W. Montroll, *Rev. Mod. Phys.* 25, 353-89 (1953).

23. R. B. Griffiths, *J. Math. Phys.* 8, 478-84 (1967).

denoted by angular brackets as

$$\langle X \rangle = E[X] = \sum_{\sigma} X(\sigma) P(\sigma). \quad (4)$$

Griffiths²⁴ proved the following set of inequalities:

$$\langle \sigma_k \sigma_l \rangle \geq 0 \quad \text{for all } k, l = 1, 2, \dots, n \quad (5)$$

and

$$\langle \sigma_k \sigma_l \sigma_u \sigma_v \rangle - \langle \sigma_k \sigma_l \rangle \langle \sigma_u \sigma_v \rangle \geq 0 \quad \text{for all } k, l, u, v = 1, 2, \dots, n. \quad (6)$$

In fact, these inequalities have been proved for the case of more general H_0 by Griffiths²⁴ and extended by Kelly and Sherman.²⁵ According to Kelly and Sherman: "the physical consequences of (6) are far reaching," when we have the interaction strength $J_{uv} (\geq 0)$ between sites u and v . A further extension of this model in which the spin variable σ may take on the $p + 1$ values $p, p - 2, p - 4, \dots, 2 - p, -p$ is given by Griffiths.²⁶

In this note, we will extend the validity of inequalities (5) and (6) to the case where the spin vector $\sigma^T = (\sigma_1, \sigma_2, \dots, \sigma_n)$ has multivariate Gaussian distribution with mean vector zero and variance-covariance matrix A . In this case the space of spin configurations will be the n -dimensional Euclidean space, and the partition function will be defined by

$$Z = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dF(\sigma_1, \dots, \sigma_n) \exp(-\beta H_0), \quad (7)$$

where

$$\begin{aligned} dF(\sigma_1, \dots, \sigma_n) &= [|A^{-1}|^{1/2} / (2\pi)^{n/2}] \exp[-(\sigma^T A^{-1} \sigma)] d\sigma_1, \dots, d\sigma_n \\ &= f(\sigma) d\sigma_1, \dots, d\sigma_n, \end{aligned} \quad (8)$$

where A^{-1} is the inverse matrix of A , $|A^{-1}|$ denotes the determinant of A^{-1} , and σ is the transpose of the vector σ^T .

We can obtain a closed form for Z in the special case

$$H_0 = -J_0 \sum_{i < j} \sigma_i \sigma_j$$

by the use of the following:

Lemma 1: Any square matrix M can be decomposed uniquely as the sum of a symmetric matrix S and a skew matrix T .

24. Ibid.

25. D. G. Kelly and S. Sherman, *J. Math. Phys.* 9, 466-84 (1968).

26. P. B. Griffiths, *J. Math. Phys.* 10, 1559-65 (1969).

We obtain

$$H_\sigma = -J_0 \sigma^T [(uu^T - I)/2] \sigma, \quad (9)$$

where u^T is the transpose of the $n \times 1$ vector of units denoted by u and I is the $n \times n$ identity matrix.

In this case, it can be easily seen that

$$Z = |A^{-1}|^{1/2} |A^{-1} - \beta J_0 (uu^T - I)|^{1/2}, \quad (10)$$

and the Gibbs probability density function $g(\sigma) = g(\sigma_1, \dots, \sigma_n)$ on the space of configurations is given by

$$g(\sigma) = (|W^{-1}|^{1/2} / (2\pi)^{n/2}) \exp\{-\sigma^T W^{-1} \sigma / 2\}, \quad (11)$$

where

$$W^{-1} = A^{-1} - \beta J_0 (uu^T - I). \quad (12)$$

If $X(\sigma) = X(\sigma_1, \dots, \sigma_n)$ is any random variable defined on this probability space, we define the thermal average by

$$\langle X(\sigma) \rangle = E[X(\sigma)] = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} X(\sigma) g(\sigma) d\sigma. \quad (13)$$

Definition 1: We shall refer to (11) as the *Gaussian spin configuration model* in the classical case.

Definition 2: If we further specialize to the case where the variance-covariance matrix A is given by

$$A = \begin{bmatrix} \lambda & \nu & \nu & \dots & \nu \\ \nu & \lambda & \nu & \dots & \nu \\ \vdots & \vdots & \vdots & & \vdots \\ \nu & \nu & \nu & \dots & \lambda \end{bmatrix} \quad (14)$$

then we shall refer to the corresponding Gibbs probability density function as that of an *equicorrelated Gaussian spin configuration model* in the classical case.

Remark: We note that $\lambda \geq 0$, since it corresponds to the variance of the spin in any site, and ν can be either nonnegative or nonpositive since it corresponds to the covariance of the spins between any two sites. In order that (8) is a well-defined (nonsingular) probability density function, we will require that A be a positive definite matrix. This will imply that

$$\begin{aligned} \lambda &> 0, \\ -[1/(n-1)] < \nu/\lambda = \rho < 1. \end{aligned} \quad (15)$$

We will now extend the validity of Griffiths' inequalities (5) and (6) for equicorrelated Gaussian spin configuration models, with an assumption on βJ_0 . It is not known whether this assumption can be eliminated. Before we state our result we will give two lemmas, which are needed in the proof of the theorem.

Lemma 2: For $-[1/(n-1)] < \theta < 1$,

$$[I + \theta(uu^T - I)]^{-1} = \frac{1}{1-\theta} I - \frac{\theta}{1-\theta} \frac{1}{1+(n-1)\theta} uu^T.$$

Lemma 3: For any Gaussian random variables X_1, X_2, X_3 , and X_4 ,

$$\langle X_1 X_2 X_3 X_4 \rangle = \langle X_1 X_2 \rangle \langle X_3 X_4 \rangle + \langle X_1 X_3 \rangle \langle X_2 X_4 \rangle + \langle X_1 X_4 \rangle \langle X_2 X_3 \rangle.$$

Theorem: In the case of an equicorrelated spin configurations model, with the condition

$$-\frac{\rho}{(1-\rho)[1+(n-1)\rho]} \leq \lambda \beta J_0 < \frac{1}{(n-1)[1+(n-1)\rho]}, \quad (16)$$

we have

$$\langle \sigma_k \sigma_l \rangle \geq 0 \quad \text{for all } k, l = 1, 2, \dots, n,$$

and

$$\langle \sigma_k \sigma_l \sigma_u \sigma_v \rangle - \langle \sigma_k \sigma_l \rangle \langle \sigma_u \sigma_v \rangle \geq 0 \quad \text{for all } k, l, u, v = 1, 2, \dots, n.$$

On Bonferroni-Type Inequalities of the Same Degree for the Probability of Unions and Intersections

Milton Sobel²⁷ V. R. R. Uppuluri

For any collection of exchangeable events $A_1, A_2, \dots, A_k$, the Bonferroni inequalities are usually stated in the form

$$\text{Max} \{N_0, N_2, \dots, N_{k_e}\} \leq P \left\{ \bigcup_{i=1}^k A_i \right\} \leq \text{Min} \{N_1, N_3, \dots, N_{k_o}\}$$

where $N_0 = 0$, $k_e(k_o)$ is the largest even (odd) integer $\leq k$,

$$N_\nu = \sum_{\alpha=1}^{\nu} (-1)^{\alpha-1} \binom{k}{\alpha} P_\alpha \quad (\nu = 1, 2, \dots, k),$$

and $P_\alpha = P\{A_{i_1} A_{i_2} \dots A_{i_\alpha}\}$ for any collection of α events. We may regard N_ν as being of the ν th degree because it involves $P_1, P_2, \dots, P_\nu$; hence the lower and upper bounds above are never of the same degree. In a report, Sobel and Uppuluri²⁸ developed the following improved lower and upper bounds of the same degree.

27. Consultant.

28. M. Sobel and V. R. R. Uppuluri, *On Bonferroni-Type Inequalities of the Same Degree for the Probability of Unions and Intersections*. Technical Report No. 150a, School of Statistics, University of Minnesota (1971).

Theorem: For any fixed degree $\nu \leq k$,

$$\text{Max}\{L_0, L_2, \dots, L_{\nu_e}\} \leq P\left\{\bigcup_{i=1}^k A_i\right\} \leq \text{Min}\{L_1, L_3, \dots, L_{\nu_o}\},$$

where $\nu_e(\nu_o)$ is the largest even (odd) integer $\leq \nu$, for $0 \leq j \leq \nu \leq k$;

$$L_{\nu-j} = \sum_{\alpha=1}^m (-1)^{\alpha-1} \binom{k}{\alpha} P_{\alpha} + \sum_{\alpha=m+1}^{\nu} (-1)^{\alpha-1} a_{\alpha} P_{\alpha},$$

with

$$a_{\alpha} = \sum_{\beta \geq \alpha+j-\nu} \binom{j}{\beta} \binom{k-j}{\alpha-\beta} \text{ and } m = \min(j, \nu-j).$$

For degree $\nu = 2, 3$, and 4 these results are given explicitly. A related problem is to get lower and upper bounds for the probability of the intersection of events, P_k , for large k in terms of $P_1, P_2, \dots, P_{\nu}$. These are also derived and given explicitly for $\nu = 2, 3$, and 4. Applications of these inequalities to incomplete Dirichlet type I integrals and to equicorrelated multivariate normal distributions are indicated.

Sample Size Requirement

K. O. Bowman

The previous annual report²⁹ described the construction of tables for determining sample sizes for a one-way analysis of variance and for a randomized block design. The tables were published as ORNL reports^{30,31} and were subsequently published in the open literature.^{32,33} Because many requests were received for tables to accommodate larger experimental designs, the tables have been extended.³⁴

The earlier tables provided sample sizes for numbers of groups equal to 2 (1) 6. This has been extended to 7 (1) 11 (2) 15 (5) 30 (10) 60. For the randomized block design this was accompanied by a reduction in the number of observations per cell to 1 (1) 5 and by an increase in the levels of type I risk to four ($\alpha = 0.01, 0.05, 0.10$, and 0.20).

Distributional Properties of Estimators

K. O. Bowman

To a large extent models constructed in the applied sciences are not members of those classes which admit of appealing theoretical properties. As a consequence, serious errors can arise from assuming that

29. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 141-42.

30. M. A. Kastenbaum, D. G. Hoel, and K. O. Bowman, *Sample Size Requirement: Test of Equality of Several Gaussian Means*, ORNL-4468 (1969).

31. M. A. Kastenbaum, D. G. Hoel, and K. O. Bowman, *Adequate Sample Sizes for Randomized Block Designs*, ORNL-4527 (1970).

32. M. A. Kastenbaum, D. G. Hoel, and K. O. Bowman, *Biometrika* 57, 421-30 (1970).

33. M. A. Kastenbaum, D. G. Hoel, and K. O. Bowman, *Biometrika* 57, 573-77 (1970).

34. K. O. Bowman, *Sample Size Requirement: Continuation*, ORNL-4712 (1971).

standard statistical techniques may be applied to situations in which those appealing properties do not obtain. With more precise information on the low-order moments of estimators, however, approximate quantiles of the distributions of the estimators can be computed and serious errors avoided. It is along these lines that research has been conducted on (1) the distributional properties of estimators arising in what has become known as Fisher's Linkage Problem³⁵ and (2) the distributional properties of the skewness statistic, $\sqrt{b_1}$, arising in samples from nonnormal populations.

Fisher's Linkage Problem. This problem can be embedded in the following categorical structure; given four categories A, B, C, D with observed occurrences of a, b, c, d ($a + b + c + d = n$) and theoretical relative frequencies $(2 + \theta)/4, (1 - \theta)/4, (1 - \theta)/4, \theta/4$, respectively, what are the best methods of estimating θ ? It is shown that although the parameter θ can assume all values in the open interval $(0, 1)$, most estimators (including maximum likelihood, minimum chi-square, and linear estimators) assume a finite set of values for different sample configurations which are *estimator oriented*.

The higher-order terms of the moments of $\hat{\theta}$ (the maximum likelihood estimator) were obtained for the bias, variance, and third and fourth central moments, including coefficients as high as those of order n^{-9} .³⁶ This was achieved through the computerization of the Taylor expansion of $\hat{\theta}$ as a bivariate series in terms of the statistics $t_1 = (a - 2b - 2c - d)/n$, $t_2 = d/n$ and the expectation of appropriate terms in this and its second, third, and fourth powers. It was discovered that, distributionally, the maximum likelihood estimator enjoys few advantages over other estimators, and in fact very large samples are needed to achieve near-normality (in the sense of the skewness and kurtosis coefficients). Details are given in Bowman and Shenton.³⁷

The skewness statistic, $\sqrt{b_1}$. Attention was concentrated on samples of finite order, n , from Pearson type I distributions, that is, from distributions whose densities are proportional to $x^{a-1}(1-x)^{b-1}$, $0 < x < 1$. Using Taylor series expansions, the first four moments of $\sqrt{b_1}$ were tabulated to terms of order n^{-6} for sample sizes large enough to be used advantageously in the series. The bias, standard deviation (σ), skewness coefficient ($\sqrt{\beta_1}$), and kurtosis coefficient (β_2) of the estimate of skewness were tabulated for selected sample sizes and selected members of the Pearson type I family of distributions.

The general result indicates that the stability of the moment series involved deteriorates as β_2 increases from $\beta_1 + 1$ to just less than $(3\beta_1 + 6)/2$. Moreover, within the region defined by $\sqrt{\beta_1} = 0, \sqrt{\beta_1} = 2, \beta_2 = \beta_1 + 1, 2\beta_2 = 3\beta_1 + 6$, samples of size a little above 50 are large enough to pinpoint moment values up to the fourth. In this region the gradient of contours for $\sigma, \sqrt{\beta_1}, \beta_2$ is in general small, and the respective contours are remarkably similar in shape.

A detailed account of the computerized approach is given in Shenton, Bowman, and Sheehan.³⁸ It is intended to investigate the distribution of the estimate of kurtosis, b_2 , in the future.

STATISTICAL APPLICATIONS

Biology

Prenatal irradiation with fission neutrons and x rays (J. J. Beauchamp, E. B. Darden, Jr.,³⁹ and W. Friedberg⁴⁰). The results of an investigation of prenatal mortality in the mouse as influenced by irradiation

35. P. A. Fisher, *Statistical Methods for Research Workers*, p. 291, Oliver and Boyd, Edinburgh, 1936.

36. K. O. Bowman and L. R. Shenton, *Note on Fisher's Linkage Estimation Problem*, ORNL-4701 (1971).

37. K. O. Bowman and L. R. Shenton, *J. Statist. Comput. Simulation* 1 (1971).

38. L. R. Shenton, K. O. Bowman, and D. Sheehan, *J. Roy. Statist. Soc. (B)* 33 (1971).

39. Biology Division.

40. Civil Aeromedical Institute, Federal Aviation Agency, Oklahoma City, Okla.

of the embryo at the one-cell stage with fission neutrons and x rays were recently examined. Female mice which had been mated the night before were either irradiated or sham irradiated (control). Sixteen days after the treatment, the mice were killed, and the number of live fetuses was recorded for each mouse. For each dose of radiation the average number of live fetuses per mother was calculated from the observed data. From an examination of these data for the neutron radiation, it was noticed that the number of live fetuses per mother ranged between 9 and 10 for dose levels up to about 2 rads and then the number of live fetuses per mother dropped rapidly as the dose of radiation was increased. Therefore, it appeared that the relationship between radiation dose and the number of live fetuses per mother has a type of "shoulder" at the low dose levels and then drops off exponentially as the dose increases. The following function derived from target theory was proposed:

$$E(Y) = \theta_1 [1 - (1 - e^{-\theta_2 X})^{\theta_3}] ,$$

where

$E(Y)$ = expected or average number of live fetuses per mother at dose X ;

X = dose of radiation;

θ_1 = expected number of live fetuses per mother at dose $X = 0$;

$\theta_2 = 1/D_{37}$, where D_{37} is the increment of dose on the log-linear portion of the survival curve which reduces the survival by a factor of 0.37;

θ_3 = "extrapolation" number.

At each dose level X_i , $i = 1, 2, \dots, N$, there are N_i mothers, each with an observed number of live fetuses denoted by Y_{ij} , $j = 1, 2, \dots, N_i$. Let

$$\bar{Y}_i = \sum_{j=1}^{N_i} Y_{ij} / N_i ,$$

and assume that $\bar{Y}_i$ is normally distributed with mean

$$\theta_1 [1 - (1 - e^{-\theta_2 X_i})^{\theta_3}]$$

and variance σ^2/N_i . The least-squares estimates of the parameters θ_1 , θ_2 , and θ_3 were found by minimizing

$$\sum_{i=1}^N N_i \{ \bar{Y}_i - \theta_1 [1 - (1 - e^{-\theta_2 X_i})^{\theta_3}] \}^2 .$$

The final estimates of θ_1 , θ_2 , and θ_3 , calculated by iterative methods, are weighted least-squares estimates. Under the assumption that $\bar{Y}_i$ is normally distributed, these estimates are also maximum likelihood estimates. In Fig. 27 a representative set of data with the fitted curve is shown for mice irradiated with fission neutrons. Table 4 contains the estimates of the parameters along with their associated standard errors.

Fig. 27. Representative dose-response curve.

Table 4. Estimates of parameters

Parameter	Least-squares estimate	Estimated standard error of estimate
θ_1	9.86	0.21
θ_2	0.06	0.01
θ_3	1.24	0.28

Mutation frequency (D. G. Gosslee). A question of considerable importance is whether or not mutation frequencies induced by radiation are proportional to the dose of radiation. When the spontaneous mutation frequency is zero, an exact statistical test is known; but in the presence of spontaneous mutations, an exact test is not known.

Two approximate statistical tests were developed to test the hypothesis of proportionality in the presence of spontaneous mutations. In each test a statistic computed from the observed frequencies is compared with percentiles of frequency distributions in published tables. The statistic is a linear function of binomial random variables. Expressions for its standard error and its first four moments have been derived.

The first test utilizes an approximation to the normal distribution and the second an approximation to the appropriate Pearson distribution with third and fourth moments equal to the corresponding moments of the statistic. The Pearson approximation is proposed for general use. Conditions for using the normal approximation as a special case were developed.

The degree of approximation of the test depends on the mutation frequency, the size of the sample, and the dose levels and, therefore, must be evaluated for each experiment. However, either desk calculators or computer programs can be used to compute the statistics, the moments, and the degree of the approximations.

Enzyme kinetics (D. G. Gosslee). The general rate equation for the enzymic conversion of a single substrate to a single product is

where E, S, and P represent the enzyme, substrate, and product, respectively, and the k 's are reaction rate constants. Experiments involving statistical estimates of the rate constants arose from several research groups in the Biology Division.

In one series of experiments the conditions lead to the solution of the differential equation known as the Michaelis-Menten equation:

$$v_0 = \frac{SV_m}{S + k},$$

where v_0 is the initial rate of reaction, S is the concentration of substrate, V_m is the maximum rate of reaction, and $k = (k_2 + k_3)/k_1$.

The initial velocity, v_0 , is determined experimentally for a series of concentrations, S . The constants V_m and k are estimated from these data by the maximum likelihood method.⁴¹ Standard errors and confidence limits for each estimate are also calculated.

The initial velocity is not directly measured but is estimated from observations on the amount of product produced as a function of time. A spacing of time intervals was proposed to estimate v_0 as precisely as possible considering practical limits on the spacing.

Chromosome aberration models (D. G. Gosslee). It is important to determine whether the production of chromosome aberrations is a function of radiation dose, the square of the dose, or a combination of both. The fitting of a general quadratic model and the models with either the linear dose or the square dose term omitted is a routine least-squares calculation. However, the variances of the estimates of the number of aberrations for a given dose are not constant, and regressions calculated under this assumption are not efficient. Weighted least-squares methods were used assuming that the numbers of aberrations for a given dose have a Poisson frequency distribution.

Reciprocals of the estimated variances at each dose are used as weights to obtain efficient estimates of the coefficients for each term in the model. In this case the sum of squares of the weighted deviations from the model is approximately distributed as chi-square and is used to test the goodness of fit of each model.

41. C. I. Bliss and A. T. James, *Biometrics* 22, 573-602 (1966).

Existing computer programs have been used to estimate the coefficients and their standard errors and to calculate the sums of squares of deviations.

Cell size distribution of mouse thymocytes (Claudia Lever and D. G. Gosslee). The purpose of the investigation was to examine possible changes during development and aging in the distribution of cell volume of mouse thymocytes. Distribution counts were made of cell suspensions from thymus donors in the age range of a few hours to 84 weeks. A Coulter counter was used to count numbers of cells in 25 size intervals.

The calculations required to analyze the counts were programmed and tested using a time-share computer. The counts were then processed using the IBM 360-75. The total distribution is composed of two overlapping distributions. Estimates of mean cell volume for each component showed a dependency on the age of the donor.

Applications of quantitative stereology to lens cell data (W. E. Lever and J. N. Dumont⁴²). When electron microphotos of tissue sections are obtained, the experimenter is interested in estimating the ratio of surface areas to tissue volume and the number of spherical items in the tissue relative to the volume of the tissue.

Based on information given in *Quantitative Stereology*,⁴³ ratio formulas were given to estimate the following four properties of a lens cell relative to the volume of the cell: the surface area of the nucleus and the respective numbers of spheres of pigment, vesicles, and pits. Each of these estimates is calculated by placing a two-dimensional grid of lines over several microphotos of tissue sections and counting the intersections of the lines with the areas of interest, counting the intersections of the lines which lie in the areas of interest, and counting the number of items of interest in the picture.

Variance formulas were developed for each of the ratio estimates using the properties of the Poisson and binomial distributions.

Effect of hypophysectomizing on the proportion of labeled lens cells in newts (W. E. Lever and T. Connelly⁴⁴). Three experiments concerned with the effect of hypophysectomizing on the proportion of cells in newt lens which can be labeled have been analyzed. Each experiment was conducted under different conditions.

One group of newts were given a sham treatment, and another group of newts were hypophysectomized. Then, both eyes of the newt were sectioned and divided into three areas. The total number and the number of labeled dorsal and ventral cells were then counted for each area.

The results of these experiments indicated hypophysectomizing did affect the rate of labeling, but the direction of the change was affected by the conditions under which the experiment was conducted.

Secondary disease (heterologous): Design VIII (T. J. Mitchell, C. C Congdon,⁴⁴ R. E. Toya,⁴⁴ M. A. Kastenbaum,⁴⁵ and D. A. Gardiner). Previous reports^{46,47} have described the experimental design and the preliminary statistical analysis of "Design VIII," the latest in a series of experiments which have been conducted to determine conditions that minimize mortality due to secondary disease in mice which have been lethally irradiated and then injected with rat bone marrow.

The initial statistical analysis detected a decrease in 90-day mortality with an increase in cell dose over the dose range 20 million to 100 million cells. However, the effect of age of donor was inconsistent from one replicate of the experiment to the other.

42. Biology Division.

43. E. E. Underwood, *Quantitative Stereology*, Addison-Wesley (1970).

44. Biology Division.

45. Now at Tobacco Institute, Washington, D.C.

46. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, p. 103.

47. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 160-62.

Table 5. Design VIII: 15 day mortality

	AGE OF DONOR (days)			
	15	30	45	60
REP 1	2/30	1/30	10/30	0/30
REP 2	11/30	2/30	1/30	1/30

Design VIII: 15 day Mortality.

Further examination of the data suggested that this difference between replicates was due to the effect of early deaths (before 15 days), so it was decided to analyze separately the 15-day mortality and the 15-to-90-day mortality.

The 15-day mortality is shown in Table 5 as a function of age of donor for each replicate. Both the 45-day-old donors in replicate 1 and the 15-day-old donors in replicate 2 had unusually high 15-day mortality. In the first case, nine of the ten mice dead at 15 days had been injected from a single pool of donor marrow; in the second case, six of the nine mice dead had been injected from a single pool. Statistical analysis showed no relationship of 15-day mortality to either age or cell dose. Rather, it appears that the unexpected high 15-day death strikes at random and is associated with some unknown property of the marrow pool other than age of donor.

The 15-to-90-day mortality, which we arbitrarily call "secondary disease mortality," is defined by:

$$P = \frac{\text{number dying between 15 and 90 days}}{\text{number alive at 15 days}}$$

The analysis was performed using Berkson's minimum logit χ^2 technique,⁴⁸ in which the data are transformed to $y = \log [P/(1 - P)]$ before fitting the polynomial in age and log dose. When P is 0 or 1, Berkson's "2n rule"⁴⁹ is applied, and P is replaced by $1/2n$ or $1 - 1/2n$, respectively, where n is the number alive at 15 days. The fitting is done by weighted least squares, with weights proportional to $nP(1 - P)$.

Results for the two replicates agreed well. The hypothesis that cell dose has no effect was rejected at the 0.025 level of significance. However, the nature of the dependence of 15-to-90-day mortality on dose of cells is different for different donor ages. This can be seen in Fig. 28, where the fitted equation for P is plotted in terms of cell dose. This equation should be regarded only as an empirical data-smoothing function, not as a theoretical model for mortality.

The fitted response curves shown in Fig. 28 suggest that, for the range of age and dose considered in this experiment, relatively low secondary disease mortality can be achieved at all cell doses with 30- or 45-day-old donors, or at doses greater than about 60 million cells with 15- or 60-day-old donors. These points form a region of low secondary disease mortality in the factor space, as shown in Fig. 29. Within this region, about 84% of the 163 mice alive at 15 days survived to 90 days. Outside this region, about 57% of the 104 mice alive at 15 days survived to 90 days. (Given these two regions, the probability of such a large difference being observed, in the absence of a true difference, is 1×10^{-5} . However, a conventional hypothesis test would not be valid here, since the data that would be used in the test have been used to define the two regions, thus influencing the hypothesis itself.)

48. J. Berkson, *J. Amer. Statist. Ass.* 39, 357-65 (1944).

49. J. Berkson, *J. Amer. Statist. Ass.* 50, 130-62 (1955).

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Fig. 28. Design VIII: fitted response curves, secondary disease mortality.

Fig. 29. Design VIII: region of low secondary disease mortality.

Fluorescence from an excited solution of random dipoles (T. J. Mitchell and R. Hemminger⁴⁴). Numerical methods have been applied to evaluate, for several values of k and A , the multiple integral:

$$F^{(k)}(A) = \int_{R_k} e^{-v_k} f(v) dv,$$

where

$$f(v) = e^{-A(v_1^{-2} + v_2^{-2} + \dots + v_k^{-2})} \left(\frac{1}{3} + c_1 e^{-\lambda_1} + c_2 e^{-\lambda_2} \right),$$

$$c_{1,2} = \frac{1}{3} \pm (v_1^{-2} + v_2^{-2} - 2x)/6S,$$

$$\lambda_{1,2} = A(v_1^{-2} + v_2^{-2} + x \pm S),$$

$$S = [v_1^{-4} + v_2^{-4} - v_1^{-2}v_2^{-2} + x^3 - x(v_1^{-2} + v_2^{-2})]^{1/2},$$

$$x = (v_1^{2/3} + v_2^{2/3})/(v_1^{2/3} - v_2^{2/3})^4,$$

and R_k is the set of points $(v_1, v_2, \dots, v_k)$ such that

$$0 < v_1 < v_2 < \dots < v_k < \infty.$$

The functions $F^{(k)}(A)$ arise in an approximate calculation of the time-dependent polarization of fluorescence from a solid solution of random dipoles initially excited by a plane-polarized flash. More precisely, A is proportional to time, and $F^{(k)}(A)$, a monotonic decreasing function, is the time course of excitation on an arbitrary dipole given that it had unit excitation at time zero. Its excitation is lost to its k nearest neighbors by Förster transfer.⁵⁰ The k -fold integration in the definition of $F^{(k)}(A)$ represents an average over all positions of these k nearest neighbors.

For fixed k and A , our initial approach was to evaluate the integral by means of the following Monte Carlo procedure. First, the appropriate transformations were made to change the region of integration into a k -dimensional unit cube. Then successive evaluations of the integrand were made at points chosen randomly from a uniform distribution within this cube. The mean of N evaluations, $\bar{y}_{(N)}$, was then the estimate of the integral $F^{(k)}(A)$. Unfortunately, the integrand is such that at $k = 7$, even when $N = 60,000$, the standard error of $\bar{y}_{(N)}$ was about 4% of $\bar{y}_{(N)}$. To achieve a relative standard error of about 1%, therefore, would require N to be nearly 1,000,000. The situation was found to become worse for increasing values of k . Since it was planned to evaluate $F^{(k)}(A)$ for more than 20 values of A and then repeat the procedure for several values of k , the prospects for success at a reasonable cost were not good.

For that reason, we discarded the original approach and tried an alternative Monte Carlo method. We first note that the integrand is dominated by e^{-v_k} and the integral of e^{-v_k} over the region of integration is

50. Theodor Förster, "Delocalized Excitation and Excitation Transfer," p. 93 in *Modern Quantum Chemistry Part III: Action of Light and Organic Crystals*, ed. by O. Sinaoglu, Academic, New York, 1965.

1. If we draw points $(v_1, v_2, \dots, v_k, v_{k+1})$ uniformly from the region R^* : $\{(v_1, v_2, \dots, v_k) \in R_k, 0 < v_{k+1} < e^{-v_k}\}$, then the proportion of these points which satisfy the condition $C: v_{k+1} < e^{-v_k} f(v_1, v_2, \dots, v_k)$ estimates the integral $F^{(k)}(A)$. This is simply the estimate of a binomial probability, so its standard error (relative to the mean) is:

$$E = \{[1 - F^{(k)}(A)] / n F^{(k)}(A)\}^{1/2}.$$

For values of A which are of most interest, relative errors of less than 1% are possible for $N = 20,000$. Moreover, this accuracy is independent of k . An added advantage was found to be that in many cases it is possible to determine whether C is satisfied without having to calculate f entirely, so more computer time was saved.

To apply this method, it was necessary to choose points uniformly from R^* . This can be done by letting v_k be the sum of k independent exponentially distributed random variables; that is,

$$v_k = - \sum_{i=1}^k \ln(x_i),$$

where each x_i is chosen from a uniform distribution on the interval $[0, 1]$. Then order a random sample of $(k-1)$ independent uniform $[0, 1]$ variables: $u_1 < u_2 < \dots < u_{k-1}$, and let $v_i = u_i v_k$, $i = 1, 2, \dots, k-1$. Finally, let $v_{k+1} = e^{-v_k} u$, where u is chosen from a uniform $[0, 1]$ distribution.

After the functions $F^{(k)}(A)$ were determined, it was desired to calculate the integrals:

$$I^{(k)}(r) = \frac{1}{r^2} \int_0^\infty e^{-A/r^2} F^{(k)}(A) dA.$$

These integrals are simply related to the polarization of the fluorescence from the solid solution of dipoles when they are excited by a *steady* polarized light. The parameter r is proportional to the concentration of dipoles.

Fortunately, it is possible to integrate over A directly first, to obtain the expression:

$$I^{(k)}(r) = \int_{R_k} e^{-v_k} g(v) dv,$$

where $g(v) \leq 1$. The integrand is again dominated by e^{-v_k} , and the procedure described above can again be applied, with f replaced by g .

Chemically induced *ad-3* mutations (T. J. Mitchell and H. V. Mallings⁵¹). Data from three experiments have been analyzed to determine the relationship between MMS-induced *ad-3* mutations in conidia and the concentration of MMS (methyl methanesulfonate). The observed mutation frequencies as originally recorded are given in Table 6.

Within each experiment, a log-log plot of these data indicates the straight-line relationship:

$$\log p = a + b \log c, \tag{1}$$

Table 6. Forward mutation frequencies

Expt. No.	Mutation frequency $\times 10^6$ at MMS concentration of -				
	3.0 mM	5.0 mM	10.0 mM	15.0 mM ^a	20.0 mM
12-62 ^b		2.58	9.32	13.48	40.14
12-63 ^c		39.2	182.4	312.8	730.8
12-64 ^c	13.3	28.6	94.9	160.9	366.7

^aShould be 13.3 (see text).^b60-min treatment with MMS.^c300-min treatment with MMS.

where p is the mutation frequency and c is the concentration of MMS. The statistical problem was:

1. to estimate the slope b for each experiment,
2. to determine whether or not these slopes are equal, and
3. to determine whether or not the slopes differ significantly from 1, that is, whether p is directly proportional to c .

In each experiment, the number (x) of purple colonies (presumptive *ad-5* mutations) observed at each concentration of MMS was assumed to follow a binomial distribution with parameters N and p , where N is the total number of surviving colonies and p is the mutation frequency. Because N is extremely large and p is small, the distribution of x is well approximated by the Poisson distribution:

$$P(x) = e^{-Np} (Np)^x / x! \quad (2)$$

In a given experiment, with data taken at concentrations $c_1, c_2, \dots, c_k$, the likelihood corresponding to particular values of a and b in (1) is:

$$L = \prod_{i=1}^k e^{-Np_i} (Np_i)^{x_i} / x_i! \quad (3)$$

where $p_i = \exp(a + b \log c_i)$. Those values of a and b which maximize L (or, equivalently, $\log L$) are called the maximum likelihood estimates $\hat{a}$ and $\hat{b}$. They are found by solving the equations:

$$\begin{bmatrix} \sum x_{i0} & \sum x_{i0} \log c_i \\ \sum x_{i0} \log c_i & \sum x_{i0} (\log c_i)^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum x_{i0} \log p_{i0} \\ \sum x_{i0} \log c_i \log p_{i0} \end{bmatrix} + \begin{bmatrix} \sum (x_i - x_{i0}) \\ \sum (x_i - x_{i0}) \log c_i \end{bmatrix} \quad (4)$$

iteratively, where p_{i0} is the current estimate of p_i and $x_{i0} = Np_{i0}$. The iterative procedure can be started by setting $x_{i0} = x_i$ and $p_{i0} = x_i/N$; convergence is usually obtained after five or six iterations. The solution vector $(\hat{a}, \hat{b})$ has the following approximate variance-covariance matrix:

$$V = \begin{bmatrix} \sum \hat{x}_i & \sum \hat{x}_i \log c_i \\ \sum \hat{x}_i \log c_i & \sum \hat{x}_i (\log c_i)^2 \end{bmatrix}^{-1} \quad (5)$$

where $\hat{x}_i = n_i \hat{p}_i = n_i \exp(\hat{a} + \hat{b} \log c_i)$. Thus the approximate standard error of $\hat{b}$ is the square root of the lower right-hand element in the matrix V .

The goodness of fit of the straight line can be evaluated by forming the ratio $L_{rel} = L_1/L_2$, where L_1 is the likelihood obtained by setting $p_i = \exp(\hat{a} + \hat{b} \log c_i)$ in expression (3) and L_2 is the likelihood obtained by setting $p_i = x_i/n_i$ in expression (3). That is, L_1 is the maximum likelihood that can be achieved assuming the straight-line relationship (1), while L_2 is the maximum likelihood that can be achieved without making the straight-line restriction. Thus, the smaller L_{rel} , the less plausible is the straight-line relation. To test whether L_{rel} is "too small" we can make use of an approximation due to Wilks,⁵² by which $-2 \log L_{rel}$ is assumed to have a chi-square distribution with $k - 2$ degrees of freedom.

When this test was made for the three experiments in Table 6, a highly significant lack of fit was found in each case. When the contribution of each experimental point to Wilks' lack-of-fit statistic was studied, it was found that in each experiment, the data at $c = 15.0$ were responsible for the failure of the straight-line fit. In every case, the observed mutation frequency was less than it should have been. Further investigation by the experimenter then revealed that the worker who was responsible for preparing the MMS solutions had repeatedly prepared solutions with a concentration of 13.3 instead of 15.0 as specified. When the value 15.0 in Table 6 was changed to 13.3, it was found that the straight-line representation gave a good fit in every experiment. (It was, however, necessary to omit the concentration 3.0 in experiment 12-64 to avoid a significant lack of fit there.)

The calculated slopes, with their estimated standard errors, are given below:

Expt	Slope	Std. error of slope
12-62	2.12	0.24
12-63	2.04	0.08
12-64	1.87	0.04

It is quite obvious that these slopes are all greater than 1. Moreover, these three slopes are not different from one another at the 0.10 level of significance ($0.10 < P < 0.25$). The analysis on which the latter conclusion was based assigned to each slope a weight inversely proportional to the estimated variance of that slope. The weighted estimate of the common slope is 1.91 with a standard error of 0.04.

Genetic control of immunopoiesis (T. J. Mitchell and C. F. Gottlieb⁵¹). It has been observed that immunopoiesis in AKR mice (compared with C3H mice) is defective.⁵³ To study the genetics of this defect, appropriate crosses were made to produce $(C3H \times AKR)F_1$, $C3H \times F_1$, $AKR \times F_1$, and F_2 mice. These four groups plus the two parental types were the six genetic classifications used in this study.

Appropriate concentrations of AKR spleen cell suspensions were mixed with sheep erythrocytes, and equal aliquots of the resulting suspension (containing 2.5×10^7 spleen cells and 5×10^8 sheep erythrocytes) were injected into appropriate recipient mice which had been previously x-irradiated with 800 R. After six days of culture, spleens of recipient mice were assayed for direct plaque-forming cell (PFC) responses using the localized hemolysis-in-agar technique.

Five experiments were performed, using either five or six recipient mice of each genetic group in each experiment. The statistical problem was to analyze the data for differences among genetic groups, with emphasis on testing appropriate genetic models for consistency with the data.

The $\log_{10}$ transformation was applied to all responses initially. This transformation appeared to give the same "spread" of the data within each of the six genetic classifications.

52. S. S. Wilks, *Ann. Math. Statist.* 9, 60-62 (1938).

53. Perkins et al., *J. Nat. Cancer Inst.* 46, 845 (1971).

The first three experiments were done without regard to grouping by sex, since it had been assumed that sex differences were negligible. To check this assumption, the last two experiments were conducted with three males and three females in each genetic group. As expected, no significant difference in response between males and females was found. Differences in overall level of response from experiment to experiment were found to be statistically significant, indicating that a pooling of the animals in each genetic group over all experiments would tend to mask differences among genetic groups. There was, fortunately, no interaction detected between genotypes and experiments; that is, genotype *differences* were essentially the same from experiment to experiment.

The data were then reduced to a 5 (experiments) $\times$ 6 (genotypes) table in which each entry was the average $\log_{10}$ response for the (usually five or six) animals in that group. Experiment-to-experiment variation was taken to be random. A two-way analysis of variance (ANOVA) was applied to this table, and the appropriate F test for differences among genotypes was made. These differences, which were found to be statistically significant at the 0.001 level, can be adequately explained by the following model:

$$\mu_2 = \frac{1}{2}\mu_1 + \frac{1}{2}\mu_3,$$

$$\mu_4 = \frac{1}{2}\mu_5 + \frac{1}{2}\mu_3,$$

$$\mu_6 = \frac{1}{4}\mu_5 + \frac{1}{2}\mu_3 + \frac{1}{4}\mu_1,$$

where

μ_1 = mean response for AKR,

μ_2 = mean response for AKR $\times$ F_1 ,

μ_3 = mean response for F_1 ,

μ_4 = mean response for C3H $\times$ F_1 ,

μ_5 = mean response for C3H,

μ_6 = mean response for F_2 .

Under this model, the least-squares estimates of μ_1 , μ_3 , and μ_5 are:

$$\hat{\mu}_1 = 3.54,$$

$$\hat{\mu}_3 = 4.13,$$

$$\hat{\mu}_5 = 4.43.$$

A comparison of the observed genotype means with those based on the fitted model is shown below:

Genotype	Mean		Observed - Fitted
	Observed genotype	Fitted model	
AKR	3.60	3.54	0.06
AKR $\times$ F_1	3.81	3.83	-0.02
F_1	4.23	4.13	0.10
C3H $\times$ F_1	4.26	4.28	-0.02
C3H	4.48	4.43	0.05
F_2	3.88	4.06	-0.18

A statistical F test indicated no lack of fit for this model ($0.10 < P < 0.25$).

The last part of the analysis consisted in reparameterizing the model and determining a confidence interval for one parameter which was of particular interest.

Estimation of permeation by glycerol (V. R. R. Uppuluri and J. M. Dolan). One of the central tenets of cryobiology is that in order for a protective solute to prevent freezing injury it must permeate the cell. Experiments are performed in the Biology Division with respect to the protection of ox red blood cells by glycerol.

Let $S(t)$ denote the amount of glycerol that permeated the cell at time t . Hitherto,⁵⁴ the following equation was used to describe the kinetics:

$$\frac{dS(t)}{dt} = PA \left[\frac{M_S}{1000} - \frac{S(t)}{V(t)} \right],$$

where P is the permeability constant for glycerol, A is the cell surface area, M_S is the osmolal concentration of glycerol in the extracellular medium, and $V(t)$ is the relative volume of water in the erythrocyte at time t . This model was used to obtain $S(t + \Delta t)$ from the estimated values of $S(t)$ and $V(t)$.

The investigator now wishes to consider the equation:

$$\frac{dS(t)}{dt} = -a + b \ln S(t),$$

and the problem is to find $S(T + \Delta t)$ given a , b , Δt , and $S(T)$. This can be accomplished by using the tables of $E_1[Z]$ computed by D. K. Trubey,⁵⁵ as follows:

$$E_1[S(T + \Delta t)] = E_1[S(T)] - b \Delta t e^{-a/b},$$

where

$$E_1[Z] = \int_Z^\infty \frac{e^{-x}}{x} dx.$$

Random breakage of single-stranded homopolymeric nucleic acid molecules (V. R. R. Uppuluri and W. H. Olson⁵⁶). Nucleic acids comprise chains of sugar moieties, each carrying one of four bases, connected by phosphate linkages. The fundamental building block, base-sugar-phosphate, is called a nucleotide. The sugar-phosphate bonds may be broken by a number of physical and chemical methods. The probability that a given bond may be broken depends, for some methods, on the nature of the adjoining nucleotides. If we consider the case where all nucleotides are the same (homopolymer), we are led to the assumption that each of the finite number of outcomes of this breakage process is equally likely.

The breaking agent is alkali. Alkaline hydrolysis may be visualized as follows: long chains of polymers are floating about, relatively far apart, in a solution of very much smaller hydroxyl ions; the polymers and hydroxyl ions are continually colliding; no breakage results from most of these collisions, but occasionally a favorable configuration is achieved, and the bond is hydrolyzed (broken).

54. *Biol. Div. Annu. Progr. Rep. June 30, 1971*, ORNL-4740, p. 23.

55. D. K. Trubey, *A Table of Three Exponential Integrals*, ORNL-2750 (1959).

56. McGill University.

Let us consider chains of polymers with $a + 1$ nucleotides (and a bonds); let b ($\leq a$) of these bonds be broken, so that the polymer is broken into $b + 1$ pieces. Let N_i , $i = 1, 2, 3, \dots$, denote the number of pieces that contain exactly i nucleotides, so that $N_1 + N_2 + N_3 + \dots = b + 1$. It is of interest to find the expected value $E[N_i]$ and the variance of N_i , denoted by $\text{Var}[N_i]$. They may be obtained by the use of indicator random variables, as follows: Let

$$\chi_\alpha(i) = \begin{cases} 1 & \text{if the } \alpha\text{th piece has exactly } i \text{ nucleotides} \\ 0 & \text{otherwise} \end{cases}$$

Then $N_i = \chi_1(i) + \chi_2(i) + \dots + \chi_\alpha(i) + \dots + \chi_{b+1}(i)$, and one can show that

$$E[N_i] = (b + 1) \binom{a-i}{b-1} / \binom{a}{b}$$

and

$$\text{Var}[N_i] = E[N_i] - \{E[N_i]\}^2 + (b + 1) b \binom{a-2i}{b-2} / \binom{a}{b}.$$

Chemical Technology

Proposed experiment design for LMFBF head-end studies (T. L. Hebble, Claudia Lever, and V. C. Vaughan⁵⁷). An experiment design is proposed for LMFBF head-end studies to determine the effect of plutonium content, fuel oxygen-to-metal ratio, and burnup on two head-end steps, voloxidation and dissolution. A fourth process variable, power level, is a function of reactor operation and will be treated as a covariate. These variables will be related to measured responses such as weight gain, percent of material reduced to less than a certain mesh, and percent of tritium remaining with the fuel. This series of experiments conforms to a central composite factorial design in three variables and is divided into three blocks. The total number of runs necessary to answer several posed questions varies from a minimum of 12 (in block 1) to about 36, depending on the conclusions that can be drawn after completion of the first block. To hold the number of experiments to a minimum, only mixed oxide fuels will be considered.

Ecological Sciences

Effect of acclimation temperature on heat death of juvenile coho salmon (J. J. Beauchamp, E. A. Hirst,⁵⁸ and C. C. Coutant⁵⁹). A study was conducted to investigate the effect of acclimation and elevated water temperature on survival times of juvenile coho salmon. For this experiment, 16 groups of 20 fish each were subjected to various water temperatures above the temperature at which the fish were originally acclimated. Six of the groups were acclimated at 10°C and the remaining ten groups were acclimated at 14°C. Over a period of two weeks the number of dead fish and the observed times to death were recorded for the two acclimation temperature groups. The observations are censored, since the fish were observed for only two weeks and there were no recorded times to death greater than two weeks, or 20,160 min. It was

57. Chemical Technology Division.

58. Director's Division and Ecological Sciences Division.

59. Ecological Sciences Division.

desired to investigate the change in time to death for the various acclimation and elevated temperature groups.

A preliminary investigation was made to determine if the times to death followed a normal or log normal distribution by looking at a plot on probability paper of the empirical distribution of the time to death for the different experimental groups. The Kolmogorov-Smirnov test of goodness of fit was applied to the acclimation and elevated water temperature groups where complete observations were available on all of the fish in order to test the normal or log normal assumption. The results from this test indicated that the distribution of the times to death is neither normal nor log normal over the entire range of temperatures.

A nonparametric procedure was used to compare the different acclimation and elevated temperature groups, since the distribution of times to death was unknown. By using a nonparametric procedure the conclusions would not depend upon the distribution function of the times to death. The procedure used the estimation of the median time to death for each temperature group. The following modification was applied to avoid overestimating the median and its associated confidence limits:

If k fish die between the two observation time points t_1 and t_2 (where $t_1 < t_2$), then the i th fish was assumed to have died at

$$t_1 + i \frac{t_2 - t_1}{k + 1}$$

for $i = 1, 2, \dots, k$. This modification is equivalent to assuming that the distribution of deaths is uniform over the interval from t_1 to t_2 . For example, if one fish died between times t_1 and t_2 , then it was assumed that the time of death of the fish was equal to $(t_1 + t_2)/2$. Then the median and a 95% confidence interval for the median were estimated for each group. The results of this estimation lead to the following conclusions:

1. For both groups of acclimation temperatures there is a significant decrease in the median time to death as the elevated temperature increases.
2. The relation between elevated temperature and median time to death appears to be different for the two acclimation temperature groups.
3. The relation between median time to death and elevated temperature appears to be exponential for both acclimation temperatures when the elevated temperature is greater than 21°C.

Although the data considered here did not appear to follow the normal or log normal distribution, by the use of nonparametric techniques it was still possible to obtain a valid statistical analysis free of an assumption about the distribution.

Effect of an herbicide on the weight loss of leaf litter (J. J. Beauchamp, Carol MacCain,⁶⁰ and M. Wittkamp⁶¹). Recently a study was conducted by members of the Ecological Sciences Division to evaluate the effect of a particular herbicide on the rate of leaf litter decomposition, as measured by weight loss. For the design of this experiment, six medium-sized tulip poplar trees were selected from the site of interest. Three of these trees received no herbicide and served as controls, and the three remaining trees were injected with a defoliant herbicide which contained arsenical cacodylic acid. The amounts of herbicide injected were $x/3$, x and $3x$, where x represents recommended commercial dose, and these were designated as treatments 1, 3, and 9 respectively. As the leaves fell, they were collected from each tree, air dried, and

60. Department of Biology, Emory University, and Ecological Sciences Division.

placed in mesh bags. These litter bags were randomly placed among the natural litter beneath a stand of mature tulip poplars, each bag in its own 1-m² plot. There were a total of 64 litter bags randomly assigned to four series denoted by A, B, C, and D. Each series included three replicate bags from one control tree (C1) and treatments 1, 3, and 9. In addition, each series also included two replicate litter bags from the two remaining control trees (C2 and C3). These remaining controls were used to estimate the tree-to-tree variability, since trees and treatments were confounded for control C1 and treatments 1, 3, and 9.

The initial time point in the experiment was assumed to be the time when the litter bags were placed among the natural litter on the forest floor. During the complete 16-week period of the experiment, the litter bags from each series were weighed every fourth week for a total of four times; for example, the bags of series A were weighed at the end of weeks 1, 5, 9, and 13; the bags of series B were weighed at the end of weeks 2, 6, 10, and 14; etc. By assuming an exponential relationship to exist between weight remaining and time, the observed data for the period of weeks 2 to 16 were used to estimate the rate of weight loss. An analysis of variance was performed on the estimated rates, and the following are some of the conclusions: (1) the treatment effect was not found to be significant and (2) the series effect was found to be significant. An analysis of the rates for the three controls yielded similar conclusions; that is, the three controls were not significantly different, but the series effect was significant.

An additional analysis of variance was performed on the observed weight remaining over time for this experiment. From this analysis the factor, times within a series-treatment combination, was highly significant, the series factor was significant, and the treatment factor was significant. An additional analysis was performed on the observed weight remaining over time for the three controls, and the results of this analysis again showed that the three controls were not significantly different. Some possible reasons for the discrepancies between the conclusions of these analyses are: (1) In the first analysis, a simple exponential relation was assumed to exist between weight remaining and time. (2) The reduction of the weight data to a single statistic for each litter bag may be covering up a treatment difference.

As a final investigation, a regression analysis was performed on the dose of herbicide vs the mean weight at each dose. From this analysis the lack of fit was not found to be significant, but the slope of the regression line was found to be significantly different from zero, implying the presence of a treatment effect.

Application of probit analysis to an ecological problem (J. J. Beauchamp, S. H. Bowen,⁶¹ and C. C. Constant⁵⁹). With the increased demand for electricity and the concern over the effect nuclear power stations may have upon the environment, some members of the Ecological Sciences Division, in consultation with some statisticians from the Mathematics Division, have been investigating the effects of temperature upon certain groups of fish. One such investigation involved an interesting application of probit analysis to study the effects of water temperature on the outcome of feeding competition between warm- and cold-water fishes. In order to determine the effect of temperature acclimation on feeding competition between two fish species, a relative performance test was selected in which both species were fed simultaneously in the same tank. Four tanks, each separated into three compartments, were used for the experiment. Four bluegills and four rainbow trout were put into each compartment. The fish in two compartments were used for testing, and the fish in the third compartment were kept for observation and to replace any of the test fish that died. The fish were acclimated to approximately 15, 18, 20, 21, 22, or 24°C for 14 days at each temperature and then fed approximately 20 food units at each feeding. The fish were fed in this fashion for ten days, and the total number of food units captured by each species was recorded. At the lower temperatures, the trout captured most of the food units, but as the temperature

61. Great Lakes Colleges Association research participant, Ecological Sciences Division.

increased, the bluegills captured a larger portion of the food. Therefore, we are interested in the relationship between water temperature and the proportion of food units captured by the two species under investigation. Since it is assumed that all of the food units are captured by the bluegills or trout, we may center our attention on one species (e.g., bluegill). For bluegills, the water temperature vs percent food units captured followed a sigmoid function within the temperature range under investigation. That is, at the lower temperatures the bluegills captured only a small portion of the food units, and toward the upper range of temperatures there was an increase in the proportion captured by the bluegill to the point where they captured most of the food units at the highest water temperature. The purpose of the experiment was to estimate the temperature of "equal competition," where "equal competition" is defined as the temperature at which each species of fish captures 50% of the food units.

The estimation of the temperature of "equal competition," T_{50} , is equivalent to the estimation of an LD_{50} in an experiment to investigate the relation between the variables of dose and percent mortality, where the LD_{50} is defined as that dose at which one expects 50% of the animals to die. This equivalence is accomplished by associating the variables of dose and percent mortality to the variables of water temperature and percent of food units captured respectively. Therefore, from the observed total number of food units fed and the number captured by the bluegills at each water temperature, the techniques of probit analysis were used to estimate T_{50} and its associated confidence limits. We cannot extrapolate beyond the range of temperatures considered because of lethal effects. The application of probit analysis to this particular estimation problem has been quite helpful to the ecologists, since probit analysis is a technique with which the ecologist is familiar, for example, in the estimation of LD_{50} 's.

Application of canonical analysis to an ecological problem (J. J. Benichamp and G. U. Jirikson⁶²). In two previous reports^{62,63} the results of a simulation study investigating the multivariate statistical technique of canonical analysis were given. A major advantage of multivariate statistical analysis is that it takes into account the statistical dependence which may exist between the members of a set of observed random variables, whereas a univariate statistical analysis of each observed random variable separately would ignore this dependence. Recently, the Statistics Department has applied canonical analysis to the investigation of a set of data arising from research in the ecological sciences.

Fish which had been acclimated at a standard temperature (16°C) were shocked by being placed in tanks with water at warmer temperatures (26, 28, and 29.5°C) for 5 min and then returned to the 16°C water. In addition to the above three groups, a control group of fish was taken from the 16°C water, placed in another tank of water at 16°C, and then returned to the 16°C water. After 5, 30, 60, or 240 min, blood sera were collected from the fish, and measurements on five proteins were taken.

The five measurements from each blood sample constitute a vector of multivariate data. By using canonical analysis the vector of the original five measurements may be reduced to a set of independent random variables which emphasize the differences between the different groups under consideration. This reduction is accomplished by a simple linear transformation; the new independent variables are referred to as the canonical variates. From the method used to calculate the canonical variates, it may be shown that the first two canonical variates do the best job of comparing the different groups and the remaining canonical variates contribute little to the comparison. The first two canonical variates, for each observation vector, may be considered as the coordinates of a point on a two-dimensional plot. In addition, a circle of uncertainty may be drawn around the transformed mean vector for each group, recognizing the fact that the measurements of the proteins are subject to statistical variation.

62. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, p. 71.

63. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, pp. 133-36.

The means of the first two canonical variates for the fish which were shocked at four different temperatures (16, 26, 28, and 29.5°C) and removed for examination 5 min after reacclimation are shown in the portion of Fig. 30 labeled "recovery time = 5 min" with the 95% circles of uncertainty for the different groups. The general overlapping of the circles of uncertainty indicates no clear-cut effect of temperature. The second portion of Fig. 30 shows a plot for the fish shocked at the same four temperatures but allowed to reacclimate 4 hr before being examined. Here, however, there is a distinct separation of the circles of uncertainty, indicating a significant effect of temperature on the blood sera of the fish when they are allowed a longer time to recover.

Additional analysis was done by investigating differences among recovery time groups within the fixed temperature. In Fig. 31 a plot is given of the 95% circles of uncertainty for control fish which were all "shocked" at 16°C but allowed to recover for 5 min, 30 min, 1 hr, and 4 hr. The overlapping of the circles of uncertainty indicates no essential difference due to the amount of recovery time. When the fish shocked at 28°C are considered, the picture changes considerably. From the lower portion of Fig. 31, an investigation of the circles of uncertainty shows the 5- and 30-min recovery time groups are significantly different from the rest but the 1- and 4-hr recovery time groups are not different from each other.

An experimenter could not be expected to detect phenomena of the kind illustrated in this example by examining sets of five interrelated measurements individually. The reduction to two independent canonical variates makes it relatively easy.

Litter decomposition study (Claudia Lever and J. J. Deschamps). The purpose of this experiment was to study the effects of different organisms present in the soil on the decomposition of litter from different species of trees. The experimental area was divided into 14 plots, and the following soil treatments were assigned to the plots at random: three plots with night crawlers plus soil flora, three plots with native earthworms plus soil flora, three plots with microarthropods plus soil flora, two plots with soil flora, and three plots as inside controls. Because each plot in the experimental area was fenced in, two unfenced control plots outside the experimental area were compared with the three original control plots to test for fencing effects. Since the plots with the night crawlers produced erratic results, these data were not included in the analysis.

Nine bags of litter from each species were placed on each plot. The species were tulip poplar, hickory, black gum, and dogwood. Approximately every two months, all the bags of litter were weighed, and one bag of each species from each plot was selected for further analysis. These bags were dried, and the dry weight of each bag was compared with the initial dry weight to obtain the percent of dry weight remaining.

It was hypothesized that the litter would decompose exponentially,

$$w = k_0 e^{-kt}$$

where

w = weight remaining,

k_0 = initial weight, and

t = time.

Then $\log w = \log k_0 - kt$; that is, the log of weight remaining should be a linear function of time.

Since the plots of the data supported this hypothesis, a straight line was fitted for each plot for each species. Estimates of the slopes, or rates of decomposition, were analyzed to see if there were significant differences among different species and among different treatments. The analysis of variance tests indicated

Fig. 30. Circles of uncertainty for various recovery times.

Fig. 31. Circles of uncertainty for various water temperatures.

highly significant ($P < 0.001$) differences in the rates of decomposition among the different species. The differences among the treatments were highly significant ($P < 0.001$) for the black gums and significant ($P < 0.10$) for the dogwoods. The differences among the treatments for the tulip poplar and hickory were not significant. For these tests, the estimate of error was the variance among plots having the same treatment and species combination.

Snail radiation sensitivity (F. L. Miller, Jr., and J. L. Cooley⁶⁴). The preceding annual reports^{65,66} have described an experiment to chronically expose the freshwater aquatic snail *Physa heterostrophus* to radiation insult.⁶⁷ During the past year, interest has centered on snails which received 0 or 1 rad/hr, since the differences between these experimental groups are subtle. We have tested the hypothesis that the snails in each of the two experimental groups produced the same egg capsule size distribution each week throughout their lifetime. Kolmogorov-Smirnov statistics revealed that the distributional form changed markedly during the first weeks of the study, stabilizing at about the age of "maturity." Further analyses compare the two dose groups.

Metals and Ceramics

Stainless steel irradiation experiment (T. L. Hebble, N. C. Cole,⁶⁸ G. M. Goodwin,⁶⁸ and R. C. King⁶⁸). The stainless steel irradiation experiment reported previously⁶⁹ has been modified to take into account changes in operation of the Idaho EBR-2 reactor and reflect shifts in emphasis. The basic factorial design remains the same. However, one pin originally planned to be replaced 213 days after its October 1970 insertion date is not scheduled to be removed until January 1972. The replacement pin contained a partial replication of the first pin to provide a measure of experimental error. Under this new schedule of operation, it will not be possible for the replacement pin to meet the increased fluence level created by the lengthened period in the reactor for the first pin. Specimen arrangement was revised to provide the necessary replication and to place greater emphasis on welds identical to those which will be used in the reactor vessel at the Fast Flux Test Facility (FFTF) in Richland, Washington.

Steam corrosion of electropolished Incoloy 800 (T. L. Hebble and J. P. Hammond⁶⁸). Steam corrosion of electropolished Incoloy 800 specimens as measured by weight gain is adequately represented by the empirical model

$$W = A + \frac{T}{B + CT},$$

where

W = weight gain, mg/cm²,

T = time, hr, and

A , B , and C are parameters to be estimated from the data.

64. Institute of Ecology, University of Georgia, Athens, Ga.

65. Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4661, p. 164.

66. Math. Div. Annu. Progr. Rep. Dec. 31, 1969, ORNL-4514, p. 106.

67. J. L. Cooley and F. L. Miller, Jr., *Radiat. Res.* 47, 716-24 (1971).

68. Metals and Ceramics Division.

69. Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4661, p. 168.

Table 7. Least-squares estimates of parameters

Specimen	A (mg/cm ²)	B (hr cm ² mg ⁻¹)	C (cm ² /mg ¹)
800-1-2E	2.22 ± 0.215	330 ± 55.6	0.256 ± 0.0125
800-1-3E	2.56 ± 0.166	405 ± 57.1	0.266 ± 0.0100
800-2-2E	4.95 ± 0.070	1080 ± 163	0.661 ± 0.0256
800-2-3E	4.73 ± 0.042	1710 ± 196	0.755 ± 0.0178

Data consisted of weight gain measurements on four electropolished Incoloy 800 specimens which were subjected to a steam atmosphere for 598 days, two specimens (800-1-2E and 800-1-3E) at 1100°F (595°C) and two specimens (800-2-2E and 800-2-3E) at 1200°F (650°C). Parameter estimates obtained from the data by the method of least squares are given in Table 7 with corresponding standard errors. Curves representing the model and the observed data for each specimen are shown in Figs. 32 and 33. The corrosion rate,

$$\frac{\partial W}{\partial T} = \frac{B}{(B + CT)^2},$$

at 5000 hr is about three times the rate at 10,000 hr and six times the rate at 15,000 hr.

Self-irradiation damage of plutonium solid solutions (T. L. Hebble and V. J. Tennery^{6,8}). An empirical mathematical model, used to represent the lattice parameter in studies of self-irradiation damage of (U_{1-x}Pu_x)N solid solutions, was fitted to x-ray diffraction data from five sample compositions: $x = 0.19, 0.38, 0.58, 0.79$, and 1.00 . This model is of the form

$$\frac{\Delta a}{a_0} = A(1 - e^{-Bt}),$$

where

a_0 = lattice constant, Å;

$\Delta a = Y - a_0$

= change in lattice parameter at time t , Å;

Y = observed lattice parameter at time t , Å;

t = time, days;

A and B are coefficients to be estimated.

The lattice constant, a_0 , and coefficients were estimated from the data by the method of least squares.

Plutonium content (mole fraction)	Estimate of coefficient				a_0	Standard error ($\times 10^{-5}$)
	A ($\times 10^{-3}$)	Standard error ($\times 10^{-4}$)	B ($\times 10^{-3}$)	Standard error ($\times 10^{-4}$)		
0.19	1.14	3.0	1.65	6.1	4.89063	6.8
0.38	1.59	2.7	2.26	5.9	4.89448	11.0
0.58	2.31	2.6	1.79	2.9	4.89990	6.9
0.79	2.14	2.4	2.53	4.2	4.90392	8.4
1.00	2.22	0.57	3.12	1.7	4.90482	7.6

Fig. 32. Corrosion of electropolished Incoloy 800 in steam at 1100°F.

Fig. 33. Corrosion of electropolished Incoloy 800 in steam at 1200°F.

The curves and data are displayed in Fig. 34.

The original model was expanded to include plutonium content as a variable:

$$\frac{\Delta a}{a_0} = A(2 - e^{-Bt} - e^{-Cx^2}),$$

Fig. 34. Radiation self damage in $(U_{1-x}Pu_x)N$ solid solutions.

where x is a mole fraction of plutonium, C is another coefficient to be estimated, and the remaining terms are defined as before. Using all observations, the least-squares estimates of the coefficients with standard errors are

$$a_0: 4.8876 \pm 0.0001\%$$

$$A: 0.00406 \pm 0.000030,$$

$$B: 0.000795 \pm 0.000028,$$

$$C: 3.24 \times 10^4 \pm 730.$$

Figure 35 shows that the expanded model does not readily account for self-irradiation damage at the extremes of plutonium content but should be useful in the $x = 0.40$ to 0.80 range.

Statistical analysis of mechanical properties of SS308 welds (T. L. Hebble and N. C. Binkley⁶⁸). A statistical analysis of mechanical properties data from welds made by joining stainless steel 304 plates with 308 filler metal showed that carbide agglomeration did not significantly change yield strength, percent elongation, or tensile strength of the solution-annealed specimens. Seventy-five specimens were cut from welds consisting principally of SS308 and were randomly divided into three groups of twenty-five. Each group was assigned one of three levels of specimen preparation: (1) as welded, (2) solution annealed, and (3) solution annealed plus carbide agglomeration. Several levels of aging time (100 and 1000 hr), aging temperature (600 to 1200°F), and test temperature (600 to 1200°F) were applied to each group.

The statistical analysis of the data consisted in preparing analysis of variance tables for three balanced sets of data, each set being arranged for the purpose of testing specific hypotheses. The residual mean square was used as an estimate of experimental error to test these hypotheses.

One set which included all of the 100-hr test data displayed a highly significant variation due to specimen preparation for all three responses that is attributed solely to the differences between the welded specimens and the average of the solution-annealed specimens. Annealing caused the yield strength to drop

Fig. 35. Radiation self damage in $(U_{1-x}Pu_x)N$ solid solutions.

from 31,700 psi to an average of 23,000 psi. The tensile strength dropped about 3000 psi, and the percent elongation increased from 21.6 to 25.9%. Carbide agglomeration did not significantly alter the solution-annealed specimens. These significant effects are illustrated in Figs. 36 and 37, which show plots of yield strength and tensile strength as functions of test temperature for each level of specimen preparation. Figure 37 also illustrates a significant preparation times temperature interaction.

A second data set consisted of those specimens which were aged and tested for 1000 hr. In the case of yield strength, the significant preparation mean square is attributed to the differences between the as-welded and the solution-annealed specimens. This annealing caused the yield strength to drop from 31,200 psi to an average of 21,700 psi. Carbide agglomeration did not significantly alter the annealed specimens. Increasing the aging and testing temperature from 600 and 1200°F produced a real decrease in both yield strength (from 32,500 to 19,100 psi) and tensile strength (from 63,200 to 33,500 psi).

The third data set consisted of data from those 100- and 1000-hr test specimens that were both aged and tested at the same temperatures: 1000, 1100, and 1200°F. The purpose of this set of data was to test the effect of aging time on the three responses. The analysis of variance indicated that only in the case of tensile strength did aging time have a real effect.

MINT-1 transducer calibration (F. L. Miller, Jr., and R. B. Fitts⁶⁶). The MINT-1 (Mechanical Interaction) capsule contains two transducers which are used to measure the length of a prototype fuel element being tested in the poolside facility of the Oak Ridge Research Reactor. The calibration of these transducers was made more difficult because the operating temperature of the transducers is only

Fig. 36. Effect of test temperature on yield strength.

Fig. 37. Effect of test temperature on tensile strength.

approximately known. The operating temperature was assumed to be less than 270°F, and calibration runs were made on both transducers at room temperature and at 270°F. Least-squares fits were made of voltage to linear and quadratic functions of position. The linear fits were preferred (although quadratic components were statistically significant at the 0.05 level for the room-temperature calibrations) because the inverse relationship (predicting position from a measured voltage) is easier to handle, and the quadratic component made very little difference from a practical standpoint. There is no theoretical justification for the linear model adopted, and a factor of 10 increase in the estimated variance of the 270°F data may have masked a quadratic effect there. Calculation schemes were set up so that once the operating temperature is determined, the appropriate calibration line for that temperature can be interpolated, or can be extrapolated if the operating temperature is higher than 270°F.

Uranium nitride experiment data analysis (F. L. Miller, Jr., O. W. Russ, B. Fleischer,⁶⁸ and K. R. Thoms⁷⁰). Two instrumented uranium nitride experiments, UN-4 and UN-5, are currently in the poolside facilities of the Oak Ridge Research Reactor. Both experiments contain thermocouples which are periodically sampled by an automatic recording device called a Dextir recorder. The recorder scans each thermocouple of an experiment in turn for 3 min every 6 hr. These data are recorded on magnetic tape and processed daily by a computer.

The problem is to develop a method of detecting aberrant thermocouples. Catastrophic failure of a thermocouple is easy to detect; what is needed is a way to detect subtle shifts in a thermocouple which could trigger malfunctions of the experiment. We have implemented a system which does not protect against all possible forms of failure and does not use all available information but does seem to make a reasonable compromise between universality of coverage and complexity of programming.

Both of the experiments contain three fuel pins, and each fuel pin is monitored by ten thermocouples. There are four pairs of thermocouples in the NaK surrounding each pin to measure heat transfer and two thermocouples on the cladding of the fuel pin. The position of the experiment with respect to the face of the reactor is adjusted to hold the temperature of one of the cladding thermocouples of the middle pin at a desired temperature. Unfortunately, the positioning is not dynamic, and the temperatures measured by the cladding thermocouples drift slowly up or down between positionings of the experiment (which may be several days apart). The direction of the drift is determined by the position of the fuel pin with respect to the constantly changing reactor flux pattern.

This drift makes control charts on average cladding temperature or average difference in temperature within a calorimeter pair difficult to compute because of the adjustments which would be necessary. The difference between the temperatures indicated by the two cladding thermocouples of a fuel pin is relatively free of drift, however, and we are monitoring it with control chart techniques.

Even though the average temperature indicated by a thermocouple drifts, the variance of this average remains relatively constant. The variance of a thermocouple seems to be a good indicator of its reliability, and we monitor the variance of each of the thermocouples with control chart techniques. Average differences between cladding thermocouples and average variances of thermocouples were obtained from past data, and 95% control limits were computed for them. In the daily processing of the Dextir recording, an average difference or variance is flagged if it is outside its control limits. This gives the personnel who are monitoring the experiment an early warning system.

Uranium oxide reactor fuels (F. L. Miller, Jr., O. W. Russ, and R. B. Fitts⁷¹). Analysis of a portion of the data collected during the SG-3 experiment indicated a 10% difference in heat generation rates between

70. Reactor Division.

71. Metals and Ceramics Division.

two experimental reactor fuel pins. A more detailed examination of this potentially important finding has been initiated.

The SG-3 capsule contained two uranium plutonium oxide fuel pins. The material was prepared by the sol-gel process and formed into microspheres (the spherepac pin) or dried and cold pressed (the pellet pin). The spherepac pin produced more heat than the pellet pin for equal temperature. Each pin was monitored by 12 thermocouples - one in the center of the fuel pin, three around the cladding, and four pairs of thermocouples in the NaK surrounding the pin to measure heat transfer. The experiment was in the poolside facility from December 15, 1969, to March 26, 1970. During this time the Dextir recorder obtained about 1500 sets of 30 scans of the 24 thermocouples. We chose 261 of these sets, ensuring that every temperature hold was represented at least once. We fitted low-order polynomials in combinations of one thermocouple against another. For example, we fitted center temperature as a quadratic function of average cladding temperature. By examination of residuals, we have been able to detect anomalous behavior in the recorder and in the thermocouples and changing flux patterns in the reactor due to the insertion of another experiment nearby. The variability of the points has been sharply reduced, and the difference between the fuel pins has been sharpened.

ORNL-NSF Environmental Program

An index of pollution (V. R. R. Uppuluri and Patricia MacLean⁷²). An index of pollution for the use of the general public is proposed. This index is defined as the relative proportion of pollutants that exceed the threshold values (e.g., set by the EPA) to the total number of pollutants observed. At a given place, based on past data, one can empirically estimate the probability that each pollutant exceeds the corresponding threshold value. By using these estimates, one can determine the probability that on a given day the index takes suggested values. Computer programs are available to compute these probabilities.

UT Memorial Research Center

Erythropoietin bioassay (T. J. Mitchell and A. L. Kretchmar⁷³). When mice are placed in cages covered with silicone rubber membranes, the oxygen level in the cages is greatly reduced. As a consequence, red blood cell production in these mice is sharply increased. When the mice are subsequently returned to a normal atmosphere, they have more red cells than they need, so that the bone marrow essentially stops red cell production for a period of time. This makes these animals particularly suitable for the assay of erythropoietin, which stimulates red cell production. If an unknown dose of erythropoietin is administered, followed by an injection of radioactively marked iron (⁵⁹Fe), the amount of ⁵⁹Fe incorporated into the new red blood cells is taken to be a measure of the amount of erythropoietin present in the unknown dose.

Data from this assay procedure are typically badly behaved. The variation is considerable, and nearly every assay indicates the presence of "outliers," or mice, whose percent ⁵⁹Fe uptake sharply disagrees with the others in the same group. Usually, these outlying observations are on the high side, so they represent mice that, for some reason, have unusually high uptakes.

Some investigators apply their own informal outlier rejection techniques. These are seldom discussed, or even admitted, in their publications; the only clue is the suspiciously low standard errors that are reported. Other investigators transform the response, usually by taking its logarithm. Of these, some also transform the dose to log dose.

72. ORAU Student Trainee.

73. University of Tennessee Memorial Research Center.

We have recently made a study of some of the statistical aspects of this assay procedure, using data obtained by researchers at the University of Tennessee Memorial Research Center, who have considerable experience in this area. The object of the study was to determine the effect of transforming the dose and/or the response and, if possible, to settle on a "best" procedure. Only the logarithmic transformation, which is the one most commonly used, was considered, so that comparisons were made among the four dose-response relationships:

1. mean response vs dose,
 2. mean response vs log dose,
 3. mean log response vs dose,
 4. mean log response vs log dose.
- (1)

The data used in this study came from regular weekly assays for erythropoietin over the period from July 11, 1969, to October 17, 1969. A total of 145 groups of 5 mice each were considered. Of these 145 groups, 25 had been given saline and served as controls; the remaining 120 groups had been given erythropoietin at various known dose levels up to 1.0 unit.

The dose-response relationships (1) were compared with respect to the requirements given by Finney⁷⁴ for the "statistical validity" of a bioassay. These are the assumptions upon which the mathematical derivations of potency estimates and their confidence intervals are based.

We concluded that the statistical assumptions can best be met by applying the logarithmic transformation to both the response and the dose. This judgment is based principally on the fact that the log transformation of the response is necessary to stabilize the standard deviation and on the observation that the corresponding log transformation of the dose appeared to improve the linearity of the dose-response relation.

In addition, the relative merits of the mean and the median as measures of group response were investigated. Both were found to be equally effective in discriminating among doses. The median is easier to use and is less affected by "outliers," but there is no easy method for estimating its standard deviation as there is for the mean.

Y-12

Maintenance study for Excello turning and boring tape controlled machines (W. E. Lever). An investigation is being conducted to evaluate the effectiveness of a preventive mechanical maintenance program for Excello turning and boring tape controlled machines in the Y-12 Plant. The study is based on production and repair time data which are collected daily and stored at the Computing Technology Center. From these records the frequency of production times between breakdowns, breakdown repair times, and preventive maintenance repair times are tabulated against time intervals appropriate for the respective operations. These tabulations are updated on a monthly basis.

Two approaches were used to evaluate the program. The first approach was to simulate the system based on the three observed frequency distributions, for production times between preventive maintenances of 25 to 500 hr.

The results of this approach proved somewhat surprising. As the preventive maintenance period was increased, the average number of breakdowns observed generally decreased, and the average time between

74. D. J. Finney, *Statistical Method in Biological Assay*, 2d ed., pp. 395-403, Hafner, New York, 1964.

breakdowns uniformly increased. These results indicated that short-term preventive maintenance may actually be decreasing the operating efficiency of the machines.

The second approach involved the fitting of a probability distribution to the observed time-between-breakdown distribution. The optimum preventive maintenance period was then determined from theoretical results based on the failure rate of the fitted distribution. The theoretical results are available in the literature.

An examination of the observed time-between-breakdown distributions indicated the two-parameter Weibull distribution was excellent for the approximating distribution.

The cumulative distribution function of the two-parameter Weibull distribution is given by

$$F(t) = \int_0^t (\alpha/\beta)(X/\beta)^{(\alpha-1)} e^{-(X/\beta)^\alpha} dX, \alpha, \beta > 0,$$

with failure rate given by

$$q(t) = (\alpha/\beta)(t/\beta)^{(\alpha-1)}.$$

The preventive maintenance policy which appears to be optimum for the n machines is to perform preventive maintenance every t_0 hours regardless of the number of breakdowns which have been repaired since the last preventive maintenance. Then it can be shown⁷⁵ that the preventive maintenance period is given by

$$t_0 = \begin{cases} t^* : \int_0^{t^*} t q'(t) dt = T_p/T_m \text{ if } q(t) \text{ is increasing after some point,} \\ \infty : \text{if } q(t) \text{ is not increasing after some point,} \end{cases}$$

where T_m is the expected cost associated with a breakdown and T_p is the expected cost associated with preventive maintenance.

When the Weibull distribution was fitted to the observed time-between-breakdown distributions, which are updated monthly, the estimate of α was consistently between 0.6 and 0.65 with an error of less than 0.05.

The estimate of α less than 1 implies the time-between-breakdown distribution has a decreasing failure rate and preventive maintenance does not seem to be justified, especially on a short-term basis.

Since the results of both approaches led to the conclusion that preventive maintenance was not justified, recommendations were made to stop preventive maintenance when possible.

These recommendations were made for the machine as a whole unit. As more data are collected, recommendations will be made for individual systems within the machines.

Procedure for determining theoretical optimum mean values for a three-stage process (W. E. Lever and Norma Hull). The outcomes, X_1, X_2, X_3 , produced at three stages of a production process in the Y-12 Plant are believed to be described by a trivariate normal probability distribution with mean vector $\mu = (\mu_1, \mu_2, \mu_3)$ and covariance matrix Σ . In order that the product of this process meet specifications, (X_1, X_2, X_3) must obey the following restrictions:

$$X_1 \geq A, \tag{1}$$

75. R. E. Barlow and L. C. Hunter, *Operations Res.* 8, 90-100 (1960).

$$X_2 \geq B \quad (2)$$

$$X_3 \geq C, \quad (3)$$

$$D_2 \geq X_1 + X_2 + X_3 \geq D_1. \quad (4)$$

Based on the trivariate normal model, an investigation was initiated to determine the range of values of μ which would yield the largest probabilities of the process meeting specifications. Since the actual value of Σ was not known, the investigation was based on an estimate of Σ obtained from observations made on the process.

A computer program written to compute the necessary probabilities used a subroutine designed to numerically integrate trivariate integrals according to the Romberg method.

A preliminary look at the probabilities for various values of μ indicated the contours of constant probability were elliptical in shape and the larger probabilities tended to be near the region defined by $\mu_1 + \mu_2 + \mu_3 = (D_1 + D_2)/2$.

The probability program was then modified to generate a series of 3^3 factorial designs in μ , with each succeeding design covering a smaller area in the μ space. Each of these designs was set up to concentrate on the region around $\mu_1 + \mu_2 + \mu_3 = (D_1 + D_2)/2$.

The first design was centered at a point which was believed to be in the general region of maximum probability. A quadratic polynomial in μ was then fitted to the calculated probabilities, and the center of the contour system, which was also the maximum point of the fitted polynomial, was determined. The next design was then centered at this point. This method was used for each of the succeeding designs, and the center point of the final contour system was taken as the optimum value for μ . A series of six designs was found to be sufficient to determine the optimum value for μ .

Since this determination had to be related to other phases of the process, probabilities were computed for a narrow range of values of μ around the calculated optimum value, and the maximum and minimum probabilities for this range were reported.

STATISTICAL PROGRAMMING

The Time-Sharing Computer Terminal

E. Leach

The Statistics Department of the Mathematics Division is presently using the time-sharing services of Rapidata Incorporated, who acquired on December 1, 1971, the New York-based computer interests of Boeing Computer Services Incorporated, the former time-sharing service used by the Statistics Department.

The time-sharing service is available through regular telephone service which allows immediate access to computers situated in New York, New Jersey, Long Island, Boston, Philadelphia, and San Francisco. The remote terminal installed onsite consists of one standard 100-word/min model 33 Teletype machine and one General Electric TDM 114A40 data set. The service is also available through an IBM 2741 communications terminal. The time-sharing service is used for running programs written either in FORTRAN or BASIC language that require little central processing unit and input-output time.

Figure 38 shows the usage in connect time of the time-sharing facility by month from November 1, 1970, through October 31, 1971. Figure 39 shows the use in CP units of the time-sharing facility by month for the same period. A CP unit is defined as being one central processing unit second or 1.33 input-output seconds.

Fig. 38. Connect time of time-sharing service.

Fig. 39. CP units of time-sharing service.

Conversational Remote Batch Entry Terminal

E. Leach

The IBM 2741 communications terminal located in the Statistics Department of the Mathematics Division continues to be used on the average of 30 hr per month for submitting jobs through the CRBE system. The system has proven to be a handy device in aiding the debugging of programs and for submitting jobs for quick turnaround time on the computer.

The programs submitted through the CRBE system consist of programs written in the FORTRAN IV, OMNITAB, or BASIC programming language.

During the last year there have been ten different users submitting programs through the CRBE terminal located in the Statistics Department. Figure 40 indicates the usage of the CRBE terminal by month for the period of November 1, 1970, through October 31, 1971.

Fig. 40. Use of CRBE terminal.

A Use of the FORMAC Symbolic Manipulation Language

T. C. Tucker J. J. Beauchamp

To obtain and program the partial derivatives of a function for nonlinear least-squares regression by NONLIN or a similar code is often very time-consuming. Further, as the complexity of the function increases, so does the possibility of error. We are investigating the FORMAC symbolic manipulation language as a possible aid in the solution of such problems.

We have concluded that FORMAC can be helpful. The language has the capability of differentiation of functions of several variables with respect to any subset of those variables. Derivatives of most common functions are standard within the FORMAC system, and nonstandard functions and derivatives can be defined in general terms.

The partial derivatives obtained by FORMAC are not always suitable for programming. For example, the relatively simple function

$$f = (a - x^{-1}) e^{ax},$$

using straightforward FORMAC coding, would have the partial derivative

$$\frac{df}{da} = e^{ax} + (a - x^{-1}) x e^{ax}.$$

Failure to expand the parenthetical expression and simplify could lead to substantial error in numerical evaluation if df/da is small compared with e^{ax} . It is possible to force such an expansion in FORMAC, thus solving this problem. A function, however, could contain the product of a pair of functions of n and m terms, some of which cancel. In this case, expansion would result in replacing an expression of $n + m$ terms by one with $n - m$ terms.

Thus a single-pass FORMAC solution is not generally good. Analysis of the initial results and reprogramming to cause simplification would be better, and the CRBE system is useful for this approach.

We are also investigating the possibility and desirability of using PL/1 with FORMAC to produce directly the FORTRAN subroutine required by NONLIN. Alternatively, the FORTRAN program NONLIN might be replaced by a PL/1 version. In this case, FORMAC could obtain the numerical values required, and the regression could be completed in a single computer run.

Fisher's Exact Test

D. A. Gardiner J. G. Sullivan

A FORTRAN program was written to evaluate the probability in Fisher's Exact Test for a 2×2 contingency table. The algorithm utilizes a recursion relationship between the successive probabilities which must be summed and thereby minimizes the number of factorials that are evaluated.

Factorials are evaluated by direct multiplication rather than by logarithms or by approximations. The numbers are manipulated in the form $a \cdot 10^b$ by scaling a between 0.1 and 1.0 and storing a separately from the integer b .

Contingency tables based on samples as large as 12,000 have been handled successfully by the program.

General-Purpose Programs

Norma Hull

The STATPAK⁷⁶ programs which were not programmed in double precision are being changed to double precision. NONLIN, a linear/nonlinear estimation program in STATPAK, has been revised to allow the user to set limitations on any of the parameters specified by the model used.

Kolmogorov-Smirnov Statistics

F. L. Miller, Jr.

A series of subroutines have been written to compute Kolmogorov-Smirnov statistics for both comparison with a known distribution and comparison of two empirical distributions. They differ from the IBM Scientific subroutine package programs⁷⁷ in that statistics are computed to test both one- and two-sided hypotheses.

76. Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL 4661, p. 177.

77. System/360 Scientific Subroutine Package (360A-CM-03X), (1968).

LOGNORM

Norma Hull J. J. Beauchamp

A computer program, LOGNORM, was written to perform a log normal regression⁷⁸ on a set of data. Input to the program is the number of data points, title of the problem, format for the data, and the data. The program consists of two main parts. The first part of the program changes the input data by means of a logarithmic transformation and performs a linear regression analysis on the data. Output from the first part of the program consists of the usual linear regression statistics.

The second part of the program takes the results from the linear regression portion and uses them to calculate the necessary constants and expressions described in "Log Normal Regression."⁷⁸

The program will also produce several useful plots to help interpret the results of the program graphically.

Application of a Gradient Search Method for Minimization of a Sum of Squares Surface

Norma Hull J. J. Beauchamp D. A. Gardiner

The program GRADIENT⁷⁹ has been adapted to find the minimum point on a sum of squares surface subject to nonlinear equality or inequality constraints. For the case when the partial derivatives of the objective function are nonlinear in the parameters to be estimated, a subroutine has been added to allow the user the option of defining these partial derivatives. For this particular problem the objective function is the sum of squares function.

The adapted program has been used with several sets of data, the most complex problem being a function involving 14 independent variables and 37 parameters subject to four equality constraints.

The output shows the value of parameters, objective function, partial derivatives, values of the constraints, and the sum of squares throughout the search procedure. When the sum of squares for successive steps has a difference less than an input tolerance value, the search procedure stops, and the final values are printed.

Conversion of Computer Programs

Norma Hull

Several programs previously written in the BASIC programming language have been converted to the FORTRAN IV programming language to be used on the IBM/360 computers. These programs were run repeatedly on a time-sharing computer through the use of a remote terminal until the central processing unit time and the input/output time became too excessive for the programs to be run economically.

Mouse Body Weight Analysis

E. Leach

A third computer program was written for the mouse body weight analysis experiment.⁸⁰ The program produces plots that give a comparison of the weights of both sexes for the different ages at which they were weighed. The user of the program must specify the group numbers and the litter orders of the animals that

78. J. J. Beauchamp and Norma C. Hull, "Log Normal Regression," this report.

79. GRADIENT was written by K. E. Cross at the Computing Technology Center.

80. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 175.

are to be included in the analysis. An analysis is done over all groups and litter orders specified for both sexes. The analysis provides the average weight of the animals for each sex at each weighing date, over all groups and litter orders included in the analysis. These average weights with their standard deviations are plotted for both sexes on the same plot. A printout of the average weights and standard deviations from the analysis is also produced. Any combination of the group numbers and the litter orders can be specified as input for the program.

Pathology Data Files

E. Leach

Several programs have been written in the BASIC programming language to create various combinations of pathological data files. The data of primary interest are the age at death of the animals in the experiment and the diseases that are found present in the animals. A coding system is used which gives a code to each animal for each disease. The five codes used are: 0, no sample was taken; 1, disease was not the cause of death; 2, disease was the possible cause of death; 3, disease was not the cause of death, but was present; and 4, disease was not present.

The master file, either a punched paper tape or a stored file, consists of the ages at death of all of the animals in the experiment in age order and will not change for the different diseases within an experiment. The disease tape, a punched paper tape, consists of the codes for each animal for a given disease.

One of the programs written combines the master file and the disease tape and creates a data file which includes only the animals with the codes specified by the user of the program. Another program allows the user to combine experiments and creates a data file in age order with the codes of each animal included. The data files created from these programs are used as input to other statistical programs written in the BASIC programming language.

Pathology Data Control: Percent Incidence and Diagnosis Lists

E. Leach

A program LISDIAG has been written for a biologist to summarize the autopsy records kept on the animals included in an experiment and for computing other statistical analyses on the experiment.

For each experiment the mean age at death and the standard error of the mean age at death are computed with all animals included. For each sex the total number of animals, the mean age at death, and the standard error of the mean age at death are computed. A list of 46 different diagnoses or combinations of diagnoses is produced for each experiment. For each of the diagnoses the number of animals with the diagnosis, the percent incidence for the diagnosis, the mean age at death, and the standard error of the mean age at death are computed for the males and females within an experiment.

Data Processing of Litter Box Collections

Claudia Lever J. J. Beauchamp Norma Hull T. Grizzard⁸¹

The presence of trace elements in the leaves, limbs, and other parts of trees varies considerably during different seasons of the year and for different species. This variation was measured by analyzing material collected from 80 plots in a forested area. The 80 plots were classified into four forest types: pine,

81. Ecological Sciences Division.

pine-oak-hickory, oak-hickory, and other hardwoods. They were then subclassified according to the density of the forest and the size of the trees so that there were 13 different forest types, with the number of plots per type ranging from 2 to 14.

Litter boxes 1 m² in area were placed at random in each plot. Nine times during the year July 1, 1969, to July 1, 1970, everything that had fallen in the boxes was collected. The collection intervals ranged from two weeks during the fall to about three months over the winter. This material was divided into leaves, limbs, and other and then dried and weighed. The percent of nitrogen present was determined for each of the three parts for each box. Then a sample was taken from each part, and the parts per million (ppm) of calcium, magnesium, sodium, potassium, and phosphorus were determined. The percents present of these elements were calculated from the ppm and the sample dry weights.

For each of the 13 forest types for each collection the means and standard errors of the dry weights of leaves, limbs, and other were calculated. The means and standard errors of the percent of each of the six elements were also calculated.

The means were punched on cards so they could be plotted in different combinations. This was useful since most of the interpretation of the results was based on visual comparison of the plots rather than a formal statistical analysis. The mean dry weights were plotted against time in days, with a separate plot for each forest type but with leaves, limbs, and other on the same plot. The means of the percents of each element were also plotted against time in days. The plots for each of the four major forest types showed different patterns, that is, different peak collection periods, different shapes of the curves, etc., but the subclassified forest types within each major type showed the same overall pattern. Therefore, the subclassification scheme was dropped, and the plots were divided into just four groups with 6 to 35 plots in a group.

The means and the standard errors of the dry weight collected and the percents of the elements were recalculated, and new plots were made of the means. The dry weight of each element was also estimated from the percent of the element present and the total dry weight collected.

The means and standard errors of the dry weights were also calculated with an adjustment for the different lengths of the collection intervals. This was done for the dry weights of all material collected and for the dry weights of each element. The plots of these means gave a better indication of the rate of accumulation of material, while the other plots gave the total weight of each collection.

PITFALL I

Norma Hull

The PITFALL I⁸² programs are being used by the Ecological Sciences Division to process and analyze environmental monitoring data. The programs have been revised to accept more data than they would originally accept. Some unusual cases have been processed by making changes in the programs to allow for more flexibility. Some of the data of very small magnitude or variation have been scaled upward to provide a better analysis of the data.

Walker Branch Watershed Data Analysis

Norma Hull F. L. Miller, Jr.

Programs have been written to correlate the rainfall and streamflow measurements taken in the Walker Branch Watershed. Autocorrelations and cross correlations are calculated. The data are measurements of

82. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970, ORNL-4661, p. 178.*

streamflow from both weirs and measurements of rainfall from five rain gages scattered across the watershed. Measurements are made every 5 min. A program has been written to combine the rain gage measurements to estimate rainfall in the two branches. These data, along with the streamflow measurements, have been placed on tape for further analysis.

Statistical Test of Changes due to Irradiation

T. L. Hebble Norma Hull

A computer program has been written to test, statistically, changes in diameter of fuel pins due to fast flux irradiation. Tolerance limits are computed to test the changes in the 0 to 180° and the 90 to 270° measurement planes and the overall average change. Confidence intervals about a single position are easily obtained from the output. Graphical output includes a plot of the observations, the average changes for each measurement traverse, and the overall average change with tolerance limits.

Mathematical Research Seminars

- Anselone, P. M. (Oregon State University), "Approximate Solutions of Integral and Operator Equations," October 15, 1971.
- Bernstein, Barry (Illinois Institute of Technology), "Volterra Integral Equations in Blood Circulation Measurements," October 28, 1971.
- Chang, S. J. (Mathematics Division, ORNL), "Several Aspects of the Mathematical Theory of Viscoelasticity," September 24, 1971.
- Coveyou, R. R. (Mathematics Division, ORNL), "Twenty Questions," November 5, 1971.
- Dolan, J. M. (Mathematics Division, ORNL), "On the Relationship between Initial-Value Problems and Oscillation Theory," October 8, 1971.
- Madsen, N. K. (Bettis Atomic Power Laboratory), "Discretization Error Estimates for Transport Problems," December 9, 1971.
- Nelson, Paul (Mathematics Division, ORNL), "A New Method for the Hybrid Solution of Partial Differential Equations," October 22, 1971.

Statistical Seminars

Frome, E. L. (Emory University, Atlanta, Georgia), "Spectral Analysis of Phono-Cardiogram," November 4, 1971.

Kastenbaum, M. A. (The Tobacco Institute, Washington, D.C.), "Some Statistics in the Smoking and Health Controversy," April 15, 1971.

MacLean, Patricia M. (ORAU Summer Student Trainee), "Probabilities and Pollution Indices," August 5, 1971.

Miller, F. L. (Mathematics Division, ORNL), "A Recent Meeting in Southwest Virginia," June 24, 1971.

Mitchell, T. J. (Mathematics Division, ORNL), "A Recent Meeting in Southwest Virginia," June 24, 1971.

Rao, C. R. (Indian Statistical Institute, New Delhi, India), "Statistics in Research and Decision Making," August 2, 1971.

Professional Activities

Bowman, Kim O., Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.

Brooks, A. A., Member, ACM SIGPLAN Committee for Symposium on Data Structures in Programming Languages.

Coveyou, R. R., Referee, *Nuclear Science and Engineering*, for several SIAM journals, and for several ACM journals.

Coveyou, R. R., Reviewer, *Mathematical Reviews* and *Computing Reviews*.

Funderlic, R. E., Referee, Society for Industrial and Applied Mathematics.

Gardiner, D. A., Member, Editorial Advisory Board, *Journal of Statistical Simulation and Computation*.

Gardiner, D. A., Editorial Board, *Communications in Statistics*.

Gardiner, D. A., Editor-Elect, *Technometrics*.

Gardiner, D. A., Chairman-Elect, Section on Physical and Engineering Sciences, American Statistical Association.

Gardiner, D. A., Member, Regional Committee on Statistics, Southern Regional Education Board.

Gardiner, D. A., Consultant, Office of Director of Regulation, U.S. Atomic Energy Commission.

Gardiner, D. A., Lecturer, Visiting Lecture Program in Statistics, Committee of Presidents of Statistical Societies.

Gove, N. B., Editor, *Computer Physics Communications*.

Gove, N. B., Member, Nuclear Data Project Advisory Board.

Heath, M. T., Referee, Society for Industrial and Applied Mathematics.

Hebble, T. L., Member, Advisory Board to Section on Physical and Engineering Sciences of the American Statistical Association.

Leinius, R. P., Reviewer, *Computing Reviews*.

Lever, W. E., Referee, *Biometrics*.

McCulloch, K. D., Referee, *Atomic Energy Review*.

Mitchell, T. J., Referee, *Technometrics* and *Sankhya*.

Mitchell, T. J., Consultant, University of Tennessee Memorial Research Center.

Mitchell, T. J., Instructor, University of Tennessee Oak Ridge Resident Graduate Program.

Nelson, P., Referee, *Nuclear Science and Engineering*.

Nelson, P., Reviewer, *Mathematical Reviews* and *Computing Reviews*.

Nestor, C. W., Referee, *Computing Reviews*.

Nestor, C. W., Referee, *Nuclear Science and Engineering*.

Penny, S. K., Member, Defense Atomic Support Agency Cross Section Working Group.

Penny, S. K., Member, Shielding Subcommittee, Codes and Formats Subcommittee, and Nuclear Codes Task Force of the Cross Section Evaluation Working Group, Brookhaven National Laboratory.

Penny, S. K., Reviewer, *Nuclear Science and Engineering*.

Uppuluri, V. R. R., Referee, *Annals of Mathematical Statistics*, *Journal of the American Statistical Association*, and *Biometrics*.

Uppuluri, V. R. R., Consultant, Medical Division, Oak Ridge Associated Universities.

Uppuluri, V. R. R., Visiting Professor, University of Minnesota.

Whitesides, G. E., Member, Committee for Nuclearly Safe Pipe Intersections for Solutions of Fissile Materials, American Nuclear Society.

Whitesides, G. E., Treasurer, Mathematics and Computations Section of the American Nuclear Society.

Whitesides, G. E., Chairman, Committee for the Validation of Computational Methods for Nuclear Criticality Safety, American Nuclear Society.

Whitesides, G. E., Executive Committee, Mathematics and Computations Section of the American Nuclear Society.

Whitesides, G. E., Member, Committee to Write Guide for the Storage of Low Enriched Uranium, American Nuclear Society.

Whitesides, G. E., Referee, *Nuclear Science and Engineering*.

Whitesides, G. E., Referee, *Nuclear Applications and Technology*.

Mathematics Division Publications

- Anderson, V. E. (with C. E. Klotz), "Monte Carlo Investigation of the Imprisonment of Resonance Radiation: The Doppler-Broadened Line," *J. Chem. Phys.* (1971).
- Anderson, V. E. (with J. E. Turner), "Relativistic Ground-State Energy Eigenvalues of the Electron-Dipole System," *Nuovo Cimento Soc. Ital. Fis.* 1B, 149-54 (February 1971).
- Anderson, V. E. (with L. G. Christophorou and D. L. McCorkle), "Swarm-Determined Electron Attachment Cross-Sections as a Function of Electron Energy," *J. Phys. & At. Mol. Phys.* (1971).
- Barish, J. (with T. W. Armstrong), "Calculated Activation of Copper and Iron by 3-GeV Protons," *Nucl. Sci. Eng.* 41, 443 (1970).
- Barish, J. (with R. G. Alsmiller, Jr., F. S. Alsmiller, and Y. Shima), *MUON Transport and the Shielding of High-Energy (≤ 500 GeV) Proton Accelerators*, to appear in *Proc. International Congress on Protection against Accelerator and Space Radiation, CERN, Geneva, April 26-30, 1971* (also available as ORNL-TM-3353, April 1971).
- Bartine, D. E., and J. Barish (with R. G. Alsmiller, Jr., F. R. Mynatt, and W. W. Engle, Jr.), *Low-Energy Electron Transport with the Method of Discrete Ordinates*, in *Proc. National Symposium on Natural and Manmade Radiation in Space, Las Vegas, Nevada, March 1-5, 1971* (also available as ORNL-TM-3318, February 1971).
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- Beauchamp, J. J. (with R. C. Dahlgren and Y. Tanaka), "Effects of Simulated Fallout Radiation on Reproductive Capacity of Rescue," to appear in *Proceedings of the Third National Symposium on Radioecology*.
- Beauchamp, J. J. (with Helen Vodopick, Elizabeth M. Rupp, C. L. Edwards, and F. A. Goswitz), "Spontaneous Cyclic Leukocytosis and Thrombocytosis in Chronic Granulocytic Leukemia," to appear in *New England Journal of Medicine*.
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- Barish, J. (with R. W. Roussin and R. G. Alsmiller, Jr.), *Shielding against Neutrons in the Energy Range 15 to 75 MeV*, ORNL-TM-3459 (December 1971).
- Bartine, D. E., and J. Barish (with R. G. Alsmiller, Jr., F. R. Mynatt, and W. W. Engle, Jr.), *Low-Energy Electron Transport with the Method of Discrete Ordinates*, ORNL-TM-3438 (1971) (dissertation).
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- Bowman, Kimiko O., *Sample Size Requirement: Continuation*, ORNL-4712 (August 1971).
- Bowman, Kimiko O. (with L. R. Shenton), *Tables of Moments of the Maximum Likelihood Estimator of the Parameter p for the Zero Truncated Binomial Distribution*, ORNL-4747 (November 1971).
- Brooks, A. A., *Adoption of Generalized Record Format*, ORNL-CF-71-1-9 (January 1971).
- Brooks, A. A., *Project for Information Processing*, ORNL-CF-71-5-37 (May 1971).
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