ORNL-4661
UC-32 – Mathematics and Computers

MATHEMATICS DIVISION
ANNUAL PROGRESS REPORT
FOR PERIOD ENDING DECEMBER 31, 1970

OAK RIDGE NATIONAL LABORATORY

operated by

UNION CARBIDE CORPORATION

for the

U.S. ATOMIC ENERGY COMMISSION

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce, Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.65

ORNL 4661
UC-32 — Mathematics and Computers

Contract No. W-7405-eng-26

MATHEMATICS DIVISION
ANNUAL PROGRESS REPORT
for Period Ending December 31, 1970

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

APRIL 1971

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
operated by
UNION CARBIDE CORPORATION
for the
U. S. ATOMIC ENERGY COMMISSION

Reports previously issued in this series are as follows:

ORNL-2283	Period Ending February 28, 1957
ORNL-2652	Period Ending August 31, 1958
ORNL-2915	Period Ending December 31, 1959
ORNL-3082	Period Ending December 31, 1960
ORNL-3264	Period Ending January 31, 1962
ORNL-3423	Period Ending December 31, 1962
ORNL-3567	Period Ending December 31, 1963
ORNL-3766	Period Ending December 31, 1964
ORNL-3919	Period Ending December 31, 1965
ORNL-4083	Period Ending December 31, 1966
ORNL-4236	Period Ending December 31, 1967
ORNL-4385	Period Ending December 31, 1968
ORNL-4514	Period Ending December 31, 1969

Contents

MATHEMATICAL RESEARCH

COMPUTING APPLICATIONS

SYSTEMS PROGRAMMING

COMPUTER SERVICES

Pearl N. Coffey, L. S. Finch, R. L. Finch, T. A. Gardner, Jr., L. G. Hodge, J. E. Parham, S. O. Smith, and C. S. Williams

MATHEMATICAL STATISTICS

Mathematical Research

THEORETICAL ASPECTS OF NEUTRON TRANSPORT

Paul Nelson

Consider steady-state linear particle transport in a slab of finite thickness. Let γ denote the maximum expected number of secondary particles emitted per collision. Then one expects physically that there is some $\gamma_1 > 1$ such that the system is subcritical for $\gamma < \gamma_1$, where "subcritical" means the steady-state transport equation has a nonnegative solution for any combination of internal and external particle sources. We have considered the problem of establishing this result under conditions of maximum generality on the cross section and scattering law.[1]

An obvious extension of the problem described in the preceding paragraph is the problem of characterizing, for given $\gamma \geqslant \gamma_1$, those source functions (if any) which yield a nonnegative solution of the steady-state transport equation. This leads to the mathematical problem of characterizing those real $\lambda > 0$ and positive y such that

$$\lambda x = Tx + y$$

has a positive solution x, where T is a positive linear operator on some ordered linear space and x, y are elements of this space. Under suitable restrictions, it has been shown[2] that this is possible if, and only if, y is annihilated by the *absolute value* of any generalized eigenvector of T^* (adjoint of T) associated with a positive eigenvalue which is not less than λ and which has an associated positive eigenvector. If the underlying space is L^p, this yields the result that such x exists if, and only if, y is almost everywhere zero on a certain set which depends on λ but is otherwise fixed. Work is currently proceeding on the problem of directly characterizing these "critical sets" in the particular case of T an integral operator.

MODELS OF NUCLEAR REACTOR ECONOMICS

Paul Nelson Gale Young[3]

This is a continuation of an item which was last described in the 1967 annual report.[4] We have shown how to solve "Problem D" of this reference for a positive discount rate and without the assumption that one reactor type have both larger specific fuel inventory and larger specific operating cost, provided that

1. P. Nelson, "Subcriticality for Transport of Multiplying Particles in a Slab," to appear in *J. Math. Anal. Appl.*
2. P. Nelson, "Positive Solutions of Positive Linear Equations," submitted to *Proc. Am. Math. Soc.*
3. Director's Division.
4. *Math. Div. Ann. Progr. Rept. Dec. 31, 1967,* ORNL-4236, p. 7.

both reactor types are breeders and the given power demand is such that both reactor types become self-sustaining within the planning period.

APPLICATIONS OF THE METHOD OF INVARIANT IMBEDDING

Paul Nelson D. W. Altom Carla L. Armstrong

We have continued to explore applications of the particular version of invariant imbedding[5] which was mentioned in the 1969 annual report,[6] with particular emphasis on applications to problems arising from fields other than linear particle transport. One of the most interesting applications has been to the numerical solution of partial differential equations by hybrid computer.[7,8] We explored the possibility of using this technique to solve a boundary-value problem for a large system over a long interval. One possible numerical difficulty occurring in this approach was isolated, and a method for avoiding it was devised.[9] The relationship between this version of invariant imbedding and that used by some other workers was clarified.[10]

ALGEBRAIC AND TRANSCENDENTAL EQUATIONS

A. S. Householder[11]

The book on nonlinear equations mentioned in the previous annual report has now appeared.[12]

The paper on the Padé table which had been submitted to the *Journal of Linear Algebra and Its Applications* was recalled in order to incorporate in it certain improvements and extensions. The revision is now in press with a slightly different title.[13] The revision includes the simplification of some of the proofs and a new derivation of the Frobenius identities that are fundamental to the *qd* algorithm for solving algebraic and transcendental equations.

A sequel[14] to this paper has been submitted to the same journal. Fundamental to the treatment in the Padé paper are certain determinants that arise in a natural way from either a single power series (Hankel determinants) or from pairs of power series (bigradients). The fundamental, and apparently new, theorem related the determinants of the two types when the single series is the expansion of the quotient of the other two. Recent results of G. W. Stewart, former ORAU Fellow now at the University of Texas, extend and generalize the method of Sebastião e Silva, adding to its flexibility and showing it to be applicable to the treatment of transcendental equations. These results suggest the introduction of determinants of a class

5. P. Nelson and M. R. Scott, "Internal Values in Particle Transport by the Method of Invariant Imbedding," to appear in *J. Math. Anal. Appl.*

6. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 7.

7. P. Nelson, "Application of Invariant Imbedding to the Solution of Partial Differential Equations by the Continuous-Space Discrete-Time Method," *Proc. 1970 SJCC, AFIPS* **36**, 397–402 (1970), AFIPS Press.

8. P. Nelson and D. W. Altom, "On the Use of Invariant Imbedding within the Continuous-Space Discrete-Time Method: Digital Simulation," to appear in the *Proc. of Conf. on Hybrid Computation, Munich, September 1970.*

9. P. Nelson and C. L. Armstrong, "Accurate Analysis of Long Two-Point Boundary-Value Problems by Invariant Imbedding," submitted to *Comm. ACM.*

10. P. Nelson and M. R. Scott, "The Relationship between Two Variants of Invariant Imbedding," to appear in *J. Math. Anal. Appl.*

11. Consultant.

12. A. S. Householder, *The Numerical Treatment of a Single Nonlinear Equation,* McGraw-Hill, viii + 216 pp., 1970.

13. A. S. Householder, "The Padé Table, the Frobenius Identities, and the qd Algorithm," *Linear Algebra and Appl.* 3 (1970).

14. A. S. Householder, "Multigradients and the Zeros of Transcendental Functions," *Linear Algebra and Appl.* 4 (1971).

apparently not previously considered, being called multigradients, that are formed from an arbitrary set of power series in a natural extension of the formation of bigradients from only two. These, in turn, lead to a class of functionals, called reduced linear combinations (RLC), that are themselves power series and lend themselves to a rather interesting calculus. These RLC's simplify the representation of certain tables that occur in Stewart's work, and exhibit at a glance the fact that Stewart's general method includes as special cases not only the algorithm of Sebastião e Silva, but also the *qd* algorithm, and, indeed, show that these two algorithms, though quite different in appearance, are actually, in a certain sense, identical.

At the request of the editors of *SIAM Review,* the factorization paper previously mentioned was revised and made into a strictly expository paper.[15] The new results were written up separately[16] and will appear shortly in *Numerische Mathematik.*

KWIC INDEX FOR NUMERICAL ANALYSIS

A. S. Householder[11]

The preparation of a KWIC Index for Matrices in Numerical Analysis was announced in the last annual report, of which one volume had already appeared. This included only papers for which the senior authors had names occurring alphabetically up through the J's. A second volume, completing the alphabet, has now appeared. Also being printed is a similar volume listing items dealing with nonlinear equations, algebraic and transcendental.

Each item gives the name(s) of the author(s), title of the article or book, and name of the journal or publisher, as well as, in many cases, references to abstracting and reviewing journals where abstracts and reviews have appeared. Work is continuing in the way of making corrections where errors are discovered, adding abstract and review references, and keeping the listing up to date. At some future date, it is planned to issue a single volume containing all listings including foreign titles not hitherto translated, and otherwise brought up to date as far as possible.

INVARIANTS OF FINITE GROUPS

G. K. E. Haeuslein

We consider a field $K = k(x_1, ..., x_n)$ of algebraic functions in n algebraically independent variables x_1, ..., x_n with coefficients in the field k. Let G be a finite group of linear transformations with coefficients in k acting on the k space with basis $\{x_1, ..., x_n\}$. G extends in a natural way to a group of k automorphisms of K by letting $\sigma f(x_1, ..., x_n) = f(\sigma x_1, ..., \sigma x_n)$ for $f \in K$, $\sigma \in G$. A polynomial $f \in K$ is called an invariant of G if $\sigma f = f$ for all $\sigma \in G$. For Abelian groups A, Fischer[17] described as early as 1915 a method for the determination of the field K^A of all invariants of A, but for arbitrary G no general method is known.

We investigated the case of a finite group G having an Abelian normal subgroup A of prime index. We first construct the field K^A of all invariants of A. Then we try to find a transcendence basis of K^A over k such that G induces a group of linear transformations on the k space spanned by the basis of K^A. This group, G', will be a homomorphic image of the Abelian factor group G/A, and we can apply Fischer's

15. A. S. Householder and G. W. Stewart, "The Numerical Factorization of a Polynomial," *SIAM Rev.* **13** (1971).
16. A. S. Householder, "Generalizations of an Algorithm of Sebastião e Silva," *Numer. Math.* **16**, 375–82 (1971).
17. E. Fischer, "Die Isomorphie der Invariantenkorper der endlichen abelschen Gruppen linearer Transformationen," *Nachr. Akad. Gottinger Wiss.*, 1915, pp. 77–80.

method to compute $(K^A)^{G'} = K^G$. This program could be carried out successfully for prime indices $\leqslant$ 19.[18]

GEOMETRIC PROPERTIES OF SOLUTIONS OF THE DIFFERENTIAL SYSTEM $x' = Ax$

Manuel Feliciano, Jr.

A flat is a subset of n-dimensional vector space of the form $v + L_0$, where v is a fixed vector and L_0 a subspace. Its dimension is that of L_0. A flat is proper if it is not also a subspace.

Let A be a real constant n by n matrix and $x = x(\tau)$ a vector satisfying the vector-matrix differential equation

$$x' = Ax \qquad \left({}' = \frac{d}{d\tau}\right),$$

$$x(0) = c\ .$$

The solution flat to the problem is the lowest dimensional flat that contains x. The dimension of x is that of the solution flat.

It is well known that the dimension of x is the rank of $(x', x'', ..., x^{(n)})$. This matrix can be expressed by

$$Ae^{A\tau}(c, Ac, ..., A^{n-1}c) = Ae^{A\tau}K\ .$$

It can be shown directly that the dimension of x is the rank of K if A is nonsingular. Also the solution flat is proper if A is singular and c has a nonzero component in the subspace belonging to the zero proper value of A.

The Jordan form of a matrix usually leads to a decomposition of the space into direct sums of subspaces. This "Jordan decomposition" of the space is not unique. The initial vector of the problem can be used to obtain a Jordan decomposition relative to A and c. Using such a decomposition the solution flat of the problem can be determined easily.

SEVERAL RELATIONS FOR COMPARISON OF THE GENERAL RATE THEORY AND THE *BKZ* THEORY[19]

S. J. Chang

Several theories were suggested recently by different authors for the mathematical representation of the time-dependent behavior of the general nonlinear materials. In particular for the general rate theory and the *BKZ* theory, we obtain a set of differential equations which should be satisfied by the stress components under two specific types of flow. This set of conditions provides a natural way to compare the two theories.

18. G. K. Haeuslein, "On the Invariants of Finite Groups Having an Abelian Normal Subgroup of Prime Index," *J. London Math. Soc.* (in press).

19. S. J. Chang and L. J. Zapas, "Several Relations for Comparison of the General Rate Fluid and the BKZ Fluid," to be presented at the Winter Annual Meeting of the Society of Rheology, Salt Lake City, Utah, Feb. 1–3, 1971, and to be submitted to the *Transactions* for publication.

It is found that the differential conditions are identical for the two theories in shear rates only in the range of second-order flow. The two theories will show significant differences for larger shear rates.

NONHOMOGENEOUS DIFFERENTIAL EQUATIONS

J. M. Dolan

Configurations of initial-value problems associated with oscillatory and nonoscillatory solutions[20] of the nonhomogeneous differential equation

$$(ry')' + qy = f \quad \text{on } [a, \infty)\,, \tag{1}$$

where a is a real number, r, q, and $f \in C[a, \infty)$, $r > 0$, and $f \equiv 0$ on $[a, \infty)$ were considered when the homogeneous differential equation

$$(ry')' + qy = 0 \tag{2}$$

is (i) oscillatory; (ii) nonoscillatory.

In particular, if η and θ, respectively, denote the set of nonoscillatory and oscillatory solutions of (1) and

$$\eta_{t_0} = \left\{ \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \in E^2 \;;\quad y(t_0) = a_0\,, \quad ry'(t_0) = a_1\,, \quad y \in \eta \right\}, \tag{3}$$

$$\theta_{t_0} = \left\{ \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \in E^2 \;;\quad y(t_0) = a_0\,, \quad ry'(t_0) = a_1\,, \quad y \in \theta \right\}, \tag{4}$$

for $t_0 \geqslant a$, then η_{t_0} is convex[21] and θ_{t_0} is convex if (ii) holds for Eq. (2). The methods employed permit one to obtain polygonal approximations to the sets η_{t_0} and θ_{t_0}. Examples were found which show that some of the results obtained were the best possible in a certain sense.

Under the assumption that q eventually has constant sign on $[a, \infty)$, the asymptotic properties of nonoscillatory solutions of (1) were studied and interesting results were obtained with the help of the auxiliary function

$$F_\lambda(x) = \lambda + \int_a^\lambda f(t)\, dt\,, \qquad x \geqslant a\,, \qquad \lambda \text{ real}\,.$$

These results relate the quantitative and qualitative properties of (1).

20. C. A. Swanson, *Comparison and Oscillation Theory of Linear Differential Equations,* Academic, New York, 1968.
21. H. G. Eggleston, *Convexity,* Cambridge, 1958.

THE SPECTRUM OF SINGULAR DIFFERENTIAL OPERATORS: NUMERICAL APPROXIMATION, QUALITATIVE BEHAVIOR, AND AN APPLICATION TO TOEPLITZ MATRICES

John V. Baxley[22]

Although finite difference methods have been used extensively for solving regular boundary value problems for differential operators, relatively little has been done in the singular case. The basic difficulties in the singular case have to do with the number and character of the boundary conditions which may be imposed. In ref. 23, the singular second-order Sturm-Liouville differential operator $\tau u = -[m(x)]^{-1}[p(x)u']'$ on the interval $0 < x < 1$, where 0 is allowed to be a singular end point, is the object of study. The extension method of Friedrichs is used to obtain two (in general distinct) self-adjoint operators in Hilbert space. Boundary condition descriptions of these operators are found, the operators are shown to be strictly positive with compact inverses, and finite difference operators are introduced whose eigenvalues approximate the eigenvalues of the given differential operators.

In ref. 24, the ideas and results of ref. 23 are extended to higher order differential operators which are basically iterates of the Sturm-Liouville operator of ref. 23.

Due to work of Toeplitz and Szego in the early years of this century and because of applications in statistics and analytic function theory, Toeplitz matrices have received considerable attention in the last 20 years. One of the basic problems concerns the asymptotic behavior of the extreme eigenvalues of $n \times n$ finite sections of Toeplitz matrices as $n \to \infty$. S. V. Parter originated the idea of attempting to first interpret the eigenvalue problem for the $n \times n$ finite section as an equivalent eigenvalue problem for a finite difference operator and then discover if the finite difference operator was a consistent approximation to some differential operator. In ref. 25, this idea is used in conjunction with the results of ref. 24 to obtain new results (which generalize earlier results of J. V. Baxley and I. I. Hirschman) in the case of Toeplitz matrices associated with Laguerre polynomials and to recover known results of Hirschman in the case of Toeplitz matrices associated with Jacobi polynomials.

Motivated by interest in the spectral structure of quantum mechanical operators, in particular the Schrodinger operator, mathematicians and theoretical physicists have devoted considerable attention to obtaining qualitative results about the spectrum of singular differential operators. Such results conclude the qualitative character of the spectrum from a knowledge of the behavior of the coefficient functions of the operator. An enormous literature has grown up over the last sixty years concerning the singular second-order Sturm-Liouville operator. Only recently have attempts been made to extend these results to partial differential operators and higher-order ordinary differential operators. M. S. P. Eastham[26] has obtained one of the nicest generalizations (to higher-order ordinary differential operators) to date. Some preliminary work, not yet in a form for publication, has led to interesting results complementary to those of Eastham and, in addition, some tentative and as yet fragmentary results for singular partial differential operators.

---

22. Research Participant, Wake Forest University, Winston-Salem, N.C.
23. J. V. Baxley, "Eigenvalues of Singular Differential Operators by Finite Difference Methods, I," submitted for publication.
24. J. V. Baxley, "Eigenvalues of Singular Differential Operators by Finite Difference Methods, II," submitted for publication.
25. J. V. Baxley, "Extreme Eigenvalues of Toeplitz Matrices Associated with Certain Orthogonal Polynomials," submitted for publication.
26. M. S. P. Eastham, "The Least Limit Point of the Spectrum Associated with Singular Differential Operators," *Proc. Cambridge Phil. Soc.* 67, 277–81 (1970).

Computing Applications

INTRODUCTION

A. A. Brooks

On September 1, 1970, 45 members of the Scientific Applications Department of the Computing Technology Center were transferred to the Mathematics Division at the Oak Ridge National Laboratory and merged with approximately 35 applications programmers. This group now forms the Computing Applications Department. The responsibilities of the new department include providing technical and scientific programming services to the Oak Ridge National Laboratory and providing services in the area of nuclear codes to Union Carbide Nuclear Division in Oak Ridge. In the interest of preserving continuity in reporting, a number of the items are reported in the annual report which were carried out or begun by members of the department prior to the time of the transfer.

The annual report is organized by the divisions which sponsored the work. In the case where work was sponsored by two or more divisions, it is included in a section entitled Interdivisional Projects.

In some cases the name of an individual in the sponsoring division is given for purposes of identfication.

BIOLOGY DIVISION

Small Sample Properties of Estimators for the Gamma Distribution

Kim O. Bowman

The gamma distribution

$$f(x) = (x/a)^{\rho-1} \exp(-x/a)/a\Gamma(\rho)$$

is widely used in statistical application, such as life-testing procedures, weather modification experiments, and the like. Fairly comprehensive sets of tables of the moments of the maximum likelihood estimators and Thom's estimators were prepared, and the distributional properties of each were studied.[1] The study shows how misleading it is to accept so-called large sample variance, etc., where there is no evidence of any kind to warrant their validity. The previous work[2] has given good approximations to the means, variances, skewness

1. L. R. Shenton and K. O. Bowman, "Remarks on Thom's Estimators for the Gamma Distribution," *Monthly Weather Rev.* 98(2) (1970); K. O. Bowman and L. R. Shenton, "Small Sample Properties of Estimator for the Gamma Distribution," CTC-28 (1970); L. R. Shenton and K. O. Bowman, "Tables of the Moments of the Maximum Likelihood Estimators of the Two Parameter Gamma Distribution," Reports of Statistical Application Research, *Union of Japanese Scientists and Engineers (JUSE)* 17 (1970).

2. K. O. Bowman and L. R. Shenton, "Properties of Estimators for the Gamma Distribution," CTC-1 (1968).

parameters β_1, β_2 in *small sample estimation.* With these we are now able to approximate the percentage points of the distributions, which is under study.

Sponsor: Biology Division J. L. Liverman

Continued Fraction for the Polygamma Function

Kim O. Bowman

If the logarithm of the gamma function is written in the form

$$\ln \Gamma(z) = -z + \left(z - \frac{1}{2}\right) \ln z + \frac{1}{2} \ln (2\pi) + J(z)\,, \tag{1}$$

then the Stieltjes continued fraction for $J(z)$ is given by

$$J(z) = \frac{\frac{1}{12}}{z+}\,\frac{\frac{1}{30}}{z+}\,\frac{\frac{53}{210}}{z+}\,\frac{\frac{195}{371}}{z+\ldots}\,,$$

and expression (1) holds for $R(z) > 0$.

We derived continued fractions of the Stieltjes type for the derivatives of ln $\Gamma(z)$,[3] that is, the polygamma functions defined by

$$\psi^{(n)}(z) = \frac{d^{n+1}}{dz^{n+1}} \ln \Gamma(z)\,, \qquad (n = 0, 1, 2, \ldots)\,.$$

Sponsor: Biology Division J. L. Liverman

Study on the Distribution of Indices of Diversity

Kim O. Bowman

Several measures of diversity in populations (and samples) have been used by ecologists and information theoreticians. For example, ecologists have used Shannon's information statistic

$$h_s = -\sum p_i \ln p_i\,,$$

Simpson's distance measure

$$h_{si} = \sum p_i^2 \qquad \text{(or its root)}\,,$$

and Brillouin's combinatorial type measure

$$h_b = n^{-1} \ln n!/n_1! \ldots n_k!\,.$$

3. K. O. Bowman and L. R. Shenton, "Continued Fractions for the Psi Function and Its Derivatives," *SIAM J. Appl. Math.* (in press).

Distributional properties of these are studied from three points of view: (1) the exact distribution is found by sample configuration enumeration; (2) approximate distributional properties are found through Monte Carlo simulations; (3) asymptotic moments are developed and their uses in assessing departures from normality considered. It is brought out that no one method is adequate for the parameter space in general and that asymptotic moment developments are generally markedly unstable. However, the distribution of h_s is remarkably close to normal when the category probabilities follow MacArthur's model.

The study illustrates methods of gaining insight into some of the complex distributional problems associated with multinomial structures, many of which defy neat mathematical formulation.

Sponsor: Biology Division — J. L. Liverman

CHEMICAL TECHNOLOGY DIVISION

Nuclear Safety Evaluation of Various Designs for the LMFBR Fuel Reprocessing Dissolver

J. R. Knight W. R. Cobb[4]

The ANISN[5] and KENO[6] codes were used to evaluate the effects of various parameters on the nuclear safety of LMFBR dissolver designs. Three basic designs – a vertical cylinder, a slab, and a horizontal cylinder – were studied. The parameters were varied and included fuel concentration, external concrete reflection, and stainless steel content of the fuel. Other factors considered were boron content, nitric acid concentrations, and variation in thickness of some of the stainless steel vessel walls. These studies have indicated that several possible systems can be operated in a nuclearly safe manner.

Sponsor: Chemical Technology Division

CHEMISTRY DIVISION

Analysis of the Range and Angular Distribution of Recoil Nuclei in I4C(EVAP)

O. W. Hermann R. L. Hahn[7]

A special version of the analysis code I4C, named I4C(ANG), is being developed to provide further treatment of the excited nucleus during the evaporation process.[8] Laboratory-system vector velocities of the recoil nucleus are calculated after each particle is emitted; from these calculations the final recoil angle and energy of the residual nucleus of each history is obtained and stored on tape. Then the stored results are analyzed for any requested product nucleus to obtain kinetic energy and angular distributions. Combined with range-energy theory,[9] these values are also used to calculate the fraction of product nuclei that recoil out of the target within specified angular intervals. The input allows variation in the interval sizes and upper and lower energy and angular limits for each nucleus requested. The analysis routines are

---

4. Reactor Division.
5. W. W. Engle, *A User's Manual For ANSIN*, K-1693, Mar. 30, 1967.
6. G. E. Whitesides and N. F. Cross, *KENO – a Multigroup Monte Carlo Criticality Program*, CTC-5, Sept. 10, 1969.
7. Chemistry Division.
8. R. L. Hahn and O. W. Hermann, *Inclusion of Fission and Charged Particle Emission in Nuclear Reactions; Calculated Energies, Angles, and Ranges of Recoil Nuclei*, ORNL-TM-3179 (to be published).
9. J. Lindhard, M. Scharff, and H. E. Schiott, *Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd.* 33(14) (1963).

included, both as a single overlay branch of I4C and as a separate code, allowing later computer runs to be made with input data changes – but without repeating the more lengthy evaporation computation. Indications are that the additional physics applied through this code is necessary to obtain a more favorable comparison with experimentation.

A slight extension of this treatment for analysis of the evaporated particles[10] is under consideration.

Sponsor: Chemistry Division R. L. Hahn

Consideration of Fission Competition During Particle Evaporation from the Excited Nucleus, in I4C(EVAP)

O. W. Hermann R. L. Hahn[7]

A significant modification of the evaporation routine of the analysis code I4C[11] was developed which considers competition between the processes of fission and particle evaporation in excited nuclei. This calculation includes the effects of particle emission in both the intranuclear cascade model[12] and the compound-nucleus model[13] as performed by MECC and the previous version of I4C; in addition, it includes the probability of fission for the heavy elements as determined by Sikkeland et al.[14]

Treatments of the compound nucleus[14,15] have been developed based upon models, which consider neutron emission and fission in heavy nuclei, but do not include the emission of charged particles. However, recent experimental studies[16] show that ^{231}Pa bombarded with 35- to 63-MeV protons have significant proton and alpha particle emission. A more detailed theoretical discussion[17] explains the possible reasons for this deviation from the description of previous theory. Further refinements are being developed to calculate the kinetic energy and angular distributions of product nuclei in the hope that these calculations may be compared more readily with experimentation. Results of the refinements will be reported[18] with a more detailed discussion.

Sponsor: Chemistry Division R. L. Hahn

Tape Editing and Plotting

F. D. Hammerling

A PL/1 program was written to process and edit a seven-track data tape produced by an ACL-820 on-line data acquisition device. The data were generated by a cyclotron experiment and were in groups of

---

10. R. W. Peele, *Sorting Evaporated Particles or Residual Nuclei According to Angle,* Memo to R. G. Alsmiller, Jr., and M. P. Guthrie (September 1970).

11. H. W. Bertini, M. P. Guthrie, and O. W. Hermann, *Instructions for the Operations of Codes Associated with MECC3, a Preliminary Version of an Intranuclear Cascade Calculation for Nuclear Reactions,* ORNL-4564 (to be published).

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

13. L. Dresner, *EVAP – a Fortran Program for Calculating the Evaporation of Various Particles from Excited Compound Nuclei,* ORNL-CF-61-12-30 (December 1961).

14. T. Sikkeland, A. Ghiorso, and M. J. Nurmia, *Phys. Rev.* **172,** 1232 (1968).

15. J. D. Jackson, *Can. J. Phys.* **34,** 767 (1956).

16. R. L. Hahn, K. S. Toth, and M. F. Roche, *Chem. Div. Ann. Progr. Rept. May 20, 1970,* ORNL-4581, pp. 28–30.

17. R. L. Hahn, *Chem. Div. Ann. Progr. Rept. May 20, 1970,* ORNL-4581, pp. 30–32.

18. R. L. Hahn and O. W. Hermann, *Inclusion of Fission and Charged-Particle Emission in Nuclear Reactions; Calculated Energies, Angles, and Ranges of Recoil Nuclei,* ORNL-TM-3179 (to be published).

three 24-bit words which represented an event (alpha, x ray, time lapse). The data were edited for missing items, correct order, overflow, etc., by looking at particular bits of the word and then collected in groups according to experiment.

The edited and collected data were then written on a scratch disk and read by a second job step which was a FORTRAN program written to plot histograms of the data.

Sponsor: Chemistry Division C. E. Bemis

CIVIL DEFENSE RESEARCH PROJECT

Analysis of Time-Varying Active-Passive Civil Defense Mixes

M. T. Heath

Several computer programs have been written for the Civil Defense Research Project as part of their project to evaluate the cost and effectiveness of various active-passive defense mixes. The programs simulate energy attack by submarine-launched multiple warhead missiles, active response by interceptors, and passive defense of the population by various kinds of blast shelters. Existing blast damage codes are utilized to calculate fatalities, but new algorithms have been developed and implemented to allow the attack and defense to be time dependent. This is a more realistic approach since the vulnerability of the population decreases as a function of time as the people reach shelter by walking, and permits investigation of such questions as the dependence of vulnerability on proximity to the sea and whether active defense can be used as a cover for people as they move to shelter.

Sponsor: Civil Defense Research Project C. M. Haaland

Evaluation of Active-Passive Interaction in Defense Against Submarine-Launched Ballistic Missiles

D. W. Altom J. V. Wilson[19] C. M. Haaland[19] C. V. Chester[19]

The Research Triangle Institute in North Carolina developed the FORTRAN program ANCET[20] (Analytical Nuclear Casualty Estimation Technique) to assist in sensitivity analyses of civil defense systems and components. Implementation of ANCET was within a CDC-3600 computing environment.

We adapted ANCET to our IBM/360 computing environment. We ran several standard test cases in order to confirm in part the accuracy of the adapted program. During this time we isolated and corrected several errors in the original ANCET program.

Civil Defense investigators used ANCET to calculate casualties and mortalities due to prompt and fallout effects for assumed nuclear attacks against large cities of the United States.

To aid these investigators we developed and implemented certain graphical display capabilities. In particular, graphs of various types of data superimposed upon maps of the United States as well as fallout contour maps for various nuclear attacks may be obtained. Certain of the graphs available may be used to verify the accuracy of the data bases and to establish suitable locations for the placement of antiballistic missile batteries.

Sponsor: Civil Defense Project

---

19. Civil Defense Research Project.

20. Research Triangle Institute Project OU-230-2, October 1967. OCD Work Unit 4113E. Prepared for the Office of Civil Defense, U.S. Department of the Army, Contract No. OCD-PS-64-56.

Ballistic Trajectory Calculations

Kay C. Chandler   C. M. Haaland[21]   C. W. Nestor, Jr.

For a given maximum range measured along a great circle on the earth's surface, the total energy for a ballistic missile trajectory was computed. Choosing shorter ranges, we then calculated an alternate set of lofted and depressed trajectories having higher and lower apogees, respectively, than the minimum energy trajectory at the maximum range. At each intermediate range, we solved a transcendental equation for the lofted and depressed reentry angles α_l and α_d where $0° \leqslant \alpha_d < \alpha_l < 90°$. We also calculated the time of flight and the apogee for both trajectories.

Each of these variables (reentry angle, time of flight, and apogee) was plotted against the range on a single plotting area using three different ordinate scales. All three resulting curves were parabolic in shape with the upper and lower branches corresponding to the lofted and depressed trajectories, respectively. An example is shown in Fig. 1. The plotting was done using the ORNL Graphics Package ORGRAPH.[22]

Sponsor: Civil Defense Research Project

---

21. Civil Defense Project.
22. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 9.

ORNL-DWG 71-2033

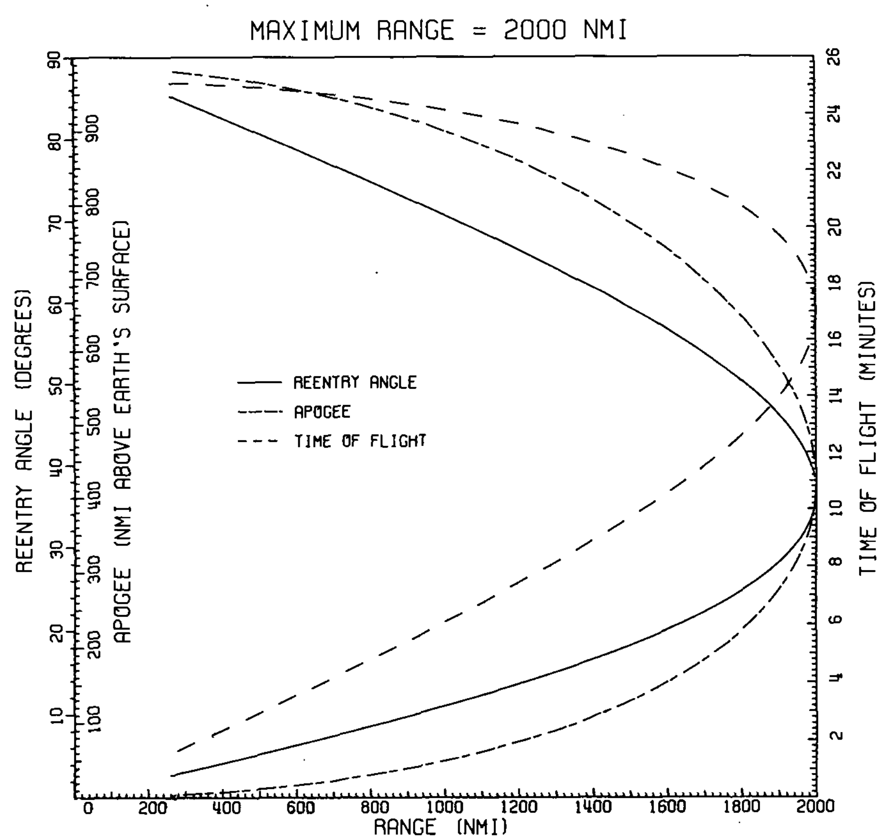

Fig. 1. Example of ballistic missile trajectories.

DIRECTOR'S DIVISION

Monte Carlo Calculations of Neutron Decay

G. W. Morrison J. T. Mihalczo[23]

The O5R[24] Monte Carlo neutron transport code has been modified to provide the neutron weight or various reaction rates as a function of time after the injection of a source neutron into a subcritical multiplying assembly. The source neutron and subsequent fission neutrons are sorted into time intervals up to a specified time T_{max} or until loss by absorption or leakage. All neutrons of a fission chain are traced until loss before another source neutron is introduced.

All the necessary cross sections are stored in fast storage, and a form of importance sampling is used at large times to assure that adequate statistics over many decades of decay are obtained. The decay in nonmultiplying assemblies can also be calculated.

This calculational method may be used for the interpretation of neutron time-dependent experiments.

Sponsor: Director's Division

ECOLOGICAL SCIENCES DIVISION

Numerical Methods for Ecologists

A. A. Brooks J. B. Mankin R. V. O'Neill[25]

A numerical methods manual is being written to aid ecologists in understanding numerical analysis and scientific applications of computers. This manual is intended to provide an introduction to numerical techniques to the ecologist who is unfamiliar with computing and to provide practical hints and a reference to existing programs and their use to those ecologists who are moderately familiar with computing. Chapters on interpolation, integration, linear and nonlinear algebraic equations, eigensystems, linear and nonlinear ordinary differential equations, partial differential equations, and sensitivity analysis are included. Emphasis is placed on practical application and the difficulties encountered in numerical computation.

Sponsor: Ecological Sciences Division

Modeling of the Energy Transfer Through a Forest Canopy

J. B. Mankin M. Reeves G. S. McNeilly
R. V. O'Neill[25] C. E. Murphy[26]

The transfer of energy within and above a forest canopy can be viewed as mechanical and thermodynamic processes. These energy processes are primarily those of a molecular diffusion of heat and moisture through a fluid, the absorption of solar and long-wave radiation, and the transfer of sensible and latent heat from the leaves and the soil. They are interacting processes which are described by coupled partial differential equations, and their solution yields a knowledge of the microclimate within the forest.

---

23. Y-12 Critical Experiments Facility.
24. D. C. Irving et al., *O5R, a General Purpose Monte Carlo Neutron Transport Code*, ORNL-3622 (February 1965).
25. Ecological Sciences Division.
26. School of Forestry, Duke University.

The transfer of heat and moisture through the canopy can be viewed as a diffusion process. Therefore, these processes can be described by nonlinear diffusion equations such as

$$\frac{\partial \varphi}{\partial t} = \frac{\partial}{\partial z}\left[K(t, z)\frac{\partial \varphi}{\partial z}\right] + s(t, z),$$

where φ is the quantity of interest (e.g., temperature), $K(t, z)$ is the diffusivity, t is the time variable, and z is the vertical displacement within the canopy. The source terms $s(t, z)$ are obtained by computing the transfer of heat and moisture from the leaves and soil to the air.

The heat transfer through the leaves can be obtained by a heat balance of the conductive, convective, and radiant heat processes acting upon the leaves. The moisture transfer from the leaves is a function of vapor pressure, and the leaves are assumed to be at their saturation vapor pressure.

A code has been developed to solve for the temperature and moisture profiles through the canopy as a function of time. It is also necessary to calculate a number of other quantities; for instance, the diffusivity is a function of the wind profile. These quantities are computed by programs developed at Duke University.[27]

Sponsor: Ecological Sciences Division

Infiltration of Water into Soils

G. S. McNeilly M. Reeves III E. E. Miller[28]

If it is assumed that (1) Darcy's law is valid, (2) the conductivity of the soil is dependent on pressure head and position in the soil, and (3) the equation of continuity is valid with the water capacity being dependent on pressure head and position in the soil, then the infiltration of water into soil can be described by the equation[29]

$$C(h, z)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h, z)\frac{\partial h}{\partial z}\right] + \frac{\partial}{\partial z}K(h, z),$$

where $C(h, z) = \partial\theta/\partial h$ is the water capacity of a particular scanning curve, $K(h, z)$ is the hydraulic conductivity, θ is the volumetric water content, h is the pressure head, and $0 > z > -L$ is the position in the soil between the surface and the ground water level.

The flow equation defined above is well known and has been investigated previously.[29] However, the present investigation will extend the model to include hysteretic behavior of $C(h, z)$ and $K(h, z)$, the effect of a crust at the soil surface, and a time-varying crust boundary condition to simulate the effect of variable rainfall and runoff.

Sponsor: Ecological Sciences Division

---

27. C. E. Murphy and K. R. Knoerr, "Modeling the Energy Balance Processes of Natural Ecosystems," Research Report, International Biological Program, Analysis of Ecosystems Project, Deciduous Forest Biome Subproject, Grant 383-6102, 1969–1970.

28. International Biological Program participant, Departments of Physics and Soils, University of Wisconsin.

29. F. D. Shisler and A. Klute, *Soil Sci. Soc. Amer. Proc.* 29(5), 489 (1965).

Recovery Time of an Ecosystem

M. Reeves III M. T. Heath R. V. O'Neill[25]

The recovery time of an ecological system may be defined as the time required to reach steady state after a disturbance to the system. The main objective here is to study the relation of this quantity to the structure of the system. Insight into this relation should provide some practical guides for changing the recovery time. A secondary objective is to provide the necessary computer program.

For this study, we have adopted a compartment model with linear donor-dependent flows. Recovery time is then inversely proportional to the real part of what we have called the crucial eigenvalue of the matrix of flow coefficients. This crucial root is characterized by a real part which is next to the smallest in magnitude relative to all of the other eigenvalues.

Perturbation theory was applied to this problem in two ways. First, all of the off-diagonal elements were considered to be the perturbations. In this case, the physical interpretation was very straightforward, but the agreement of crucial roots as calculated rigorously and through perturbation theory was very poor in most cases. Second, a small perturbation to one of the flows was considered. Here the physical interpretation was very obscure, and hence no calculations were made.

We are now beginning a sensitivity analysis where the sensitivity of an eigenvalue to change of a given matrix element is defined as the derivative of that eigenvalue with respect to the appropriate matrix element.

Sponsor: Ecological Sciences Division

ORNL RESAP Adaptation

J. D. Amburgey F. D. Hammerling

A program for the least squares analysis of gamma spectra involving intermixed standard samples (RESAP)[30] which was written at the Computing Technology Center was adapted to the Mathematics Division's equipment. A program was written for the CDC 160A to convert paper tape data to magnetic tape in the format required by RESAP. Since the paper tape data have usually contained several errors, a program was written to edit the mag tape, and hopefully produce an error-free tape to be processed by RESAP.

Sponsor: Ecological Sciences Division Daniel J. Nelson

Linear Compartmental Analysis of Ecosystems

R. E. Funderlic M. T. Heath

The kinetics of a linear compartmental system may be expressed by a system of differential equations $\dot{x} = Ax$, where A is the matrix of transfer coefficients and x is the vector of concentrations in the compartments. Such a system has the usual exponential solution depending on the eigenvalues and eigenvectors of A. Important problems in ecology and other disciplines where such systems occur are the stability of the system, the rate of decay of the transient solution, and the sensitivity of the solution to

30. A. A. Brooks, A. Hume, and B. J. Handley, *RESAP – a Program for the Least Squares Analysis of Gamma Spectra Involving Intermixed Standard Samples*, CTC-25 (March 1970).

changes in the coefficients or other system properties. Under the assumption of conservation of mass or energy, the nonzero eigenvalues of A have negative real parts, and thus the solution is stable, that is, it tends to a constant with increasing time. This constant is an eigenvector corresponding to the eigenvalue zero, which is always a root since A is singular. One measure of the recovery time of the system from a perturbation (e.g., injection of a pollutant) is the magnitude of the real part of the nonzero root closest to zero. Call this root the crucial root. If the matrix B obtained by deflating the zero root(s) from A is essentially positive (i.e., is irreducible and has nonnegative off-diagonals), then the following theorem[31] provides upper and lower bounds on the crucial root, which is real in this case.

Theorem. If the matrix B is essentially positive, then the crucial root lies between the minimum and maximum column sums of B.

By an appropriate scaling (diagonal similarity transformation), these bounds can be improved in the best possible way as shown in the next theorem.[31]

Theorem. If the matrix B is essentially positive, then there is a nonsingular diagonal matrix D having nonnegative entries such that the column sums of the matrix DBD^{-1} are all equal to the crucial root.

This last expression is equivalent to a system of n nonlinear equations in n unknowns, where n is the order of B. Information concerning the sensitivity of the crucial root may be obtained from this system, which has a particularly simple form for some kinds of ecological systems.

Sponsor (partial): Ecological Sciences Division — R. V. O'Neill

ORNL-NSF ENVIRONMENTAL PROGRAM

An Electricity Supply-Demand Prediction System

T. J. Tyrrell D. Chapman[32]

We have started the development of an environmentally oriented electricity supply-demand prediction system. Traditionally, such systems have been developed by utility companies and various government agencies, using input-output and ordinary least squares techniques. In addition to the basic price and policy change responses of a typical prediction system, we have incorporated supply-mix and energy-form-substitution factors into our model. We have chosen a simultaneous estimation technique using regression analysis. Our primary innovation, however, is that our system is designed so that its output is readily usable in other prediction systems, such as, for example, a pollution by-product prediction system.

Sponsor: Environmental Program, Energy Group — R. S. Carlsmith

GENERAL ENGINEERING AND CONSTRUCTION DIVISION

Symbolic Manipulation of Matrices in Structural Mechanics

T. C. Tucker W. C. Stoddart[33]

The finite element method for solving problems in structural mechanics involves matrices which describe the force/deflection vector relationships. In principle, these matrices may be obtained by either

31. Richard S. Varga, *Matrix Iterative Analysis*, pp. 258, 261, Prentice-Hall, 1962.

32. Environmental Project, Energy Group.

33. General Engineering and Construction Division.

analytical or numerical means. In practice, although the analytic representation is often desirable, numerical means are very predominant. The large amount of algebraic manipulation required for the analytical derivation is both tedious and susceptible to error. We have investigated the FORMAC symbolic manipulation language as a means to overcome these difficulties.

The problem chosen for study was the transformation of the stiffness matrix for a curved quadrilateral element from an abstract coordinate system into the polar coordinate system. In this case, the original stiffness matrix K was a symmetric 8×8 matrix. The transformation matrix R was an 8×8 matrix. The desired result was the symmetric 8×8 matrix $R^T K R$.

We wrote a subroutine for a FORMAC program which performs this multiplication for any conformable matrices R and K, where K is symmetric. Although FORMAC allows subscripted variable names, it does not provide for array variables. However, by using the string-handling capabilities of the PL/I language and calling certain FORMAC library subroutines explicitly, we were able to write the subroutine so that its effective operands are matrices. The sample problem, including definition of the initial matrices and simplification of the terms of the result, required less than 15 machine-use seconds on the IBM 360/91. It is believed that a significant reduction in computer time will be achieved by using this analytic result rather than the current numerical transformation.

Further application of FORMAC to structural mechanics is currently under consideration.

Sponsor: General Engineering and Construction Division — W. C. Stoddart

SINDA-3G

D. W. Altom T. C. Tucker G. H. Llewellyn[33]

We have implemented one version of the Thompson Ramo Wooldridge Systems Improved Numerical Differencing Analyzer,[34] SINDA-3G, on the IBM 360 systems at ORNL. This is a programming system which is used at many NASA and AEC installations for heat transfer, fluid dynamics, and stress analysis.

We have used the version coded by the Idaho Nuclear Corporation for the IBM 360. All features of the system are available with the exception of the plotting features.

Sponsor: General Engineering and Construction Division — G. H. Llewellyn

HEALTH PHYSICS DIVISION

Health Physics

G. S. McNeilly Peggy G. Fowler

An investigation is in progress to determine the more critical radionuclides (in terms of internal and external dose to humans) produced by nuclear fission reactors. Since the number of nuclides produced in the core of a nuclear fission reactor is approximately 500, an efficient data-handling system is necessary.

A program, SEARCH, using the Battelle-Northwest Isotropic Data Tape[35] as a data base has been written. SEARCH, in addition to information retrieval capability, edits the master file with additions and

---

34. Chrysler Improved Numerical Differencing Analyzer for 3rd Generation Computers, Technical Note TN-AP-67-287, Chrysler Corporation Space Division, New Orleans, 1967.

35. R. L. Reynolds, BNWL-551 (1967).

corrections and checks key words and record format for correctness. The nuclear structure data of the Battelle tape have been complemented by the addition of ICRP biological half-life data.[36] Other quantities of interest to dose calculations can be easily appended.

Sponsor: Health Physics Division

Routine Atmospheric Releases of Short-Lived Radioactive Nuclides

M. Reeves III   Peggy G. Fowler   K. E. Cowser[37]

In siting and operating nuclear facilities, it is desirable to predict the transport of radioactive materials. We consider a routine situation in which radioactive materials are being continuously emitted into the atmosphere, rather than an accidental situation. Hence, our results will be annual averages relative to atmospheric stabilities, wind speeds, and wind directions.

Some releases will contain relatively short-lived members of radioactive decay chains, which necessitates the consideration of several factors. For example, radioactive production and decay processes will occur both in the atmosphere and on the ground. Also, the washout and fallout processes by which the materials reach the surface will be characterized, in general, by different washout coefficients and deposition velocities for different members of the decay scheme.

By generalizing the Gaussian plume analysis,[38] to take into account the radioactive production and decay processes,[39] we have developed expressions of the ground-level air concentration, deposition rate, and ground concentration for each isotope of a radioactive decay chain. These expressions have been coded in double-precision FORTRAN IV. A description of the mathematical analysis, the numerical analysis, and the computer program is being published as an ORNL-TM report.

Sponsor: Health Physics Division

Heat Transfer Analysis of Radioactive Waste Disposal in Natural Salt Formations

W. D. Turner   R. L. Bradshaw[37]

The thermal effect on the geological environment is one of many questions arising from the project on radioactive waste disposal in natural salt formations.[40] There are many variables which will influence the temperature distribution in a radioactive waste repository, and the effects of these variables must be analyzed in designing such a facility. In order to determine their effects on the temperature distribution, solutions have been obtained for models evaluating the size of rooms, separation between rooms, spacing between wastes in each room, and backfilling the disposal rooms with crushed salt.

A versatile code, the Mine Management Program, is being developed to predict the most economical waste container spacing while ensuring that the temperature throughout the facility does not exceed a specified maximum value. In estimating the temperature distribution in the formation, one must accurately

---

36. *Health Phys.* 3 (June 1960).

37. Health Physics Division.

38. D. H. Slade, *Meteorology and Atomic Energy, 1968,* TID-24190 (1968).

39. D. R. Vondy, *Development of a General Method of Explicit Solution to the Nuclide Chain Equations for Digital Machine Calculations,* ORNL-TM-361 (1962).

40. *Health Phys. Div. Ann. Progr. Rept. July 31, 1970,* ORNL-4584, pp. 16–36.

model the rooms, the sources, the stratigraphic formation, the boundary conditions, the thermal properties, etc. Solutions have been obtained for a spectrum of problems which have been used to study the effects of these variables. As new data for the proposed facility become available, work will continue toward developing a model or group of models which will most accurately and economically predict the temperature distribution throughout the repository.

The heat conduction code HEATING[41] is currently being used to perform most of the heat transfer calculations. Detailed information and results on some of the models that have been studied are presented in the Health Physics Division's annual report.[42]

Sponsor: Health Physics Division R. L. Bradshaw

Dose from Gamma-Ray Sources

G. G. Warner W. S. Snyder[37]

We made extensive amendments to the internality of the man phantom described in ALGAM.[43] New bones – scapulae and clavicles – were added; newer regions for both red and yellow marrow were defined; the definitions of the sections of the gastrointestinal tract were strengthened by describing the walls of each section as well as its contents; and nasal passages were described. We used ALGAM to estimate internal dose to the man phantom from 12 monoenergetic photon sources located uniformly in the liver, both kidneys, the lungs, and the contents of the stomach, the small intestine, the upper large intestine, and the lower large intestine. From the decay schemes of seven isotopes of iodine, we computed doses from sources of each isotope in the bladder, the stomach, the small intestine, the upper large intestine, the liver, the gonads, and the thyroid. Other radioisotopes simulated as sources were ^{239}Pu, a point 0.4 cm deep in cheek; ^{75}Se uniform in liver; and three monoenergetic "isotopes" in the nasal passages.

We compiled a variation of ALGAM which restricted its output to the histories in the bladder wall and a few other organs. This variation estimated dose from monoenergetic photons uniformly distributed in the contents of a bladder being continuously filled at a constant rate from 0 to 525 ml in 9 hr. Another variation gave estimates from 12 monoenergetic sources in the fixed contents at each of seven volumes: 0, 50, 100, 200, 300, 400, and 500 ml. We computed a third variation in which the decay schemes of ^{203}Hg and ^{197}Hg were used as sources of photons in a continuously filling bladder from 0 to 280 ml in 4.8 hr. The volume of the contents of the bladder was picked according to the distribution $e^{-\lambda_r t}(1 - e^{-\lambda_i t})$, where 0 hr $< t <$ 4.8 hr, λ_r is a retention constant, and λ_i is an input constant.

We compiled yet another variation of ALGAM in which the output was amended to give depth dose estimates[44] as well as dose estimates to the internality of the man phantom from cloud sources of photons. L. T. Dillman[44] supplied us with a code which can calculate the photon energy spectra incident upon the phantom from initially monoenergetic cloud sources, and we used these spectra with their accompanying probability distributions as sources. It was necessary to write a subroutine which gave the proper angular

41. W. D. Turner and J. S. Crowell, *Notes on HEATING – an IBM 360 Heat Conduction Program*, CTC-INF-980 (November 1969).

42. *Health Phys. Div. Ann. Progr. Rept. July 31, 1970*, ORNL-4584, pp. 25–31.

43. 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).

44. L. T. Dillman, "Radiation Dose Estimation for Immersion in a Radioactive Cloud," *Health Phys. Div. Ann. Progr. Rept. July 31, 1970*, ORNL-4584.

distribution for photons impinging on the phantom. Runs were made for 12 monoenergetic clouds and for clouds which each contained the two principal decay photons of ^{85}Kr, 0.305 and 0.1495 MeV.

Sponsor: Health Physics Division W. S. Snyder

Absorbed Fractions of Gamma-Ray Energy

G. G. Warner W. S. Snyder[37]

Using a method developed by Berger[45] for the calculation of buildup factors for proton energies, a computer code was written to calculate the fraction of emitted energy absorbed per gram of target organ at a distance from an isotropic source in another organ by

$$B(\mu x)\frac{\mu_a}{4\pi x^2}e^{-\mu x} ,$$

where $B(\mu x)$ is the buildup factor for a given energy, μ is the attenuation coefficient, x is the distance between source and target, and μ_a is the energy absorption coefficient. Because absorbed fractions calculated in this manner are conservative when compared with those estimated with ALGAM,[46] we used this method to provide fractions where the statistics of the fractions estimated by ALGAM were poor.

Sponsor: Health Physics Division W. S. Snyder

Effective Energy

G. G. Warner L. T. Dillman[47]

EFFEC, a computer code we helped to develop,[48] was run to produce effective energies, E's, for ^{75}Se and ^{99m}Tc; then we used the output to calculate dose to a target organ T in man from sources of each radionuclide in several source organs S by

$$\text{Dose}_T = \frac{51.15}{\text{Mass}_T}\sum_S [(\mu\text{Ci-days})_S E_{T\leftarrow S}] ,$$

where μCi-days is a residence parameter supplied by the client.

Sponsor: Health Physics Division

Plutonium Body Burden Estimation

L. W. Gilley R. C. Durfee

A computer program was written to estimate intakes and body burdens of persons exposed to plutonium. The two different power functions, $aT^{-\alpha}$ and $a[T^{1-\alpha} - (T-1)^{1-\alpha}]/(1-\alpha)$, were used in estimating the body burdens, where T represents time. The program adjusts the parameter α within

45. M. J. Berger, "Energy Deposition in Water by Photons from Point Isotropic Sources," MIRD Pamphlet No. 2, *J. Nucl. Med. Suppl.* **1** (February 1968).

46. 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).

47. Consultant, Ohio Wesleyan University.

48. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 20.

specified limits depending upon a comparison of experimental data with calculated results. A second code similar to the first was written to produce a different parameter adjustment and therefore a different calculated curve for a given set of experimental data. Both codes allow input data to be punched in an easily usable free form style. The user may plot his final results on the mechanical plotter if desired.

Sponsor: Health Physics Division W. S. Snyder

INSTRUMENTATION AND CONTROLS DIVISION

DEXTIR Data Acquisition Systems, General Description

G. J. Farris[49] O. W. Russ, Jr. R. E. Textor[50]

Beckman Instrument Company's DEXTIR data systems are used at the Reactor Division (9201-3, Y-12), the Oak Ridge Research Reactor (ORR), and the High Flux Isotope Reactor (HFIR) for rapid, accurate collection of experimental data. Each basic system consists of the Central Processing Unit (CPU), up to 100 collection boxes having 25 analog and 25 digital inputs, and connecting party-line coaxial cable allowing up to a mile's distance between data boxes and CPU. Boxes are scanned sequentially in continuous or 5-, 15-, 30-, or 60-min intervals in approximately 3 sec per box, and data are recorded on magnetic tape by the CPU. Each scan records the day of year, box number, time of day, and 25 analog and 25 digital inputs. The magnetic tape containing 24 hr (or a weekend) of data is sent to the ORNL Computing Center for overnight processing by the IBM 360/75 DEXTIR program to optionally scale the digital data, convert the analog millivolt data into engineering units, and print, plot (Calcomp or CRT), or punch output for return to the experimenter. The Y-12 DEXTIR CPU has a PDP-8 computer attached for immediate data conversion and remote readout in engineering units on a Teletype unit at the experiment location. The Laboratory's Instrumentation and Controls Division[51] is responsible for the installation, operation, and maintenance of the DEXTIR systems, and programming support for data reduction is provided by the Mathematics Division's Computing Applications Department.

Sponsor: Instrumentation and Controls Division

MAN PROGRAM

Estimation of Virus Counts

Kim O. Bowman

The problem of estimating the total number of virus particles in a given preparation was considered in order to determine the optimal counting procedure. The data were successfully fitted to a modified geometric distribution with consideration to size of counting area. The counting procedure was determined, which is optimal with respect to minimizing the variance.

Sponsor: MAN Program W. W. Harris

---

49. Now with Union Carbide Corp., South Charleston, W.Va.
50. Leave of absence at Drexel Institute of Technology.
51. Instrumentation and Controls Division annual reports for 1965 through 1970.

MATHEMATICS DIVISION

Development of a General-Purpose Nonlinear Programming Algorithm for Linear Constraints

G. W. Westley

An effective procedure has been developed to solve the following problem.

Find a minimum value of $f(x_1, ..., x_n)$ subject to the m constraining conditions

$$f_i(x_1, ..., x_n) \leqslant 0 \ ,$$

where each of the f_i is a linear function.

The program is an extension of an earlier version.[52] The extensions allow the user to start the procedure from parameter estimates that do not satisfy the constraints and to allow the procedure to converge on a criterion based on the accuracy required in the x_i parameters.

The primary version of the routine requires that the gradient of the function be known in closed (i.e., function) form. However, a version has been developed that eliminates this requirement. This later version has been successfully used to solve several physical parameter estimation problems.[53,54] Both versions of the program have recently been published.[55] This publication also contains a detailed description of the method used in the minimization technique.

The most effective use of the program will be in the analysis of economic modeling problems where there are a large number of constraints and where many of the constraints are expected to be binding at the solution.

The program has been compared with other published techniques and has been found to be more effective than most.[56]

Sponsor: Mathematics Division

Development of a General Geometric Programming Algorithm

G. W. Westley

A procedure has been developed to solve the engineering design problem given below.

Find a minimum cost value of

$$U(t) = \sum_{i=1}^{n_0} c_i \left(\prod_{j=1}^{m} t_j^{a_{ij}} \right)$$

subject to the L constraining conditions

$$g_k(t) = \sum_{i=N_{k-1}+1}^{n_k} c_i \left(\prod_{j=1}^{m} t_j^{a_{ij}} \right) \leqslant 1 \ .$$

52. G. W. Westley and J. A. Watts, CTC-39 (1970).
53. G. W. Morrison, R. F. Haglund, C. Pearson, and G. W. Westley, *Phys. Rev.* **15** (1970).
54. T. G. Miller, G. W. Morrison, and G. W. Westley, *Phys. Rev.* **15** (1970).
55. G. W. Westley, ORNL-4644 (in press).
56. A. R. Colville, IBM Report No. 320-2949 (1968).

The standard restrictions of $t_j > 0$ and $c_i > 0$ are imposed. However, the latest published[57] attempt to remove the $c_i > 0$ restriction has been examined. In some cases the standard procedure can be used to solve the more general problems.

The program written to implement the procedure has been tested on an extensive series of problems.[58] The results indicate that the program is significantly faster (in terms of equivalent computer usage time units) than the previously published version.[59] The algorithm and the program have both been published.[60]

Sponsor: Mathematics Division

FORTRAN FREEFORM Input

R. C. Durfee

We have written a FORTRAN input package, FREEFORM, for the IBM 360 which will allow programmers to read input information without using FORMAT statements. The input package consists of a set of three function subprograms which read real, integer, and alphameric data, respectively. The only restriction on the input items is that they be separated from one another by blanks. The functions may be used with either the IBM FORTRAN IV compiler or the ORNL FORTRAN compiler.

Sponsor: Mathematics Division

FORTRAN Dynamic Storage Allocation

R. C. Durfee

We have written two assembly language subroutines, GETCOR and FRECOR, which may be called from FORTRAN subroutines during execution to allocate and release core storage. Those variables for which core storage is to be allocated must be arguments to the FORTRAN subroutines. Before any FORTRAN subroutine can return to its caller, it must first release all core storage allocated to any of its arguments. Through the use of GETCOR, FRECOR, and variable dimensioning, users will now be able to run jobs with a minimum of core storage thereby allowing better memory utilization of the IBM 360/91 computer. Also with smaller memory requirements some jobs may fall into a better CLASS with faster turnaround. These two subroutines may be used with either the IBM FORTRAN IV compiler or the ORNL FORTRAN compiler.

Sponsor: Mathematics Division

General Purpose Simulation System, GPSS/360

R. C. Durfee

We have received and made available for general use the IBM-distributed programming system General Purpose Simulation System, GPSS/360. GPSS is a simulation program that provides an effective means of

---

57. M. Avriel and A. C. Williams, *SIAM J.* 19(1) (1970).
58. C. J. Frank, Westinghouse Report 64-1HO-129-R1 (1964).
59. C. J. Frank, Westinghouse Report 64-1HO-129-R2 (1964).
60. G. W. Westley, ORNL-4650 (in preparation).

testing, evaluating, and manipulating a proposed system under various conditions in a laboratory environment. The real system's behavior is modeled by a computer program, which reacts to various operating conditions in a manner quantitatively similar to the system itself. Hours, weeks, or even years of simulated activity can be examined on a computer in a matter of minutes. Of course, computer simulation is not a precise analog of the actual system, and thus careful judgment should be exercised by the user in setting up a good model and interpreting the results. GPSS features a simple flowchart language for describing the problem or system to be simulated. When this description is presented as input to the computer, the program automatically carries out the simulation.

The program itself resides on a disk so that it may be referenced with the proper set of control cards. User's manuals[61] are available from the ORNL computer librarian, and persons familiar with GPSS/360 are available for consultation.

Sponsor: Mathematics Division

Numerical Inversion of the Laplace Transform

Sandra H. Merriman F. W. Stallmann[62]

The proposed method of finding the inverse of a Laplace transform, as described in last year's annual report,[63] has been tested successfully on numerous functions.

Sponsor: Mathematics Division

Free Thermal Convection in Molten Metals

T. C. Tucker Carla L. Armstrong J. Smith[62]

We have continued the study of free thermal convection in a horizontal, concentric circular annulus.[64] Of the three methods of solution proposed previously, boundary layer theory has received the least attention, primarily because other methods have appeared more promising than we anticipated. We have initiated work on a numerical finite difference calculation.

We found, however, that expansion methods seem quite promising. From the results of the small-parameter expansion previously reported, we concluded that development of a double expansion in the Grashof and Prandtl numbers was feasible. We found that all nonzero terms of the expansions are included in

$$\Psi = G^{-1/2} \sum_{i=1}^{\infty} G^i \sum_{j=0}^{i-1} P^j \Psi_{i,j} , \tag{1}$$

$$\Phi = \Phi_{0,0} + \sum_{i=1}^{\infty} G^i \sum_{j=1}^{i} p^j \Phi_{i,j} , \tag{2}$$

61. *General Purpose Simulation System/360, Application Description Manual,* GH20-0186 (1969); *General Purpose Simulation System/360, Introductory User's Manual,* GH20-0304 (1969).

62. Consultant, University of Tennessee.

63. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 5.

64. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514.

where P is the Prandtl number, G is the Grashof number, Ψ is the dimensionless stream function, and Φ is the dimensionless temperature function. The coefficient functions $\Psi_{i,j}$ and $\Phi_{i,j}$ are defined by recursive sequences of linear partial differential equations. Further, both $\Psi_{i,j}$ and $\Phi_{i,j}$ are separable functions of radius and angle (in polar coordinates), and the angular dependence is expressible by trigonometric polynomials of order i.

We obtained analytic expressions for the radial functions through terms in G^2 (i = 2), using the FORMAC symbolic mathematics interpreter to do much of the tedious and repetitious differentiation, summation, and collection of terms. We wrote a computer program to obtain numerical results from these expressions. The results of one calculation are shown in Fig. 2.

From this work we concluded the following:

1. Terms through G^2 are sufficient up to about $G = 10^4$ for $\tau_0 = 0.5$ (τ_0 is the ratio of inner radius to outer) and up to about $G = 10^7$ for $\tau_0 = 0.8$. These limits are nearly independent of Prandtl number.
2. For values of τ_0 closer to unity, the radial functions could not be evaluated accurately.
3. The heat transport calculated from the truncated expansion provides a good measure of the applicability of the expansion. Theoretically, the heat transport across any concentric cylindrical surface is independent of the radius, but that calculated from the truncated expansion varies with radius. We found this variation becomes unacceptably large at, or before, the Grashof number at which the stream and temperature functions become unreliable.

Since this attempt at an expansion solution had yielded so much information, we developed a procedure for developing terms in higher powers of G by numerical means.

This approach is desirable because the coefficient functions need to be determined only once for any radius ratio, and calculations for various Grashof and Prandtl numbers are then quite simple. For a direct two-dimensional finite difference calculation, however, the entire, usually lengthy, calculation must be repeated if any parameter is changed.

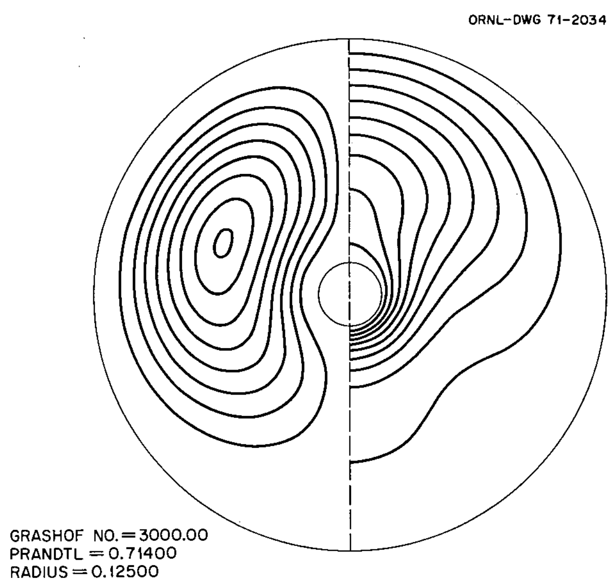

Fig. 2. Contour plot of results of an analytic expansion using terms through G^2. The closed lines on the left represent streamlines. Flow is counterclockwise. On the right are lines of constant temperature at equal increments. The inner cylinder is hot. The Prandtl number corresponds to air.

We used the FORMAC system to facilitate obtaining the recursively defined ordinary linear differential equations defining the radial portions of each function. Then we used a PL/I program to convert the FORMAC output into FORTRAN statements in punched cards. Using this procedure, we generated the punched cards for all terms through G^6, a total of 113 functions, in about 20 min on the 360/91. Similarly, we obtained cards for terms through G^9 with Prandtl number zero.

We developed an explicit method for solving the fourth-order ordinary difference equation with Dirichlet boundary conditions. This method is at least 50 times faster than iterative procedures.

We combined the FORMAC-generated difference equations with the explicit method of solution to obtain the desired numerical results. From these calculations we have concluded:

1. Numerical results can be obtained, through terms in G^2, which differ from the analytical solution by less than 1 part in 10^7.
2. The coefficients of terms from G^2 through G^9 almost form a geometric progression. Thus, there is an effective radius of convergence in terms of Grashof number for the double expansion.
3. Within the radius of convergence, there does not appear to be any limit to the inner-outer radius ratio.

We are considering various means for extending the expansion solution past the presently limiting Grashof number. As one approach, we are trying to apply the theory of analytic continuation. As a second approach, we are considering functional approximation in the space spanned by the coefficient functions of the expansion.

Sponsor: Mathematics Division

Family of Heat Transfer Programs

R. C. Durfee C. W. Nestor, Jr.

We have continued the development of a family of heat transfer programs described in last year's report.[65] We have written two programs, ORTHIS and ORTHAT,[66] which are designed to solve steady-state and transient heat-conduction problems in two-dimensional geometries (x-y, r-z, or r-θ). Thermal properties, heat-generation rates, and boundary conditions may be functions of position, time, or temperature.

In the development of the steady-state program, we have studied the effects of various approximations in the case where the thermal conductivity is a function of temperature. The difference equations are derived from the application of Gauss' theorem to each element of volume surrounding a mesh point; when the thermal conductivity is a function of temperature, it must be evaluated on the interfaces between the volume element and its neighbors. Comparison of the solution of the difference equations with the analytic solution of a simple model problem shows that the truncation error does not decrease with decreasing mesh size if thermal conductivity is assumed constant over an entire mesh volume.[67]

We have also studied the effects of various boundary conditions on the rate of convergence of the iterative solution of the difference equations, using model problems similar to those investigated by Stewart

---

65. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 12.

66. *O*ak *R*idge *T*ransfer of *H*eat *i*n *S*teady State; *O*ak *R*idge *T*ransfer of *H*eat *a*t *T*ransient.

67. Similar results are discussed by R. E. D. Stewart and F. C. Wessling, Jr., Sandia Laboratories Report SC-RR-70-334, June 1970.

and Lick.[68] We consider a cylinder, infinite in length, with a uniform heat source and a mixed condition at the outer boundary:[69]

$$a[T(R) - T_{\text{ext}}] = \left.\frac{dT}{dr}\right)_{r=R} . \tag{3}$$

In addition, the thermal conductivity is a linear function of temperature:

$$k(T) = k_0[1 + \alpha(T - T_0)] . \tag{4}$$

For small values of a [Eq. (3) above], variations in α have a large effect on the rate of convergence; the larger the value of a, the smaller the effect of α. Typical results are shown in Fig. 3, where we have plotted the number of iterations required to reduce the error by a factor of 10 vs the overrelaxation parameter β.

In the transient program we had initially used the Peaceman-Rachford alternating-direction-implicit (ADI) procedure described by Varga,[70] but found instability occurred when the mesh size was small even though our time steps were fairly short. We modified the ADI scheme to include a predictor-corrector process, using approximate temperatures on neighboring mesh lines generated by extrapolation of past

68. G. W. Stewart III and D. W. Lick, *Comm. ACM* 11, 639 (1968).

69. T_{ext} is an external temperature.

70. R. S. Varga, *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, N.J., 1962.

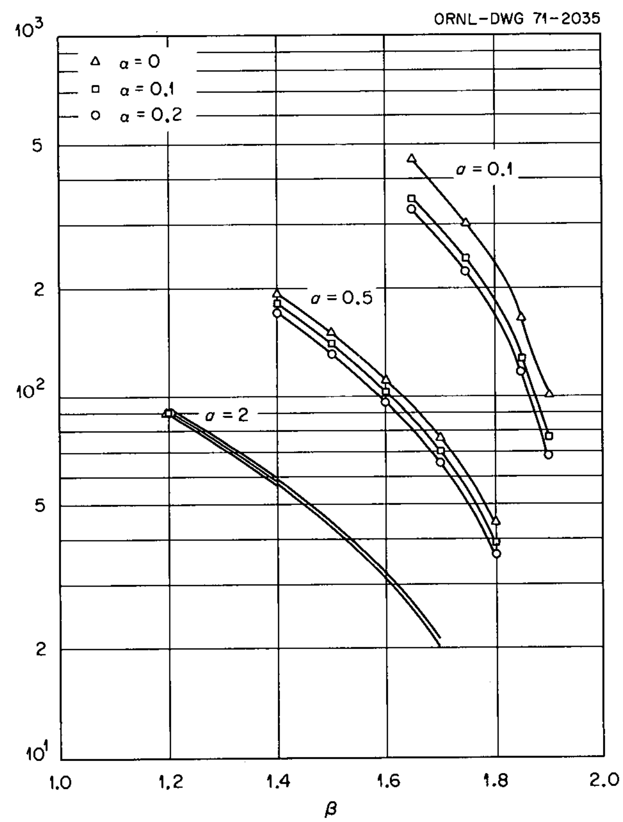

Fig. 3. Number of iterations required for error reduction by a factor of 10.

temperatures. The improvement in stability was excellent; in one problem, 180 time steps were required to integrate over a time interval that required 2000 time steps using an explicit method. The agreement in temperatures calculated by the two methods was also good.

We have included an approximate treatment of nodal freezing and melting in the transient program. We obtained satisfactory agreement between the results of a calculation with our program and the results of a calculation[71] with another program in which the latent heat of fusion was simulated by increasing the specific heat over a small temperature range close to the melting point.

Sponsor: Mathematics Division

ORDEAL: General Purpose System

T. D. Calton

We expanded the ORDEAL[72] programming language by including new procedures for the approximation of definite integrals and for the smoothing of data. The procedures involved the use of subroutines from IBM's System/360 Scientific Subroutine Package (Version III). The new capabilities include: (1) the integration of a polynomial, (2) numerical integration using the trapezoidal rule, Simpson's rule, or one of several Gaussian quadrature formulas, (3) data smoothing by unweighted averaging of neighboring points, and (4) data smoothing by certain least squares polynomials.

The first phase of ORDEAL development is complete, and a user's manual[73] has been published. A second manual[74] cataloging in detail the procedures available in ORDEAL will be forthcoming.

We compiled a list of proposed improvements to ORDEAL. These include: (1) more complex arithmetic expressions, (2) additional data and program management capabilities, and (3) a conversational mode for terminal users. Approval to implement some or all of the proposed improvements has not yet been granted.

Sponsor: Mathematics Division

Spectrum Analysis

A. F. Joseph G. W. Chandler

The user's manual for the SPECTRAN system has been published. Included in the improvements are additional peak finding and peak fitting routines, as well as other user-requested options. Also the spectrum code from Argonne National Laboratory is available for use.

Sponsor: Mathematics Division

---

71. M. Siman-Tov, personal communication.

72. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 9.

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

74. M. Feliciano, C. W. Nestor, N. B. Gove, and T. D. Calton, *ORDEAL Catalog of Procedures,* ORNL-4506, Vol. II (in preparation).

Computer Graphics

Kay C. Chandler	J. D. McDowell
G. W. Chandler	T. D. Calton
Linda P. Helton	E. G. Grohman[75]
M. Feliciano	Ruth B. Hofstra
N. B. Gove	Marie H. Eckart

The manual for the graphics package ORGRAPH[76] has been revised with more examples. A number of improvements and additions have been made. Polar plots have been added, and a printer plot option and a contour plot option are being tested. We made several thousand net migration rate graphs for the Urban Growth Patterns Project.

Sponsor: Mathematics Division

Forms Writer

V. A. Singletary

We wrote a FORTRAN IV program[77] that can generate rectilinear forms of varying complexity on either the pen-and-ink plotter or the cathode-ray tube. In addition to the lineal aspect of the form, textual information may be inserted within the form. Figure 4 illustrates some of the program capabilities.

Sponsor: Mathematics Division

ORNL Computer Center Accounting System

T. D. Calton

The ORNL computer center accounting system[78] described in last year's annual report is now a working reality. Operation under the new accounting system began in July 1970. Detailed reports of the computing center charges may be generated on a weekly or a monthly basis.

The accounting system maintains all accounting files on disk storage with copy on a disk and on magnetic tape. A programmer's activity file for appropriate Mathematics Division personnel is maintained and reported to the management of the Mathematics Division.

We modified accounting programs of the Neutron Physics and Physics Divisions to permit access to data within our accounting files.

Other Mathematics Division programmers contributing to this effort were V. A. Singletary, D. W. Altom, C. L. Armstrong, and R. B. Hofstra.

Sponsor: Mathematics Division

---

75. Knoxville College, Knoxville, Tenn.
76. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 9.
77. V. A. Singletary, *Forms Writer,* ORNL-TM-3290 (to be published).
78. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 10.

ORNL-DWG 71-2036

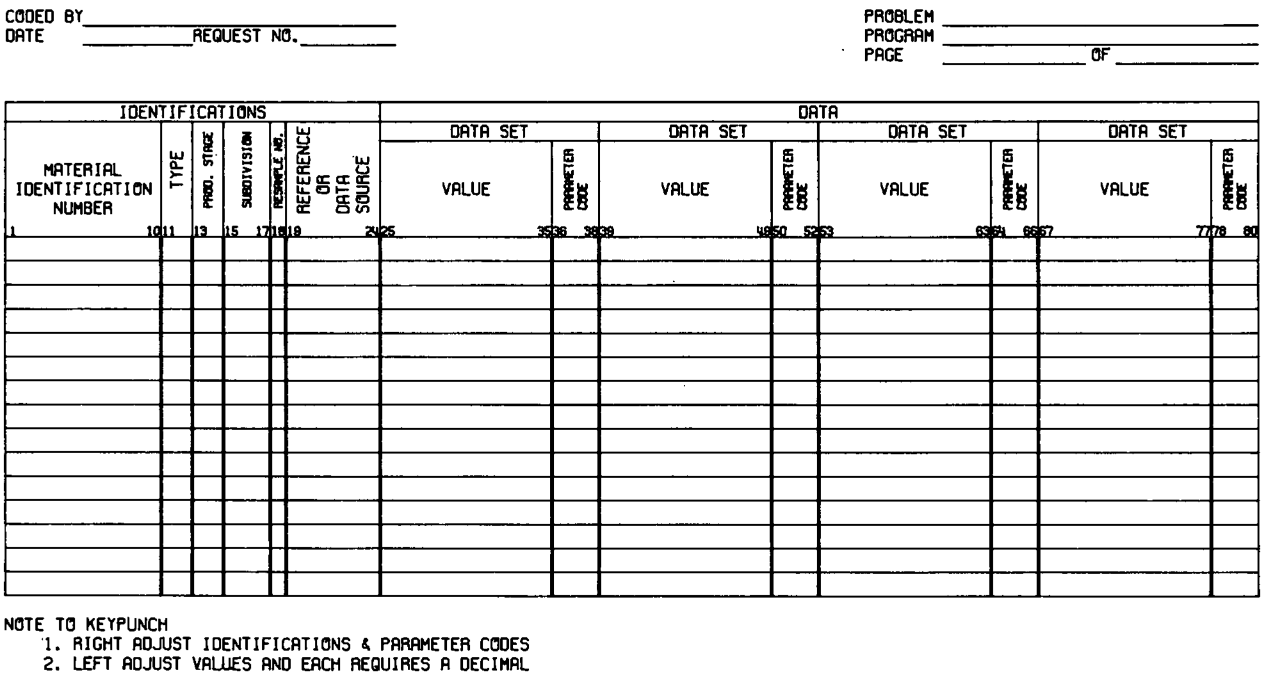

Fig. 4. Sample form generated by the forms writer.

CRBE Public Library

Carla L. Armstrong

We added an assortment of files to the CRBE public library (PUBLC) that allows the CRBE user not only to access and execute subroutines within the Computing Technology Center Numerical Analysis Library[79] and the programs ADSEP[80] and SADS[81] but also to access information describing the required input, the expected output and its disposition, and any user-supplied subroutines peculiar to the subroutine or program being described.

Moreover, there exists within PUBLC as files driver programs (i.e., programs that read in the requisite data, call the desired subroutine, and perform various dispositions of the output) for the subroutines ALLMAT, HOUSEH, VALVEC, ORTHOG, ORTHPT, and CNLLS.[79]

Sponsor: Mathematics Division

Miscellaneous Services

Marie H. Eckart Ruth B. Hofstra Betty Hurt

The Mathematics Division supplies a number of routine computer services to programmers of other divisions. Included among these were FORTRAN 360 classes held during the spring and summer. The

79. G. W. Westley and J. A. Watts, *The Computing Technology Center Numerical Analysis Library,* CTC-39 (October 1970).

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

81. A. Hume and A. A. Brooks, *The SADS Program – Statistical Analysis of Data Subsets* (October 1969).

FORTRAN subroutine library has been maintained, and portions of it have been placed on a data cell for general use.

Sponsor: Mathematics Division

METALS AND CERAMICS DIVISION

Electromagnetic Fields Due to a Current Encircling a Ferromagnetic Tube

C. C. Lu   C. V. Dodd[82]

We have attempted to solve the nonlinear Maxwell equations for the system involving ferromagnetic materials. The problem is simplified by assuming isotropic media, that is, $\mathbf{B} = \mu(B)\,\mathbf{H}$, with axial symmetry. For the case of a long tube encircled by a concentric current, the final differential equations of two variables for the vector potential can be solved by relaxation methods. For comparison studies we have written two programs, differing in treatment of the boundary conditions. They yield similar results, although the final desired convergence is not yet fully attained.

Sponsor: Metals and Ceramics Division   C. V. Dodd

Nondestructive Test for Measuring the State of Heat Treatment in Closure Welds

C. C. Lu   C. V. Dodd[82]

We have completed the first stage in the development of a nondestructive testing technique to measure the properties of resistance-welded closures on chemical munition containers. The preliminary technique using a magnetic circuit measures (1) temper of the weld, (2) cross-sectional area of the weld, and (3) variation of cap height from nominal. We have made measurements of magnetic properties as a function of temper and area of samples of AISI type 1040 steel. A prototype probe to induce the magnetic circuit, link the magnetic circuit through the weld, and measure the magnetic flux through the circuit was designed and constructed. Tests performed on six sample welds demonstrated the capability for measuring the temper, area, and variations in cap height.

Sponsor: Metals and Ceramics Division   C. V. Dodd

NEUTRON PHYSICS DIVISION

A Reevaluation of Natural Iron Neutron and Gamma-Ray Production Cross Sections – ENDF/B Material 1124[83,84]

S. K. Penny   W. E. Kinney[85]

Recent data and good agreement between calculated and experimental cross sections prompted the reevaluation of natural iron neutron and gamma-ray production cross sections for ENDF/B use with the aim

82. Metals and Ceramics Division.

83. Abstract of ORNL-4617 (to be published).

84. Research partially supported by the Defense Atomic Support Agency under Union Carbide Corporation's contract with the USAEC.

85. Neutron Physics Division.

of improving angular distributions and extending inelastic level excitation cross sections. Calculations were performed and were shown to be in good agreement with experiment. Below 2 MeV, neutron elastic scattering cross sections and cross sections for inelastic scattering to levels in ^{56}Fe are obtained from experimental results. Above 2 MeV, neutron elastic scattering cross sections and cross sections for inelastic scattering to levels in ^{56}Fe up to an excitation energy of 4.116 MeV are obtained from calculations. Cross sections for inelastic scattering to the continuum are obtained from fits to experimental results. The total cross sections are the evaluated cross sections of Irving and Straker from 330 keV to 15 MeV and those of the U.K. evaluation DFN-91 from 10^{-5} eV to 330 keV. The (n,p) and (n,α) cross sections were taken from the U.K. evaluation DFN-91, while the $(n,2n)$ cross sections are those of ENDF/B material 1122. The (n,γ) cross sections were taken from U.K. DFN-91. The gamma-ray production cross sections and associated gamma-ray spectra were calculated from the evaluated (n,n') and (n,γ) cross sections together with known and assumed branching ratios.

Sponsor: Neutron Physics Division F. G. Perey

Calculation of Cross Sections for Gamma-Ray Production via Neutron Inelastic Scattering in ^{56}Fe[86]

S. K. Penny

Gamma-ray production via neutron inelastic scattering in ^{56}Fe has been calculated using the computer program HELGA.[87] These calculations have been compared with measured data, and the agreement is reasonably good.

The calculations were performed using only discrete states. The levels and branching ratios through 4 MeV were determined experimentally,[88] and the levels through 9 MeV were obtained from a shell model calculation by McGrory.[89] The unknown branching ratios were obtained in an ad hoc way by assuming knowledge of various orders of multipole radiation. The penetrabilities needed for the statistical model calculation were obtained via an optical model in which the real and imaginary well depths were linear functions of energy. The optical model parameters were obtained from fits to the neutron elastic scattering data of Kinney and Perey.[90]

Table 1 shows the comparison of experimental gamma-ray production in natural iron for 0.5-MeV gamma-ray energy intervals by Maerker and Muckenthaler[91] with these calculations and those of Celnik and Spielberg[92] in 1-MeV intervals. The calculations had to be integrated over a reactor spectrum. These calculations did not include ^{54}Fe, which would contribute approximately another 60 mb in the 1- to

86. Partially supported by Defense Atomic Support Agency under Union Carbide Corporation's contract with the U.S. Atomic Energy Commission.

87. S. K. Penny, "HELGA – a Computer Program to Calculate Gamma-Ray Production Cross Sections via the Hauser-Feshbach Model," this report.

88. A. Aspinall et al., *Nucl. Phys.* **46**, 33 (1963); A. Sperduto and W. W. Buechner, *Phys. Rev.* **134**, B142 (1964); A. D. Katsanos et al., *Phys. Rev.* **141**, 1054 (1966); G. Brown et al., *Nucl. Phys.* **77**, 365 (1966); B. L. Cohen and R. Middleton, *Phys. Rev.* **146**, 748 (1966); J. R. MacDonald and M. A. Grace, *Nucl. Phys.* **A92**, 593 (1967); P. F. Hinrichsen et al., *Nucl. Phys.* **A101**, 81 (1967).

89. J. B. McGrory, *Phys. Rev.* **160**, 915 (1967).

90. W. E. Kinney and F. G. Perey, *Neutron Elastic- and Inelastic-Scattering Cross Sections for ^{56}Fe in the Energy Range 4.19 to 8.56 MeV*, ORNL-4515 (1970).

91. R. E. Maerker and F. J. Muckenthaler, *Gamma-Ray Spectra Arising from Fast-Neutron Interactions in Elements Found in Soils, Concretes, and Structural Materials*, ORNL-4475 (1970).

92. J. Čelnik and D. Spielberg, *Gamma Spectral Data for Shielding and Heating Calculations*, United Nuclear Report UNC-5140 (1966).

Table 1. Gamma-ray production cross sections in iron for a reactor spectrum (mb)

Gamma-ray energy interval (MeV)	This calculation	Maerker's experiment	Celnik's calculation
0.5–1.0	905	600	1100
1.0–1.5	153	278	307
1.5–2.0	82	110	
2.0–2.5	83	101	198
2.5–3.0	77	74	
3.0–3.5	29	44	78
3.5–4.0	38	33	
4.0–4.5	12.7	8.7	14
4.5–5.0	8.9	5.6	
5.0–5.5	4.4	3.8	8.5
5.5–6.0	2.8	2.4	
6.0–6.5	1.7	2.1	2.0
6.5–7.0	0.6	<0.6	

1.5-MeV interval. The 0.846 gamma ray is anisotropic, which accounts for some of the discrepancy in the 0.5- to 1-MeV interval, since Maerker's measurements were for 90°.

Comparisons have also been made with the data in BNL-325,[93] with Kinney's calculations,[94] and with preliminary results from Dickens' measurements.[95] The agreement obtained with the data in BNL-325, which is all below 5 MeV, is good considering the experimental difficulties. Better agreement is obtained with Dickens' measurements for all neutron energies in the range 4 to 9 MeV and with Kinney's calculations below 5 MeV. Tables 2–4 show the comparison with Dickens' measurements for three neutron energies. The 0.846-MeV gamma ray is anisotropic by small amounts as shown experimentally, but this is not likely to be important to transport calculations as indicated by Straker.[96]

The results of the calculations have been placed in ENDF/B format and have been incorporated into the iron evaluation reported in another section of this report.[97]

Sponsor: Neutron Physics Division F. G. Perey

HELGA – a Computer Program to Calculate Gamma-Ray Production Cross Sections via the Hauser-Feshbach Model[86]

S. K. Penny

The computer program HELGA incorporates the Hauser-Feshbach model with width fluctuation corrections and continuum states in the calculation of the neutron reaction cross sections. This is done in

---

93. M. D. Goldberg et al., *Neutron Cross Sections, Vol. IIA, Z = 21 to 40,* BNL-325, 2d ed., suppl. 2 (1966).

94. W. E. Kinney and F. G. Perey, "Calculated ^{56}Fe Neutron Elastic and Inelastic Scattering and Gamma-Ray-Production Cross Sections from 1.0 to 7.6 MeV," *Nucl. Sci. Eng.* **40**, 365 (1970).

95. J. K. Dickens, private communication, 1970.

96. E. A. Straker, Technical Note, *Nucl. Sci. Eng.* **41**, 147 (1970).

97. S. K. Penny and W. E. Kinney, "A Reevaluation of Natural Iron Neutron and Gamma-Ray Production Cross Sections – ENDF/B Material 1124," this report.

Table 2. Differential cross sections for gamma-ray production via neutron inelastic scattering in iron

E_n = 5.35 MeV

E_γ (keV)	Differential cross section (mb/sr)		
	Calculation	Experiment	
		55°	90°
846	109.9	85.0	81.7
1038	5.4	5.7	5.7
1168 + 1175	1.5	2.1	2.2
1238	28.8	23.9	22.6
1811	9.9	9.3	10.6
2113	7.2	5.5	5.9
2523	5.2	5.3	4.5
3202	2.6	2.4	1.9
3445 + 3451	2.7	2.5	3.5
3548	3.4	2.0	2.2

Table 3. Differential cross sections for gamma-ray production via neutron inelastic scattering in iron

E_n = 6.40

E_γ (keV)	Differential cross section (mb/sr)		
	Calculation	Experiment	
		55°	90°
846	106.3	88.0	82.0
1038	5.6	6.5	6.1
1168 + 1175	1.1	2.5	2.1
1238	32.3	28.9	24.5
1811	8.0	9.9	8.9
2113	5.6	5.4	4.9
2523	4.2	3.5	3.4
3202	2.6	1.6	1.8
3445 + 3451	2.7	2.4	2.8
3548	2.8	2.2	2.5

Table 4. Differential cross sections for gamma-ray production via neutron inelastic scattering in iron

E_n = 8.50

E_γ (keV)	Differential cross section (mb/sr)		
	Calculation	Experiment	
		55°	90°
846	102.2	93.4	85.1
1038	7.0	7.9	6.4
1168 + 1175	0.8	2.2	1.9
1238	39.6	34.5	31.1
1811	6.6	9.2	8.5
2113	4.7	4.1	3.7
2523	3.6	2.4	2.2
3202	3.4	2.2	1.8
3445 + 3451	3.5	1.8	1.6
3548	2.1	2.0	1.4

the same way as is done in the program HELENE.[98] Direct-interaction contributions to the neutron cross sections may be read as input calculated using programs such as JULIE.[99] The gamma-ray cascade among discrete states is an integral part of HELGA, while the cascades originating in the continuum are read as input and are calculated with the program DUCAL.[100] Experimentally determined branching ratios are read as input, and all others are calculated in an ad hoc way by assuming knowledge of the probabilities of various orders of multipole radiation. Of course, gamma-ray production is calculated by weighting the cascades with the appropriate neutron cross sections and then summing.

98. S. K. Penny, *HELENE – a Computer Program to Calculate Nuclear Cross Sections Employing the Hauser-Feshbach Model, Porter-Thomas Width Fluctuations, and Continuum States,* ORNL-TM-2590 (1969).

99. R. H. Bassel, R. M. Drisko, and G. R. Satchler, *The Distorted Wave Theory of Direct Nuclear Reactions,* ORNL-3240 (1962).

100. K. J. Yost, "A Method for the Calculation of Neutron Capture Gamma-Ray Spectra," *Nucl. Sci. Eng.* 32, 62 (1968).

The excitation spectrum for each residual nucleus of the competing reactions can be divided into three regions instead of the usual two, discrete and continuum. The middle region is discrete also, but the contribution from each level in this region is weighted by the ratio of the number of levels that the continuum model could predict in a narrow energy region to the actual number of discrete levels in that energy region. In this fashion one may use discrete levels predicted by a shell model calculation presuming the spin-parity distributions to be correct, but yet assuming that the continuum model predicts the correct total number of levels.

Sponsor: Neutron Physics Division C. E. Clifford

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

N. M. Greene R. B. Perez[101] G. de Saussure[101] S. K. Penny

A knowledge of multiple-scattering effects in optically thick (several mean free paths) samples is required for an accurate determination of resonance parameters. Previously, analytical or Monte Carlo techniques have been employed for this purpose.

The present method of determining resonance parameters is based on calculating the changes in calculated vs experimental response rates compared with resonance parameter changes and using this "derivative" to drive the calculation to a converged set of parameters. Because a scheme of this type will involve several neutronics calculations, and because Monte Carlo calculations are relatively time-consuming, an alternate procedure was desired. The Monte Carlo scheme also has "indeterministic" statistical variations which can lead to difficulties.

The present scheme employs a modified version of ANISN, a one-dimensional S_n multigroup transport program. ANISN solves the transport one-dimensional Boltzmann equation numerically by setting up a network of mesh points in the energy, angle, and spatial coordinates. The scattering kernel can be expanded in Legendre polynomials to any order within reasonable computer memory capabilities and time. The other pieces of MSC are a code to evaluate cross sections at many points across a resonance and a code to calculate elastic scattering transfer matrices.

A flow chart for MSC is presented in Fig. 5.

Since there are so many options and adjustments with the S_n method, a parametric study was performed and the results compared with Monte Carlo results for the same case. To facilitate the discussion that follows, we shall name the various cases studied in the form ${}^{G}S_nP_l{}^{R}$, where the subindexes n and l indicate the number of mesh points in the angular coordinates and the order of truncation in the scattering kernel, respectively, and the superindexes G and R indicate the number of energy intervals taken (groups) and the number of space intervals defined along the thickness of the sample respectively. On the basis of the well-known relation

$$\int dE \int d\Omega \int d\mathbf{r}\, \Sigma_x(E)\, \Phi(\mathbf{r}, \Omega, E) = \int dE \int d\Omega \int d\mathbf{r}\, S(\mathbf{r}, \Omega, E)\, \Phi^{\dagger}(\mathbf{r}, \Omega, E)\,, \qquad (1)$$

where

$\Sigma_x(E)$ = macroscopic cross section for a given neutron reaction,

$S(\mathbf{r}, \Omega, E)$ = neutron source,

$\Phi(\mathbf{r}, \Omega, E)$, $\Phi^{\dagger}(\mathbf{r}, \Omega, E)$ = real and adjoint fluxes,

101. Neutron Physics Division.

ORNL-DWG 71-2037

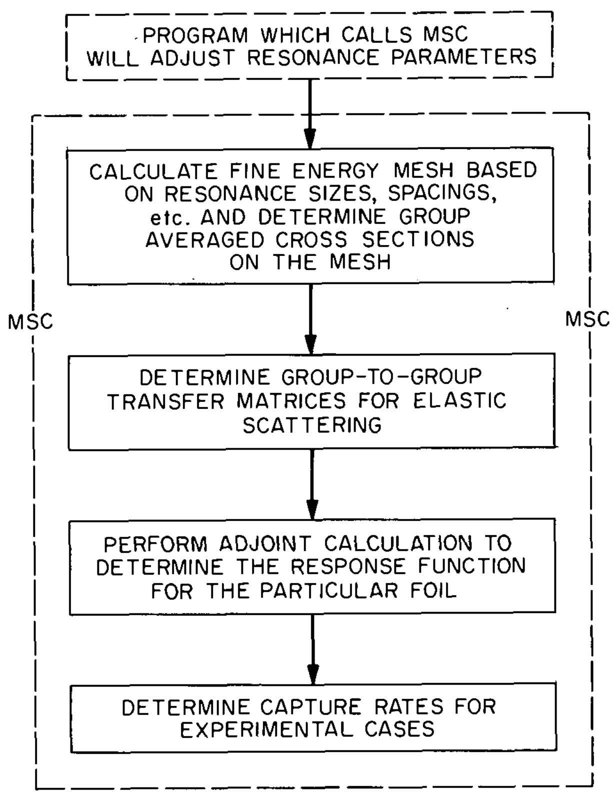

Fig. 5. MSC flow chart.

the total number of events is computed by the convolution of the neutron source and the adjoint flux. There are two reasons for the use of this procedure: (1) it eliminates the necessity for calculating the real flux for each neutron source energy, and (2) it takes advantage of the observed fact that the adjoint flux changes much more slowly with the angular and energy variables than does the real flux.

The example considered in this work was the 6.67-eV capture resonance of ^{238}U. The sample had a radius of 3.81 cm and a thickness of 1.03 mean free paths, which are dimensions that correspond to actual experimental conditions.

Several MSC calculations are shown in Table 5. Inspection of the results shows that case 11, corresponding to $^{100}S_4P_1{}^5$, compares very well with case 5 ($^{100}S_{48}P_3{}^5$), the substantial differences occurring away from the resonance energy. This indicates that only a few angle mesh points together with linear anisotropic scattering are suitable for the calculation. The effect of the number of energy points across the resonance can be exhibited by the comparison of case 6 ($^{200}S_8P_3{}^5$) and case 15 ($^{50}S_8P_3{}^5$). For the particular points shown in Table 5, the agreement found is very good; however, the results around the peak of the resonance become marginal for the 50-group case. This suggests that one could use less than 100 groups with a denser energy mesh in the vicinity of the resonance peak and still obtain good results with a considerable saving in computer storage capability and running time. Cases 14 ($^{100}S_{16}P_3{}^{25}$) and 12 ($^{100}S_{16}P_1{}^5$) show that for all practical purposes a few spatial intervals will suffice. Further calculations have shown that, in fact, for sample thickness up to 15 mils as few as two space intervals yield accurate results.

Figure 6 displays a comparison between the MSC results and a Monte Carlo calculation, which utilizes 100 energy bins and 10^4 neutron histories. The agreement for case 5 ($^{100}S_{48}P_3{}^5$) is excellent. Case 11

($^{100}S_4P_1{}^5$), which is a much shorter calculation, also yields results which are accurate enough for our purposes. Both results indicate that indeed the finite size of the sample does not invalidate the MSC one-dimensional calculations.

The calculation time shown in Table 5 does not include the time to generate the cross sections.

The time invested in the calculation of the Doppler-broadened cross section is a fraction of a second and does not add appreciably to the overall timing. The longest calculation by far is the one related to the elastic scattering transfer matrix; however, it need be calculated only once at the beginning of a set of

Table 5. MSC calculations

Case	n of S_n	l of P_l	Spatial intervals	Energy spacing (eV)	Computer time (min)	Response (captures neutron^{-1} cm^{-2})		
						5.195 eV	6.605 eV	7.505 eV
1	4	3	5	0.030	0.11	1.5188−4	3.6981−2	3.9399−4
2	8	3	5	0.030	0.11	1.4641−4	3.6952−2	3.8088−4
3	12	3	5	0.030	0.13	1.4523−4	3.6948−2	3.7838−4
4	32	3	5	0.030	0.29	1.4426−4	3.6945−2	3.7839−4
5	48	3	5	0.030	0.42	1.4443−4	3.6945−2	3.7916−4
6	8	3	5	0.015	0.21	1.4641−4	3.6946−2	3.8088−4
7	12	3	5	0.015	0.26	1.4523−4	3.6942−2	3.7839−4
8	32	3	5	0.015	0.52	1.4428−4	3.6940−2	3.7839−4
9	4	3	2	0.030	0.04	1.5188−4	3.7104−2	3.9398−4
10	4	3	10	0.030	0.13	1.5188−4	3.6961−2	3.9398−4
11	4	1	5	0.030	0.08	1.5189−4	3.6964−2	3.9404−4
12	16	1	5	0.030	0.18	1.4476−4	3.6928−2	3.7759−4
13	16	3	5	0.030	0.16	1.4475−4	3.6946−2	3.7751−4
14	16	3	25	0.030	0.68	1.4475−4	3.6918−2	3.7751−4
15	8	3	5	0.060	0.06	1.4643−4	3.70−2[a]	3.82−4[a]
16	12	3	5	0.060	0.07	1.4524−4	3.70−2[a]	3.80−4[a]
17	32	3	5	0.060	0.16	1.4426−4	3.70−2[a]	3.80−4[a]

[a]These points did not exist in the 0.060 spacing structure and are interpolated values.

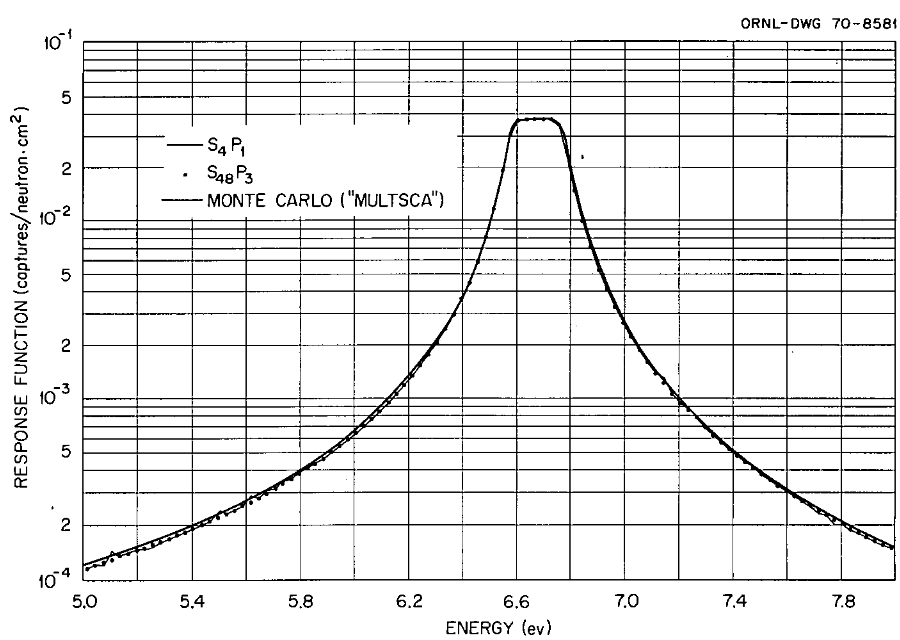

Fig. 6. Comparison between the Monte Carlo calculation and various MSC results.

iterations. Between successive iterations it is necessary only to scale the transfer matrix, which again takes about a fraction of a second. In the particular case at hand the Monte Carlo calculation run for 7.95 min is to be compared with 0.42 min for case 5 ($^{100}S_{48}P_3{}^5$) and with only 0.08 min for case 11 ($^{100}S_4P_1{}^5$).

In view of the above results, it seems then feasible to utilize deterministic codes for resonance parameter searches with thick-sample cross-section measurements used as input data.

Present work is concerned with combining the separate steps shown in Fig. 5 into a single callable code package to allow automating the resonance parameter adjustments. The existing scheme has three separate programs linked together with IBM Job Control Language.

The routines which generate the elastic scattering matrices employ a double-numerical integration for which it is possible, within the limits of the resonance problem, to determine analytic functions for the matrices. These functions have been derived and are being programmed and should greatly enhance the efficiency of MSC.

At least two independent uses for MSC have been encountered. It is in the process of being used to verify (or check) the applicability of the Nordheim treatment to filter calculations. It is also being used to determine leakage spectra from filters.

Sponsor: Neutron Physics Division — R. B. Perez, G. de Saussure

Activities Connected with the Cross Section Evaluation Working Group

S. K. Penny

Although the Cross Section Evaluation Working Group (CSEWG) of the National Neutron Cross Section Center at Brookhaven National Laboratory is composed of USAEC contractor personnel whose main interests lie with reactor calculations, there is a small number of people in CSEWG who are interested in shielding calculations and who have been very influential in adequately presenting the viewpoint of shielding. The activities reported here are largely connected with this shielding subcommittee.

A task force was formed early this year to start a system to acquire available shielding cross-section data in the ENDF/B format and to perform a check-out and review of these data. ORNL Mathematics Division involvement was in the area of (1) evaluation,[102] (2) formulating formats and procedures, (3) aiding in the draft of a formats and procedures manual, and (4) check-out of ENDF/B codes.

Other activities were associated with serving on the CSEWG Codes and Formats Subcommittee and the newly formed task force on Nuclear Model Codes.

Sponsor: Neutron Physics Division — C. E. Clifford

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

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

Two programs have been written in order to plot certain neutron cross sections from an ENDF/B[103] data tape for reference use in the experimental program at ORELA. However, the programs are equally

---

102. S. K. Penny and W. E. Kinney, "A Reevaluation of Natural Iron Neutron and Gamma-Ray Production Cross Sections – ENDF/B Material 1124," this report.

103. H. C. Honeck, *ENDF/B-Specifications for an Evaluated Nuclear Data File for Reactor Applications*, BNL-50066 (ENDF-102) (May 1966; revised July 1967).

applicable to the plotting of any cross section from the ENDF/B tape. Since the ORNL Cross Section Steering Committee expressed an interest in the programs and since that Committee is involved in protecting the general ORNL interests in neutron cross-section data, it was decided to use the programs in the future to prepare plots for general reference use as well as that of the shielding experimental program.

The program, ECSP, produces the CALCOMP plots of ENDF/B cross-section data. The program reads a specially prepared tape of cross sections vs energy produced by the other program. For the shielding experimental program at ORELA the cross sections for each element are plotted for five energy bins that range from 10^{-2} to 10^{8} eV in value. Each of the five plots per element contains the curves for the total, the elastic, and the inelastic plus the capture cross sections. The plots are logarithmic and are 15 in. wide by 10 in. high. This program makes use of the modified INTRIGUE-360, which is described elsewhere in this report.

The other program retrieves data from ENDF/B files 2 and 3 and performs the necessary calculations to place the data in the form required by the plotting program. The subroutines used have been borrowed from the SUPERTOG[104] program. The single-level Breit-Wigner formalism is used for calculation of cross sections in the resolved resonance region. The energy mesh is constructed by the program and includes 50 points for each resonance. Cross sections in the unresolved resonance region are computed by taking averages over suitable Porter-Thomas distributions of the neutron and fission widths. An energy mesh of 81 points equally spaced in lethargy over the unresolved resonance range is used. The resonance contributions are added to the smooth background cross section from ENDF/B file 3 to obtain the final cross sections. Doppler-broadened cross sections can be produced if desired using the method of the TEMPO[105] program.

Sponsor: Neutron Physics Division — E. A. Straker

The Thrust of Cross-Section Data Requirements for Reactor Shielding Calculations[106]

S. K. Penny

The requirements for cross-section data necessary to perform radiation shielding calculations have become much more stringent in the past few years. The recently acquired capabilities of calculating penetration of radiation to large depths, of efficiently handling large arrays of cross-section data, and of performing coupled neutron and gamma-ray transport calculations are some of the more important reasons for the demand for better and more detailed cross-section sets. The methods for measuring radiation energy spectra, angular distributions, and other quantities have been improved recently and hence provide a more detailed check of cross-section adequacy. Last, but not least, are programmatic requirements, such as for radiation damage and nuclear heating in the LMFBR program.

There are several types of neutron cross-section data that are most urgently needed for shielding calculations. The total cross sections at the minima between resonances in the keV or MeV energy regions are crucial for deep penetration calculations. Equally important is the angular distribution of elastic scattering at these minima. One must know the cross sections for level excitation via inelastic scattering to be able to predict neutron spectra accurately. For high energies, even the total inelastic cross section is a

---

104. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, Jr., *SUPERTOG: A Program to Generate Five Group Constants and Pn Scattering Matrices from ENDF/B*, ORNL-TM-2679 (1969).

105. K. Gregson and M. F. James, *TEMPO – a General Doppler Broadening Program for Neutron Cross Sections*, AEEW-M518 (1965).

106. Summary of paper to be published in ANS-SD-11 by Shielding and Dosimetry Division of the American Nuclear Society.

welcome quantity, since for deep penetration the tradeoff between inelastic and elastic scattering can make large differences in attentuation of neutrons. Finally, the (n,p) and (n,α) cross sections have become important because of the requirement to calculate radiation damage for the LMFBR program.

Gamma-ray production cross sections of all kinds are urgently needed for shielding. It is known now that it is not always conservative to treat the gamma rays produced by neutron capture as if they were produced at thermal energies. Primary lines cannot be used alone, and one must not be cavalier in the treatment of the continuum part of the capture spectrum. Indeed, now the requirement is that the capture gamma-ray spectra be known as completely as possible at all neutron energies where the capture cross section is significant. Since neutron inelastic scattering plays an important role in shielding calculations, the gamma rays following inelastic scattering are also important. The gamma rays following level excitation by (n,α) and (n,p) reactions at high neutron energies in the general case can be significant.

The requirements for cross-section data in such detail have made the job of the Shielding Subcommittee of the Cross Section Evaluation Working Group (CSEWG) difficult. Not only do the requirements increase the problems of evaluation, but they make nontrivial the task of data testing. The Shielding Subcommittee of CSEWG has essentially completed the establishment of formats for cross-section data and is now principally concerned with obtained evaluated sets of data and with data testing. Evaluation is to be encouraged with the proviso that particular attention be given to the cross-section requirements mentioned above. The Subcommittee is setting up an ad hoc review group to perform, from the shielding viewpoint, the Phase I data testing or initial critical review of evaluated cross-section sets sent to the National Neutron Cross Section Center (NNCSC). A checklist is being devised to aid in this initial review, and it is expected that the Radiation Shielding Information Center will provide a helping hand in the way of data transmittal, check-out, plotting, and editing for review. While the Phase II data testing is just now being formulated for CSEWG as a whole, the shielding community already has made some advances in this area. Phase II data testing is the testing of cross-section sets that have been accepted for the Evaluated Nuclear Data File (ENDF/B) for adequacy relative to needs and requirements. The shielding community has made such tests for the minima in total cross sections, and, as a result, new cross-section sets have been sent to NNCSC. The need for more work in this area is clearly indicated.

Since the experimental and theoretical capabilities in the area of determining cross sections have expanded in recent years, it is to be expected that many of the shielding cross-section requirements will at least be partially fulfilled in the near future.

Sponsor: Neutron Physics Division — C. E. Clifford

Auxiliary Routines for MORSE[107]

Margaret B. Emmett E. A. Straker[108]

As the MORSE[109] code is applied to solving neutron and gamma-ray transport problems, the desire for more diagnostic aids regarding the behavior of the sample distribution arises. Routines that can be used to obtain estimates of the fluence from the collision counters in MORSE (collision density per unit volume

---

107. Partially funded by Defense Atomic Support Agency under Union Carbide Corporation's contract with the U.S. Atomic Energy Commission.

108. Neutron Physics Division.

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

estimator) have been very useful in obtaining the fluence averaged over regions. We are continuing work in the use of visible displays of a sample of the collision density so that the regions in which events occur can be easily obtained. This involves either the CALCOMP plotting package INTRIGUE[110] or the printer plotting package.[111]

In addition to these diagnostic aids, routines have been written to provide a processed cross-section tape from a MORSE run to be used in subsequent runs. This tape may be generated in a separate program independent of a MORSE calculation.

Sponsor: Neutron Physics Division E. A. Straker

A Set of Sample Problems for MORSE – a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code[107]

Margaret B. Emmett E. A. Straker[108]

The Multigroup Oak Ridge Stochastic Experiment (MORSE) code[109] is a multipurpose neutron and gamma-ray Monte Carlo code. Because of its many options and types of problems that can be solved, it has proved useful to develop sample problems to aid new users of the code in understanding what is required for solving problems of different types. Problems involving neutrons, coupled neutron–gamma ray, fission, time dependence, albedo scattering, point estimators, and boundary crossing estimators are being investigated. SAMBO,[112] an analysis package written for use with the MORSE code, is being adapted to the problems being studied.

Sponsor: Neutron Physics Division E. A. Straker

O6R System Development[107]

C. L. Thompson

O6R[113] is a major revision of the Monte Carlo neutron transport code O5R.[114] All proposed changes to O5R have been made; the FORTRAN-IV version of O6R is complete and has been tested for shielding problems. Additions have been made to O6R, and required changes to the cross-section preparation code are complete except for two options. Other support programs for the O5R system have been rewritten for O6R.

The major change in O6R has been to make the energy structure of the cross-section input data variable rather than fixed by the code. This allows the user to have finer cross-section detail in energy regions where the cross sections vary rapidly. Also, an energy cutoff, below which isotropic scattering is used rather than the Coveyou technique, has been added to conserve storage.

---

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

111. C. L. Thompson, *A FORTRAN-360 Subroutine Package for Producing Printed Linear, Semilogarithmic or Logarithmic Graphs,* ORNL-TM-3079 (Aug. 6, 1970).

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

113. *Neutron Phys. Div. Ann. Progr. Rept. May 31, 1969,* ORNL-4433, p. 56.

114. D. C. Irving et al., *O5R, a General Purpose Monte Carlo Transport Code,* ORNL-3622 (February 1965).

NUSECT, the cross-section preparation code for O6R-ACTIFK,[115] which uses cross-section data from the ENDF/B[116] library, was rewritten to allow user-defined supergroup energy boundaries and the anisotropic energy cutoff.

Additions were made to O6R and NUSECT to provide a standard method of using the ENDF/B library data for handling inelastic scattering and gamma-ray production.[117] NUSECT will use the data available in an ENDF/B data set to produce magnetic tapes of input parameters to standard subroutine sets in O6R which process inelastic scattering and photon production. In earlier versions of O5R the user was responsible for providing his own subroutines and data for these problems.

NUSECT still does not process resonance parameters from the ENDF/B library, and the gamma-ray production routine does not process data in the form of transition probability arrays. NUSECT allows the user to select the standard O5R supergroup energy structure for his cross-section data as an option.

NUSECT uses any data appearing in files 12, 13, and 15 of an ENDF/B material to prepare input parameters to the O6R subroutines which define the parameters of gamma rays generated during the neutron transport problem. Data from the ENDF/B library are converted to microscopic gamma-ray production cross sections for each material in an O6R problem. The microscopic gamma-ray production cross-section data are used to produce macroscopic cross-section data as a table of total photon production probabilities and a table of cumulative normalized photon production probabilities for each medium in the problem. A gamma ray may be produced at each collision during the random walk, if the total production probability is nonzero.

The probability of having a gamma-ray-producing event is calculated as

$$P_{m,i}^{\text{prod}} = X_{m,i}^{\text{prod}}/X_{m,i}^{\text{total}} ,$$

where $X_{m,i}^{\text{prod}}$ is the macroscopic production cross section for medium m and neutron energy i and $X_{m,i}^{\text{total}}$ is the total macroscopic cross section.

The normalized continuous photon spectrum for each medium m is calculated as a table of probabilities

$$PJ_{m,i,j}^{\text{prod}} = X_{m,i,j}^{\text{prod}}/X_{m,i}^{\text{prod}} ,$$

where j is the photon energy index.

$X_{m,i}^{\text{prod}}$ is calculated as

$$X_{m,i}^{\text{prod}} = \sum_j X_{m,i,j}^{\text{prod}} ,$$

and $X_{m,i,j}^{\text{prod}}$ is calculated as

$$X_{m,i,j}^{\text{prod}} = \sum_{k=1}^{N} \sigma_{k,i,j}^{\text{prod}} \times \delta_k ,$$

---

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

116. H. C. Honeck, *ENDF/B-Specifications for an Evaluated Nuclear Data File*, BNL-5006 (ENDF-102).

117. D. J. Dudziak, *ENDF/B Formal Requirements for Shielding Applications*, LA-3801 (ENDF-111).

where N is the number of elements in medium m, $\sigma_{k,i,j}{}^{\rm prod}$ is the microscopic photon production cross section for neutron energy i, photon energy j, and element k, and δ_k is the partial density of element k in medium m, in units of 10^{24} atoms/cm^3.

Photon production cross sections are averaged over neutron energy intervals which may be user defined, or the O6R supergroup-subgroup structure. Cross-section data are assumed constant across each neutron energy interval, consistent with the method used to represent neutron cross sections in O6R. A standard photon energy structure is provided, as an option, or the user may define the photon energy structure.

EDITXS,[118] a program to edit O5R cross-section tapes, has been rewritten to edit O6R tapes written by NUSECT.

O6R has been debugged for fast neutron shielding problems. Thermal neutron problems and problems involving fissioning systems have not been attempted.

Sponsor: Neutron Physics Division — E. A. Straker

O6R-ACTIFK System Development[107,116]

C. L. Thompson

The standard subroutine sets, described in the discussion of O6R in this report, to interface the ENDF/B[116] inelastic and photon production data with the O5R[114]-O6R system were added to O6R-ACTIFK.[115] The cross-section processing code NUSECT[115] was extended to include routines which produced input tapes with the input parameters for inelastic collisions and photon production. Program EDITXS[118] which edits O5R cross-section tapes was revised to also edit the photon production tape.

Sponsor: Neutron Physics Division — E. A. Straker

Neutron and Secondary Gamma-Ray Induced Heat in the Ground Due to Point 12.2- to 15-MeV and Fission Sources at an Altitude of 50 Feet[107,119]

E. A. Straker[108] Margaret B. Emmett M. L. Gritzner

The energy deposited in ground due to neutrons and the secondary gamma rays has been determined as a function of range, ground depth, and time from an instantaneous point neutron source with either a fission spectrum or a 12.2- to 15-MeV energy band. In all cases, the source was at a height of 50 ft above the air/ground interface. Discrete ordinates and Monte Carlo[109] calculations illustrated that there is a significant effect on the energy deposited due to source energy distribution, but little effect due to small differences in ground composition. The importance of gamma rays produced by low-energy neutrons was found to be small for the 12.2- to 15-MeV source, but large for the fission source.[120,121]

Sponsor: Neutron Physics Division — E. A. Straker

---

118. *Math Div. Ann. Progr. Rept. Dec. 31, 1967,* ORNL-4236, p. 18.
119. Abstract of ORNL-4626 by E. A. Straker, M. B. Emmett, and M. L. Gritzner (November 1970).
120. *Neutron Phys. Div. Ann. Progr. Rept. May 31, 1970,* ORNL-4592, pp. 60, 62.
121. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 32.

Calculated Neutron Flux in Sodium[122]

C. L. Thompson

O6R-ACTIFK[115] was used to make a Monte Carlo calculation to determine the neutron flux distribution resulting from a point isotropic fission source located in the center of a 10-m-diam sphere of sodium. The purpose was to obtain data which would be helpful in evaluating the accuracy of calculations involving neutron transport in sodium.

Sponsor: Neutron Physics Division C. E. Clifford

Several Computer Programs for Analysis and Plotting of Results from Shielding Experiments Conducted at ORELA

Margaret B. Emmett E. A. Straker[108] C. E. Burgart[108]

We have written various programs to manipulate and display experimental data obtained at ORELA.[123] These programs involve the subtraction of background, conversion from channel number to energy or time scales, and providing CALCOMP plots of relevant results. In particular CALCOMP plots of the two-dimensional arrays are provided in a compact array. The plotting package INTRIGUE-360[124] is utilized. By providing many options in both the data reduction and plotting routines, the programs have great flexibility.

Sponsor: Neutron Physics Division E. A. Straker

A FORTRAN-360 Package for Producing Printed Linear, Semilogarithmic, or Logarithmic Graphs

C. L. Thompson

A FORTRAN-360 subroutine package has been written to produce printed linear, semilog, or log-log plots similar to those produced on the Calcomp Digital Incremental Plotters by the subroutine package INTRIGUE.[125] The calling sequence and input to this package are very similar to INTRIGUE, and many programs using one may use the other without change.

Sponsor: Neutron Physics Division E. A. Straker

A Revision of INTRIGUE-360, a Plotting Program for the IBM-360 System

Margaret B. Emmett

We have modified the plotting package INTRIGUE-360[124] to add greater flexibility. The height of the plot is now under user control so that the wide-scale plotter can be used. We have changed the option for

122. C. L. Thompson, *Calculated Neutron Flux Distribution Resulting from a Fission Source Located at the Center of a 10-Meter-Diameter Sphere of Sodium,* ORNL-TM-3156 (Oct. 27, 1970).

123. *Neutron Phys. Div. Ann. Progr. Rept. May 31, 1970,* ORNL-4592, pp. 55–56.

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

125. C. L. Thompson, *A FORTRAN-360 Subroutine Package for Producing Printed Linear, Semi-Logarithmic or Logarithmic Graphs,* ORNL-TM-3079 (1970).

drawing tick marks to put them on all four sides of the graph rather than on only two sides. We have added a subroutine that inserts a label within the grid lines at a user-specified location and one which inserts a numerical value within a label in a user-specified format. We have added an option allowing curves to be drawn with dashed lines as well as with solid lines.

An optional version of this package which prints all labels and titles in a large size more suitable for direct reproduction of graphs for reports is also available.

A report is in preparation and should be published soon.

Sponsor: Neutron Physics Division — E. A. Straker

Neutron-Energy-Dependent Capture Gamma-Ray Yields in ^{238}U

R. S. Booth[126] J. E. White S. K. Penny K. J. Yost[127]

Model calculations were performed to generate energy-dependent capture gamma-ray yields for ^{238}U. These calculations were compared on an absolute basis with the integral data obtained with this experiment and with differential yield data obtained with another more sophisticated experiment. The calculated gamma-ray yields differ from the experimental yields by an amount comparable with the estimated experiment errors.

The technique of performing model calculations to obtain capture gamma-ray yields in which certain parameters are determined by experiment gives one an advantage over a purely experimental approach. This advantage is strictly economic in that once the calculational parameters are fixed, neutron and gamma-ray group boundaries may be arbitrarily changed and additional calculations performed at a small cost, whereas a new experiment for each new case would entail a prohibitive cost.

The calculational methods have been reported before,[128,129] and many aspects of the experiment at the Tower Shielding Facility at ORNL have been reported by Maerker and Muckenthaler.[130]

Sponsor: Neutron Physics Division — C. E. Clifford

Application of the Discrete Ordinates Radiation Transport Method to Multidimensional Deep-Penetration Shielding Problems[131]

F. R. Mynatt

The most widely used calculational techniques for radiation transport problems requiring more than one space dimension are the Monte Carlo and discrete ordinates methods. Until recently the use of these two methods has been severely hampered by the limited capabilities of existing computers and shortcomings of the methods themselves. However, increases in the size and speed of third-generation

---

126. Instrumentation and Controls Division.

127. Purdue University.

128. K. J. Yost, "A Method for the Calculation of Neutron-Capture Gamma-Ray Spectra," *Nucl. Sci. Eng.* **32**, 62 (1968).

129. K. J. Yost, P. H. Pitkanen, and C. Y. Fu, "The Calculation of Gamma-Ray Transition Probabilities in Odd-*A* Nuclei," *Nucl. Sci. Eng.* 39, 379 (1970).

130. R. E. Maerker and F. J. Muckenthaler, *Gamma-Ray Spectra Arising from Thermal Neutron Capture in Elements Found in Soils, Concretes, and Structural Materials,* ORNL-4382 (1969).

131. Summary of invited paper presented in the Special Session on Multidimensional Transport Methods at the American Nuclear Society Meeting, San Francisco, Calif., Nov. 30–Dec. 4, 1969.

computers, together with improvements that are systematically eliminating the difficulties inherent in the methods, have resulted in both the Monte Carlo and the discrete ordinates methods now being widely used in shield design. Much of the development work on the methods has been centered at Oak Ridge, and the work on the discrete ordinates method has been concentrated in what is now the Radiation Transport Methods Section of the Mathematics Division. This paper summarizes the most important advances that have been made in the application of the discrete ordinates method to shield penetration calculations. As is usually the case, most of these advances have resulted from attempts to apply the method to specific problems, and at Oak Ridge the problems have arisen because of the needs of the radiation shielding programs carried out in the Neutron Physics Division for the Defense Atomic Support Agency and the Space Electric Power Office, with emphasis on the former. Current shielding programs for the Liquid Metal Fast Breeder Reactor (LMFBR) and for the National Aeronautics and Space Administration are benefiting from the improved techniques.

The discrete ordinates method is basically a numerical technique, with the flux obtained by successive iterations for a number of difference cells that are finite in space, angle, and energy. To date the method is limited to one- and two-dimensional problems, but many problems with three-dimensional detail can be adequately approximated in two dimensions.

As developed for criticality calculations for small highly enriched systems, the original discrete ordinates method used a "diamond-difference" technique which assumes that the average flux in a cell is the mean of the fluxes at opposing cell faces. For shielding problems, this assumption led to serious difficulties since it becomes invalid in shield regions where steep flux gradients exist, and the resulting extrapolated cell-face flux may have a negative value. This in turn results in an oscillating flux solution that may give negative values throughout all regions of the problem. Decreasing the cell size to prevent this occurrence is impractical, and the alternative of using less accurate but physically plausible integration techniques for those cells in which the negative fluxes occur has been chosen. One such technique, called the step-function method, assumes that changes in the flux occur only at the cell boundaries.[132] With this assumption the calculation gives fluxes that are always positive and greater than the true answer. A combination of the diamond-difference and step-function techniques, called a mixed-mode method, is the procedure most frequently employed in current discrete ordinates calculations. Other techniques being developed at a number of laboratories are based on a "weighted" diamond-difference method.

Another major difficulty arose from the assumption of isotropic scattering in the original method since in shields the effect of anisotropic scattering is very important in determining the deep-penetration transport. Since excessive computer storage would be required to compute a transfer cross section for all possible combinations of directional change and energy group transfer, techniques were developed by several investigators to approximate the angular dependence of each group-to-group transfer by a Legendre series. It was found that low-order (P_2, P_3) scattered approximations were sufficiently accurate for predicting measured fast-neutron dose in water.[133] Later calculations for lead and polyethylene slabs,[132,134] in which Legendre expansions up to P_8 were used, showed that a P_3 expansion would be adequate for most problems.

---

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

133. F. R. Mynatt et al., "On the Application of Discrete Ordinates Transport Theory to Deep-Penetration Fast Neutron Dose Calculations in Water," *Trans. Am. Nucl. Soc.* **9**, 366 (1966).

134. F. R. Mynatt et al., "Angle-Dependent Spectra Emergent from Slab Shields – Comparison of Two-Dimensional Discrete Ordinates Calculations with Experiment," *Trans. Am. Nucl. Soc.* **11**, 195 (1968).

A third difficulty arose from the long computer times required by the inner iteration process due to scattering within an energy group. These have been reduced by supplementing the original Gaussian iteration techniques with two convergence acceleration schemes, one based on the Chebyshev polynomials and the other on a space-dependent driving function. Also, improved convergence criteria which concentrate on the zone of interest have been developed for two-dimensional calculations.[132] The effect of convergence acceleration in the inner iterations has been demonstrated in calculations of intermediate-energy neutrons in lead[132] and by special test problems.[135]

Another difficulty which can occur in two-dimensional problems with small sources is the "ray effect," in which the predicted flux reflects oscillations corresponding to the finite directions. For many problems the use of an analytic first-collision source removes the offending discontinuity.[132] As an example, flux anomalies due to the ray effect in problems having a point source in air over a ground interface were resolved by the use of an analytic first-collision source.[136]

A difficulty related to the ray effect was encountered in attempting to calculate the effect of radiation streaming in a large-radius annular slit in a missile silo cover.[137] This problem was solved by using a biased high-order quadrature which could accurately represent the streaming paths in the slit. Frequently the calculation of experiments using external detectors also requires biased quadratures.[132]

In the calculation of the flux across a long thin unit cell (length-to-diameter ratio of about 50) with an implicit white boundary condition, the traditional mesh sweep is not suitable for converging the boundary condition. However, an alternate mesh sweep which iterates to first converge the boundary condition for each polar angle level and axial interval is successful in obtaining convergence with ten inner iterations. This technique was used in preliminary calculations for the LMFBR program.[138]

Although much progress has been made in applying the discrete ordinates method to shield penetration problems, and versions of one- and two-dimensional codes (ANISN and DOT) are now being routinely used for real design problems, it is pointed out that most of the difficulties discussed above have only been reduced to acceptable levels and have not yet been completely resolved. Much of the current work is concerned with adopting and qualifying the existing techniques for the various systems analysis under the DASA and AEC projects.

Sponsor: Neutron Physics Division's Radiation Shielding Programs for the Space Electric Power Office, the Liquid Metal Fast Breeder Reactor, and the Defense Atomic Support Agency

A Study of the Overlap Conditions Required in Sequential Discrete Ordinates Transport Calculations for a 14-MeV Point Neutron Source in a 5000-m-Radius Cylinder of Air

J. V. Pace III F. R. Mynatt

The first step in many problems encountered in nuclear weapons radiation shielding studies is a calculation that follows the transport of the radiation produced in an atmospheric burst to distant locations

---

135. E. M. Gelbard and L. A. Hageman, "The Synthetic Method as Applied to the S_n Equations," *Nucl. Sci. Eng.* **37**, 288 (1969).

136. E. A. Straker and F. R. Mynatt, *Calculations of the Effect of the Air-Ground Interface on the Transport of Fission Neutrons through the Atmosphere,* ORNL-1819 (1968).

137. F. R. Mynatt, "The Use of Two-Dimensional Discrete Ordinates Calculations to Evaluate Streaming Effects in Annular Ducts," *Trans. Am. Nucl. Soc.* **12**, 370 (1969).

138. C. E. Clifford, F. R. Mynatt, and H. C. Claiborne, *LMFBR Shielding Development Program Interim Report: Preliminary Evaluation of Techniques for Predicting the Spectra of Neutrons Transmitted by Grid Plate Shields,* ORNL-TM-2896 (1970).

on the air-ground interface. Such a calculation requires at least two-dimensional geometry so that particle interactions in both the atmosphere and the ground can be considered. The discrete ordinates DOT code is two-dimensional and would be applicable to the problem in cylindrical (r,z) geometry except that the distances involved (on the order of 5000 m) exceed those that can be covered by a single DOT calculation owing to the tremendous amount of computer storage required. This difficulty can be overcome, however, if the problem is run as several overlapping segments, a procedure called bootstrapping. A prerequisite to such an application is a determination of the overlap conditions required to give the same results that would be obtained in a single run.

The overlap conditions have been studied by performing simpler calculations for an infinite cylindrical geometry with the one-dimensional discrete ordinates code ANISN for the case of a 14-MeV point neutron source in a 5000-m-radius cylinder of air. The ANISN calculations were carried out first as a single run with approximately 170 space intervals and then as a sequence of overlapping runs, each arbitrarily limited to 60 space intervals (approximately the maximum number used in DOT). With vacuum boundary conditions, an overlap of 300 m was required for agreement within 1%, but with a properly determined albedo boundary condition, an overlap of only 30 m yielded comparable accuracy.[139]

Sponsor: Neutron Physics Division's Weapons Radiation Shielding Program for the Defense Atomic Support Agency

Discrete Ordinates Transport Calculations of the Time-Dependent Spectra of Neutrons and Secondary Gamma Rays Emerging from a Polyethylene Slab in a Pulsed Neutron Beam

W. W. Engle, Jr. C. E. Burgart[140]

In designing shields against weapons radiation, it is often necessary to calculate the dose *rates* penetrating the shield, as opposed to total doses, and since these rates will vary with time the transport code used must give time-dependent results. One such code is the discrete ordinates code ANISN-T1, which has recently been developed by treating the time derivative in the Boltzmann equation in a manner analogous to the treatment of the space and angle derivatives in the one-dimensional code ANISN.

Preliminary calculations have been performed with the ANISN-T1 both to assist in the design of an Oak Ridge Electron Linear Accelerator (ORELA) experiment, which in turn will be used to check the code, and to compare the results with those obtained from time-dependent calculations with the Monte Carlo code MORSE. Insofar as was practical, the calculations simulated the experiment, which is to consist of time-dependent measurements of the energy spectra of neutrons and secondary gamma rays emerging from a 6-in.-thick polyethylene slab that intercepts a pulsed monodirectional neutron beam. The beam will originate 50 m from the slab and will be produced by electrons impinging on a tantalum target. The beam will be normally incident on the slab and will have pulse widths of 24 nsec.

The calculations yielded the time-dependent spectra of neutrons and secondary gamma rays that emerged from the source side of the slab following one pulse, that is, the surface-integrated spectra of neutrons and gamma rays "reflected" back out of the slab. The incident neutron spectrum was taken to be

139. This work will be reported more fully in ORNL-TM-3269 (CTC-40) (to be published).
140. Neutron Physics Division.

that calculated by Alsmiller et al.[141] – and subsequently verified at ORELA[142] – for neutrons produced by 150-MeV electrons impinging on 20 radiation lengths of tantalum.

ANISN-T1 is capable of solving the coupled neutron and secondary gamma-ray problem in a single pass on the computer with no tapes; for these calculations the GAM-II neutron cross sections in 21 groups and the MUG gamma cross sections in 18 groups were employed. A time-dependent boundary source was used to describe the time and energy dependence of the neutrons entering the slab, and fine time steps were used for both the neutrons and the secondary gamma rays. The neutron velocities corresponded to the mean energy of each group, except for the thermal group, which was assigned a velocity of 2200 m/sec.

Agreement between the ANISN-T1 results and those obtained with the MORSE code, which used the same sets of multigroup cross sections, is excellent for all times and energies. As a result, any disagreement between the calculations and the experiment will cast doubt on the accuracy of the cross sections, although possible errors in the calculational techniques or in the experiment will of course have to be thoroughly investigated.

Sponsor: Neutron Physics Division's Weapons Radiation Shielding Program for the Defense Atomic Support Agency

Calculations of Neutron Transport in Iron[143]

F. R. Mynatt M. L. Gritzner
E. A. Straker[140] R. Q. Wright
L. R. Williams

When radiation transport calculations revealed that the several cross-section sets for neutron interactions and secondary gamma-ray production in iron yielded widely varying results, considerable uncertainty was associated with the shielding calculations being performed for systems utilizing iron, in particular those for missile silo covers and liquid metal fast breeder reactors. The variations in the cross-section sets stemmed from the fact that iron cross sections contain a great deal of structure not always accounted for in the measurements on which the cross-section sets are based. This structure not only must be known in detail but also must be properly treated in the cross-section processing for the calculations so that important features of the cross sections are not obscured by averages over energy intervals. Specifically, the valleys (antiresonance regions) in the total neutron cross sections, which result in neutron streaming that dominates the penetration process, must be pinpointed and properly treated in the transport process, as well as the peaks (resonance regions) corresponding to neutron interactions that result in gamma-ray production.

In an attempt to resolve the discrepancies, a series of Monte Carlo and discrete ordinates calculations of the transport of neutrons in iron were performed to investigate the various cross-section sets and the manner in which they should be used. In one series of calculations the O6R Monte Carlo code and the ANISN discrete ordinates code were used to calculate the case of a point fission source in a 1.5-m-radius sphere of iron with four different cross-section sets, thereby showing the sensitivity of the results to various aspects of the individual sets. In the same series of calculations the effect of using the cross sections in

141. R. G. Alsmiller, Jr., T. A. Gabriel, and M. P. Guthrie, *Nucl. Sci. Eng.* **40**, 365–70 (1970).

142. C. E. Burgart, E. A. Straker, T. A. Love, and R. M. Freestone, Jr., *Nucl. Sci. Eng.* **42**, 421 (1970); see also ORNL-TM-3022 (June 1970).

143. Summary of invited paper presented at the American Nuclear Society Meeting, Los Angeles, Calif., June 29–July 2, 1970.

multigroup form was investigated. Most discrete ordinates codes and some Monte Carlo codes use multigroup cross sections, but since "point" cross sections are for much finer energy intervals they can include all the detail available in the cross-section set and thus, in principle, should give more accurate results than multigroup cross sections. It was found, however, that a properly weighted multigroup set with 296 energy groups selected to fit the important valleys of the total cross sections gave results that agreed with those obtained with point cross sections.

The 296-group structure was then used for additional discrete ordinates calculations performed with the two-dimensional code DOT for comparison with two integral experiments.[144] When a cross-section set compiled by Irving and Straker[145] was used, the integral flux transmitted through a 24-in.-thick iron cylinder (20 in. in diameter) agreed within 10 to 20% of that measured at the Tower Shielding Facility for neutron energies above 50 keV. Comparisons of the calculated angle-dependent neutron spectra for a hollow spherical iron assembly (maximum iron thickness of 13.41 in.) measured at Gulf General Atomic revealed a large disagreement which has since been partially attributed to an experimental error.

Sponsor: Neutron Physics Division's Weapons Radiation Shielding Program

Preliminary Evaluation of Techniques for Predicting the Spectra of Neutrons Transmitted through the Reactor Grid Plate Shield of the Fast Flux Test Facility

F. R. Mynatt M. L. Gritzner
V. R. Cain[140] C. L. Thompson
E. A. Straker[140] L. R. Williams

As Liquid Metal Fast Breeder Reactors (LMFBR's) are increasingly considered as large-scale power plants of the future, the need for developing a refined shielding technology that will avoid the usual conservatism and its associated costs becomes imperative. It appears that this technology will be based on transport solutions by the discrete ordinates and Monte Carlo methods. As a first step toward this goal, these two methods have been applied to help solve some of the shielding problems arising in the design and construction of the Fast Flux Test Facility (FFTF), a sodium-cooled fast breeder reactor being built by Westinghouse as a predecessor to the larger LMFBR's.

The first calculations for the FFTF have investigated the effectiveness of a steel-sodium matrix below the reactor core in protecting the FFTF bottom support plate from radiation damage. The configuration, consisting of stainless steel pins immersed in sodium, was extremely difficult to simulate not only because of its complicated geometry but also because of uncertainties in the neutron interaction cross sections needed as input. Nevertheless, the three-dimensional Monte Carlo MORSE code, the two-dimensional discrete ordinates DOT code, and the one-dimensional discrete ordinates ANISN code were all applied, with approximations designed to give upper and lower limits. The resulting neutron spectra were compared with spectra measured at the Tower Shielding Facility in an experiment which simulated the actual grid plate shield design.[146]

144. The experiments were performed by F. J. Muckenthaler and R. M. Freestone, Jr., of the Neutron Physics Division.

145. D. C. Irving and E. A. Straker, "Evaluation of the Total Cross Section of Iron," *Trans. Am. Nucl. Soc.* 12(2), 924 (1969).

146. The experiment was performed by F. J. Muckenthaler, J. L. Hull, E. A. Straker, R. G. Graf, T. A. Love, and R. M. Freestone, Jr., of the Neutron Physics Division.

The results of this investigation show that in their present stage of development the transport methods are inadequate for such a complicated system; however, both the calculations and the experiments indicated a possibly severe neutron "streaming" effect (neutrons streaming from the core to the grid plate) that prompted the FFTF designers to redesign the region below the core.[147]

Sponsor: Neutron Physics Division's Shielding Program for Fast Breeder Reactors

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

K. J. Yost[140] C. Y. Fu[148]
J. E. White W. E. Ford III

Some reactor shield materials exposed to high neutron fluxes are sources of secondary gamma-ray fluxes that pose as serious a shielding problem as the radiations produced within the reactor itself. Thus for a shield to be properly designed, the number and energy of the secondary gamma rays produced by neutron interactions in the materials of interest must be known as a *function* of the energy of the interacting neutrons. Because ^{181}Ta and natural tungsten are being considered as gamma-ray shields for reactors that will be used to provide auxiliary electrical power on spacecraft and because weight limitations will require that the shield be as close to the reactor as possible, it is particularly important that the secondary gamma-ray production in these elements be known. A calculational program now under way is attempting to provide neutron-energy-dependent capture gamma-ray yields for ^{181}Ta and the various isotopes in natural tungsten, and preliminary results for neutron energies up to approximately 1 MeV are available.

In performing these calculations existing experimental data were utilized in making a parametric fit to the thermal spectrum with the code DUCAL. Select DUCAL parameters which described the thermal spectrum were used to generate capture spectra for higher energy capture states. When available, the primary gamma-ray lines resulting from resonance capture were incorporated into the calculation. Most of the energy-level information was found in the Nuclear Data Tables; however, spins and parities for ^{182}Ta had to be supplemented by a nuclear model calculation.[149] Having coalesced the DUCAL spectra, the resultant yields were converted to a multigroup energy structure and combined with the appropriate neutron reaction cross sections to obtain secondary gamma-ray production cross sections. These cross sections were used in coupled neutron and gamma-ray transport calculations corresponding to measurements made at the Tower Shielding Facility. Comparisons of the measured and calculated results for the thermal and epithermal reactor beams show good agreement in shape.

Sponsor: Neutron Physics Division Shielding Program for the Space Electric Power Office (SEPO)

The Importance Distribution of Neutron Reactions Relative to Their Contribution to the Secondary Gamma-Ray Dose Transmitted by Tungsten and Laminated Lithium Hydride and Tungsten Shields

J. V. Pace III F. R. Mynatt

In designing SNAP reactor shields, which have stringent weight limitations, it is important to know in what regions of the shield the secondary gamma rays contributing to the exit dose are produced, what

147. This work is described in more detail in ORNL-TM-2896, *LMFBR Shielding Development Program Interim Report: Preliminary Evaluation of Techniques for Predicting the Spectra of Neutrons Transmitted by Grid Plate Shields,* by C. E. Clifford, F. R. Mynatt, and H. C. Claiborne (1970).

148. Consultant from the University of Tennessee.

149. C. Y. Fu and K. J. Yost, "A Unified Model of Odd-Odd Nuclei for Nuclear Data Generation and Analysis," *Nucl. Sci. Eng.* **41**, 193 (1970).

neutron interactions produce the gamma rays, and what the energies of the interacting neutrons are. Since tungsten and lithium hydride are frequently proposed as gamma-ray and neutron shields, respectively, for SNAP reactors, a study has been made of the importance distribution of neutron reactions relative to the secondary gamma-ray dose transmitted through these materials when they are used in specific shield configurations exposed to a SNAP reactor source. The configurations studied were comprised of tungsten alone, of tungsten preceded and followed by lithium hydride, and of tungsten with lithium hydride on either side. The source was assumed to have the neutron energy spectrum measured at the Tower Shielding Facility for a SNAP experimental reactor.

For each configuration studied both an adjoint calculation and a forward calculation were performed with the one-dimensional discrete ordinates code ANISN. In the adjoint calculation a given exit gamma-ray dose response was assumed, and the probability that a gamma ray of a given energy originating at a given position in the shield would contribute to that dose was calculated. In the forward calculation the penetration of neutrons from the reactor to positions throughout the shield was determined. The results from these two calculations, convoluted with selected gamma-ray production data, reveal the origin of the exit secondary gamma-ray dose as it is distributed in space and neutron energy.

The results from this study will be published in a forthcoming report.[150]

Sponsor: Neutron Physics Division's Radiation Shielding Program for the Space Electric Power Office (SEPO)

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

W. E. Ford III

Coupled calculations of the transport of neutrons and the production and transport of secondary gamma rays are facilitated by a FORTRAN IV program called POPOP4, which converts spectra of secondary gamma rays produced by neutron reactions to multigroup production cross sections.[151] A library of secondary gamma-ray data which can be used by POPOP4 has been assembled for a number of nuclides of interest in radiation shielding studies and is available on a BCD-formatted magnetic tape from the Radiation Shielding Information Center. The initial and first update compilation contains a total of 223 data sets, each set consisting either of intensities of the secondary gamma rays resulting from neutron-nucleus interactions (referred to as "yields") or of secondary gamma-ray production cross sections for neutron-nucleus interactions (referred to as "x-sects."). A data set is identified with a six-digit number: the first and second digits identify the atomic number of the target nucleus, the third digit the mass number of the target nucleus, the fourth digit the type of neutron reaction, and the fifth and sixth digits the literature source of the data.

Before the data on the BCD-formatted tape can be used in POPOP4, it must be transferred to a binary tape, for which a retrieval program identified as the POPOP4 Library Tape Maker is available.[152] This program can also update a binary library tape, make or update a BCD-formatted library tape, and list or punch selected data sets on a library tape.

---

150. J. V. Pace III and F. R. Mynatt, *The Importance Distribution of Neutron Reactions Relative to Their Contribution to the Secondary Gamma-Ray Dose Transmitted by Tungsten and Laminated Lithium Hydride and Tungsten Shields,* ORNL-TM-3270 (CTC-41) (to be published).

151. 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).

152. W. E. Ford III and D. H. Wallace, *The Use and 'Testing' of Al, Fe, Ni, Cu, and Pb Secondary Gamma-Ray Production Data Sets From the POPOP4 Library,* CTC-20 (1970).

If the data set read by POPOP4 is an x-sect. set, POPOP4 converts it from the form in which it is received to an energy group structure required for the calculation in which it is to be used. If the data set is a yield set, POPOP4 converts the yields to a multigroup structure and then multiplies the multigroup intensities by input multigroup neutron reaction cross sections to obtain the multigroup secondary gamma-ray production cross sections.

The POPOP4 library data set titles and literature sources in the initial compilation have been published elsewhere.[153]

Sponsor: Neutron Physics Division's Radiation Shielding Programs for Defense Atomic Support Agency and Space Electric Power Office

The Use and Testing of Selected Secondary Gamma-Ray Production Data Sets from the POPOP4 Library

W. E. Ford III D. H. Wallace[154]

The data sets included in the POPOP4 library for the production of secondary gamma rays by neutron capture and inelastic-scattering reactions in aluminum, iron, nickel, copper, and lead have been evaluated by comparing secondary gamma-ray pulse-height spectra calculated with the various data sets with measured pulse-height spectra.[153] In each calculation the data set to be tested was converted to secondary gamma-ray production cross sections with the POPOP4 code.[151] Another program, the Sample Simple Coupling Code, then combined the production cross sections with P_N neutron and gamma-ray cross sections to provide a P_N coupled cross-section set for use in a transport calculation with the discrete ordinates code ANISN.[152] Finally, the gamma-ray angular flux from the ANISN calculation was converted to a pulse-height spectrum with a FORTRAN IV code called LINFOLD, which also compared the calculated and measured pulse-height spectra.[152]

The measured spectra were obtained in a series of experiments performed at the Tower Shielding Facility.[155,156] Thin slabs of the materials being investigated were exposed to neutron beams from the Tower Shielding Reactor II, with cadmium and boron filters introduced in the beam in different runs to alter the spectrum of neutrons impinging on the samples. A NaI(Tl) detector was used to measure the secondary gamma-ray spectra.

Most of the data sets evaluated were for secondary gamma rays produced by neutron captures. Six such sets were tested for aluminum, four sets each for iron and nickel, three for copper, and two for lead. One set of inelastic-scattering gamma-ray data was tested for each of the elements except for copper, for which no data were available.

Graphical comparisons of some of the calculated and experimental spectra have been published elsewhere.[152] Since at present there is a dearth of secondary gamma-ray data, especially for neutron energies above thermal, the general lack of agreement shown by the lead and copper comparisons was

---

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

154. Applied Science Department, Computing Technology Center, Union Carbide Corporation, Oak Ridge, Tenn.

155. R. E. Maerker and F. J. Muckenthaler, *Gamma-Ray Spectra Arising from Thermal-Neutron Capture in Elements Found in Soils, Concretes, and Structural Materials,* ORNL-4382 (1969).

156. R. E. Maerker and F. J. Muckenthaler, *Gamma-Ray Spectra Arising from Fast-Neutron Interactions in Elements Found in Soils, Concretes, and Structural Materials,* ORNL-4475 (1970).

expected. As the first step in an iterative process, these comparisons show which data sets yield the best results and the elements for which additional data are most needed.

Sponsor: Neutron Physics Division's Radiation Shielding Program for the Defense Atomic Support Agency and Space Electric Power Office

Application of the Discrete Ordinates Method to Electron Transport

D. E. Bartine R. G. Alsmiller, Jr.[140]
F. R. Mynatt W. W. Engle, Jr.
J. Barish

The transport of low-energy (of the order of a few MeV) electrons through matter is important in the shielding of manned space vehicles that orbit through the Van Allen electron belt. A code that treats this transport by means of Monte Carlo methods is available,[157] but because of the poor statistical accuracy which can be obtained, a nonstatistical method of calculation is needed. To fill this need, the method of discrete ordinates has been adapted to the transport of low-energy electrons.

In principle, the discrete ordinates code ANISN may be used to transport electrons by the simple expedient of introducing into the code differential cross sections for electron-nucleus elastic collisions, electron-nucleus bremsstrahlung-producing collisions, and electron-electron collisions. In practice, however, these cross sections are quite different from those which 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 successfully to transport electrons. In the Monte Carlo treatment of electron transport, the individual electronic collisions are not considered, but rather the theories of multiple Coulomb scattering and continuous slowing down are used to group together a large number of collisions.[157]

In applying ANISN to electron transport calculations, the individual electronic collisions are treated except that those electron-electron collisions which result in very small energy transfers (of the order of the average ionization potential of the atom) are treated using the continuous slowing-down theory. The differential cross sections for electron-nucleus elastic collisions and electron-nucleus bremsstrahlung production are taken from standard sources.[158,159] The differential cross section given by Moller[160] is used to describe electron-electron collisions which result in large energy transfers, and the usual stopping-power formula[161] with the energy loss due to large energy transfers subtracted out is used to treat electron-electron collisions which result in small energy transfers.

The transmitted electron spectrum calculated with ANISN for the case of 1-MeV electrons normally incident on a 0.11-g/cm^2-thick aluminum slab are in excellent agreement with an experimental spectrum[162] for energies below 0.85 MeV and are in approximate agreement for higher energies. The applicability of the method to thicker shields and higher energies remains to be tested.

Sponsor: Neutron Physics Division's Radiation Shielding Program for the National Aeronautics and Space Administration

---

157. M. J. Berger and S. M. Seltzer, *ETRAN, Monte Carlo Code System for Electron and Photon Transport through Extended Media,* NBS-9836, NBS-9837 (1968).
158. C. D. Zerby and F. S. Keller, *Nucl. Sci. Eng.* 27, 190 (1967).
159. H. W. Koch and J. W. Motz, *Rev. Mod. Phys.* **31**, 920 (1959).
160. C. Moller, *Ann. Physik* **14**, 531 (1932).
161. M. J. Berger and S. M. Seltzer, *Tables of Energy Losses and Ranges of Electrons and Positrons,* NASA-SP-3012 (1964).
162. D. H. Rester and W. E. Dance, *Investigation of Electron Interactions with Matter,* L.T.V. Report No. 0-71000/6R-18 (1966).

Discrete Ordinates Calculations of the Lateral Spread of High-Energy Neutron Beams (≤400 MeV) and Earthshine

R. G. Alsmiller, Jr.[140] M. L. Gritzner
F. R. Mynatt J. V. Pace
J. Barish

In the design of high-energy accelerators, it is often necessary to consider the transport of high-energy nucleons through very thick shields. A Monte Carlo transport code has been used for such studies for several years, but because of statistical considerations its usefulness for problems involving very deep penetrations is limited. The applicability of the one-dimensional discrete ordinates code ANISN to calculations of the penetration of neutrons with energies considerably higher (≤400 MeV) than those encountered in reactor shielding calculations was studied for the cases of broad incident neutron beams with encouraging results.[163,164]

Subsequent studies have been carried out with the two-dimensional code DOT for the cases of zero-width beams of 100- and 400-MeV neutrons normally incident along the axis of a cylindrical shield of silicon dioxide with 5% water by weight. The shield radius and thickness were assumed to be 500 and 1500 g/cm^2, respectively. The results include the omnidirectional neutron flux per unit energy as a function of depth and radius in the shield and the neutron and photon dose equivalents as a function of depth and radius in the shield.

DOT calculations have also been performed to study the diffusion of neutrons and secondary gamma rays through the ground below the shielded target area of an accelerator to an outside area (an effect referred to as "earthshine"). The results, together with those for the cylindrical shields, are published elsewhere.[165]

Although there are no experimental data with which to compare these calculations, the method of discrete ordinates does seem to be a satisfactory method for two-dimensional problems involving high-energy neutrons.

Sponsor: Neutron Physics Division's Radiation Shielding Program for High-Energy Accelerators

Nuclear Safety Evaluation of Various Designs for the LMFBR Fuel Reprocessing Dissolver

J. R. Knight W. R. Cobb[166]

The ANISN[167] and KENO[168] codes were used to evaluate the effects of various parameters on the nuclear safety of LMFBR dissolver designs. Three basic designs – a vertical cylinder, a slab, and a horizontal cylinder – were studied. The parameters were varied and included fuel concentrations, external concrete reflection, and stainless steel content of the fuel. Other factors considered were boron content, nitric acid concentrations, and variations in thickness of some of the stainless steel vessel walls. These studies have

163. R. G. Alsmiller, Jr., et al., *Nucl. Sci. Eng.* **36**, 251 (1969).
164. R. G. Alsmiller, Jr., et al., *Nucl. Instr. Methods* **72**, 213 (1969).
165. R. G. Alsmiller, Jr., et al., *The Lateral Spread of High-Energy (≤400 MeV) Neutron Beams and Earthshine,* ORNL-TM-3025 (1970).
166. Reactor Division.
167. W. W. Engle, *A User's Manual For ANISN,* K-1693 (Mar. 30, 1967).
168. G. E. Whitesides and N. F. Cross, *KENO – a Multigroup Monte Carlo Criticality Program,* CTC-5 (Sept. 10, 1969).

indicated that several possible systems can be operated in a safe nuclear manner. Other minor changes in the program have caused the core requirements to be reduced to 300 K bytes.

Sponsor: Neutron Physics Division

Completion of I4C, a General Code for Various Analyses of Intranuclear Cascade Calculations

O. W. Hermann M. P. Guthrie[140] G. W. Perry[169]

The requested version of I4C[170] was completed and used in a series of production cases. This IBM/360 code includes, with several extensions, four analysis codes[171] which had a substantial fraction written in FAP for the IBM/7090. I4C contains about 4500 FORTRAN statements and requires a region size of 1040 K. This code is being included in the group of codes[172] for analyses and calculations of intranuclear cascades,[173] which will be available soon for external distribution.

The analyses are performed on results of computed reactions of protons, neutrons, or π^+ or π^- mesons incident on a target from ^{4}He to ^{239}Pu. The printed results of I4C include angular, energy, and momentum distributions of residual nuclei, cascade-particle energy spectra for various angular intervals, cross sections for various multiplicities of emitted particles, differential cross sections of cascade particles, energy spectra of evaporated particles, cross sections of nuclei remaining after evaporation, distribution of angular momentum in the nucleus after the cascade, and other results of interest. The calculations have been extended to incident particle energies as high as 3500 MeV.

Sponsor: Neutron Physics Division H. W. Bertini

Revisions in the MUG Program for Producing Photon Transport Cross Sections

J. R. Knight D. K. Trubey[174]

The MUG program[175] has been revised to include two changes. The first change is a modified way of computing the energy-dependent absorption cross sections. These cross sections are now obtained from the integral over the group limits of the product of the pointwise energy, times the pointwise Compton absorption cross section, plus similar terms for the photoelectric and pair-production cross sections. This change yielded significant improvements in the absorption cross-section values.

The second change is a revision which allows data for photoelectric and pair-production cross sections to be read directly from an ENDF/B file 23 data tape, in addition to the other data options previously available. Other minor changes in the program have caused the core requirements to be reduced to 300 K bytes.

Sponsor: Neutron Physics Division

---

169. Formerly with Mathematics Division.
170. An acronym for Intranuclear Cascade Calculation Combined Analysis Codes.
171. H. W. Bertini, H. E. Francis, and M. P. Guthrie, *Instructions for the Operation of Codes Associated with the Low-Energy Intranuclear Cascade Calculation,* ORNL-3844 (March 1966).
172. H. W. Bertini, M. P. Guthrie, and O. W. Hermann, *Instructions for the Operation of Codes Associated with MECC3, a Preliminary Version of an Intranuclear Cascade Calculation for Nuclear Reactions,* ORNL-4564 (to be published).
173. H. W. Bertini, *Monte Carlo Calculations on Intranuclear Cascades,* ORNL-3383 (April 1963).
174. Formerly with the Neutron Physics Division.
175. J. R. Knight and F. R. Mynatt, *MUG – a Program for Generating Multigroup Photon Cross Sections,* CTC-17 (Jan. 20, 1970).

Calculated Activation of Copper and Iron by 3-GeV Protons

J. Barish T. W. Armstrong[140]

Using NMTC,[176] an estimate of the residual photon dose rate and the neutron leakage induced in an accelerator magnet by a beam of 3-GeV protons is computed.[177] The magnet was approximated as an infinite cylinder of copper surrounded by iron. Monte Carlo methods were used to calculate the nucleon-meson cascade, the residual nuclei production, and the photon transport.

Sponsor: Neutron Physics Division, Activation of an Accelerator Magnet Project T. W. Armstrong

Calculation of the Long-Lived Induced Activity in the Soil around High-Energy Accelerator Target Areas – II

J. Barish R. G. Alsmiller, Jr.[140] T. A. Gabriel[140]

Nucleon-meson cascade calculations were carried out and estimates of the induced activity in the soil surrounding high-energy accelerator target areas were obtained. Computation was performed for 200- and 500-GeV protons incident on a lead target and for 500-GeV protons incident on a beryllium target.[178]

Sponsor: Neutron Physics Division, Design of Neutrino Channel Project for the National Accelerator Laboratory R. G. Alsmiller, Jr.

Eyges-Dublin-Shape

J. Barish R. G. Alsmiller, Jr.[140]

In the shielding of high-energy accelerators, it is often necessary to consider the transport of high-energy muons through matter. Based on the transport theory of Eyges,[179] three codes – Eyges, Dublin, and Shape – were written to carry out such computations. Calculations have been performed for both Stanford[180,181] and the National Accelerator Laboratory.[182,183] Work on the codes is continuing in an effort to make them more applicable to a wider range of problems.

Sponsor: Neutron Physics Division, Muon Transport Project R. G. Alsmiller, Jr.

---

176. W. A. Coleman and T. W. Armstrong, *The Nucleon-Meson Transport Code, NMTC,* ORNL-4606 (October 1970).

177. T. W. Armstrong and J. Barish, *Calculated Activation of Copper and Iron by 3-GeV Protons, Neutron Phys. Div. Ann. Progr. Rept. May 31, 1970,* ORNL-4592; ORNL-TM-2902; *Nucl. Sci. Eng.* **41**, 443–61 (1970).

178. T. A. Gabriel, R. G. Alsmiller, Jr., and J. Barish, *Calculation of the Long-Lived Induced Activity in the Soil around High-Energy Accelerator Target Areas – II,* ORNL-4599 (October 1970).

179. L. Eyges, *Phys. Rev.* 74, 1534 (1948).

180. R. G. Alsmiller, Jr., and J. Barish, *High-Energy (<18 GeV) Muon Transport Calculations and Comparison with Experiments,* ORNL-TM-2439 (1968); *Nucl. Instr. Methods* **71** (1969).

181. R. G. Alsmiller, Jr., and J. Barish, *High-Energy (<18 GeV) Muon Transport Calculations and Comparison with Experiments – II,* ORNL-TM-2669 (1969); *Neutron Phys. Div. Ann. Progr. Rept. May 31, 1970,* ORNL-4592.

182. R. G. Alsmiller, Jr., M. Leimdorfer, and J. Barish, *High-Energy Muon Transport and the Muon Backstop for a 200 GeV Proton Accelerator,* ORNL-4322 (1968).

183. R. G. Alsmiller, Jr., and J. Barish, *High-Energy Muon Transport and the Muon Backstop for a Multi-GeV Proton Accelerator,* ORNL-4386 (1969).

Calculations Evaluating Several Methods for Reducing the Residual Photon Dose Rate around High-Energy Proton Accelerators

J. Barish T. W. Armstrong[140]

Using the codes NMTC,[176] OGRE,[184] and O5R,[185] calculations were carried out to evaluate several methods for reducing the residual photon dose rate inside an accelerator tunnel due to the activation of the concrete tunnel walls by thermal neutrons from a 3-GeV proton beam located on the axis of an iron cylinder.[186]

Sponsor: Neutron Physics Division, Reduction of the Residual Photon Dose Rate around High-Energy Proton Accelerators Project — T. W. Armstrong

PICTURE: An Aid in Debugging GEOM Input Data

D. C. Irving[187] G. W. Morrison

A computer program, PICTURE,[188] was written to aid in preparing correct input data for the O5R[189] general geometry routine GEOM. PICTURE provides a printed view of the arbitrary two-dimensional slices through the geometry. By inspection of these "pictures," one may determine if the geometry specified by the input cards is indeed the desired geometry.

An example of a complex geometry is given in Fig. 7. A two-dimensional slice across the geometry is shown in Fig. 8. This printed output shows the presence of all the quadric surfaces.

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 Format

R. Q. Wright S. N. Cramer D. C. Irving[187]

A computer program, UKE, has been written to translate neutron cross sections on computer tape from the United Kingdom Atomic Energy Authority Nuclear Data Library[190,191] to the Evaluated Nuclear Data File ENDF/B.[192] The code will translate UK-library smooth cross-section data, as well as secondary angular and energy distributions, to the ENDF/B format. No resonance parameters, thermal-scattering data, or photon data are considered, however. The secondary angular distributions are translated as differential scattering probabilities only, and no Legendre expansion coefficients are given.

---

184. D. K. Trubey, S. K. Penny, and M. B. Emmett, *OGRE-P2, a Monte Carlo Program for Computing Gamma-Ray Leakage from Laminated Slabs with a Distributed Source,* ORNL-TM-237 (August 1962).

185. D. C. Irving et al., *O5R, a General Purpose Monte Carlo Transport Code,* ORNL-3622 (February 1965).

186. T. W. Armstrong and J. Barish, "Calculations Evaluating Several Methods for Reducing the Residual Photon Dose Rate around High-Energy Proton Accelerators," *Neutron Phys. Div. Ann. Progr. Rept. May 31, 1970,* ORNL-4592; ORNL-TM-2768 (November 1969).

187. Present address: Savannah River Laboratory, Aiken, S.C.

188. D. C. Irving and G. W. Morrison, *PICTURE – an Aid in Debugging GEOM Input Data,* ORNL-TM-2892 (1970).

189. D. C. Irving, R. M. Freestone, and F. B. K. Kam, *O5R, a General Purpose Monte Carlo Neutron Transport Code,* ORNL-3622 (1965).

190. K. Parker, *The Aldermaston Nuclear Data Library as at May 1963,* AWRE-0-70/63 (May 1963).

191. K. Parker, *The Format and Conventions of the U.K.A.E.A. Nuclear Data Library,* unpublished (June 1965).

192. 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.

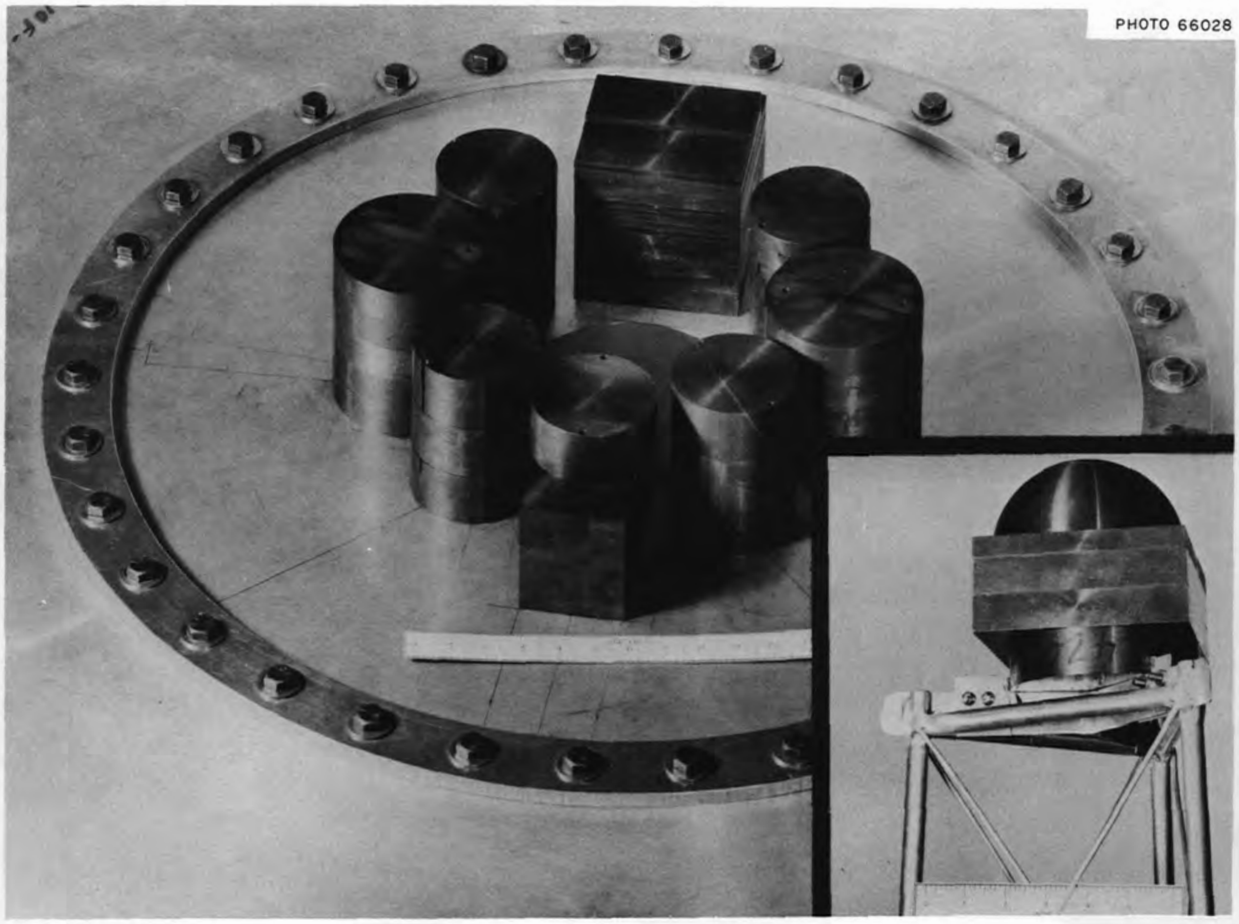

Fig. 7. Critical 93.2% ^{235}U enriched uranium metal assembly with eight-unit upper section and an irregularly shaped centerpiece (inset). The unit at the top of the photograph is an approximate parallelepiped whose base is 5 by 5 in. and whose height varies in three steps (5.14, 5.27, and 4.39 in., front to back); the opposite unit is a parallelepiped with a 3- by 5-in. base and a 3.51-in. height topped by a 3.60-in.-diam by 1.70 in. cylinder; the four small cylinders are 3.59 in. in diameter and 5.11 in. high; and the two large cylinders are 4.5 in. in diameter and 5.3 in. high. The centerpiece, which penetrated the hole in the support diaphragm, consists of a 4.5-in.-diam by 1.11 in. cylinder topped by a parallelepiped with a 5.00- by 5.00-in. base and a 2.25-in. height and by a hemisphere with a 2.39-in. radius.

UKE is documented in ORNL-TM-2880, where general information is presented concerning the format of the two libraries, along with a detailed description of the translation from the UK secondary energy distribution laws to those of ENDF/B. Programming details and a user's guide are also presented.

Sponsor: Neutron Physics Division D. K. Trubey

Retrieval of ENDF/B Elastic and Inelastic Scattering Cross Sections

R. Q. Wright

A program has been written to retrieve "smooth" neutron elastic and inelastic scattering cross sections and angular distributions from ENDF/B[192] tapes. Input to the program consists of incident neutron energies and incident energy spread. Interpolation is used to obtain Legendre coefficients (for

ORNL-DWG 71-2038

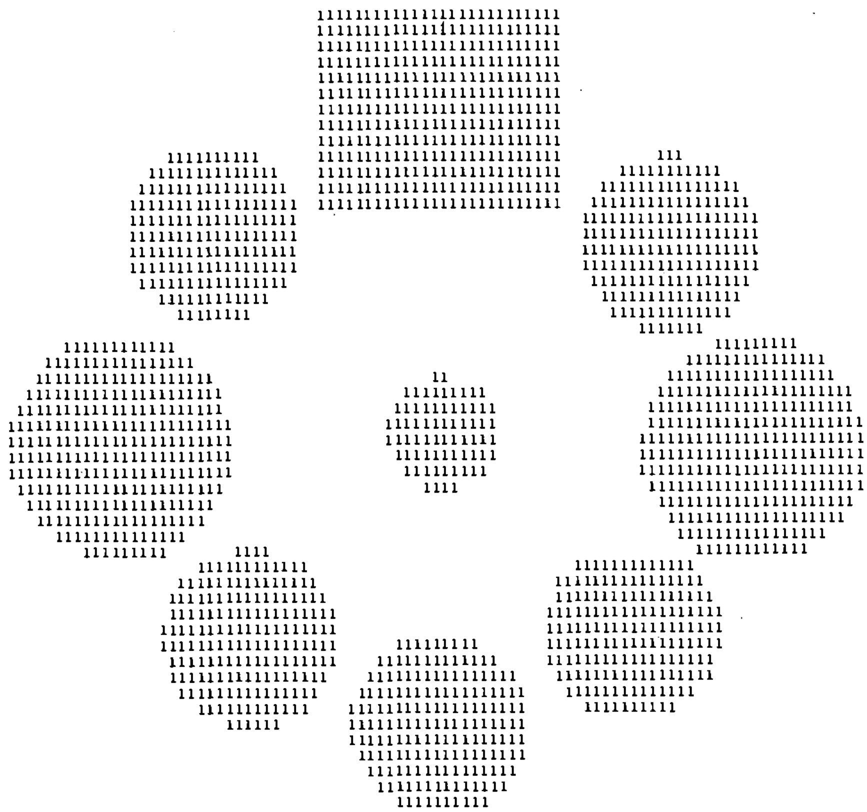

Fig. 8. PICTURE output of a horizontal slice through the assembly shown in Fig. 7.

center-of-mass angular distributions) in units of millibarns per steradian from the ENDF/B data. Output from the program consists of "smooth" elastic and inelastic cross sections as given on the ENDF/B tape plus the Legendre coefficients at each incident neutron energy. Results have been obtained for carbon, iron, silicon, sodium, magnesium, aluminum, and vanadium. Perey and Kinney have used the results to compare their experimental data with ENDF/B.

Sponsor: Neutron Physics

F. G. Perey
W. E. Kinney

PLOTFB, a Plotting Program for ENDF/B Data

R. Q. Wright

The PLOTFB[193] program was received from the National Neutron Cross Section Center, Brookhaven National Laboratory, Upton, New York. The program is designed to interpret BCD or binary data in the ENDF/B[192] standard (rather than alternate) format and to present the interpreted data in the form of

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

listings and/or plots. Data may be requested by material number and/or ZA number and file number. The Brookhaven version was operational on the CDC-6600 computer and utilized the CALCOMP-835 plotter. Extensive modifications were required to convert the program to the IBM-360/75-91. The plotting routines were rewritten to utilize the ORNL cathode ray tube plotter (CRT). The basic routines for the CRT plotter have been described in ORCID Memo 29/360, May 10, 1968. The BPLOT[194] package (a generalized FORTRAN plot package for the IBM 360) was also incorporated, and the BNL plotting routines were removed. The program is designed to eventually handle all files in the ENDF/B format:

1–7	Neutron interaction data
12–16	Photon production data
23–27	Photon interaction data

At the present time, the processing routines are only available for files 1–5, 7, and 23 (file 5 can be listed but not plotted). The remaining routines are still in the process of being developed and debugged. Also, work is presently under way to implement the photon production files (12–16), and the routines are now partially operational.

Sponsor: Neutron Physics — D. K. Trubey

Updating of the DLC-2 Cross Section Library

R. Q. Wright

Fifty-two materials in the ENDF/B[192] Version II library have now been processed by SUPERTOG,[195] and the DLC-2 99-group neutron cross-section library[196] has been updated.

DLC-2 was generated from nuclear data in either point-by-point or parametric representation as specified by ENDF/B. These data were averaged over each specified group width. The explicit assumption was made that the flux (weighting function) per unit lethargy was constant. When resonance data were available, resolved and unresolved resonance contributions were calculated and used. DLC-2 consists of fine-group constants such as one-dimensional reaction arrays (absorption, fission, etc.), P_n elastic scattering matrices, and inelastic and $(n,2n)$ scattering matrices which were generated, combined, and written on tape as card images in the ANISN[197] format.

DLC-2 represents a P_8 approximation to elastic scattering angular distributions. The data have a 100-group structure with energy-group boundaries identical to those in the GAM-II[198] library, with a group 1 upper-boundary energy of 14.92 MeV and a group 99 lower energy of 0.414 eV. The group-to-group transfer matrices reflect only downscatter in energy, and group 100 serves as a "sink" group, itself having no data to describe absorption, fission, and scattering.

The nuclides in DLC-2 are those which have been released as Category I ENDF/B by the National Neutron Cross Section Center, Brookhaven National Laboratory.

Sponsor: Neutron Physics Division — R. W. Roussin

---

194. R. Q. Wright, *BPLOT, a Generalized Fortran Plot Package for the IBM 360,* TIDBITS, Vol. 4, No. 6, June 1968.

195. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, Jr., *SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B,* ORNL-TM-2679 (September 1969).

196. RSIC Data Library Collection, DLC-2: 99-Group Neutron Cross Section Data Based on ENDF/B, Miscellaneous Informal Notes, ORNL-CF-5-20.

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

198. G. D. Joanou and J. S. Dudek, *GAM-II: A B_3 Code for the Calculation of Fast-Neutron Spectra and Associated Multi-Group Constants,* GA-4265 (1963).

High-Energy Cascade Code

Arline H. Culkowski, A. F. Joseph
H. Bertini[140], T. C. Tucker
N. B. Gove, M. Feliciano, Jr.
Kay C. Chandler

Several features have been added to HECCI[199] to account for scattering absorption, charge exchange, and single and double pion production. Cross-section data have been included in the form of polynomial fits. Particle production probabilities have been included as tables and used with interpolation procedures. The sampling techniques conserve energy and nuclear matter.

Some of the polynomial fits were done with ORDEAL; some were done with the interactive graphics routines of C. E. Hammons.

Sponsor: Neutron Physics Division

Monte Carlo Calculations of High-Energy Nucleon-Meson Cascades

Kay C. Chandler, T. W. Armstrong[140]

Nucleon-meson transport calculations that utilize Monte Carlo techniques in conjunction with the intranuclear-cascade-evaporation model for treating nonelastic collisions have been carried out for a variety of problems (e.g., ref. 200). This method of calculation was previously restricted to particle energies $\lesssim 3$ GeV because of limitations imposed by the particular intranuclear-cascade model used.[201] To enable transport calculations to be performed for high-energy sources, the calculational model has been extended to higher energies by using an extrapolation model[202] to obtain the description of products from nonelastic collisions $\gtrsim 3$ GeV.

To test the validity of this new high-energy nucleon-meson transport code, the cascade induced in a target composed of alternating iron slabs and air gaps by 19.2-GeV/*c* protons and by 30.0-GeV/*c* protons has been calculated and compared with experimental data[203,204] for the same configurations. Good agreement between the calculations and experiments has been obtained. The new code has been used to compute the induced activity and flux spectra in the moon due to galactic and solar cosmic ray bombardment. The results of the calculations have been used to estimate the cosmic ray exposure age of various Apollo samples and to aid in the interpretation of some of the Apollo measurements.[205]

---

199. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 33.

200. T. W. Armstrong and K. C. Chandler, "Calculation of the Radionuclide Production in Tissue by Solar-Flare Bombardment," *Neutron Phys. Div. Ann. Progr. Rept. May 31, 1970,* ORNL-4592, p. 89.

201. Hugo W. Bertini, *Phys. Rev.* **188**, 1711 (1969).

202. T. A. Gabriel, R. G. Alsmiller, Jr., and M. P. Guthrie, *An Extrapolation Method for Predicting Nucleon and Pion Differential Production Cross Sections for High-Energy (>3 GeV) Nucleon-Nucleus Collisions,* ORNL-4542 (1970).

203. A. Citron, L. Hoffman, C. Passow, W. R. Nelson, and M. Whitehead, *Nucl. Instr. Methods* **32**, 48 (1965).

204. A. VanGinneken, National Accelerator Laboratory, P.O. Box 500, Batavia, Ill.; private communication.

205. T. W. Armstrong and R. G. Alsmiller, Jr., "Calculation of Cosmogenic Radionuclides in the Moon and Comparisons with Apollo Measurements," paper submitted to the Second Annual Lunar Science Conference to be held in Houston, Texas, Jan. 11, 1971.

This method of calculation has also been applied to determine the depth dependence of the absorbed dose and dose equivalent in tissue induced by galactic proton bombardment.[206]

Sponsor: Neutron Physics Division

NUCLEAR DATA PROJECT

LEVEL Scheme Plotting Program

T. J. Tyrrell W. B. Ewbank[207]

We have written a program for the IBM/360 to prepare nuclear level scheme charts with either the pen-and-ink Calcomp plotters or the cathode ray tube plotter. Each drawing is made up of one or more "ladder" diagrams (see Fig. 9) with gamma-ray transition lines. The input for this program consists of a few cards giving information about the arrangement of the drawing, followed by a card for each level and a card for each transition. The diagram in Fig. 9 required 73 input cards.

Sponsor: Nuclear Data Project D. Horen

Atomic Mass Adjustment

N. B. Gove Ruth B. Hofstra
T. D. Calton Judy B. Ritts[208]
A. H. Wapstra[209]

We have written a computer program to perform a least-squares fit to all available nuclear reaction Q values and mass doublets, using the atomic masses as unknowns. This leads to a system of about 5000 equations in 1720 unknowns. A set of subroutines was written to find and remove singly determined masses from the system. This leads to about 4000 equations in about 700 unknowns, which decomposes into two systems of about 300 and 400 unknowns. The fitting procedure involves inverting a 300×300 normal matrix and a 400×400 normal matrix. The Choleski inversion method was used in double (REAL*8) precision. From the resulting atomic mass values, new reaction Q values and mass doublets were calculated. We wrote programs to make Calcomp plots of certain Q values and separation energies so as to demonstrate systematic trends.

A portion of one of the mass tables is shown in Fig. 10; one of the Calcomp plots is shown in Fig. 11.

This work was supported in part by the Nuclear Data Project and by the Instituut voor Kernphysisch Onderzoek.

Sponsor: Nuclear Data Project

206. T. W. Armstrong, R. G. Alsmiller, Jr., and K. C. Chandler, "Monte Carlo Calculations of High-Energy Nucleon-Meson Cascades and Applications to Galactic Cosmic-Ray Transport," paper to be presented at the National Symposium on Natural and Man-Made Radiation in Space to be held in Las Vegas, March 2–5, 1971.

207. Nuclear Data Project.

208. Now with U.S. Steel, Pittsburgh.

209. Instituut voor Kernphysisch Onderzoek, Amsterdam, Netherlands.

ORNL-DWG 71-2039

A=207 Drawing 3, Part 1

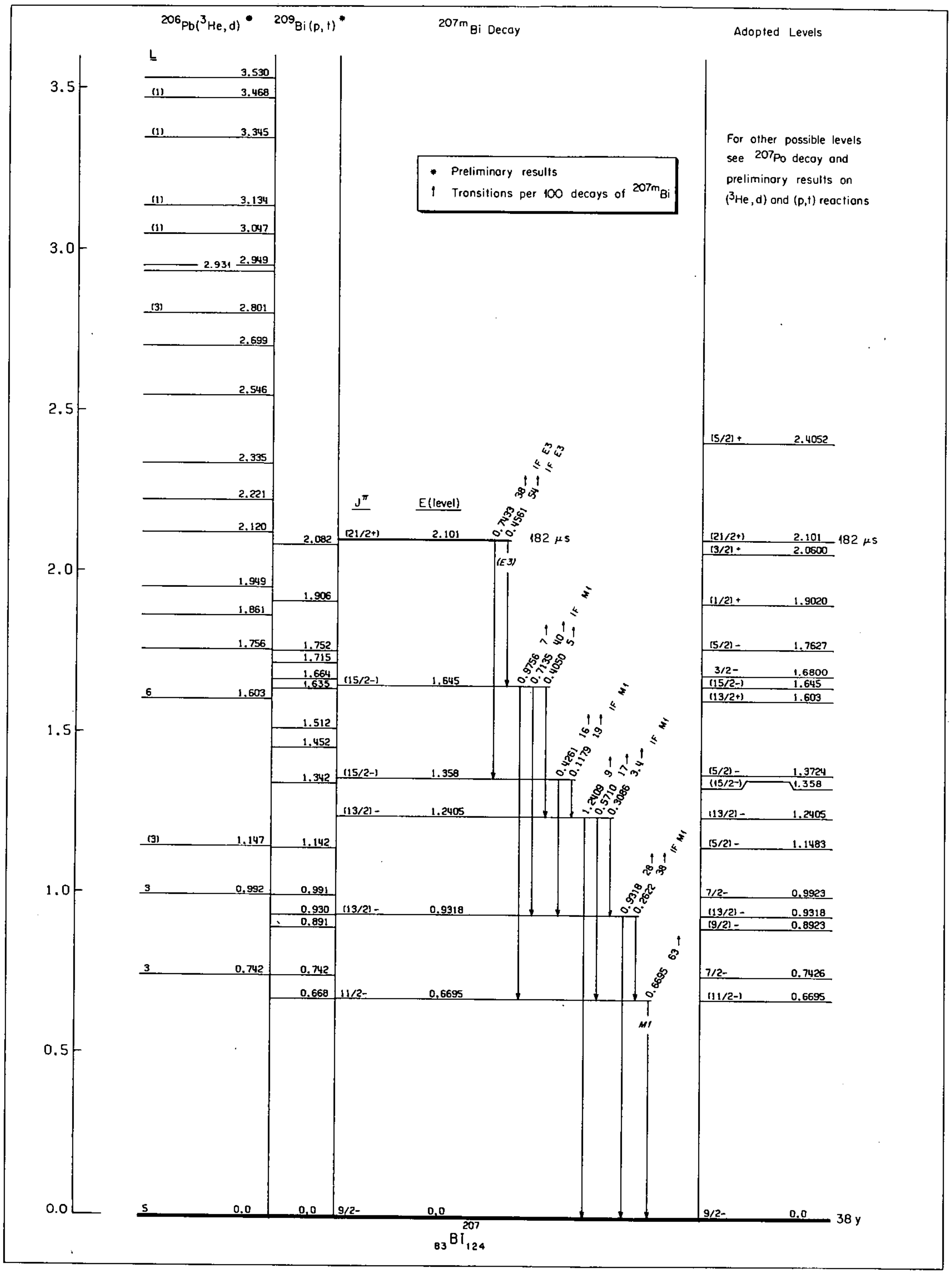

Fig. 9. Nuclear level scheme.

ORNL-DWG 71-2040

REACTION		Q-VALUE		ADJUSTED Q-VALUE		REFERENCE	LAB	DG	V/S
1H(N,G)2D		2224.62	0.15	2224.64	0.04	65PR06		1	0.1
		2224.63	0.20			65CO20,62KN1	CAN	1	0.0
		2224.61	0.07			66GR10		1	0.3
		2224.67	0.05			67TA03		1	-0.6
2D(G,N)1H		-2224	2.5	-2224.64	0.04	65RY01,50M56	WIS	U	-0.2
		-2227	3			65RY01,53N12		U	0.7
2D(N,G)3T		6257.6	0.3	6257.59	0.13	69PR06		1	-0.0
		6258	2			64TR05		U	-0.2
2D(D,P)3T		4029	12	4032.95	0.11	65RY01,49T23	CIT	U	0.3
		4034	6			64SP12	MIT	1	-0.1
		4033.7	1.7			670D01		1	-0.4
2D(D,N)3HE		3260	9	3269.13	0.12	65RY01,49T23		-	1.0
		3269	11			65RY01,56D41	WIS	-	0.0
		3264	7			AVERAGE		1	0.7
3T(B-)3HE		18.64	0.04	18.65	0.04	69SA21*59P78		1	0.1
3T(P,N)3HE	1019.3	-764.03	0.15	-763.82	0.05	61RY5	ZUR	1	1.4
		-764.34	0.37			64BO10	NRL	1	1.4
		-763.77	0.08			64SA12	ZUR	1	-0.6
4H(G,N)3T		5200	1700	2900	500	62AR5		F	-1.3
		2900	500			69MI10		2	
3HE(D,P)4HE		18380	10	18353.76	0.35	64MA57	MEX	F	-2.6
		18382	15			64MA57	MEX	F	-1.8
		18350.1	3.9			670D01		1	0.9
4HE(N,G)5HE		-890	50			*66LA04		2	
4HE(P,G)5LI		-1965	50			*65MA32		2	
5H(B-)5HE		19700	SYST	22400	800	66LA04,S		U	2.7
		22400	800			68Y006		3	
6LI(N,A)3H		4794	6	4783.5	0.7	67DE15		1	-1.7
6LI(P,A)3HE		4017	12	4019.7	0.7	65RY01,49T16	CIT	1	0.2
		4021	5			65RY01,51W26	WIS	1	-0.2
		4023	2			65RY01,53C02	BIR	1	-1.6
		4028	10			62MA2	MEX	1	-0.8
		4025	6			64SP12	MIT	1	-0.8
6LI(D,A)4HE		22376	14	22373.5	0.8	65RY01,53P28	RIC	1	-0.1
		22396	12			65RY01,53C02	BIR	1	-1.8
		22403	12			64MA57	MEX	1	-2.4
6LI(P,T)4LI		-18700	300			65CE03		2	
6HE(B-)6LI		3509.8	3.8			63J004		2	
6LI(P,N)6BE		-5061	17	-5070	5	62FR16		-	-0.5
		-5074	13			67H001		-	0.3
6LI(H,T)6BE		-4306	6	-4306	5	66WH01		-	-0.0
6LI(P,N)6BE		-5070	5			AVERAGE		2	
7LI(P,A)4HE		17364	11	17347.4	0.9	65RY01,51W05	CIT	1	-1.5
		17352	9			65RY01,53C02		1	-0.5
		17345	13			65RY01,53F18	RIC	1	0.1
		17357	14			64SP12	MIT	1	-0.6
		17373	6			64MA57	MEX	F	-4.2
7LI(T,A)6HE		9788	30	9836.5	3.8	65RY01,54A35	CRI	F	1.6
6LI(N,G)7LI		7250.2	0.5	7250.7	0.5	68SP01,69RA10		1	1.0
6LI(D,P)7LI		5028	2	5026.1	0.5	65RY01,53C02	BIR	1	-0.9
		5035	5			61JA23	MEX	1	-1.7
		5024	7			64SP12	MIT	1	0.3
6LI(T,D)7LI		986	7	993.1	0.5	54A35		1	1.0
7LI(H,A)6LI		13322	10	13327.7	0.6	64MA57	MEX	F	0.5
6LI(H,D)7BE		136	3	112.7	0.5	64MA57	MEX	F	-7.7
7LI(T,H)7HE		-11184	30			69ST02,67ST04		2	
7LI(P,N)7BE	1880.4	-1644.17	0.22	-1644.22	0.07	61RY5	ZUR	1	-0.2
		-1643.66	0.26			65RY01,63GA09	WIS	1	-2.1
		-1644.28	0.08			70RO07	MAR	1	0.7
7B(B+)7BE		12170	100			*67MC14		2	
8BE(A)4HE		94.5	1.4	91.88	0.05	65RY01,53J28	WIS	U	-1.8
		93.9	0.8			65RY01,56F45	CIT	U	-2.5
		91.88	0.05			68BE02		1	0.1
6LI(T,P)8LI		790	11	801.4	0.9	54A35		U	1.0
6LI(H,P)8BE		16824	12	16787.8	0.8	64MA57	MEX	F	-3.0
6LI(H,[illegible]B		-1974.8	1.0			58D78 ,65RY01	CAN	2	
7LI(N,G)8LI		2032.8	1	2032.9	0.7	67RA24		-	0.1
7LI(D,P)8LI		-192	1	-191.8	0.7	65RY01,51W26	WIS	-	0.2
		-188	7			64SP12	MIT	U	-0.5
7LI(N,G)8LI		2032.7	0.7			AVERAGE		2	
7LI(H,D)8BE		11795	13	11761.7	0.9	64MA57	MEX	F	-2.5
8HE(B-)8LI		10700	120			*66CE01		3	
9BE(P,A)6LI		2130	10	2125.4	0.7	65RY01.51C64	CHI	U	-0.4
		2125	4			65RY01.51W26	WIS	1	0.1
		2126	2			65RY01,53C02	BIR	1	-0.3
		2144	6			64SP12	MIT	F	-3.1
		2125.4	1.8			670D01		1	0.0
6LI(A,P)9BE		-2125.6	1.2	-2125.4	0.7	65DR28		1	0.1
6LI(A,N)9B		-3974	12	-3975.2	1.0	63MF08		U	-0.1
7LI(T,P)9LI		-2397	20	-2397	5	64MI04	HAR	U	-0.0
9BE(D,A)7LI		7162	10	7151.5	0.8	65RY01,51W05	CIT	1	-1.0
		7153	3			65RY01,53C02	BIR	1	-0.5
		7157	8			64SP12	MIT	1	-0.6
		7162	4			64MA57	MEX	1	-2.6
7LI(H,P)9BE		11215	15	11202.3	0.8	64MA57	MEX	F	-0.8

Fig. 10. Sample of mass adjustment table.

ORNL-DWG 71-2041

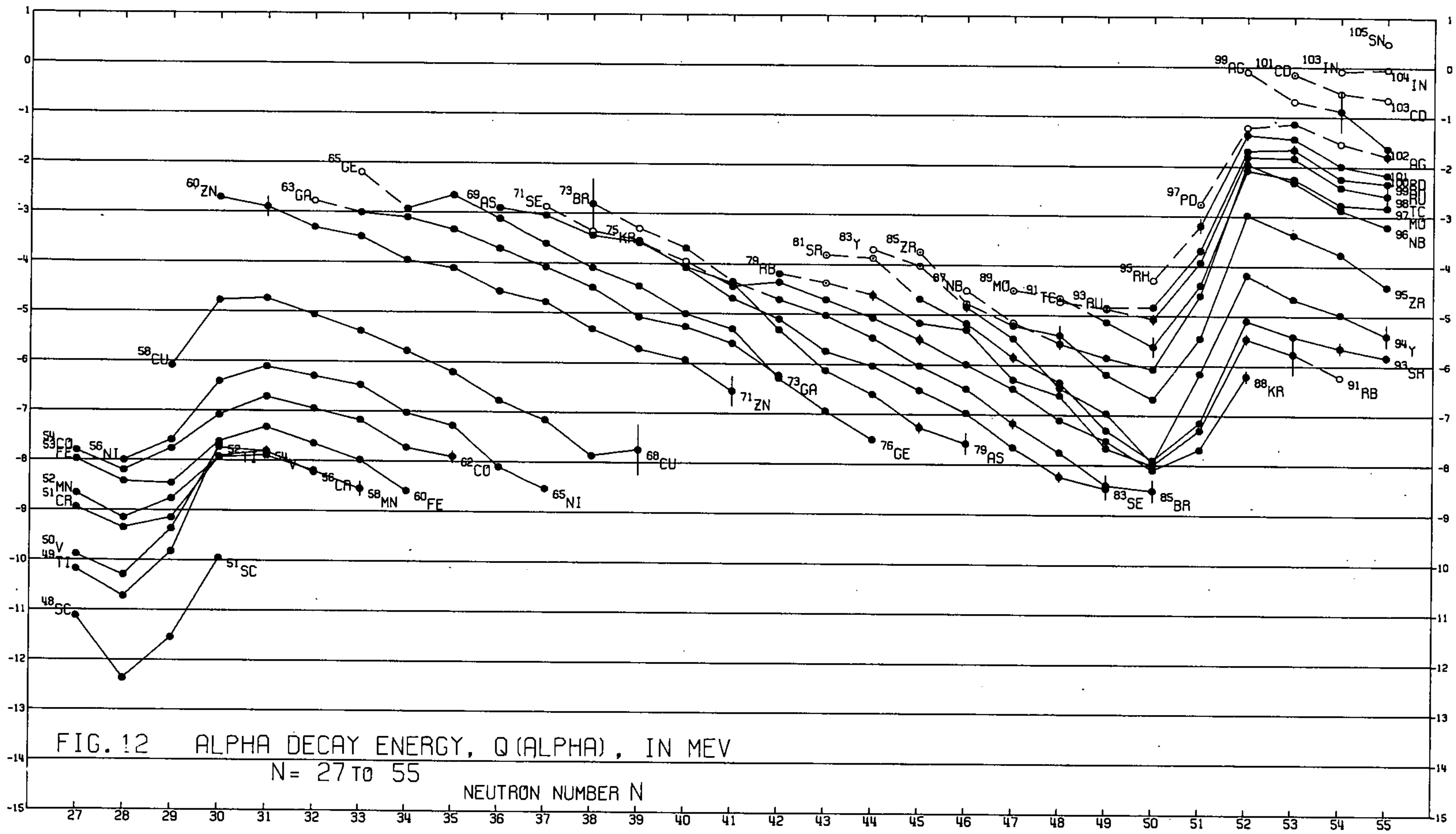

Fig. 11. Alpha decay energy, Q(alpha), in million electron volts, N = 27 to 55.

OPERATIONS DIVISION

Estimation of Radiation Doses Following a Reactor Accident

F. W. Stallmann[210] F. B. K. Kam[211]

A computer program is being developed which evaluates the radiation damage to a receptor at given location and time if a reactor accidentally releases radioactive material into the air. One major part of this program consists of a fast numerical integration routine which determines the total gamma radiation from a cloud of radioactive material. This part is completed and ready for use. The remainder of the program is designed to cover the movement of the cloud and the release and decay of the radioisotopes.

Sponsor: Operations Division

PHYSICS DIVISION

Spiral Reader

R. D. McCulloch

The Spiral Reader (SR) constructed by LRL for the University of Tennessee was delivered in June 1970. The SR is sited at ORNL and will be maintained and operated by ORNL and University of Tennessee personnel. The SR is a semiautomatic digitizing machine to be used in the measurement of bubble chamber photographs; it will greatly expand the measuring capability of the ORNL-UT High-Energy Physics Group, as the measurement rate of the SR is expected to be 20 to 30 times the rate of a conventional measuring machine now in use.

Programs written at LRL have been rewritten and tested for the calibration of the SR. The SLAC version of the LRL program, POOH, is being rewritten to perform data filtering and track matching. The filtered data from POOH will be input to the conventional spatial reconstruction program TVGP.

It is estimated that the SR will be measuring film by mid-December 1970. It is hoped that the ORNL version of POOH will be rewritten and fully checked out for production use by February 1971.

Sponsor: Physics Division Hans Cohn

Renormalized Finite-Nuclear Brueckner Theory

M. R. Patterson R. L. Becker[212]

A set of codes which produces Pauli-corrected two-body nuclear matrix elements has been developed during the last several years.[213] These matrix elements are distinguished by the fact that very realistic nuclear potentials, such as the Hamada-Johnston potential, are used in the relative–center-of-mass interaction. The careful evaluation and transformation of these matrix elements are very time-consuming on the computer.

---

210. Consultant, University of Tennessee.
211. Operations Division.
212. Physics Division.
213. R. L. Becker and M. R. Patterson, ORNL-4513 (May 1970).

Considerable effort has been spent during the last year in speeding up those codes which transform and Pauli-correct the relative matrix elements, resulting in a code which is about an order of magnitude faster than the previous version. This fact makes practical the calculation of properties of larger nuclei than those previously considered. The emphasis thus has shifted to calculation of the relative matrix elements as the most expensive step. The latter has been speeded up by about 5%, and further modifications are not being considered at the present time. Various approximations were considered during the year; however, their use offers no advantage over options already available in the code.

The final step of these codes is use of the two-body matrix elements to compute observable nuclear properties such as binding energy or nuclear spectra. Significant second-order contributions to these observables have been computed and are presently included in the codes. Their presence has enhanced agreement with experiment.

A new method of computation of the fractional occupancy (renormalization) of virtual hole states[214] has recently been incorporated in the final code. This new method reduces the required storage for cases presently studied and will allow consideration of a larger number of single-particle states in future studies.

Sponsor: Physics Division

Numerical Lagrangian Partial Derivatives

F. D. Hammerling

The subroutine DLAG[215] which performs two variable Lagrangian interpolations was modified to calculate numerical partial derivatives. This subroutine will permit the calculation of partial derivatives of tabular functions. The partial derivatives are useful in applying Newton's method or gradian techniques to the solution of equations involving the tabular function. It is hoped this version will replace the old version in our library in the near future.

Sponsor: Physics Division

Nonrelativistic Hartree-Fock Calculations

C. W. Nestor, Jr. T. A. Carlson[212]

Using a nonrelativistic Hartree-Fock program,[216,217] we have calculated electron binding energies and wave functions for several excited states of ionized neon. Comparison with the observed spectrum of electrons photoelectrically ejected from neon shows that the calculated energies are in reasonably good agreement with the observed energies, but that calculated transition probabilities do not agree with the observed intensity ratios. This situation is in accord with the findings of Sinanoglu,[218] who points out that a better treatment of electron correlation is necessary if one is to obtain agreement of theoretical and observed transition probabilities.

---

214. R. J. McCarthy and K. T. R. Davies, *Phys. Rev. C* I.5, 1644 (May 1970).

215. G. W. Westley and J. A. Watts, *The Computing Technology Center Numerical Analysis Library,* CTC-39 (October 1970).

216. Charlotte Froese, *Can. J. Phys.* **41**, 1895 (1963).

217. C. W. Nestor, Jr., ORNL-CF-70-11-31 (1970).

218. O. Sinanoglu, *Comments on Atomic and Molecular Physics* **2**, 73 (1970).

It is worth noting that several of these calculations were initially very difficult to make converge to a satisfactory level of self-consistency. C. F. Fischer[219] has described a method for improving the convergence of these calculations; unfortunately, this method leads to somewhat higher total energies, and thus in some sense wave functions calculated with her procedure are not as good as other wave functions.

Sponsor: Physics Division — T. A. Carlson

Single-Particle States for Asymmetric Fission

C. C. Lu   C. Y. Wong[212]

We have extended a simple single-particle model, proposed previously[220] for the overlapping ellipsoids of different sizes and shapes, to take into account spin-orbit interactions and other corrections. With a suitable choice of basis, the Hamiltonian is diagonalized to obtain the eigenenergies. The purpose of the present investigation is to study how the single-particle states will be affected by the asymmetry of the two fissioning parts, with a hope of explaining why the mass distributions for low-energy fission of transuranium nuclei are asymmetric.

Sponsor: Physics Division — C. Y. Wong

Relativistic Hartree-Fock-Slater Calculations

C. C. Lu   Linda P. Helton
C. W. Nestor, Jr.   T. C. Tucker
T. A. Carlson[212]

Using the Hartree-Fock-Slater program described previously,[221] we have calculated electron binding energies, wave functions, and other properties of interest for the ground states of all elements with atomic numbers from 2 to 126. The results of these calculations were issued as a Laboratory topical report.[222]

We have made extensive revisions to the program for the maintenance of the wave function library stored on an IBM 2314 disk pack. Magnetic tape copies of this library are now made on a regular schedule to serve as backup in case of disk pack trouble.[223]

The calculation of electron densities[224] for the atom as a whole has been added to the program library on the 2314 disk pack. This new program permits the retrieval of total electron densities (punched on cards for further use, if desired) given the library serial number of the atom. We have also modified the existing output subroutines to provide electron densities at the origin, at the nuclear surface, and averaged over the nuclear volume for s and $p_{1/2}$ electrons.

---

219. C. F. Fischer, *Can. J. Phys.* 46, 2435 (1968).
220. C. Y. Wong, *Phys. Letters* 308, 61 (1969).
221. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 39.
222. C. C. Lu et al., ORNL-4614 (December 1970).
223. *Math Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL 4514, p. 38.
224. Sponsor of this improvement was G. M. Stocks, Metals and Ceramics Division.

To facilitate the comparison of predicted x-ray energies with experimental data, we have written a computer program[225] which calculates x-ray energies from the one-electron eigenenergies stored on the 2314 disk pack and tabulates the calculated energies, the observed energies, and the percentage difference.

Sponsor: Physics Division T. A. Carlson

REACTOR DIVISION

Pressure Vessel Stress Analysis

A. J. Edmondson[226] V. A. Singletary D. E. Arnurius

The program representing the pressure solution to the cylinder-to-cylinder pressure vessel configuration has been obtained to give the best comparison with experimental results.[227,228] Reasonable agreement exists not only with the experimental results but with finite-element results as well. The pressure program is considered to be complete and will be mated with programs representing the solutions of other loading arrangements of the cylinder-to-cylinder configuration when they become available. These programs are most useful in parameter studies.

Sponsor: Reactor Division

Heavy Section Steel Technology Programs

Carla L. Armstrong

We converted the FORTRAN programs CTMESH-1, HOLD-1 Plane Stress, and HOLD-1 Plane Strain as references in Report WCAP-7368[229] to run within our IBM 360/75-91 computing environment. Except for several cards that require minor alteration, the programs will compile using either the FORTRAN IV compiler or the FORTRAN 360 compiler.

We did this work in support of the AEC-funded Heavy Section Steel Technology Program, the purpose of which is to develop a quantitative means of ensuring the safety against fracture of large steel nuclear pressure vessels.

Sponsor: Reactor Division

Stress Analysis of MSBR Graphite

D. W. Altom J. A. Carpenter S. J. Chang

The stress analysis of irradiated graphite for the core design of the MSBR is continuing. The previous work[230–232] was improved to include the effect of a variable creep coefficient arising from a nonuniform

---

225. C. W. Nestor, Jr., ORNL-CF-70-3-20 (1970).

226. Consultant to Reactor Division from the University of Tennessee.

227. *Math. Div. Ann. Progr. Rept. Dec. 31, 1968,* ORNL-4385, p. 39.

228. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 44.

229. C. Visser, S. E. Gabrielse, and W. Van Buren, *A Two-Dimensional Elastic-Plastic Analysis of Fracture Test Specimens, Heavy Section Steel Technology Program Technical Report No. 4,* WCAP-7368 (October 1969).

230. S. J. Chang, C. E. Pugh, and S. E. Moore, *Viscoelastic Analysis of Graphite under Neutron Irradiation,* ORNL-TM-2407 (October 1968).

231. *MSR Program Semiann. Progr. Rept. Feb. 28, 1969,* ORNL-4396, pp. 229–31; ibid., *Feb. 28, 1970,* ORNL-4548, pp. 218–21.

232. S. J. Chang, J. A. Carpenter, and D. W. Altom, *Viscoelastic Analysis of Irradiated Graphite with Variable Creep Coefficient,* ORNL-TM (to be published).

temperature distribution. The resulting calculation has shown significant improvement, especially when the dose level is high and the temperature difference throughout the body is large. A computer program, VATCRP, is completed for the present analysis. It can include the previous one as a special case if the parameter is appropriately adjusted. Numerical results are shown in Figs. 12–14.

Sponsor: Reactor Division, Molten Salt Breeder Reactor

Time-Dependent Behavior Studies of Stainless Steel under Elevated Temperature[233,234]

S. J. Chang

It is intended in the present investigation to formulate a mathematical model to represent the time-dependent behavior of the stainless steel under elevated temperature for the purpose of LMFBR components design. Many papers concerning the mathematical theory of creep (or flow) have been reviewed and examined during the period of investigation. The development of an analytical form for the representation has been initiated.

Sponsor: Reactor Division, Liquid Metal Fast Breeder Reactor

Calculation of Energy Requirements for Buildings on a District Heating System

M. T. Heath

As part of a project sponsored by the Department of Housing and Urban Development, a computer program was written which calculates the energy requirements for a given collection of buildings over a given time period. The specific use of the program in this project was to simulate the operation of a district

233. *Informal Progress Report on Structural Design Methods for LMFBR Components for Period Ending May 31, 1970,* ORNL-CF-70-6-14, pp. 23–24.

234. Ibid., *for Period Ending June 30, 1970,* ORNL-CF-70-6-48, pp. 12–13.

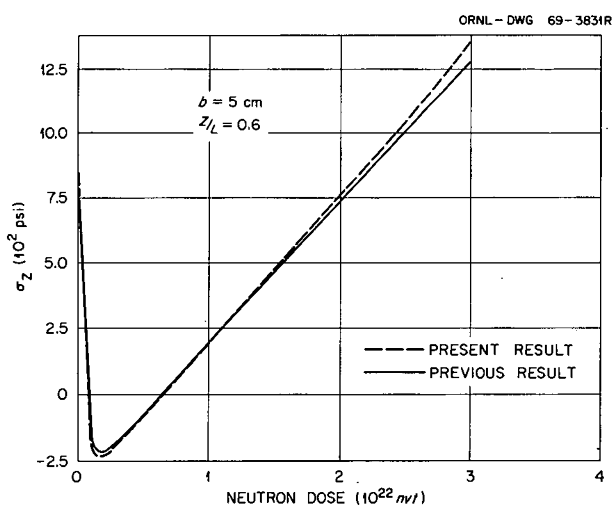

Fig. 12. Axial stress at the outer surface as a function of fluence level.

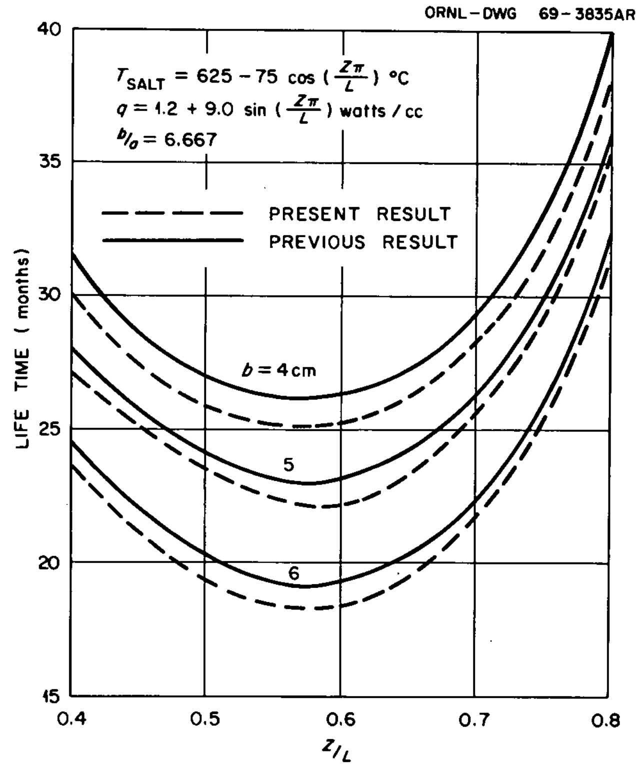

Fig. 13. Lifetime of MSBR graphite core cylinders as a function of axial position according to the volumetric distortion criterion.

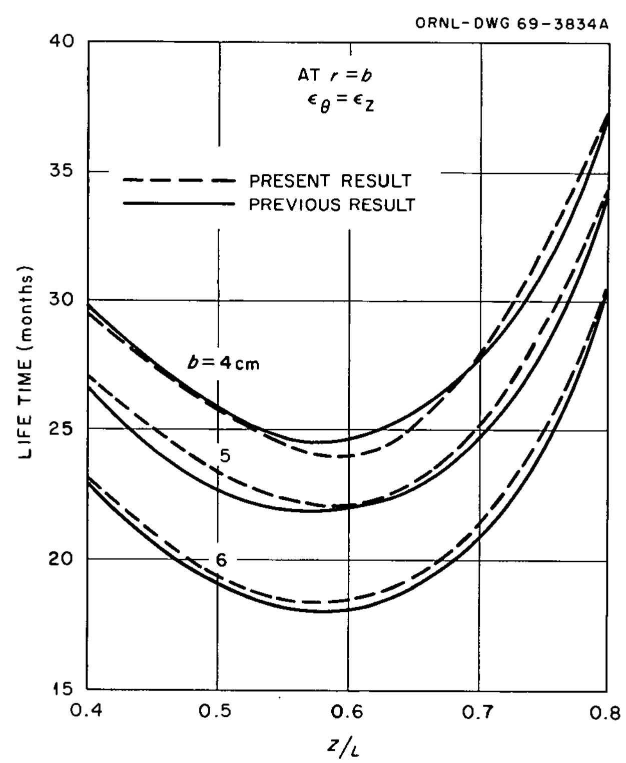

Fig. 14. Lifetime of MSBR graphite core cylinders as a function of axial position according to the axial strain criterion.

heating system so that the feasibility of using a nuclear reactor as energy source could be evaluated. A single building or an entire city may be included, and both thermal and electrical loads are computed. In addition to input concerning the physical properties of the buildings, the program uses weather information taken from U.S. Weather Bureau data for the desired location.

For each kind of building the basic calculation is that of the thermal energy balance during a given hour. This quantity is the difference between heat losses and gains inside the building. The value obtained is the amount of heat which must be added or removed in order to maintain a specified comfort level (temperature and humidity) in the building. The heat losses and gains considered are those due to transmission, ventilation, infiltration, electrical power use, humidity regulation, solar radiation through glass, and latent and sensible heat of occupants. From the heat balance the thermal and electrical demands on the district system can be determined, depending on the kinds of heating and cooling employed. Values for longer time periods are computed by summing over consecutive hours.

The author acknowledges valuable contributions to the development or testing of this program by A. A. Brooks, A. B. Fuller, and A. J. Miller (project coordinator); J. W. Megley;[235] and M. J. Wilson.[236]

Sponsor: Reactor Division

Economic Analysis of Development Proposals for Desalting Processes

G. W. Westley R. A. Carter W. G. S. Fort[237]

The Office of Saline Water (OSW), an agency in the U.S. Department of Interior, has the responsibility of planning and directing all governmental activities in the area of desalination. This analysis hopes to provide OSW with an economic tool for allocating available funds to development proposals, specifically those intended to improve established desalination processes.[238]

Theoretically, the relative value of a proposed development project can be characterized by a numerical Cost Effectiveness Index (CEI), which is a function of the estimated funding requested by the project proposal and the predicted benefits derived from the successful project completion. It is postulated that a subset of the collected proposed projects can be identified as the subset to receive primary funding by the OSW. This subset is determined by an Accumulated Benefits Evaluation (ABE), which attempts to maximize the actual benefits derived from a given subset of projects. The CEI will be discussed first.

To evaluate different development proposals on an equal basis, compatible cost models must be used for the various process types. This requirement is met through a series of cost models that use compatible design materials whenever possible.[239–241] Each cost model is coupled with a parameter optimization procedure that allows cost reductions, resulting from a project proposal, to be evaluated on an optimal plant-design basis. Thus, the effect of a development proposal is the net total of the cost reductions on an optimal design plant in each process type affected by the proposal.

The above gives a means of computing a cost reduction resulting from a project. However, this cost reduction must be weighted by the estimated need for the cost reduction. This weighting is accomplished

235. Present Address: Boston Edison, Boston, Mass.

236. Present Address: I. C. Thomasson and Associates, Nashville, Tenn.

237. Reactor Division.

238. W. G. S. Fort and I. Spiewak, *The Facilitation of OSW Management Decisions,* ORNL-67-7-48 (July 24, 1967).

239. *Multistage Flash Desalination Plant Cost Model* (to be published).

240. *Vertical Tube Evaporator Desalination Plant Cost Model* (to be published).

241. *Electrodialysis Desalination Plant Cost Model* (to be published).

by implementing a water-demand model which attempts to predict the future water requirements for a specific process type as a function of time. The estimated benefit for a development proposal is the product of the cost reduction attained and the estimated volume of water required in that specific process type.

Since different development proposals would probably begin at different times, both the funding required and benefits from the project must be discounted back to a fixed time. Thus, the CEI value for a specific development proposal is

$$\mathrm{CEI} = \sum_j \frac{\text{discounted benefits from the proposal in process } j}{\text{discounted funding for the proposal}},$$

where j assumes the values of process types affected by the development proposal.

The above is a simplistic discussion of a CEI value. In any realistic model, options would exist to evaluate a specific development proposal on: (1) a process type at different production capacities, (2) different feedwater types, and (3) different fiducial intervals for the project. Thus, a development proposal can be characterized by a series of CEI values.

Since funding limits are less than infinite, only a subset of the collected development proposals can be funded. Ideally, the primary subset to be funded would be that which maximizes the actual benefit derived from the proposed project list under the preset funding limitations. If all of the projects were independent, the best subset simply would be that with the highest CEI values. But normally, the projects are interdependent. Thus, the effect of implementing several development proposals in a process type is not necessarily equal to the effects of implementing each project autonomously. One assumes that the project proposal having the largest CEI value should be funded. The remaining project proposals are evaluated in order of decreasing CEI value as long as the sum of the discounted benefits derived from the project subset, minus the total discounted funding for the project subset (the actual benefit derived), continues to increase. The resulting subset is designated as the primary funding project proposal list.

It should be emphasized that the above indices are first iterations in an attempt to use computers to aid in the OSW management decision process.

Sponsor: Reactor Division I. Spiewak

Stress Analysis Using Finite Element Techniques

J. S. Crowell

The finite element concept is a basis for the numerical treatment of problems of structural analysis.[242] During the past several years the finite element method has become one of the most powerful tools of the structural engineer. The method can also be applied to nonstructural-type problems such as heat conduction and fluid flow.

Many of the finite element computer programs at ORNL were obtained by the Reactor Division. These programs have been used to help analyze prestressed-concrete reactor vessels, components of reactor piping systems, and other problems of interest to the Applied Mechanics Section of the Reactor Division. Most of the responsibility of converting, maintaining, correcting, and extending these programs has been borne by individuals who are in the Mathematics Division.

---

242. O. C. Zienkiewicz, *The Finite Element Method in Structural and Continuum Mechanics*, McGraw-Hill, 1967.

Several plotting programs have been written to aid the users of some of the finite element programs assimilate the rather large amount of printed output. Plots may be machine-generated showing stress contours, principal stresses, and displacements.

Sponsor: Reactor Division — J. M. Corum

Finite Element Programs for the Reactor Division

J. S. Crowell   Peggy G. Fowler   B. V. Stout[243]

Several programs which use the finite element technique for analyzing structural problems are maintained by the Mathematics Division. At the request of and with the assistance of members of the Reactor Division, these programs have been made operational in Oak Ridge, extended, and corrected during the last four years. Some of these programs were written specifically for the Reactor Division by outside groups under subcontract with ORNL.

A brief categorization of the most-used programs is as follows:[244]

Two-Dimensional Analysis of Elastic Solids. SAFE-PLANE, SAFE-AXISYM, and SAFE-PCRS are the first programs which were used. In 1969 SAFE-2D largely supplanted the above three and is used for most two-dimensional applications. All these programs were written by a group at General Atomic Division of General Dynamics, as were all the programs whose names begin with SAFE-. Another program, commonly called Wilson's code, has been used extensively by several groups in Oak Ridge. These programs have been and are being used to solve axisymmetric and plane stress analysis problems for complex structures.

Two-Dimensional Viscoelastic Analysis of Concrete Structures. The two programs in this category are SAFE-CREEP and SAFE-CRACK, with the latter one being the most recent work. These programs have been used by the Reactor Division's Applied Mechanics Section to study the behavior of reactor pressure vessels under specific loading conditions.

Finite Element Analysis of Thin Shells. A general thin shell analysis program, JOINT, was modified by a group at the University of California at Berkeley to perform the analysis of thin-walled tee joints. This program has been in use by the Reactor Division for approximately two years.

Three-Dimensional Analysis of Elastic Solids. The SAFE-3D computer program is applicable to general three-dimensional geometries. The program has been used in analyzing a concrete reactor pressure vessel and thick-walled steel pipe joints. The treatment is restricted to static analysis.

Sponsor: Reactor Division — J. M. Corum, R. C. Gwaltney, S. E. Moore, F. J. Witt

DEXTIR Data Reduction Programming

O. W. Russ, Jr.

Programs were written for Reactor Division projects of dryer-superheater development (water-steam and potassium systems) for NASA, fission products deposition loop, and experimental stress analysis of

---

243. Summer employee at CTC.

244. Specific references as to user's manuals and descriptive reports have been omitted. It is suggested that interested persons contact the author for references for any of the listed programs.

thin wall tees, and are being developed for failed fuel mockup tests for the LMFBR. The DEXTIR-collected experimental data are converted into such parameters as a single- and two-phase heat fluxes, heat inputs and losses, qualities, flows, specific volumes, densities, viscosities, Reynolds numbers, mass flow rates, gas concentrations, diffusion coefficients, radiation counts, strains, pressure drops, and temperature distributions, the results to be output in printed format, punched cards, and Calcomp or CRT plots. The POOLSID1 computer program,[245] originally written to read manual data from punched cards from Metals and Ceramics Division's SolGel-1 fuel capsule tests (ORR), to print and Calcomp-plot temperature differences, heat generation rates, linear power levels, and elapsed operating times, was modified to read DEXTIR scanned data directly from magnetic tape and further adapted to reduce DEXTIR data from SolGel-2, -3, and UN-3 fuel capsule tests (ORR). Programs for Reactor Division's GCFR 04-p9 (ORR) and HTGR HRB-2 (HFIR) fuel capsule tests are in progress to print and Calcomp-plot parameters during the 8-hr ORR pressure cycle every eight weeks and the yearly steady-state cycle updated monthly, and to print and plot running averages, maximum temperatures, temperature profiles, and other parameters over the three-week HFIR operating cycles.

Sponsor: Reactor Division

One-Group Neutron Cross Sections Using the GAM-II Code with an Input Flux Spectrum

R. Q. Wright

One-group neutron cross sections for 113 nuclides were produced using the GAM-II code[246] with an input flux spectrum. The principal reactions of interest were (n,γ), $(n,2n)$, (n,p), and (n,α), but cross sections were obtained for other reactions when data were available. Five different flux spectra were used to weight the cross sections:

LMFBR blanket spectrum
LMFBR core spectrum
HFIR spectrum
EBR-II blanket spectrum
EBR-II core spectrum

The basic sources of cross-section data were the ENDF/B,[247] GAM-II, and UK[248] libraries. ENDF/B was used whenever data were available, and the other libraries were used only when the data were not available in the ENDF/B library. The first step in the process was to run the SUPERTOG[249] code to produce 99-group cross sections in the GAM-II update format. The next step was to run the GAM-II update program to produce an updated GAM-II cross-section tape. The final step was to run the GAM-II code to generate the spectrum-averaged one-group cross sections. When GAM-II cross sections were used, the first two steps

245. Written by Ruth B. Hofstra, Mathematics Division.

246. G. D. Joanou and J. S. Dudek, *GAM-II: A B_3 Code for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants*, GA-4265 (1963).

247. 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.

248. K. Parker, *The Aldermaston Nuclear Data Library as at May 1963*, AWRE-0-70/63 (May 1963).

249. R. Q. Wright, J. L. Lucius, N. M. Greene, and C. W. Craven, Jr., *SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B*, ORNL-TM-2679 (September 1969).

were not required. Data from the UK library were first processed by the UKE[250] code to translate from the UK format to the ENDF/B format.

Sponsor: Reactor Division H. T. Kerr

Updating of the GAM-II and 100-Group XSDRN Cross-Section Libraries

R. Q. Wright

Forty-five materials in the ENDF/B[247] version II library have now been processed by SUPERTOG,[249] and the GAM-II[246] and XSDRN[251] libraries have been updated. Since most materials which have resonance parameters are processed twice – once as infinite dilution and once as a resonance nuclide – the total number of nuclides involved is 72.

Transmission of data from ENDF/B to GAM-II is accomplished in three steps:

1. The SUPERTOG code is run with the results placed either on punched cards or magnetic tape by input option. The format is described in the instructions for the GAM-II update program. The first eight cards are not provided by SUPERTOG and must be added later.
2. A retrieval program is run which provides the first eight cards and merges the contents of two or more SUPERTOG tapes onto a single tape in a format acceptable by the GAM-II update program.
3. A modified version of the GAM-II cross-section tape update code is run generating a 99-group GAM-II cross-section tape.

The 100-group XSDRN tape is generated by an auxiliary program from the GAM-II tape, and data for one thermal group are added in this step. The 100-group XSDRN cross sections have been used by the Reactor Division to perform XSDRN calculations for ENDF/B phase II data testing.

Sponsor: Reactor Division J. D. Jenkins

Reactor Division Cooperative Code Development

G. W. Cunningham III T. B. Fowler[237] D. R. Vondy[237]

Oak Ridge National Laboratory is participating in an inter-installation cooperative effort directed at achieving efficient exchange of code blocks. This effort is in support of development of the LMFBR concept (fast breeder) and is funded by the Reactor Physics Branch of the Reactor Development and Technology Division of the AEC. The specific contributions made in this effort were as follows:

1. Evaluation of the needs of and the restrictions imposed by local computers and their operation.
2. Contributions to the ground rules in this effort such as programming requirements to ease the burden of implementing outside codes as well as implementing our code blocks by other installations.
3. Implementing the evolving standard interface data files to permit coupling of code blocks. Thus, routines have been written to convert cross-section data from files used locally to a form used by new code blocks being exchanged.

---

250. 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).

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

4. Development of miscellaneous computer programming to facilitate checking out new code blocks. Thus, effort has gone into a two-point neutron spectrum calculation which was used to implement and debug depletion and fuel-management code blocks and to aid in understanding requirements for communicating data and control instructions.

Sponsor: Reactor Division

CITATION Code Development

G. W. Cunningham III T. B. Fowler[237] D. R. Vondy[237]

CITATION,[252] a nuclear reactor analysis code, is being upgraded prior to a new release to other installations and to support local use. This effort included the following:

1. Extension of the diffusion-theory treatment in up to three space dimensions to cover the periodic or repeating boundary condition. This boundary is needed, for example, in certain situations to close the circle in the θ dimension of R-θ or R-θ-Z geometry. Routines were programmed to add the capability to solve simultaneously the flux values along a row of points with end coupling within the framework of the code. This added formulation was carried through routines which perform neutron balance and perturbation calculations.
2. Criticality search procedures were extended to add flexibility in the support of developing fuel-management analysis capability. The indirect-search technique of solving a series of eigenvalue problems, with nuclide concentrations changed after each, was implemented. Nonlinear dependence of the multiplication factor on search nuclide concentrations was studied, and suitable formulations were implemented with constraints as found necessary from a broad range of test problems. A significant extension was made to the direct-search procedure in the code; by this technique, iteration is directly toward a desired critical condition. The extension allows simultaneous increase in the concentrations of some nuclides and decrease in others. Thus, the heavy metal content of fuel rods may be held fixed as a constraint.
3. Some work was done in accounting for nuclide concentration changes on a finer scale than that upon which macroscopic cross sections are calculated for neutronics problems.
4. Other areas of effort include provision for solving fixed-source problems, as arising in analysis of reactor startup, and code changes found to be desirable from user experience.
5. An auxiliary program to the CITATION code is used for processing cross-section data, for example, conversion from other formats; this was reprogrammed to add flexible dimensioning of data arrays to minimize storage requirements and to contain the data associated with the maximum of one or more dimensions in a given storage allocation.

Sponsor: Reactor Division

---

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

ESP, a General Monte Carlo Reactor Analysis Code

S. N. Cramer J. L. Lucius R. S. Carlsmith[237]
M. L. Tobias[237] G. W. Perry[253]

ESP[254] contains many of the transport and collision routines of O5R,[255] but it has been specialized to a general reactor analysis code by including a detailed resonance energy cross-section treatment. This resonance treatment, together with the O5R general geometry description, gives ESP the ability to handle complicated energy-space problems. The code is linked to the ENDF/B[247] system and may be run in its entirety with only one deck setup and computer pass. The analysis of neutron histories is performed in the computer core for those quantities usually wanted in reactor calculations. Included are cross sections and fluxes averaged over arbitrary energies and spatial regions.

The development of ESP has continued throughout the year with emphasis on the following items:

(1) The first production version of ESP has been completed. A code report written by S. N. Cramer is currently being reviewed for publication.

(2) A path-length estimation of flux and flux-dependent quantities has been added to the code. This estimation permits good results to be obtained in optically thin regions, including internal voids.

(3) A maximum execution-time option has been added that allows the user to specify a time which, if exceeded, will effect the termination of the program with complete results printed, based on batches completed. Without this option, an inaccurate estimate of the time required to complete the calculation could result in a significant expenditure of computer time with no useful results obtained.

(4) The ESP version of the RAFFLE[256] geometry package has been revised to treat a fixed-source neutron-detector problem.

(5) The renormalization of weights between batches has been eliminated and replaced with renormalization of the splitting, Russian roulette, and fission-production weights.

(6) The source routine has been revised to allow an almost completely arbitrary source description, as well as many specific distributions, by input option.

(7) The inelastic-scattering treatment has been revised to accommodate ENDF/B version II data.

(8) Data management procedures have been revised to achieve a more efficient interface with the ENDF/B libraries.

(9) The unresolved resonance treatment and that segment of the data management procedure linking the treatment to the ENDF/B libraries has been revised, as required, to process new data.

(10) Several reactor bench-mark problems have been calculated with ESP. The homogeneous and full-core mockups of the ZPR-III Assembly 48 Reactor are currently being calculated. These ZPR calculations use a periodic array[257] version of the generalized geometry package and a fictitious scattering version of the transport routine which eliminates the tracking of neutron histories across the many thin plates of the ZPR-III core.

---

253. Former employee; present address, Middle South Utilities, New Orleans, La.

254. S. N. Cramer et al., *ESP, a General Monte Carlo Reactor Analysis Code,* ORNL-TM-3164 (to be published).

255. D. C. Irving et al., *O5R, a General Purpose Monte Carlo Neutron Transport Code,* ORNL-3622 (February 1965).

256. O. W. Hermann and R. S. Carlsmith, *RAFFLE: A Monte Carlo Code for Calculation of First Flight Collision Probabilities,* ORNL-TM-1699 (December 1966).

257. G. W. Morrison, *ARRAY GEOM,* this report.

(11) A preliminary investigation has been made of the problems associated with including the $S(\alpha, \beta)$ thermal neutron scattering package[258] into ESP.

(12) An investigation of the spatial distribution of neutron capture through thin uranium foils has been started. This work is in connection with the calculation of capture gamma-ray production in uranium using broad-group cross sections. The ESP code should produce a more nearly correct spatial capture distribution due to the fine energy group structure in the resonance calculations.

Sponsor: Reactor Division

ARRAY GEOM

G. W. Morrison

The O5R[255] generalized geometry routine GEOM has been rewritten to permit complex geometrical arrays composed of repeatable units to be specified with a minimum of input data. The basic repeating unit is the ZONE, which in turn may be composed of many blocks, each having several quadric surfaces.

ARRAY GEOM has been used with the ESP Monte Carlo code to analyze the SPR-III Assembly 48 critical experiment.[259] The core of Assembly 48 is composed of identical fuel assemblies. The specification of this geometry using GEOM would require specifying each of the fuel assemblies for a total of over 300,000 input GEOM data cards. ARRAY GEOM required only one assembly to be specified.

Sponsor: Reactor Division

Monte Carlo Analysis of Heterogeneity Effects in ZPR-III Assembly 48

G. W. Morrison   M. L. Tobias[237]

A cooperative effort has been undertaken in the LMFBR program concerning the analysis of heterogeneity effects in ZPR assemblies. The first step in the joint study has been a comparison between representative quantities obtained by one-dimensional discrete ordinates calculations, which was performed by Atomic Power Development Associates[260] with the ESP Monte Carlo calculations.[254,261] The ESP code was revised to accept the same P_0 multigroup cross sections as used by APDA. Figure 15 shows a comparison between the one-dimensional ANISN code and ESP for the so-called "normal" drawer of ZPR-III Assembly 48.

Sponsor: Reactor Division

Monte Carlo Calculation of Optimum Detector Spacing for Superheavy Element Detection

G. W. Morrison   M. L. Tobias[237]

The ESP[254] Monte Carlo neutron transport code was used to aid in the design of a device for detecting the possible existence of superheavy elements in nature.[261] The apparatus, planned by the Chemistry and

---

258. G. W. Morrison, L. W. Petrie, Jr., and R. S. Carlsmith, *A General Scattering Law Kernel Using S(α,β) Data from ENDF/B,* this report.

259. W. G. Davey, *Proceedings of the International Conference on Fast Critical Experiments and Their Analysis,* ANL-7320 (1966).

260. T. A. Pitterle, E. M. Page, and M. Yamamato, *Analysis of Sodium Reactivity Measurements; Volume II Sodium Void Calculations,* APDA-216, vol II (June 1968).

261. M. L. Tobias et al., paper presented to the Workshop–Seminar on *Monte Carlo Methods and Computer Codes for Radiation Transport in Shielding Applications,* ORNL-RSIC-29 (to be published).

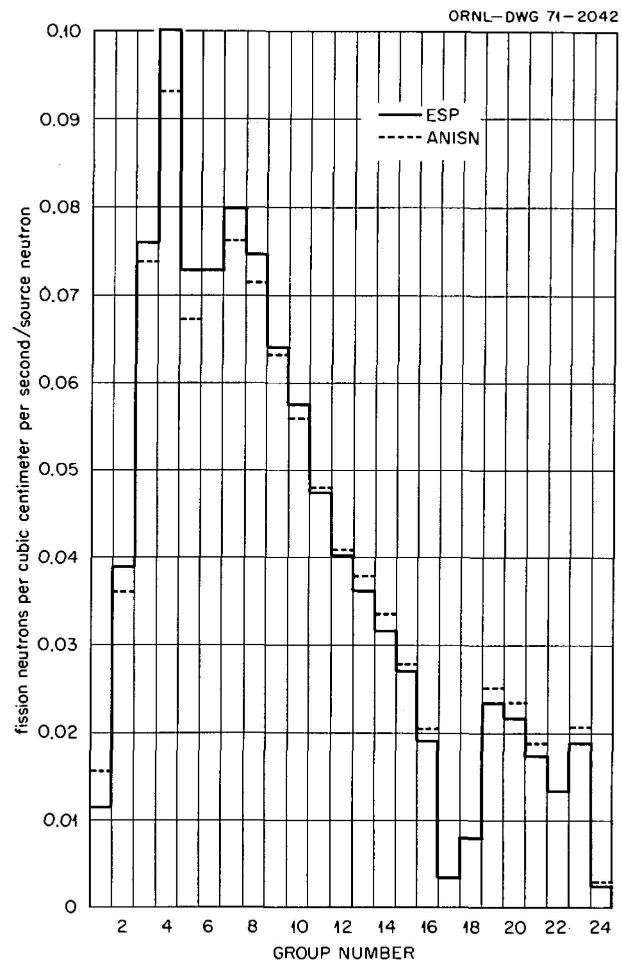

Fig. 15. Fission rate in the fuel drawer of ZPR-3 assembly 48 as a function of group number.

Physics Divisions of Oak Ridge National Laboratory, is essentially a set of concentric cylinders of finite length, in which a ring (or rings) of cylindrical neutron detectors is to be placed. The object of the calculations was to determine the relative advantages of the use of various materials, and of different sizes and locations of detectors in order to maximize the sensitivity of the device. Because of the geometrical complexity, the exact description was possible only in a Monte Carlo code having general geometry capabilities.

Several sets of calculations were performed to give the optimal design.

Sponsor: Reactor Division

A Free-Gas Scattering Kernel for the ESP Monte Carlo Neutron Transport Code

G. W. Morrison R. S. Carlsmith[237]

A free-gas scattering kernel has been written for the ESP Monte Carlo code.[254] This kernel is used to describe the interaction of neutrons of low energy (<1 eV) with solid and gaseous moderators. The assumption is made that the thermal speed distributions are Maxwell-Boltzmann. Sampling from the

Maxwell-Boltzmann distribution follows the prescription given in ref. 262. The flux in an infinite medium of mass 12 has been computed with the free-gas kernel and with analytic results. The results obtained by the free-gas kernel show excellent agreement with the analytic results (see Fig. 16).

Sponsor: Reactor Division

Improvements to Resolved Resonance Treatments in GAM-II and XSDRN

N. M. Greene R. Q. Wright

The Nordheim integral treatment[263] is a numerical method for calculating effective cell resonance cross sections, which has received widespread use in the design of thermal and intermediate reactors where simpler treatments are mainly inapplicable. However, as with many complex formulations, subtle approximations *in its application* can introduce serious inaccuracies.

The three approximations in the GAM-II,[246] TONG,[264] and XSDRN[251] versions of the Nordheim treatment which were looked at in the present study are:

1. the wing correction,
2. possible inadequacies in the integration mesh,
3. spatial self-shielding.

Wing correction. The extent of the wing correction is shown in Fig. 17. A primary resonance range is determined (E_1, E_2) over which the effects of resonance shielding, Doppler broadening, etc., are calculated. But to conserve time, the "wings" are integrated analytically (non-Doppler broadened) and parceled out to the groups containing E_1 and E_2, with 50% of the total integral in each. This clearly gives an incorrect distribution of the cross sections. A better approach is to include the wings in the background data. This correction requires that the basic data processing code know enough about the Nordheim treatment to determine (E_1, E_2). The code SUPERTOG[249] has been modified to these ends. The wing correction in the Nordheim treatment is then suppressed.

Integration mesh. The range (E_1, E_2) is divided into N points, equally spaced in lethargy, and the cross section $\sigma(E)$ and weighting function in the fuel lump $W(E)$ are evaluated thereon for a trapezoidal numerical integration. Typically, codes force N to lie between 100 and 1000 points. One hundred points has been found inadequate for narrow resonances, because too few points are taken in the neighborhood of the resonance peak. An infinite dilution calculation showed errors of 7% in some groups for ^{239}Pu with the GAM-II energy structure. On the other hand, forcing at least 400 points gave agreement in all groups to less than 1% with a more exact treatment. For this reason, the present XSDRN code forces N to lie between 400 and 500 points. Note that significant Doppler broadening would tend to soften these requirements, however.

Spatial self-shielding. Normally an average cross section *in a fuel lump* would be defined by

$$\bar{\sigma}^g_{\text{lump}} = \frac{\int_g dE\, \sigma(E)\, W(E)}{\int_g dE\, W(E)} .$$

262. R. R. Coveyou et al., *J. Nucl. Energy* 2 (1956).

263. L. W. Nordheim, "The Theory of Resonance Absorption," in *Symposium on Applied Mathematics*, vol. XI, 1961.

264. D. R. Vondy and T. B. Fowler, *Computer Code TONG for Zero-Dimensional Reactor Depletion Calculations*, ORNL-TM-1633 (June 1967).

This is zone averaging. When a cell is smeared, this cross-section definition will be multiplied by a flux disadvantage factor, defined by the average lump flux divided by the average cell flux in a volume sense; that is,

$$\bar{\sigma}^g_{\text{cell}} = \bar{\sigma}^g_{\text{lump}} \frac{\bar{\phi}^g_{\text{lump}}}{\bar{\phi}^g_{\text{cell}}} .$$

Note that when the two equations are combined

$$\bar{\sigma}^g_{\text{cell}} = \frac{\int_g dE\, \sigma(E)\, W(E)}{V_{\text{lump}}\, \bar{\phi}^g_{\text{cell}}} ,$$

where V_{lump} is the lump volume. If the flux in the cell is assumed to be $1/E$, the above equation becomes

$$\bar{\sigma}^g_{\text{cell}} = \frac{\int_g dE\, \sigma(E)\, W(E)}{\Delta u_g} \left(\frac{V_{\text{cell}}}{V_{\text{lump}}} \right) .$$

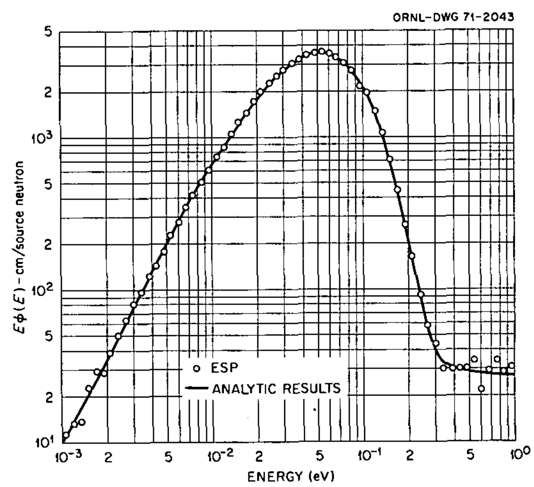

Fig. 16. Infinite media flux per unit lethargy for a mass 12 free gas plotted as a function of energy for the ESP results and the analytic results.

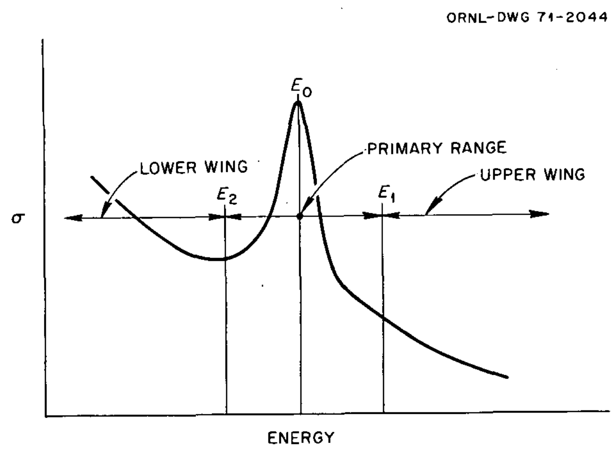

Fig. 17. Calculational regions for Nordheim integral treatment.

The volume ratio is accounted for in the cell number density definition, and the normal definition for the resonance cross section is the first ratio in this equation. But if one notes, as suggested by J. H. Marable,[265]

$$\bar{\phi}^g_{\text{cell}} = \frac{V_{\text{mod}}\,\bar{\phi}^g_{\text{mod}} + V_{\text{lump}}\,\bar{\phi}^g_{\text{lump}}}{V_{\text{cell}}}$$

$$= a\,\bar{\phi}^g_{\text{mod}} + (1-a)\int_g dE\,\sigma(E)\,W(E)\,,$$

where $a \equiv V_{\text{mod}}/V_{\text{cell}}$, and only assumes $\bar{\phi}_{\text{mod}} \sim 1/E$ (more reasonable), it follows that the input of one extra parameter a allows a better definition of a "cell" cross section. The present XSDRN resonance routines use this formulation.

The limits of $a = 0$ and $a = 1$ are interesting. In the latter case, the treatment reduces to the old method. In the former case, a zone weighting is accomplished such as would be desired if the cross sections are to be used in an explicit spatial mockup of the cell.

Sponsor: Reactor Division M. L. Tobias

S_n Parametric Study for a Selected LMFBR

N. M. Greene W. R. Cobb[237]

Before applying a theory to a new area, a study is generally required which defines the required orders of approximation and the effects of those approximations. The present study attempts to define the limits on the application of S_n theory to typical LMFBR problems.

The effects of varying the energy-group structure, the angular quadrature, the cross-section expansion order, and the spatial mesh were studied. Infinite-medium, cell, and zone weighting techniques were used to obtain cross-section data. Final results were compared with diffusion theory results for an identical case.

The reactor chosen for analysis was patterned after an "advanced" 1000-MW(e) UO_2-PuO_2 fueled LMFBR described in GEAP-5618.[266] This reactor can be mocked as a cylinder (see Fig. 18) which is 10 ft in diameter by 6½ ft high. A 3-ft-high "zoned" core contains ~70,000 fuel pins located in a hexagonal array; the inner core zone is 5 ft in diameter; the outer core zone forms a 1-ft-thick annulus around the inner core zone. Completely surrounding the core is a 1-ft-thick fertile blanket consisting mainly of depleted uranium and the coolant. The entire assembly is in turn surrounded by a 6-in. reflector layer of coolant and structural material. The principal codes used in the analysis were: XSDRN,[251] ANISN,[267] DOT,[268] and CITATION.[269]

All cross-section weighting calculations were made with XSDRN starting with 100-group data which were obtained from ENDF/B.[270] The final broad-group cross-section sets of 30, 15, and 5 energy groups

---

265. J. H. Marable, private communication.

266. *Comparison of Two Sodium-Cooled 1000 MWe Fast Reactor Concepts – Task I Report of 1000 MWe LMFBR Follow-On Work,* GEAP-5618 (1968).

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

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

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

270. H. C. Honeck, *ENDF – Evaluated Nuclear Data File Description and Specifications,* BNL-8381 (1964).

were used in ANISN, DOT, and CITATION mockups of the reactor in one and two spatial dimensions.

Table 6 is a tabulation of some results of the study. All results are for a one-dimensional radial traverse of the reactor and use a "buckling" approximation to account for the axial leakage.

For a given set of cross sections, reasonably "converged" values for k_{eff} and reaction rates are attained with an S_4P_1 calculation. ("Convergence" is used in the sense that a higher-order approximation, for example, $S_{16}P_3$, will not give very different results.)

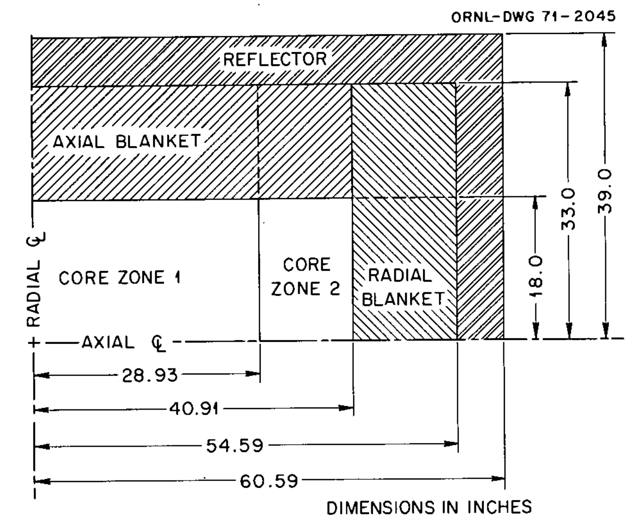

Fig. 18. Mockup for LMFBR (GEAP-5618).

Table 6. Summary of Results for a One-Dimensional Cylindrical Mockup of a Selected LMFBR

Calculation	Code	Number Energy Group	Cross-Section Weighting	Type Calculation	Number Spatial Intervals	k_{eff}	Absorptions: Core 1	Absorptions: Core 2	Absorptions: Radial Blanket	Absorptions: Reflector	Fission Source: Core 1	Fission Source: Core 2	Fission Source: Radial Blanket
1	XSDRN	100	Fine Group	S_8P_1	50	0.98986	0.46385	0.33912	0.13019	7.522×10^{-3}	0.50321	0.42899	0.057656
2	XSDRN	100	Fine Group	S_8P_3	50	0.98993	0.46359	0.33949	0.13003	7.513×10^{-3}	0.50288	0.42956	0.057494
3	ANISN	30	Inf Med	S_4P_0	50	1.00033	0.46127	0.35254	0.12364	6.194×10^{-3}	0.49992	0.44713	0.053264
4	ANISN	30	Inf Med	S_4P_1	50	0.99060	0.46438	0.33943	0.12964	7.092×10^{-3}	0.50401	0.42927	0.057302
5	ANISN	30	Inf Med	S_4P_2	50	0.99076	0.46398	0.34001	0.12941	7.081×10^{-3}	0.50353	0.43015	0.057061
6	ANISN	30	Inf Med	S_4P_3	50	0.99070	0.46398	0.33996	0.12943	7.084×10^{-3}	0.50353	0.43008	0.057084
7	ANISN	30	Inf Med	S_6P_3	50	0.99038	0.46501	0.33933	0.12937	6.995×10^{-3}	0.50471	0.42924	0.056413
8	ANISN	30	Inf Med	$S_{16}P_3$	50	0.99022	0.46496	0.33922	0.12936	7.002×10^{-3}	0.50468	0.42912	0.056406
9	ANISN	30	Cell	S_4P_3	50	0.99106	0.46410	0.34003	0.12939	7.083×10^{-3}	0.50374	0.43025	0.057054
10	ANISN	30	Cell	S_6P_3	50	0.99075	0.46506	0.33943	0.12942	7.004×10^{-3}	0.50485	0.42945	0.056439
11	ANISN	30	Zone	S_4P_3	50	0.99099	0.46389	0.33977	0.12979	7.368×10^{-3}	0.50353	0.43021	0.057235
12	ANISN	30	Zone	S_8P_3	50	0.99077	0.46426	0.33918	0.12997	7.376×10^{-3}	0.50399	0.42938	0.057387
13	ANISN	30	Inf Med	S_4P_3	39	0.99063	0.46378	0.34000	0.12964	7.082×10^{-3}	0.50334	0.43012	0.057176
14	ANISN	30	Inf Med	S_4P_3	30	0.99097	0.46403	0.33994	0.12994	7.054×10^{-3}	0.50364	0.43001	0.057293
15	ANISN	30	Inf Med	S_4P_3	15	0.98868	0.46414	0.33742	0.13175	6.327×10^{-3}	0.50398	0.42663	0.058062

More dramatic differences are noted on comparing cross-section weighting schemes. The cell-weighting results agree well with the infinite-medium results; the calculated flux traverses across the tiny cells were flat in the important energy regions. However, zone weighting produces a marked improvement in the reflector absorptions. An investigation showed a significant difference in the center spectrum vs the outside spectrum of the reactor.

The calculations were relatively insensitive to the spatial mesh. The very crude 15-interval mesh yielded a reasonable value of k_{eff}, but had inaccurate reaction rates.

The group-structure studies were made chiefly with two-dimensional calculations. The 30- and 15-group energy structures were picked to define predominant peaks and depressions in the core spectrum, but the 5-group structure could not define the spectrum very well. Results obtained from two-dimensional S_n (DOT) and diffusion (CITATION) calculations indicate that even a crude structure can give reasonable values of k_{eff}, but that reaction rates suffer.

Figures 19–22 present some of the effects of different approximations on the spatial variation of the neutron flux and the fission source.

The results of this study were presented at the ANS Summer 1970 meeting in Los Angeles.

Sponsor: Reactor Division

Gas Behavior in Molten-Salt Reactors

T. C. Tucker   C. C. Webster   H. A. McLain[237]

Inert gas bubbles are continuously injected into and removed from the circulating fluid of a molten-salt reactor to remove gaseous fission products, especially xenon and tritium.[271] We have developed a computer code to describe the behavior of these gas bubbles throughout the circulating salt loop.

We assume a known total concentration of gas at each point of the salt loop (a closed network of parallel paths). We wish to know how much gas is in salt solution, how much is in the bubbles, and at what rate the gas moves from one phase to the other. Ignoring surface tension effects, the amount of gas in solution can be determined from

$$\frac{dc}{dt} = -ka(C - Hp) , \tag{1}$$

where

C = concentration of gas dissolved in salt,

k = mass transfer coefficient,

a = surface area of gas-liquid interface,

H = Henry's law constant,

p = partial pressure of the gas.

The interface area, a, is a function of the number and size of bubbles present. The mass transfer coefficient, k, is a function of physical properties of both gas and salt, the size of the salt container, and rate of salt

271. R. J. Kedl, *MSR Program Semiann. Progr. Rept. Feb. 28, 1969,* ORNL-4396, pp. 92–94.

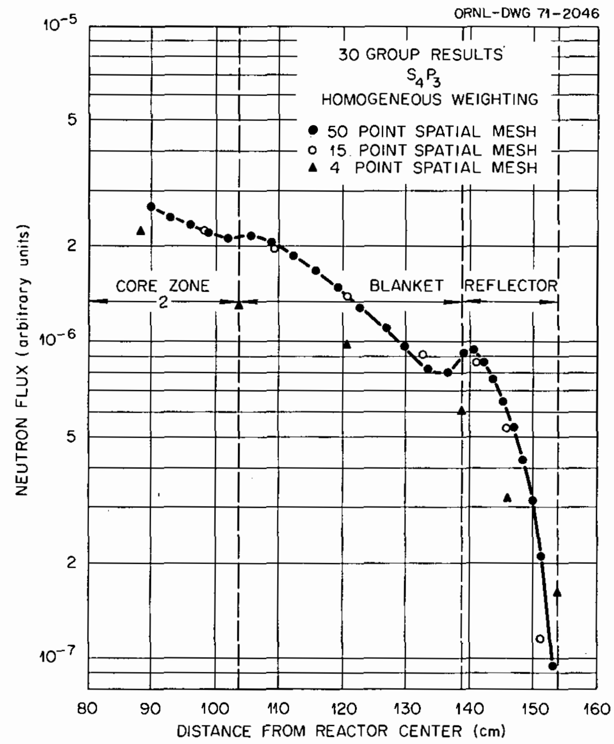

Fig. 19. Radial flux variation, 2.61 to 3.35 keV.

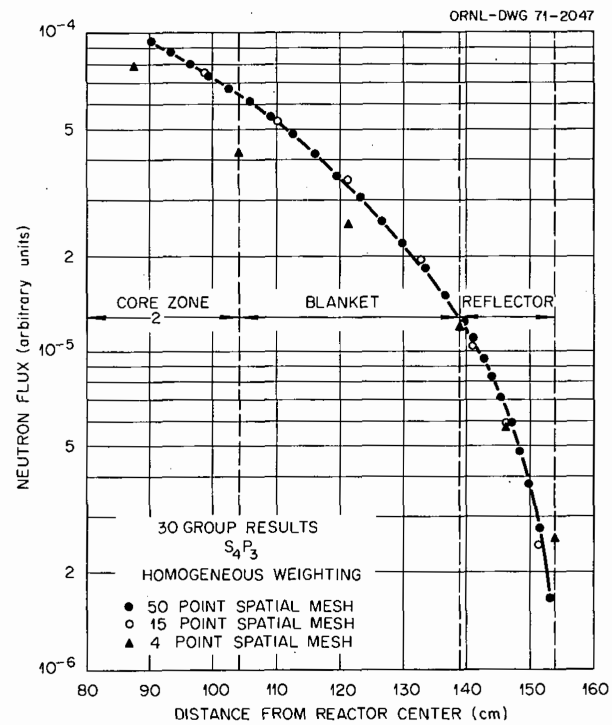

Fig. 20. Radial flux variation, 19.3 to 24.8 keV.

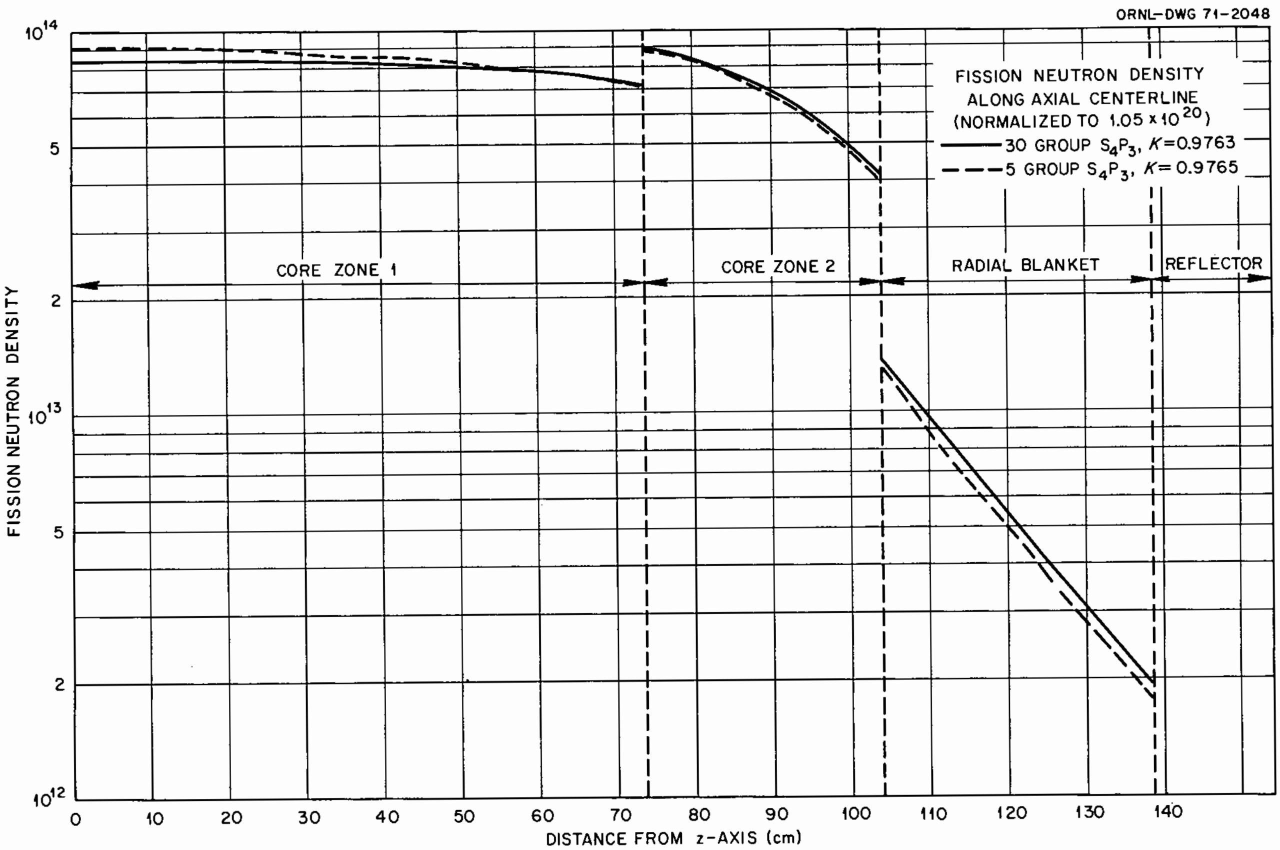

Fig. 21. Radial variation of fission source.

flow. At present, three distinct correlations for k are in use. The Henry's law constant, H, is a function of temperature, which, along with the pressure, p, is a function of location within the salt loop.

We have divided the network into a number of segments. Some of these segments represent junctions of two or more incoming streams. The properties at the end of the segment are calculated by assuming perfect mixing. For the remaining segments, Eq. (1) is modified to the following function of position:

$$\frac{dc}{dx} = -Mk\theta^{2/3}(C - Hp) , \tag{2}$$

where

x = the variable of position, either a length or a volume,

M = a function of the segment of the flow loop relating position to time,

θ = the specific volume of the bubbles.

Starting with an assumed dissolved gas concentration at some point in the network, we calculate successive concentrations from Eq. (2) using the Bulirsch-Stoer algorithm, or by using weighted averages for junction points. Upon returning to the starting point, we generally observe a different concentration than that assumed. We iterate until a specified difference in these values is obtained.

The results are printed so that a flow chart with cutouts can be overlaid. Thus the values for any point of the flow loop are evident to the engineer without possible ambiguity or translation error.

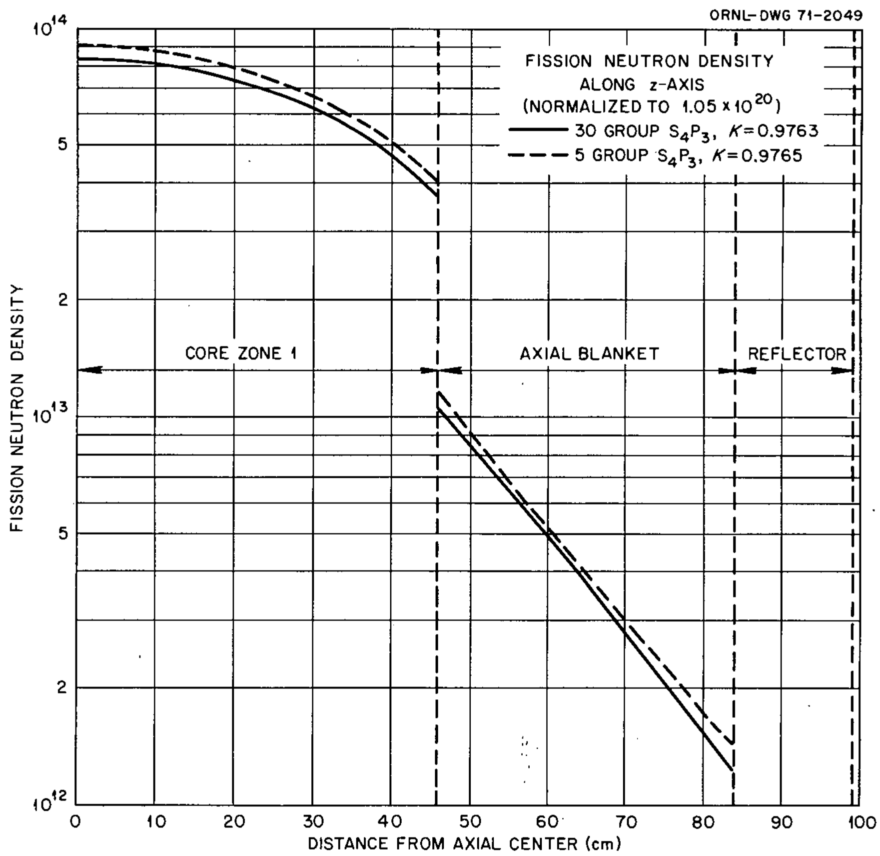

Fig. 22. Axial variation of fission source.

We designed the code to be evolutionary in nature so that revisions in reactor design or other data would require relatively little recoding. Recent data describing the bubble size distribution and mass transfer of gases to and from bubbles flowing concurrently with liquids[272] are being incorporated into the code.

Sponsor: Reactor Division H. A. McLain

REACTOR CHEMISTRY DIVISION

Fission Product Diffusion Program

C. C. Webster

A program for solving one-dimensional linear and nonlinear diffusion problems (prepared by Gulf General Atomic in FORTRAN V language for use in a Univac computer) has been adapted to ORNL's IBM 360 computer in the FORTRAN IV language. The program is capable of solving a wide range of diffusion and heat transfer problems but has been adapted specifically to fission products diffusion problems within the reactor environs. It utilizes decay constants, diffusion coefficients, and mass transfer coefficients, as

272. T. S. Kress, *MSR Program Semiann. Progr. Rept. Feb. 28, 1970,* ORNL-4548, pp. 90–91.

well as the gas temperature and pressure inside and outside the outer boundary. The input capabilities are: 52 mesh points, 52 initial concentration values, 52 diffusion coefficient values, temperature data at 52 mesh points with linear interpolation between mesh points, and 4 isotopes. Calculations can be made in as many as 100 time steps. At each time step the concentration is computed as well as each quantity dependent on concentration at the last time step. Sources, temperatures, and other time-dependent parameters are computed at each time step.

Sponsor: Reactor Chemistry Division — W. E. Browning

SOLID STATE DIVISION

A Computer Program for Controlling an Autocorrelation Neutron Time-of-Flight Spectrometer

S. H. Merriman L. W. Gilley

A PDP-15/30 computer has been interfaced to a neutron time-of-flight spectrometer for the purpose of controlling the experimental apparatus and data acquisition devices. We have written programs for positioning up to eight stepping motors (thereby determining sample position and neutron detector position). Data collection programs have been written which make a quick scan of the diffracted neutron beam and which make a detailed survey of the beam, using up to 16 counters. The latter provides a cathode ray tube display of the raw TOF data in histogram form.

The information attainable in time-of-flight experiments can be increased by using computer-generated pseudorandom pulses to produce a magnetically modulated neutron beam. We are preparing a series of programs for cross-correlating the known pseudorandom sequence and the TOF data. This correlation technique will be used to extract scattering information and to determine cross sections. Previously collected data can be analyzed in a background/foreground system concurrently with data acquisition and display.

Sponsor: Solid State Division — H. A. Mook

THERMONUCLEAR DIVISION

MHD Equilibrium and Stability Computations

R. H. Fowler

Magnetohydrodynamic equilibria and their stability are being studied in collaboration with the Thermonuclear Division and in support of the ORMAK experiments. An equilibrium code has already been developed[273] to treat ideal MHD equilibria for very general geometries. The code solves the equations grad $P = \mathbf{J} \times \mathbf{B}$ and curl $\mathbf{B} = 4\pi\mathbf{J}$, with the boundary condition $\mathbf{B}\cdot\hat{\mathbf{n}} = 0$ at the conducting wall. Implicit constraints on the equilibrium may also be included.

A computer code is being developed to study the stability of ideal MHD equilibria for TOKAMAKs. The method of approach being used is linear dynamical analysis and involves obtaining the time evolution of the displacement vector $\boldsymbol{\xi}(\mathbf{r}, t)$ from the equation

$$\rho \frac{\partial^2 \boldsymbol{\xi}(\mathbf{r}, t)}{\partial t^2} = \text{grad } [\gamma P \text{ div } \boldsymbol{\xi} + \boldsymbol{\xi}\cdot\text{grad } P] + \mathbf{J} \times \mathbf{Q} - \mathbf{B} \times \text{curl } \mathbf{Q} \, ,$$

273. R. A. Dory and R. H. Fowler, *MHD Equilibria in Tokamaks and Doublets*, The Sherwood Meeting, April 1970.

where $\mathbf{Q} = \text{curl}(\boldsymbol{\xi} \times \mathbf{B})$ and $\boldsymbol{\xi}\cdot\hat{\mathbf{n}} = 0$ at the conducting wall. The input is the pressure, magnetic fields, etc., obtained from the equilibrium calculations.

Sponsor: Thermonuclear Division

Plasma Physics

G. S. McNeilly

The computer code IONS calculates the solution of the Fokker-Planck equation for a mirror-confined plasma. This solution provides an estimate of the plasma containment time as a function of various device parameters, and is thus useful in fusion feasibility studies. The numerous physical and calculational assumptions contained in the code are described in the literature.[274]

The code was originally written in LRLTRAN for a CDC 6600 and now compiles in IBM FORTRAN IV double precision and runs on OS 360.

Sponsor: Thermonuclear Division

INTERDIVISIONAL PROJECTS

Maintenance of ENDF/B Evaluated Neutron Cross-Section Data and Related Computer Programs via the ORNL Cross Section Steering Committee

S. K. Penny J. D. Jenkins[275] D. K. Trubey[276]

The ORNL Cross Section Steering Committee was formed on April 27, 1970, by a letter proposing such a jointly funded activity.[277] Many activities were already under way before the establishment of this committee but were not officially supervised nor funded jointly as is now the case.

The Radiation Shielding Information Center (RSIC) is the point of contact for the National Neutron Cross Section Center (NNCSC) and as such receives ENDF/B tapes and related computer programs for all of ORNL. The responsible personnel of RSIC, R. W. Roussin, I. J. Brown, and formerly D. K. Trubey, work closely with R. Q. Wright of the Mathematics Division to check these data tapes for errors and to notify the Steering Committee and other interested persons of the existence of the data. R. Q. Wright then places the new data in the ORNL ENDF/B library which currently resides on a disk owned by the Reactor Division.

Superficially this seems a simple and straightforward task. However, two facts complicate matters and force a continuous maintenance not only of the data file but of the utility programs which manipulate and display the data and of the processing programs which transform the data to the myriad forms required for ORNL use. These two facts are: (1) the data changes in character and quantity because of more sophisticated experiments and calculations and (2) the data formats and handling procedures change either because of (1) or because need for new types of data arises.

---

274. John Killen and Kenneth D. Marx, in *Methods in Computational Physics,* vol. 9, Academic, New York, 1970.

275. Reactor Division.

276. Director's Division, Environmental Study.

277. Letter from J. D. Jenkins, S. K. Penny, and D. K. Trubey to S. E. Beall, F. C. Maienschein, A. M. Perry, and C. E. Clifford, "Outline for the Joint Neutron Physics, Reactor Division, and RSIC Cooperative Program for Local Nuclear Data Management," April 27, 1970.

Version 2 of the ENDF/B data file involved extensive format changes, and as a consequence errors were frequently encountered on the new tapes. R. Q. Wright corrected all errors as he was notified of them or discovered them. He also changed the utility program EDIT to read the new formats, as well as the processing program SUPERTOG.[278]

With the establishment of formats and procedures for gamma-ray production cross sections[279] and the gradual influx of such data, programs had to be altered or modified. The utility program CHECKER was modified by J. L. Lucius and R. Q. Wright of the Mathematics Division.[280] The utility program EDITOR,[281] originally the program EDIT, was modified for the gamma-ray production files by C. L. Thompson of the Mathematics Division. Currently J. L. Lucius and R. Q. Wright are modifying the PLOTFB program.[282]

Currently V. A. Singletary of the Mathematics Division is converting the data for Cl, K, Mg, and Na to version 2 formats, merging the gamma-ray production files with neutron files, and correcting errors in the angular distributions for both neutrons and secondary gamma rays. It is anticipated that there will be a joint effort involving J. L. Lucius, R. Q. Wright, and M. B. Emmett to continue the work reported in this annual[283] to create an ENDF/B plotting program satisfying more general ORNL needs than the program PLOTFB.

J. L. Lucius has written an information retrieval program[284] to retrieve information about cross-section data sets, both microscopic and multigroup, available at ORNL.

The Steering Committee works with the Cross Section Evaluation Working Group of NNCSC and has members of the various subcommittees.[279] The Steering Committee has been recently joined by J. L. Lucius, F. R. Mynatt, and R. W. Roussin, who replaced D. K. Trubey.

Sponsor: ORNL Cross Section Steering Committee (Reactor and Neutron Physics Divisions)

An Index of Nuclear Data Libraries at ORNL

J. L. Lucius R. Q. Wright J. D. Jenkins[275]

A program has been initiated under the auspices of the Oak Ridge Cross Section Steering Committee to index the major cross-section libraries frequently used at ORNL.

The purpose of this index is to provide cross-section users with a current, concise, and systematic reference to cross-section data available at ORNL. To initiate this effort, a computer program called INDEX has been written to index the ENDF/B,[285] GAM-II,[286] XSDRN[287] 123-group, and XSDRN 100-group

---

278. R. Q. Wright, *SUPERTOG II, a Multigroup Neutron Cross Section Code,* this report.

279. S. K. Penny, *Activities Connected with the Cross Section Evaluation Working Group,* this report.

280. J. L. Lucius and R. Q. Wright, *CHECKER Modification,* this report.

281. C. L. Thompson, J. R. Stockton, L. M. Petrie, and R. Q. Wright, *EDITOR – an ENDF/B Cross-Section Editing and Manipulation Program,* this report.

282. R. Q. Wright, *PLOTFB, a Plotting Program for ENDF/B Data,* this report.

283. M. B. Emmett, R. Q. Wright, and S. K. Penny, *Plotting of ENDF/B Evaluated Neutron Cross Sections for General ORNL Use,* this report.

284. J. L. Lucius, R. Q. Wright, and J. D. Jenkins, *An Index of Nuclear Data Libraries at ORNL,* this report.

285. 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.

286. G. D. Joanou and J. S. Dudek, *GAM-II, a B_3 Code for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants,* GA-4265 (September 1963).

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

libraries. Also, two satellite computer programs have been written to interrogate the GAM-II and XSDRN libraries for the items of information needed for a meaningful index.

Currently, the INDEX program is being used to generate an edit of the following items of information about each material residing in the four libraries previously mentioned:

1. material name,
2. library name,
3. library identification number and the (Z, A) number of the material,
4. reaction types,
5. category,
6. format,
7. source of the data,
8. evaluator,
9. date when the data became available for use at ORNL,
10. document name and number,
11. number of resolved resonances,
12. an indication of the presence or absence of unresolved resonance data,
13. comments.

In addition to the complete edit, the INDEX program also generates selective edits and data collection functions on command.

The ENDF/B version II data recently received from the National Neutron Cross Section Center, Brookhaven National Laboratory, currently is being assimilated into the ORNL GAM-II and XSDRN libraries. At the completion of this task, the first index will be published along with documentation of the INDEX program.

Sponsor: Oak Ridge Cross Section Steering Committee (Neutron Physics Division and Reactor Division)

EDITOR – an ENDF/B Cross-Section Editing and Manipulation Program

C. L. Thompson J. R. Stockton[288] L. M. Petrie R. Q. Wright S. K. Penny

The Evaluated Nuclear Data File[285] (ENDF) is a system designed to facilitate the exchange of cross-section data between users. The ENDF/B library is a data collection normally stored on binary magnetic tape in a format that can be used as input to cross-section processing codes. A BCD (card image) format is also defined so that data may be more easily translated into the ENDF/B library and for exchanging cross-section data between laboratories.

The FORTRAN-IV program EDITOR for the IBM 360 is a revision and extension of program EDIT,[289] which was designed to print, in a readable form, the contents of ENDF/B data tapes. EDITOR allows copying, altering mode, merging, punching, and editing data in the ENDF/B format from and to binary or BCD tapes or cards.

---

288. Tennecomp Corp., Oak Ridge, Tenn.
289. *Math. Div. Ann. Progr. Rept. Dec. 31, 1966,* ORNL-4083, p. 34.

EDITOR will be extended and updated when necessary to conform to ENDF standards.

ENDF data are ordered as "materials" (element, isotope, molecule, or mixture) which contain "files" (class of data) each of which has data in "sections" (reaction type), subsections (collection of data within a section), and energy-data pairs. Materials, files, and sections bear integer labels defined by the ENDF system and are organized as units within a data set. EDITOR will process a material, file, or section, but must process a section completely since there is no method for standard reference of a subsection or data pair. EDITOR will process, alternatively, all materials, all files in a material, all of specified files in all materials, all sections of a file, all specified sections of specific files in all materials, or only those explicitly named materials, files, and sections from an ENDF/B tape as controlled by the user.

Sponsor: Neutron Physics Division and ORNL Cross Section Steering Committee (Neutron Physics and Reactor Divisions)

CHECKER Modification

J. L. Lucius R. Q. Wright

The CHECKER[290] program obtained from the National Neutron Cross Section Center, Brookhaven National Laboratory, has been made operational on ORNL computers and extended to process the photon files 12–16.

The purpose of CHECKER is to check the data on an ENDF/B[285] BCD card-image tape. The tape is primarily tested for the correctness of its structure and formats as well as the consistency of the data.

Sponsor: Neutron Physics Division and ORNL Cross Section Steering Committee (Neutron Physics and Reactor Divisions)

SUPERTOG-II, a Multigroup Neutron Cross Section Generator

R. Q. Wright

A revision of SUPERTOG,[291] designated as SUPERTOG-II, has been completed. This new package will accept ENDF/B[285] version II data. In addition, some modifications were made to the code to allow new options. With the replacement of four subroutines, SUPERTOG-II may also be used to process ENDF/B version I data.

Changes in the calculational model:

1. **Smooth cross sections.** SUPERTOG now processes the $(n,n')\alpha$, $(n,n')3\alpha$, and $(n,n')p$ reactions if data are given in ENDF/B file 3. These results are also used to generate contributions to the inelastic scattering matrix as well as being included in the total cross section.

2. **Resonance cross sections.** The resolved resonance treatment has been revised and is now equivalent to the method shown in Appendix C of ref. 285. The notation used is more nearly that used by John M. Otter.[292] This treatment treats $l = 1$ resonances correctly and provides for the multilevel scattering

290. Henry C. Honeck, *Description of the ENDF/B Processing Codes and Retrieval Subroutines, ENDF-110,* BNL-13582 (September 1967). Revised September 1970.

291. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, Jr., *SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B,* ORNL-TM-2679 (1969).

292. J. M. Otter, "Comment on the Calculation of the Scattering Cross Section for Multiple Resonances," Technical Note, *Nucl. Sci. Eng.* 28 (1967).

formula. SUPERTOG has also been modified to calculate a background which is consistent with the GAM[286]/XSDRN[287] Nordheim treatment. The unresolved resonance treatment has been modified to permit the use of energy-dependent unresolved resonance parameters (ENDF/B format modification 69-6).

3. **Inelastic and $(n,2n)$ matrices.** The inelastic scattering reactions $(n,n')\alpha$, $(n,n')3\alpha$, and $(n,n')p$ are now included in the inelastic scattering matrix if data for these reactions are given on the ENDF/B tape. SUPERTOG now processes $LF = 1$ (arbitrary tabulated function) data for secondary energy distributions.

4. **Weighting functions.** A new weighting option $1/(E\sigma_t)$ designated as $IW = 6$ is now available. The weighting function is generated by using the total cross section from ENDF/B file 3. This option cannot be used if resonance parameters are given in ENDF/B file 2.

Sponsor: Neutron Physics Division and Reactor Division

XLACS, a Program to Produce Fine-Group Averaged Cross Sections from ENDF/B Data

N. M. Greene R. Q. Wright J. L. Lucius

Work has continued on the development of XLACS, a computer program which calculates fine-group averaged cross sections from ENDF/B data.[285] The cross sections can be selectively edited or plotted. A complete set of tape manipulations (updating, editing, plotting) is provided within the single program.

The ENDF/B format is very general and allows data to be specified in several ways for practically any nuclear process. Cross sections are given in point-wise and parametric representations, depending primarily upon what data are supplied. This generality requires a corresponding and even expanded generality upon the part of processing codes which use the data. We have attempted to design flexibility into the XLACS code so new processing routines can be (relative to most codes) added easily to the basic package as these general representations of data become important.

A significant feature of XLACS is its flexible dimensioning which allows the program to reuse areas of core storage without limiting the user to a set of fixed dimensions inherent in any FORTRAN equivalencing scheme. A properly flexibly dimensioned program does not waste core and will run any problem which can be defined within the confines of available data storage. This feature, combined with an overlay scheme, allows new treatments, routines, and options to be added at very little core penalty, unless, of course, the new treatments are abnormally lengthy compared with the longest old treatment.

It is illuminating to examine the steps involved in making and updating a cross-section library tape for the *full-range* (energy sense) cross-section weighting code XSDRN.[287] Six separate computer codes must be run, and these require redundant data input, excess data handling, and a disproportionate amount of time to go from one end to the other. In schemes such as this, cross-section group structures and expansion orders are definitely limited and, in some cases, absolutely defined, *with no easy way for change.* The flexible dimensioning in XLACS eliminates the restrictions on group structures, expansion orders, number of resonances, etc. Input data are required for only one code. In addition, this code serves as a complete cross-section manipulation package for XSDRN library tapes.

The input data required by XLACS, with the exception of title cards, are read in the very efficient FIDO format which is already in use by the codes ANISN,[293] XSDRN, and DOT.[294] Treatments are provided for

1. smooth neutron cross sections,
2. elastic scattering,
3. inelastic scattering,
4. $(n,2n)$,
5. resolved resonances,
6. unresolved resonances,
7. $S(\alpha, \beta)$ thermal data.

For resonance nuclides, XLACS performs infinite-dilution calculations, but also passes resonance data for a Nordheim[295] treatment in XSDRN.

In addition to processing ENDF data as noted above, XLACS will

1. make an XSDRN cross-section library tape,
2. update an XSDRN cross-section library tape,
3. selectively edit data on an XSDRN master library tape,
4. selectively plot data on an XSDRN master library tape.

These processes are independent. One operation does not require or assume any other.

The code is being readied for release, and a report is in preparation.

Sponsor: Reactor Division and Neutron Physics Division

XSDRN: A Discrete Ordinates Spectral Averaging Code

N. M. Greene C. W. Craven, Jr.[275]

XSDRN[287] is a discrete ordinates spectral code for the generation of nuclear multigroup constants in the fast, resonance, and thermalization energy regions. It employs a variable dimensioning technique which optimizes the use of core storage. The code calculates an arbitrary number of flux moments for zero or one-dimensional systems. Several problem types are provided for, including fixed source, eigenvalue, and criticality search. Extensive cross-section libraries are available which can be reduced, using calculated fine-group fluxes, to arbitrary broad-group structures. Provisions are available to produce library tapes for several codes.

During the past year, the work with XSDRN has been general maintenance primarily, but several improvements and additions have been made including:

---

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

294. F. R. Mynatt, *A User's Manual for DOT, a Two-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering,* K-1964 (to be published).

295. L. W. Nordheim, "The Theory of Resonance Absorption," in *Symposium on Applied Mathematics,* vol. XI, 1961.

1. The code will now produce a "cooperative interface" formatted tape.[296]
2. Improvements, as discussed elsewhere in this report, to the resolved resonance routine have been made which extends the range of application of the Nordheim integral treatment.[295]
3. The S_n output options have been expanded to allow more general output.

Sponsors: Reactor Division and Neutron Physics Division

Heat Transfer Studies

W. D. Turner Peggy G. Fowler
M. Siman-Tov[297]

Many of the current projects at the Laboratory generate complex heat transfer problems whose solutions are best approximated by utilizing numerical techniques such as finite difference methods. Since many of these problems are similar in nature, it is feasible to develop and maintain a general heat transfer code or group of codes to obtain steady-state and/or transient temperature distributions.

For problems we have studied in the past, we have employed a general heat conduction code, HEATING2,[298] which is a modification of the HEATING program.[299] HEATING2 is capable of solving problems containing a maximum of 8500 nodes and is designed to solve steady-state and/or transient heat conduction problems in one-, two-, or three-dimensional Cartesian or cylindrical coordinates. Thermal conductivity, density, and specific heat may be both spatially and temperature dependent, while heat generation rates and boundary conditions may be both spatially and time dependent. The mesh spacing may be variable along each axis.

During the past year we have modified HEATING2 in order to meet some of the current needs in our heat transfer studies. This latest version, HEATING3,[300] considers radiative, natural convective, and forced convective heat transfer from a surface to an external medium whose temperature may vary both with position and time. Likewise, the code allows radiative, natural convective, and forced convective heat transfer across an internal gap.

For some transient problems the numerical technique dictates a small time step which, in turn, requires a large amount of computing time to solve the problem. As a first step toward alleviating this disadvantage, we have incorporated into HEATING3 a modification of the numerical technique which eliminates the restriction of a small time increment.[301] From our test cases, this modification appears to be useful for certain problems.

As an aid in analyzing the temperature distributions created by the code, a contour plotting program has been adapted for use with output from HEATING and HEATING3 to create isothermal plots.

---

296. G. W. Cunningham III, T. B. Fowler, and D. R. Vondy, *Reactor Division Cooperative Code Development,* this report.

297. General Engineering and Construction Division.

298. W. D. Turner and J. S. Crowell, *Notes on HEATING – an IBM 360 Heat Conduction Program,* CTC-INF-980 (November 1969).

299. R. R. Liguori and J. W. Stephenson, *The Heating Program,* ASTRA, Inc., Raleigh, North Carolina, ASTRA 417-5.0 (January 1961).

300. W. D. Turner and M. Siman-Tov, *HEATING3 – an IBM 360 Heat Conduction Code,* ORNL-TM-3208 (December 1970).

301. S. Levy, *Use of "Explicit Method" in Heat Transfer Calculations with an Arbitrary Time Step,* General Electric Research and Development Center, Schenectady, New York, GE-68-C-282 (August 1968).

Among the heat calculations we performed during the past year with HEATING3 were studies of temperature distributions in the beryllium target in the ORELA program and in shields for an orbiting nuclear space station. These studies were conducted for J. Lewin of the Neutron Physics Division.

Calculations were also conducted for a series of heat transfer problems arising from the thermal analysis of LMFBR oxide fuels. These calculations were performed for C. M. Cox, R. B. Fitts, and A. R. Olsen of the Metals and Ceramics Division.

Sponsors:	General Engineering and Construction Division	M. Siman-Tov
	Health Physics Division	R. L. Bradshaw
	Metals and Ceramics Division	C. M. Cox
	Neutron Physics Division	J. Lewin

Information Retrieval

N. B. Gove	Linda P. Helton
A. F. Joseph	A. A. Brooks
Norma A. Buhl	V. A. Singletary

We wrote an information retrieval program, ORLOOK, which can be used to search a file for specified words or strings and print out records or groups of records containing the specified items. Logical "and," "or," and "but not" requests can be used. The request format is free-form, and almost any file format may be searched. CRBE files may be searched with ORLOOK (see Fig. 23 for sample output).

We are making a comparison study of several large-scale information retrieval systems: CIRK, RECON, and SPIRES.

We are participating in the design of an information management system for environmental information.

ORNL- DWG 71-2050

```
  ORLOOK INFORMATION RETRIEVAL PROGRAM
 SEQU  79,80
 LOOK FOR 'DIFFUSION'
 FILE
                                     LIST OF ANSWERS FCUND

WAPD-TM-639               THERMAL FEEDBACK CALCULATIONS IN THE PCQ-5 FEW-        201
WAPD-TM-639               GROUP NEUTRON DIFFUSION-DEPLETICN COMPUTER             202
WAPD-TM-639               PROGRAM                                         *      203
WAPD-TM-639               01/67    SORENSEN,JN                                   204
WAPD-TM-395               THE UTILIZATION OF THE NEUTRON DIFFUSICN PROGRAM       501
WAPD-TM-395               PDQ-5                                           *      502
WAPD-TM-395               01/65    HAGEMAN,LA,PFEIFER,CJ                         503
WAPD-TM-671               M0807-A DIFFUSION THEORY FITTING PROGRAM USING        1401
WAPD-TM-671               FORTRAN-IV                                      *     1402
WAPD-TM-671               09/67    RUTHERFORD,CH                                1403
WAPD-TM-532               WIGL2-A PROGRAM FOR THE SOLUTION OF THE ONE-          2301
WAPD-TM-532               DIMENSIONAL, TWO-GROUP, SPACE-TIME DIFFUSION          2302
WAPD-TM-532               EQUATIONS ACCOUNTING FOR TEMPERATURE, XENON AND       2303
WAPD-TM-532               CONTROL FEEDBACK                                *     2304
WAPD-TM-532               10/65    HENRY,AF,VOTA,AV                             2305
WAPD-TM-532 ADDENDUM 1    01/67                                           +     2306
ANL-7319                  CANDID-1D, A ONE-DIMENSIONAL, MULTIGROUP              2901
ANL-7319                  DIFFUSION-THEORY PROGRAM FOR THE CDC-3600       *     2902
ANL-7319                  05/67    ZEMAN,JL,GREENSPAN,H,BUTLER,MK               2903
ANL-7305                  ANL-CANDID, A TWO-DIMENSIONAL, DIFFUSICN-THEORY       3001
ANL-7305                  CODE BASED ON CANDID2D                          *     3002
ANL-7305                  09/67    LEAF,GK,KENNEDY,AS,JENSEN,GC                 3003
WAPD-TM-891               WANSY-A PROGRAM TO SOLVE THE STATIC TWO-              4401
WAPD-TM-891               DIMENSIONAL GROUP DIFFUSION EQUATIONS BY              4402
WAPD-TM-891               SYNTHESIS METHODS                               *     4403
WAPD-TM-891               07/69    YASINSKY,JB,MARINACCI,JW,VOTA,AV             4404

  211 CARDS READ CONTAINING        59 RECORDS.              7 ANSWERS FOUND
```

Fig. 23. Result of ORLOOK retrieval.

We are receiving summary tapes for the 1970 census and loading data on the data cell for the Urban Growth Patterns Project. We have installed into the CRBE (Conversational Remote Batch Entry) system several programs (MOD1, MOD2, MOD3) obtained from Dual Labs, Inc. These programs can be used to retrieve and tabulate data from the census files. In addition, programs were written to use the output from the above programs to calculate rate of migration, proportion of native-born population living in the state, percent of nonwhite population in four categories, median age of native and migrant populations, and index of age influence.

Sponsor: ORNL-NSF Environmental Program and Civil Defense Research Project

Documentation of the Computing Technology Center Numerical Analysis Library[302]

G. W. Westley   J. A. Watts[303]

A collection of numerical techniques has been implemented in subroutine form for the IBM 360 system. This work is an extension of an earlier similar collection[304] which contained about half of the present subroutines. These techniques are provided in 90 primary subroutines which have been documented in a recent publication.[302] The documentation provides the necessary information for the user to effectively employ the numerical methods without having to concern himself with the programming details.

The subroutines provide numerical analysis support in the areas of interpolation, approximation, differentiation, integration, differential equations, linear algebra, nonlinear optimization, linear least squares, nonlinear least squares, sorting, searching, random number generation, scaling, plotting, and special functions.

The package has been placed on system devices at ORNL for use by the technical personnel.

As additions or modifications are verified, these will be used to update the program package.

Sponsor: Ecological Sciences Division   S. I. Auerbach
Computing Technology Center
Responsibility for maintenance has been transferred to
ORNL Mathematics Division

The Management and Analysis of Mixed Alphanumeric and Digital Information

A. Hume[305]   Peggy G. Fowler   J. Watts[306]   B. Handley[306]
M. Feezell[306]   Kim O. Bowman   A. A. Brooks

The problem of providing computer software to carry out the selection and statistical analysis of data of unspecified format or content was seriously addressed about three years ago on behalf of the Biology Division. A brief description of the earlier years' work is given to provide a continuity in reporting. It was decided to provide a data management program capable of processing records which were

---

302. G. W. Westley and J. A. Watts (eds.), *The Computing Technology Center's Numerical Analysis Library,* CTC-39 (1970).
303. Applied Science Department, Computing Technology Center.
304. R. E. Funderlic (ed.), *The Programmer's Handbook,* K-1729 (1968).
305. Formerly with UCND at CTC.
306. Currently with UCND at CTC.

specified only to the degree that they would be self-describing nested lists which were equivalent to tree structures, hierarchies, and arrays. The analysis capability would be provided by a load and execute compiler which processed a language having powerful list-processing Boolean operators for selection purposes, a frequency-count and averaging capability, and a linear regression analysis capability. It was designed to operate from the previously described records and to process incomplete records.

The data management function is contained in ADSEP – Automated Data Set Edit Program[307,308] which permits the user to:

1. define the structure and nomenclature of the hierarchical structure desired;
2. perform the usual editing functions of adding, deleting, correcting, concatenating, pooling, listing, etc., at any level of the hierarchy;
3. supply data input and data reduction procedures when the standard options will not suffice;
4. avoid the tedious detail of record structure and internal record descriptors.

The program is accompanied by a dictionary management program and subroutines should a subject-oriented multiuse thesaurus utilizing abbreviations and synonyms be desired.

The analysis capabilities are embodied in SADS – Statistical Analysis of Data Sets[309,310] which is a sophisticated language enabling the user to:

1. define subsets of his data based on complex Boolean criteria related to simple fields, lists, correlated lists, and nested lists;
2. tally and display rectangular arrays of frequency counts, means of values or expressions, and their standard deviations;
3. carry out several multiple linear regressions each having several dependent variates and display the results;
4. be unaware of missing portions of the data.

The program is designed to operate using the aforementioned thesaurus and a sequential file of records having the general format mentioned. The compiler is replete with diagnostics and error trace commands. The language can be interfaced with Fortran.

The following is a list of problems which have made use of this system:

1. Biology Division – analysis of the low-level radiation experiment data involving the anamnesis, pathology, and hematology of mice; analysis of mouse colony data (incomplete).
2. Biology Division – analysis of data from the controlled air contaminant experiments on mice.
3. Oak Ridge Gaseous Diffusion Plant – analysis of cascade pilot plant data; analysis of barrier production plant data.
4. Molecular Anatomy Project – analysis of ORNL medical histories (incomplete).

---

307. A. A. Brooks, *DSEP, a Data Set Edit Program,* K-1748 (June 23, 1968).

308. A. A. Brooks, *ADSEP, an Automated Data Set Edit Program,* CTC-34 (May 12, 1970).

309. A. Hume and A. A. Brooks, *SADS, Statistical Analysis of Data Subsets, a Status Report,* K-DP-3310 (July 26, 1968).

310. A. Hume and A. A. Brooks, *The SADS Program – Statistical Analysis of Data Subsets,* CTC-19 (Oct. 9, 1969).

The authors are indebted to M. Kastenbaum and F. Miller for frequent consulting and moral support.

Sponsors: Biology Division (principal)	A. C. Upton, M. Hanna
ORGDP	J. Snyder, J. McKeever
MAN	N. Anderson

A General Scattering Law Kernel Using $S(\alpha, \beta)$ Data from ENDF/B

G. W. Morrison L. M. Petrie, Jr. R. S. Carlsmith[275]

A general thermal scattering kernel which uses the so-called "general scattering law" data has been written. Egelstaff shows how the double-differential cross section is related to the scattering law.[311] Assuming a Fermi pseudopotential, the scattering cross section for a single scattering species can be evaluated using the first Born approximation to give:

$$\frac{d^2 \sigma}{d\Omega \, dE_f} = \frac{\sigma_h}{4\pi kT} \sqrt{\frac{E_f}{E_i}} e^{-\beta/2} \, S(\alpha, \beta) \, . \tag{1}$$

This is transformed to a probability distribution on α and β:

$$P(\alpha, \beta | E_i) = \frac{1}{\sigma^s(E_i)} \frac{\sigma_b kT}{4E_i} e^{-\beta/2} \, S(\alpha, \beta) \, . \tag{2}$$

A clever technique for sampling from a continuous distribution at n points has been formulated.[312] This technique also preserves the first $2n - 1$ moments of the distribution. Using this technique in Eq. (2) permits the rapid selection of α and β with a minimum of storage.

Sponsors: Reactor Division and Y-12 Critical Experiments Facility

PDP Computers

D. L. Wilson G. W. Chandler R. C. Durfee H. J. Hargis

We have written a variety of programs for PDP-8 and PDP-9 computers.

For the nuclear fission project of F. Plasil and H. W. Schmitt we have written programs to interface a PDP-9 with the experimental equipment.

For the I and C Division, we converted PALFTN[313] to run on the IBM 360 computers and produce program tables as well as the PDP-8 program. We have written several software systems using the Digital Equipment Corporation conversational language FOCAL.

Sponsor: Instrumentation and Controls Division and Physics Division

311. P. A. Egelstaff, *Nucl. Sci. Eng.* **12**, 250 (1962).
312. R. R. Coveyou, private communication.
313. D. L. Wilson and J. M. Jansen, *PALFTN, a 360 Program to Assemble PDP-8 PAL Programs* (report in preparation).

AECOP

Transport Calculations (HAMMER Code) for Study of Economical Advantages in Element Design Changes of Certain Savannah River Reactor Lattices

O. W. Hermann G. F. O'Neill[314]

A feasibility planning study was performed using a series of neutron transport and burnup calculations to determine the effects of major modifications to target elements in certain Savannah River reactor lattices. HAMMER[315] was used in obtaining criticality calculations, which were analyzed and recomputed as needed in the process of obtaining optimized reactor parameters and maximum safety controls.

HAMMER is a group of codes containing about 20,000 source cards; it was provided by the Savannah River Laboratory, where the major developments of the code system were made. HAMMER incorporates the programs THERMOS, HAMLET, FLOG, THOR, HERESY, and DIED with the control program CAPN as explained in the operations manual.[316] Briefly, the options of the program provide for: (1) multigroup transport reactor-cell calculations, (2) multiregion or mixed lattice source-sink model computations using the cell parameters, (3) a total reactor-material-balance edit showing effects of burnup and decay over a requested time interval, and (4) repeated passes through the complete computation with refined concentrations until convergence criteria are met. The HAMMER project required a summary of results from about 50 computer runs in addition to several trials for better optimization. A short code was written for giving empirical adjustments, and an organized summary, as well as a calculation of the equivalence of certain materials to excess reactivity. Slight changes were made in HAMMER, which reduced the number of material edit prints and provided punched data cards for the next reactor passes; these changes enhanced accuracy and saved considerable time.

Conclusions and results will be reported elsewhere,[317] giving the comparisons of the 20 to 30 most useful parameters obtained for each reactor design in addition to the input data which may be needed for further studies. Results seem to be sufficient to indicate a significant economic advantage in the modifications studied.

Sponsor: Production Reactor Group of AECOP G. F. O'Neill

Transport Calculations (HAMMER Code) for Survey Study of Transuranic Element Production of Various Power Reactors

O. W. Hermann J. P. Hamric[318]

A survey study of transuranic element production of various power reactors is being performed with the utilization of the neutron transport and burnup codes in HAMMER.[315,316] The standard BWR lattice is being analyzed first. Later studies will include other power reactor types. Already, the code has been successfully applied to lattices of certain Hanford and Savannah River reactors.

---

314. Savannah River Laboratory (assignment with AECOP).

315. An acronym for Heterogeneous Analysis by Multigroup Methods of Exponentials and Reactors.

316. J. E. Suich and H. C. Honeck, *The HAMMER System,* E. I. du Pont de Nemours and Co., Savannah River Laboratory, DP-1064 (January 1967).

317. To be published at the Savannah River Laboratory.

318. Douglas United Nuclear, Inc., Richland, Washington (assignment with AECOP).

Reactor parameters are being computed for the BWR lattice for cases with water and with steam, leading to an approximate method of computing the water-steam combination cases. In addition to other parameter comparisons, examination will be made of spectral effects in the steam region as compared with the water region. Since the sections of the BWR core remain in the reactor for a period of several years, there are relatively large quantities of potentially valuable transuranic isotopes produced. The material edit printed by HAMMER at requested intervals over this period of time gives immediate results of the isotope production. Although convergence of computer passes are slower for cases of a core life of several years than for previous cases due to large spectral and concentration changes, the results appear to be relatively good for this type of survey. One limitation to HAMMER is that cross sections for a maximum of 18 isotopes may be applied in any single case, although additional daughter products are computed. This requires several cases of different inputs followed by a careful analysis. Isotopes for which quantities presently are being calculated are ^{234}U to ^{239}U, ^{237}Np to ^{239}Np, ^{238}Pu to ^{242}Pu, ^{241}Am to ^{244}Am, ^{242}Cm, and ^{244}Cm.

The two cross-section libraries used by HAMMER were updated to the June 22, 1970, set of values. Also, the decay constants within the code were updated to values from the May 6, 1969, Chart of the Nuclides by Battelle Northwest. It was found that short cases with slight data changes could be run most easily using the IBM 2741 remote terminal.

Sponsor: Production Reactor Group of AECOP — H. P. Hamric

COMPUTING TECHNOLOGY CENTER

CNLLS – a Callable Nonlinear Least Squares Routine[319]

A. A. Brooks

This subroutine embodies the most valued features of several previous routines as well as what is believed to be a new implementation of an old convergence criterion. The program is intended for use with sums of exponentials but is not limited to this function as the function and its derivatives are provided in a callable subroutine. A calling program is provided for the input of data.

The method used is basically a Lenenberg[320] method utilizing a parabolic extrapolation to the minimum of the correction vector as suggested by Hartley.[321] Finally, after the sums of squares convergence criterion is met, the procedure minimizes the length of the partial derivative vector. It uses a single term in the Taylor's expansion in M dimensions and the Choleski method for the solution of positive definite matrices.

The program permits a wide flexibility in the employment of its algorithms including parameter correction suppression by successive sets, variable convergence criteria for each subalgorithm, and the bypassing of each subalgorithm. While experience prevents belief in a panacea, this program is based on results from several hundred nonlinear problems.

Sponsor: UCND, CTC

---

319. G. W. Westley and J. A. Watts (eds.), *The Computing Technology Center Numerical Analysis Library*, CTC-39 (Oct. 6, 1970).

320. K. Lenenberg, "A Method for the Solution of Certain Nonlinear Problems in Least Squares," *Quart. Appl. Math.* 2(2), 164 (1944).

321. H. O. Hartley, "The Modified Gauss-Newton Method for the Fitting of Nonlinear Regression Functions by Least Squares," *Technometrics* 3(2), 269 (1961).

Nuclear Physics

G. S. McNeilly

A study of both single and double differential cross sections from the reaction $^{24}Mg(\alpha,\alpha'\gamma)^{24}Mg$ has been completed.[322] Treating the excited states of ^{24}Mg as rotational levels of a deformed nucleus, fits to both the single and double differential cross sections were calculated using DWBA[323] plus Hauser-Feshbach (HF)[324] and coupled channels (CC)[325] plus HF theories.

Good agreement between the DWBA plus HF and the CC plus HF theories was obtained, with the greatest discrepancy occurring in the fits to the anisotropic coefficients of the double differential cross sections.

Sponsor: Computing Technology Center

ORGDP

Vibration Analysis

M. R. Patterson G. W. Westley J. A. Watts[326]
P. R. Coleman C. V. Smith, Jr.[327]

An analysis of the stresses induced by steady-state dynamic forces on a floor structure has been completed. Solutions which included damping in systems with about 300 degrees of freedom were obtained. The floors of two separate buildings were studied, and the computed results serve as a guide for the redesign of those buildings.

A product of these studies is a set of finite element codes for plane structures which can treat both static and dynamic problems.[328,329] These codes generate stiffness matrices, loading vectors, static reactions, normal modes of vibration, response to an arbitrary sinusoidal forcing function, dynamic reactions, and the associated shears, moments, and stresses. Both beam and plate elements are allowed. The total computer time for such a set of runs is less than 10 min.

Sponsor: ORGDP D. S. Pesce

Safe Storage and Shipment of UF_6 Containers with Varying Enrichment and Water Reflection

J. R. Knight R. G. Taylor[330]

The ANISN[331] and KENO[332] codes were used to evaluate the nuclear safety factors in the storage of large cylinders of UF_6. Variations in ^{235}U enrichment between 2 and 5% were considered. The thickness of

322. Gregory S. McNeilly, CTC-43 (1970).

323. R. H. Bassel, G. R. Satchler, R. M. Drisko, and E. Rost, *Phys. Rev.* **128**, 2693 (1962).

324. W. Hauser and H. Feshbach, *Phys. Rev.* **87**, 366 (1952).

325. T. Tamura, *Ann. Rev. Nucl. Sci.* **19**, 99 (1969) and references contained therein.

326. Computing Technology Center.

327. Consultant, Georgia Institute of Technology.

328. C. V. Smith, *Finite Element Model, with Applications to Buildings K-33 and K-31*, CTC-29 (June 1, 1970).

329. M. R. Patterson, G. W. Westley, J. A. Watts, and P. R. Coleman, *Vibration Analysis of a Floor Structure*, CTC-30 (June 10, 1970).

330. Laboratory Division, ORGDP.

331. W. W. Engle, *A User's Manual for ANISN*, K-1693 (Mar. 30, 1967).

332. G. E. Whitesides and N. F. Cross, *KENO – a Multigroup Monte Carlo Criticality Program*, CTC-5 (Sept. 10, 1969).

water between individual units in an array was varied, and optimum reactivity conditions were found. The effects of external water reflection and variation in the thickness and type of metal in the cylinder walls were also studied. These results will be applied to evaluating safe conditions for the storage and shipment of UF_6 containers.

Sponsor: Laboratory Division, ORGDP

PORTSMOUTH GASEOUS DIFFUSION PLANT

Portsmouth Criticality Safety Analysis

Nancy F. Cross   R. J. Hinton   J. L. Feuerbacher[333]

A wide variety of criticality safety calculations were performed using the KENO code. Some of the problems considered were:

1. calculations designed to determine the safety of the feed vaporization bays and to improve the safety margin;
2. investigation of the effect of concrete rather than water reflection on a 14-ton UF_6 container and to verify the safety of storing such a unit in a room having a concrete floor;
3. investigation of the criticality consequences should condensation occur in the cascade;
4. verification of the safety of planned shipping arrays and an investigation of the sensitivity of such arrays to spacing changes and various reflectors;
5. calculations to determine the criticality safety of using cheaper aluminum containers rather than Monel containers now in use;
6. a criticality safety analysis of UF_6 accumulation in a withdrawal station;
7. investigation of the criticality safety of the proposed storage of arrays of 2½-ton UF_6 containers.

Sponsor: Portsmouth Gaseous Diffusion Plant   Jack L. Feuerbacher

USAEC

Boron Isotope Separation Plant Studies

R. A. Carter   A. A. Brooks   G. I. Farris[334]

The AEC facilities[335] at Lewiston, New York, are operated by the Nuclear Materials and Equipment Corporation (NUMEC) to produce the Commission's requirement of ^{10}B. The process utilizes packed columns, and the operation is analogous to a binary fractionation. When the dimethyl ether–boron trifluoride complex (DME complex) is distilled at 100°, approximately 60% of the vapor phase dissociates

---

333. Portsmouth Gaseous Diffusion Plant.

334. Former employee, UCND.

335. G. T. Miller, R. J. Kralik, E. A. Belmore, and J. S. Drury, "Production of Boron-10," *Second United Nations Intern. Conf. on Peaceful Uses Atomic Energy,* A/CONF.15/P/1836, June 27, 1958.

into gaseous boron trifluoride and dimethyl ether. Isotopic exchange of the boron in the gas with that in the liquid phase results in the concentration of ^{10}B in the liquid phase.

The facilities were taken out of standby in 1965, and we were requested by the AEC to assist in certain aspects of the operation.[336] Our initial objectives were (1) to propose a mathematical model of the actual process, (2) to determine the technical and economic feasibility of computer control of the process, and (3) to suggest potentially desirable engineering changes to the plant facilities. It was proposed that, mathematically, the isotopic exchange process could be represented by the methods used for a squared-off gaseous diffusion cascade.[337] Although the analogy has some obvious differences, experience has shown that the treatment is reasonably accurate.

Initial operating and analytical data showed that computer control of the process was not feasible. By mutual agreement, however, we continued to participate in the evaluation of plant performance and to make engineering studies of proposed operational and plant modification. A computer program was developed to calculate for each column the number of stages and material balances for ^{10}B, total boron, and the DME complex. The program, which also provides a printout of pertinent operational data in convenient form, is being used on a routine basis.

Recently, detailed productivity calculations were made for plants of various sizes. The results of the study were used by NUMEC to determine the number, size, and arrangement of columns which would be required for an expanded plant to produce large quantities of ^{10}B at a minimum cost. A study is now in progress to determine the location and rates at which several lots of DME complex of different assays now on hand should be fed into the existing plant to realize the largest gain.

Sponsor: USAEC, Production Division — E. H. Hardison

Atmospheric Turbulence Partial Differential Equations

P. R. Coleman   S. R. Hanna[338]

A mathematical model has been devised to describe turbulence and diffusion in the atmospheric boundary layer over urban areas. We are hoping to learn more about the distributions of temperature, wind speeds, and turbulent energy in this layer.

This three-dimensional model consists of eight partial differential equations, four of which are nonlinear, in eight unknowns. We are presently considering the steady-state problem which makes the second-order equations be of the elliptic type.

Because of the importance of an accurate initial "guess" for the solution of the three-dimensional system, we plan to proceed in steps. First, solve the one-dimensional case, and use its solution as the initial guess for the two-dimensional case, etc. Currently, we are in the first step of this outline, working on the one-dimensional case.

Sponsor: Atmospheric Turbulence and Diffusion Laboratory, NOAA

---

336. Letter from C. E. Center, UCND, to S. R. Sapirie, USAEC, Feb. 12, 1965.

337. J. Shacter and G. A. Garrett, *Analogies between Gaseous Diffusion and Fractional Distillation*, K-197 Revised (June 5, 1948) (AECD-1940).

338. Atmospheric Turbulence and Diffusion Laboratory, NOAA, AEC.

Y-12

Heat Transfer in Curvilinear Coordinates

M. R. Patterson Mark Reeves III Peggy G. Fowler

Analytical and numerical results for temperature distributions in an isotropic homogeneous medium subjected to Dirichlet and convective boundary conditions have been computed. Comparison of the analytical and numerical results checked those cases of physical interest and allowed generalization of the numerical computation to include temperature-dependent thermal properties, for example, conductivity, specific heat, film coefficient, etc. Considerable experience with and codes for computation of the spherical Bessel functions were obtained from this study. The findings will be reported later.

Sponsor: Y-12 C. D. Montgomery

Digital Filtering with the Fast Fourier Transform

M. R. Patterson E. C. Long[326] F. L. Miller, Jr.

The advent of the fast Fourier transform[339] (FFT) rendered the computation of discrete Fourier transforms a relatively speedy process. For example, a set of 8192 data points can be transformed using FFT in less than 0.2 *percent* of the time previously required. The profound effect of this fact is still being felt by elements of the scientific and engineering community.

Locally the FFT capability has been applied to the filtering of time-dependent signals. The filtering process previously was done by evaluation of a convolution integral using numerical integration. However, the same result was obtained by using the convolution theorem paired with FFT.[340] Much less computer time was required, and the results are more accurate due to the reduced number of computer operations and the resultant decrease in roundoff error.

Also, the Kolmogorov-Smirnov[341] test was applied to the frequency spectra of two types of data to determine whether both types of measurement sampled from the same distribution. Information of this type was valuable because one type of measurement could be done considerably more cheaply than the other.

Sponsor: Y-12 R. R. Feezell

Information Retrieval from a Predecessor-Successor Chain

P. R. Coleman

We are writing an information retrieval program based on a predecessor-successor chain, that is, parent-offspring relationships, among a given set of elements. Although this program should have several applications, for example, genetics problems, we are currently applying it to Y-12 production problems. These problems consist, for example, of ores being mixed to make blends, which are then combined to

---

339. J. W. Cooley and J. W. Tukey, *Math. Comp.* **19**(90), 297–301 (1965).

340. M. R. Patterson, E. C. Long, and F. L. Miller, Jr., *Digital Filtering and Spectral Comparison Using the Fast Fourier Transform*, CTC-44 (Sept. 22, 1970).

341. D. A. Darling, *Ann. Math. Statist.* **28**, 823–38 (1957)

make parts, etc. The program then is to extract the "family tree" of a given element from the production chain. As examples, the history of a certain part may be desired, or upon finding a certain ore to be bad, it may be desired to know all parts which were made of this ore. Data can also be associated with each element and can be retrieved in this fashion.

Certain editing features are also being incorporated into the program to allow for continual updating, that is, the deletion of old elements and the addition of new elements.

Sponsor: Y-12 Metallurgical Development Division — Trygve Myhre

Criticality Search Package for KENO

Nancy F. Cross G. E. Whitesides G. R. Handley[342]

A search package has been designed and incorporated into the KENO code to allow criticality searches on the geometry of a system. The basic restriction is that the geometry configuration must remain constant. (If the innermost region is a sphere, it cannot be changed to any other basic configuration such as a cylinder or cube. This is true for every region in the unit.) However, the size of each region can be altered as long as it does not shrink into the next smaller region or expand into the next larger region. This enables one to search on any one or more regions simultaneously, even to expand some regions while shrinking others and/or leaving other regions unchanged. This altering procedure is continued until (1) the desired value of k effective has been achieved, (2) the specified number of iterations have been executed, or (3) a region has "bumped" into another region.

This 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 material that must be placed about a fissile unit in order to meet specified criticality conditions.

A simple array size search package is included as part of the criticality search package. It allows one to vary the array size of a given unit until (1) the desired value of k effective has been achieved, (2) the specified number of iterations have been executed, or (3) the search suggests an array size that has been calculated previously. The array search can alter all three dimensions simultaneously or alter any two while holding the other two constant. It is useful in determining the maximum safe array size for an array of given fissile units.

Sponsor: Y-12 Radiation Safety Dept., Criticality Safety — G. R. Handley

Computer Codes for X-Ray Diffraction Calculations

O. W. Hermann A. L. Coffey[343] W. E. Baucum[343]

A series of computer codes for various types of x-ray diffraction calculations were obtained, converted for the IBM 360, given major or minor modifications, and applied to many cases of interest. The function of some of these codes is to compute the angles of x-ray diffraction reflections and the Miller indexes for a given powder material, which is defined by characteristics such as chemical formula or crystalline type and lattice parameters. The reverse is computed in other codes, where a set of reflection angles or part of the diffraction pattern is input, and statistical predictions of lattice parameters for requested crystalline types

342. Y-12 Radiation Safety Department, Criticality Safety.

343. Development Division, Y-12.

are computed. One code also provides a plot of the diffraction pattern.[344] Details of the theory, operating instructions, and the programs are not presented here since this subject is covered in the literature.[344–348] A comparative study[349] of some of the codes gives a more detailed evaluation of the use of these codes in laboratory development at the Y-12 Plant. Also, some of the codes were made available for use on a CDC remote terminal at Y-12.

Sponsor: Development Division, Y-12 — A. L. Coffey

Paducah Criticality Safety Analysis

G. E. Whitesides J. R. Knight

As more nuclear reactors begin operating, a new problem arises in the criticality safety evaluation of gaseous-diffusion enrichment facilities. Uranium that has been used in reactors becomes enriched in ^{238}Pu and ^{239}Pu. Obviously, feeding ^{238}Pu and ^{239}Pu into the diffusion plant is not desirable, so a proposal was made to remove the undesired plutonium by trapping it in a CoF_2 compound. Selectively trapping the plutonium in a column required a study of the maximum pipe diameter which could be used without collecting a critical mass of plutonium. The KENO[332] program enabled us to provide data necessary to establish safe diameters and safe spacings for the array of columns to be used in the trapping operation.

Sponsor: Criticality Safety Section, Radiation Safety Department, Y-12 — G. R. Handley

Albedo-Transmission Study

G. E. Whitesides J. R. Knight Nancy F. Cross

The application of differential albedos in Monte Carlo criticality calculations has been studied in considerable detail. Primary focus has been on eliminating the tracking of neutrons in a thick reflector by substituting information obtained from deterministic solutions. Since an exact replacement of the tracking by a deterministic solution is not practical for all geometries, it was necessary to determine the effects of the approximations which were required when using differential albedos. The results of the study showed that the effect of the approximations was to produce high estimates of k_{eff} as the approximations became poorer. For criticality safety purposes, this is desirable since a high estimate is a conservative estimate. However, the study did show that, for most practical systems, the use of differential albedos gave results which were not distinguishable from results that would be obtained by actual tracking.

The most significant result has been the reduction of the computer time required to calculate k_{eff} for a reflected array of fissile material. This reduction in time and money is a direct function of the amount of

---

344. D. K. Smith, *A Revised Program for Calculating X-Ray Powder Diffraction Patterns,* University of California, Lawrence Radiation Laboratory, UCRL-50264 (June 1967).

345. D. E. Williams, *LCR-2, a FORTRAN Lattice Constant Refinement Program,* Iowa State University, Ames Laboratory, IS-1052 (October 1964).

346. C. R. Heiple, *A Computer Program for Indexing Crystals from Their X-Ray Powder Patterns,* The Dow Chemical Co., Rocky Flats Division, RFP-1292 (May 1969).

347. G. J. Werkema, *A Revised FORTRAN IV Program to Calculate Crystallographic Functions,* The Dow Chemical Co., Rocky Flats Division, RFP-1329 (May 1969).

348. K. I. Hardcastle and A. D. Stock, *J. Sci. Instrum. (J. Phys. E),* Series 2, vol. 1 (1968).

349. A. L. Coffey, *A FORTRAN IV Computer Program for Calculating Interplanar Spacings,* Y-1729 (July 1970).

neutron leakage into the reflector. The systems which have been studied exhibit a saving in time ranging from 5 to 22 times as fast as calculating the actual reflector.

Work has also been under way to apply this same type of information to the problem of an interspersed moderator between fissile units in an array. In addition to using the differential albedo data, one also uses the differential transmission data. Experience with this technique has been limited but promising. Further work is planned in this area because of the importance of studying arrays of fissile materials stored in an area which contains a fire-prevention sprinkler system.

Sponsor: Criticality Safety Section, Radiation Safety Department, Y-12 G. R. Handley

Utility Timing Routines

L. M. Petrie, Jr.

A subroutine called PULL has been written, which allows a program to set a time interval in order that iteration loops can be timed with subsequent control and modification of the algorithm if the set time interval has been exceeded. After the interval has expired, the program is interrupted and control is given to the program at a point specified in the call. The subroutine has an entry ITIME which allows the program to read the clock. The calling sequence for PULL is:

CALL PULL (IMIN, ISEC, &STNO), where IMIN is the fixed-point number of minutes in the interval, ISEC is the fixed-point number of additional seconds in the interval, and &STNO is the statement number to which control is to be given when the interrupt occurs. The interval may be canceled by another call to PULL with a new interval. After the interrupt has occurred, a new interval may be set with a new call to PULL.

The calling sequence for ITIME is:

CALL ITIME (ITOT, IINT), where ITOT is the total time in hundredths of a second from the first call (either to PULL or ITIME) and IINT is the time in hundredths of a second since the last call to ITIME.

Both ISEC and IINT are optional arguments and need not be included in the calling sequence. If &STNO is not specified and an interrupt occurs, control will be turned to the statement following the call to PULL.

If the interrupt should occur while the program is in the FORTRAN I/O routines, then no further I/O (including printing messages) can be done by the program.

Sponsor: Criticality Safety Section, Radiation Safety Department, Y-12 G. R. Handley

The Effects of Accidental Release of Fire Water Sprinklers on the Nuclear Safety of Various Arrays of Uranium Metal Parts

J. R. Knight G. R. Handley[350]

The KENO[332] criticality program has been used to evaluate the effect of water spray from fire water sprinkler systems on the nuclear safety of arrays of uranium metal parts. The results of various spray densities were obtained for arrays which varied in size, number of parts, and types of external reflection. The effects of the water spray, both between and around arrays, were determined, and conditions for

350. Technical Division, Y-12.

optimum reactivity were obtained. Criticality conditions for arrays of arrays filled with and separated by water spray were also evaluated. The results of these studies will be used for the safe arrangement of uranium metal parts in buildings which could have an accidental release of water from the fire water sprinkler systems.

Sponsor: Technical Division, Y-12

Monte Carlo Criticality Studies Using Point Cross Sections

L. M. Petrie, Jr.

A Monte Carlo code has been developed to solve criticality problems using point cross-section data. A subsidiary code has been written to process ENDF/B[351] data into the format required by the Monte Carlo code. The code assumes the cross section can be represented by a straight line between neighboring points. The code can handle the same geometries as the KENO[332] code. Anisotropic elastic and inelastic scattering are handled by scattering at discrete angles selected by a technique developed by R. R. Coveyou.[352] Use of this technique allows N angles to preserve $2N - 1$ moments.

Any of the inelastic secondary energy distributions specified by ENDF/B can be used; $(n,2n)$ reactions are handled by doubling the weight of the neutron and treating the secondary energy distribution as specified by ENDF/B. Thermal collisions are treated by using the $S(\alpha, \beta)$ data from ENDF/B, or, if this is not available, by assuming the colliding nucleus is a free gas.

Calculations have been made of some experiments done with low-enriched uranium billets of two enrichments. Annular billets of 1.97% enrichment were 40 in. long with an inside diameter of 2.6 in. and outside diameters of 5.2, 6.2, and 7.2 in. The billets were placed in both square and triangular arrays in water. Annular billets of 3.85% enrichment were 30 in. long with an inside diameter of 2.6 in. and outside diameters of 6.2 and 7.2 in. Solid billets of 3.85% enrichment were 30 in. long and 2.56, 6.2, and 7.2 in. in diameter. All the billets were placed in both square and triangular arrays with variable pitches. The calculations yielded subcritical k_{eff}'s. Analysis of the results indicated the problem might be that the ENDF/B ^{238}U absorption cross section is too large in the range from 50 to 200 keV.

Calculations have also been made of low-enriched uranium fluoride homogeneously distributed in paraffin blocks. Again, subcritical k_{eff}'s were obtained, and too much absorption in the ^{238}U seems to be the trouble here also.

Calculations have been done on highly (93%) enriched uranium metal pieces reflected by graphite and also by paraffin. These yielded k_{eff}'s that were too high. The problem here seems to be that the ENDF/B ^{235}U (material number 1102) fission cross section is too high in the range from 100 eV to 100 keV.

Further development work on the code and on the cross-section preparation program is continuing. Improved methods of treating the cross sections in the unresolved resonance region are being investigated.

Sponsor: Criticality Safety Section, Radiation Safety Dept., Y-12 — G. R. Handley
Critical Experiments Facility — E. B. Johnson, J. T. Mihalczo

---

351. H. C. Honeck, *ENDF/B*, BNL-50066 (May 1966).
352. R. R. Coveyou, private communication.

Monte Carlo Criticality Studies

Nancy F. Cross Chris S. Day R. J. Hinton J. T. Thomas[353]

Monte Carlo calculations utilizing the KENO code were conducted during the calendar year 1970 for J. T. Thomas. In addition to calculations of experimental arrangements of fissile materials, survey calculations were performed in support of nuclear criticality safety specifications. A portion of these calculated and experimental data has been reported by J. T. Thomas.[354] Other portions of the data are being utilized in support of the Nuclear Standards writing effort on the part of the American Nuclear Society. Subcommittee ANS-8, Fissionable Materials Outside Reactors, is in the process of preparing a "Guide for Nuclear Criticality Safety in the Storage of Fissile Materials."

Sponsor: Critical Experiments Facility, Y-12 J. T. Thomas

353. Critical Experiments Facility.

354. J. T. Thomas, *Uranium Metal, Monte Carlo Calculations and Nuclear Criticality Safety,* Y-CDC-7 (August 1970).

Systems Programming

OPERATING SYSTEMS ON THE IBM SYSTEM/360 COMPUTERS

T. D. Calton, R. P. Rannie
C. E. Hammons, J. G. Sullivan
G. K. Haeuslein, Carolyn P. Walker
R. P. Leinius, R. O. Williams
D. R. Winkler

Summary of System History and Changes

Operation of the IBM 360/91 and 360/75 computers was carried out using modified versions of release 17 of the IBM-supplied multiprocessing operating system (MVT). Several systems and subsystems have been generated to include new operational features and to support new devices and modes of operation.

Software maintenance continues to be a major and continuing activity due to large numbers of IBM corrections which must be applied to the IBM-supplied operating system.

Improvements can be made in the operating system only when the operating conditions of the system are understood. Accordingly, when the compulsory activities of system generation and maintenance are completed, system monitoring activities are undertaken. Two types of hardware monitors have been used during the year, but at the present time the most useful data on system operation have been obtained from the use of a software monitor adapted for use at ORNL. A significant reduction in computer memory requirement was accomplished through analysis of the data gathered from this software program. This program is presently being used to obtain data needed for the implementation of the Houston Automatic Spooling Program (HASP) system.

In addition to system improvements accomplished by adjustments of IBM-provided parameters, a number of uniquely ORNL-developed codes have been implemented as a part of the operating system on the System/360 computers. The ORNL-developed MZAP modification of the IBM SUPERZAP program has enabled system modifications and updates at ORNL that would probably not be considered without this tool. The ORNL-developed Semidynamic Dispatching has eliminated bottlenecks in the flow of jobs through the computer. Controlled Memory Allocation has not only helped to reduce computing bottlenecks but has made available a considerable quantity of hitherto unavailable large core storage memory on the IBM 360/75 computer. The number and facilities of the procedures by which the operators may interrogate and alter the status of the system have been increased. This activity is also directed toward increasing throughput, since bottlenecks occur because very fast computers tend to run ahead of the operator unless very responsive control features are provided. Logistical savings in operations such as printing dumps have been provided.

Remote accessing has increased considerably on the IBM 360/75 computer, and further increases are anticipated on both System/360 computers.

Education of system personnel, computer operators, and the user community remains a continuing task. Monitoring and "exhortation" programs have received a favorable response from users whose programs have been the object of the inquiry, and system program exchanges with other installations have been mutually helpful. The operating system presently includes modules from more than a half dozen other installations.

Implementations of release 19.6 of the operating system and HASP are being carried out. Development on further system monitoring and control programs is continuing to meet the need for control of a system of increasing complexity.

System Maintenance

System maintenance is a major and continuing activity that is needed to provide backup facilities and correction procedures for systems and data that are stored on direct access devices. Updating of cataloged procedures is carried out in order to provide efficient means for programmers to execute standardized procedures by a simple reference to this catalog.

The majority of system maintenance is involved with diagnosis of problems within the system, obtaining a correction for the program, and incorporating the correction into the system. We have applied corrections at a rate of approximately one every other day during this year.

System Monitoring

Many avenues exist for improving the operation of as large and diversified an operating system presently in use on both ORNL System/360 computers. The prime requisite for improving or even understanding the system is the ability to monitor various activities of the system.

A hardware monitor for use by the systems group was developed by the Instrumentation and Controls Division along the line of plans obtained from the computing center at the Massachusetts Institute of Technology. This portable monitor can be plugged into any two indicator light sockets on the consoles of the computers and integrates the voltage applied. Input from these two sources may be measured individually or they may be logically ORed. Output from the monitor is shown on a meter which indicates the percent of the last integration period during which voltage was applied to the indicator light.

This type of device is often referred to as a "wait state monitor" since an indicator light frequently measured is the one indicating the time the system is waiting for a time-dependent operation to complete. This value is of interest since it represents a potential for system improvement if other tasks can be put into execution during this otherwise unused time.

A simple software monitor program, MONITOR, was obtained from the Safeway Corporation. This program has been revised and extended for use on the ORNL System/360 computers. This program measures the number of times various system modules, subprograms, are used as the system processes jobs. The information provided by the MONITOR program has resulted in significant improvements in system operation in making better use of less memory and improving throughput due to a better selection of modules to be kept always resident in computer memory.

During the year the statistics gathering option within the ORNL-written accounting routine[1] has been employed on several occasions to collect data on every job step for periods of approximately one week. A

1. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 54.

program for extensive analysis of these records has been written, and data from this analysis have made a number of significant contributions to system improvements.

System Development and Operational Improvements

Semidynamic dispatching. Semidynamic dispatching (SDD) facilitates the processing of jobs through the computers by eliminating a number of bottlenecks that contribute to a loss in system utilization in the form of system wait time.

Efficient operation of computers performing independent tasks simultaneously can only occur when the tasks that perform extensive input-output operations are executed at higher priorities than compute bound tasks. Priority dispatching allows given tasks to gain access to the computer according to a priority scheme. The standard operating system does not allow individual tasks to run at different priorities.

Semidynamic dispatching automatically assigns priorities to tasks based on the input-output to compute ratio of the program being executed in that step. This reduces wait time considerably. A significant portion of the data used in establishing the priorities was obtained through analysis of the statistics records described in System Monitoring.

Controlled memory allocation. Because all of the $2048K$ ($K = 1024$) bytes of memory on the ORNL IBM 360/91 computer is of one kind, the actual speed of operation of programs on this computer is not memory location dependent. However, on the ORNL IBM 360/75 computer the $512K$ bytes of low (low memory address) memory is approximately 12 times faster than the 2048 bytes of high (high memory addresses) memory which comprises the large core storage.[2]

The standard operating system gets the requested memory for a program from the highest free memory available. The program is then loaded into the lowest portion of the memory obtained. Had no modifications been made to the operating system, only in the case of extremely large jobs and fortuitous circumstances would there be any utilization at all of the fast memory.

Modifications were made to the operating system[3] so that all programs submitted (with the exception of a special class of utility programs) would be altered to appear to be requesting all of the 360/75 user memory regardless of the user's actual request. This, together with other procedures at system initialization, made it possible to use nearly all of the available fast memory. This modification operated satisfactorily, but a great deal of effort was involved in changes to system modules which kept track of the user's true memory request for accounting purposes. Moreover, the operation was very constrained. Introduction of minor changes in the system nucleus or resident modules required changes in the initialization procedures. Perhaps the worst problem lay in the loss of the majority of the $1536K$ byte region since most jobs now being run on the IBM 360/75 computer use only a portion of this region.

The majority of these problems were overcome when modifications were made to the operating system which allowed for controlled memory allocation (CMA). The names of the supervisor programs which execute the user's programs were used to control whether the memory for the program was obtained from high memory or low memory. Since the operating system allows initiators to execute prescribed classes of jobs, it is now possible to schedule jobs into the desired memory on the basis of user-supplied job classes. The memory previously unused is now available for utility programs (many of which are now supplied via CRBE and RJE) except when a very large job needed to run on the IBM 360/75 computer.

---

2. *Math. Div. Ann. Progr. Rept. Dec. 31, 1968,* ORNL-4385, pp. 44–45.
3. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 52.

The CMA modification also proved to be very useful in the operation of the IBM 360/91 computer. The execution of several jobs on this computer tends to fragment the memory due in part to the fact that all jobs are trying to obtain memory only at the upper boundary of free memory. This can reduce the effective utilization of memory and can result in long printing operations severely dividing memory for periods which can exceed ½ hr. There might well be over 500*K* bytes of free memory, but the largest program that could be run might be as small as 150*K* bytes if this was the largest contiguous memory region. The most severe problem occurs when a small long-running (for example, 1 hr) compute bound job is executing near the center of available memory.

The introduction of CMA on the IBM 360/91 computer often produced a marked improvement. The requests for memory from the upper boundary of free memory have been reduced by over half, and the long printing jobs have been positioned at a desirable location, the upper bound of free memory. The spread of memory requests against both boundaries has allowed the consolidation of the previously fragmented memory, and more jobs can now be in execution. Of particular benefit is the execution of the long-running job with no fragmentation loss.

Another function of these system modifications is to fill the memory bytes obtained for a job with the bit pattern 01110111 (or 77 in hexadecimal notation) before loading and execution of the user's program.

The contents of users' memory had changed from all zeros to undefined with the implementation of MVT. While random values had a certain advantage over the very bad zeros (which unfortunately could be added, subtracted, multiplied, tested, shifted, etc., with often disastrous impunity), they did not help debugging procedures. Moreover, memory dump programs were obliged to consume time to print huge arrays of "garbage" characters. The 77 memory fill frequently reduced memory dumps by noting that the next so many lines were identical. Unlike zero, the arithmetic interpretation of the 77 values quickly stopped programs which tried to use them in calculations. This value also helped to stop runaway programs and was easily recognized when printed in hexadecimal, EBCDIC, or arithmetic form.

SUPERZAP. The IBM 360 Operating System consists of numerous programs most of which are stored on disk. Sometimes minor changes and corrections to these programs become necessary. IBM developed the SUPERZAP program to accomplish these modifications. We added new options to SUPERZAP and can now list partitioned data set directories, change or delete member names, and find and display the disk address of any program stored on disk.

The modified SUPERZAP program, MZAP, allows dynamic maintenance of the operating system. This permits testing of system changes from the system console. MZAP contains a feature which permits testing of changes to critical modules without the danger of destroying these system programs. Erroneous modification could require a total restoration of the operating system from backup tapes, which is a danger also faced when modifications are assembled into the system. This in-core modification feature changes only the copy of the module in memory. If utilization of this changed module verifies the change, the entire modified and now tested code may be transferred into the disk copy of the module.

GETDSCB. Additional features have been added to the GETDSCB program[1,4] used for maintenance of direct access data sets. There was a need for these features since the variety of direct access devices being supported has increased and the number of private disk packs has increased. In addition, there has been a continuing increase in the number of permanently resident public data sets. The increase in data sets created in connection with remote computing has added to the variety of data sets which must be scrutinized by the GETDSCB program.

---

4. *Math. Div. Ann. Progr. Rept. Dec. 31, 1968,* ORNL-4385, p. 43.

Development is continuing on this program to provide support for the IBM 2321 Data Cell Drive, to allow selective deletion of data sets by data set name in conjunction with creation date indicators internal to the data set, and to provide summary data on the record of data set use being created and updated by the data set monitor program.

Utility program. The ORNL tape utility program, UCHBUF,[5] was improved by the addition of more program commands for the user and a special version of the ORNL tape buffering package, BUFIN.[6] A new subroutine was added to produce a newsmessage to inform users of modifications or additions to the program and the current commands available to the user.

FORTRAN/IBM 2741. Release 17 of the System/360 operating system (IBM) does not support the IBM 2741 teletypeprinter using the *B*asic *T*elecommunications *A*ccess *M*ethod (BTAM). BTAM was modified to give reasonable support to the IBM 2741 teletypewriter used by ORNL, and several basic FORTRAN-callable assembler-language subroutines were written to enhance the operation of the IBM 2741's.

Logical record counter. Several computer users have had the need to determine the number of logical records in a data set (file of information) which was written with a variable-length format. An assembler-language program was written to solve this problem using the *B*asic *S*equential *A*ccess *M*ethod (BSAM) and the *Q*ueued *S*equential *A*ccess *M*ethod (QSAM). Each physical record is reported along with its contents of logical records accumulated with those from the beginning of the data set.

Other developments. Development has continued on the console commands and displays used on the ORNL System/360 computers. Several new types of information have been added to the display active command used to access the status of computer operation. Console commands and displays for system debugging have been added. Priorities of jobs may now be changed dynamically during execution by the operator in order to alleviate potential bottlenecks in job throughput. The ability to delete failing programs from execution has been added. This permits the system to continue operation in cases which previously required a complete restart of the computing system. The diagnosis and handling of such problems have become more important as the telecommunication load has increased, and a premium has been placed on uninterrupted operation.

The time to execute the system startup procedure has been reduced from several minutes to less than 1 min by system modifications. The need for involved operator responses during this critical startup period has been eliminated.

A saving of over 10% in the volume of printout used for memory dumps was accomplished by modifying the system to print on all of the lines of a page used in dumps. An additional dump option has been added to those already available which will dump only user-provided programs and not those obtained from the standard FORTRAN library. The FORTRAN input/output routines have had features added to aid in pinpointing errors and to facilitate debugging of problems.

Remote Computing

Terminals and work stations which are remote from the central computer facility have continued to handle an increasing volume of the input to and output from the ORNL IBM 360/75 computer. By the end of the year, the only categories of jobs being submitted to the IBM 360/75 computer through its central

5. *Math. Div. Ann. Progr. Rept. Dec. 31, 1968,* ORNL-4385, p. 47.
6. *Math. Div. Ann. Progr. Rept. Dec. 31, 1966,* ORNL-4083, p. 55.

card reader are those jobs which require tape drives, the IBM 2311 disk drives, or the IBM 2321 data cell drive.

The remote computing facilities in use on the ORNL IBM 360/75 computer at the end of last year[7] have been expanded. All remote computing programs continue to execute in the Large Core Storage portion of the computer memory which has proved quite satisfactory for these input-output bound programs. The fast core of the computer continues to remain available for the type of programs for which it is best suited, the compute bound jobs.

Operation of the IBM 2780 Data Transmission Terminal at Y-12 continued with good success throughout the year but began to impact the overall operation of the IBM 360/75 during the third quarter of the year due to difficulties with the Remote Job Entry (RJE) program. Problems related to remote computing which required a restart of the operating system on the computer were acceptable only when batch processing and a limited remote operation over and above RJE was being carried on. The need to obtain a stable remote processing program was a major reason for the implementation of the HASP system. In spite of difficulties the use of RJE has grown, and techniques for the interaction of RJE and CRBE (Conversational Remote Batch Entry system) have been developed due in large measure to an interested user community.

The IBM-supplied CRBE program has been replaced by a faster, more powerful, and more reliable version of the CRBE program which was developed at the Stanford Linear Accelerator Center (SLAC). The number of IBM 2741 communications terminals in the Laboratory has grown to 14.

Support was given in the implementation of Reactor Division's Novar 5-50 terminal. This terminal is similar to the IBM 2741 teletypewriter terminals and has several additional useful features, one of which is off-line cassette magnetic tape editing. A study of its specifications was made to verify its compatibility with the CRBE. The device is operating successfully in the CRBE system.

The reprogramming of the telephone link from the IBM 360/75 computer to the SEL 840A computer at ORIC was completed and checked out by March 1970. The reprogramming involved developing two system tasks, a reading task and a task which would gather output from a computer program and return it to the ORIC link. The link is designed so that ORIC personnel can submit the same job through either the Computer Center dispatcher in Building 4500N or the phone link with a minimal change to the user's program deck. These tasks are under control of the console operator and may be started or deleted from the computer memory as necessary.

During the fourth quarter of the year the Administrative Terminal System (ATS) was installed on the IBM 360/75. This program presently provides interaction between one IBM 2741 communication terminal at the Instrumentation and Controls Division and data stored on a 2311 disk pack at the ORNL IBM 360/75.

During December the RECON system was installed on the ORNL IBM 360/75. RECON supports a network of cathode ray tube terminals using data files stored both on 2311 disk packs and on a number of bins of the 2321 data cell drive. The data files contain information from *Nuclear Science Abstracts.* RECON is a proprietary information retrieval program developed by Lockheed Corporation for the Division of Technical Information Extension (DTIE) of the U.S. Atomic Commission. With the installation of RECON on the ORNL computers the system presently supports four remote terminals and one terminal at the ORNL central computer facility.

---

7. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 53.

Several upcoming projects will further enlarge the remote computing facilities of ORNL. Remote Job Entry facilities at the Naval Research Laboratory and the Harry Diamond Laboratories in Washington, D.C., will add two remote terminals to the IBM 360/91 computer and one more remote terminal to the IBM 360/75 computer. The arrival of the IACC PDP-10 computer will culminate in another remote entry to the IBM 360/75 computer.

The Culler-Fried system presently undergoing development at the University of California at Los Angeles will shortly be implemented on the IBM 360/75 computer to support two Culler-Fried terminals, one in the Thermonuclear Division at ORNL and one at the ORNL central computer facility.

Locally written remote processing programs are being developed in which experiments are carried out to discover other useful interactions between a variety of remote terminals and the central computers.

Local Education and Training Activities

The problem of operator training[7] remains a significant one as new features are added to the operating system and new programs for remote computing are incorporated into the computer operations. A close liaison is maintained between the Computer Operations and the Programming Systems Departments as the complexity of the computing endeavor grows. In addition to operator training courses there have been courses for computer operator supervisors. A study on training relating to computer users, programmers, and operators is presently under way.

A major avenue for improvement in computer throughput is through education of the user community in more optimal methods of utilizing the computer. Most users are quite willing to make changes for the common good, but the problem remains one of bringing ways of improvement to their attention. Computerized techniques are not being neglected in this endeavor. One example of this is a small portion of the system accounting routine which now prints an additional series of messages at the termination of a job when the user did not make economical use of the computer memory he reserved for his job. The response to this computerized message has been encouraging and has resulted in an improvement in user memory utilization.

Another example of user education is found in results from the use of the data set monitoring program developed in the systems group. This program monitors and records the activity of user data sets stored on disks. Users who are thereby presented with statistics on the use of data sets are usually quite willing to relinquish infrequently used space to users with more active programs.

A teleprocessing seminar was given to several members of the Mathematics Division in order to promote familiarity with remote terminal concepts which are becoming increasingly important. Topics which were studied in detail during the two-week period were:

1. What is teleprocessing?
2. New concepts in computer hardware about teleprocessing
3. Data transmission codes
4. Data transmission methods (phone lines)
5. General text structure
6. Several remote station configurations
7. Methods of error detection

System Program Exchange Outside the Laboratory

A major source of useful concepts for the improved operation of the System/360 operating system is to be found in discussion and exchanges with system programmers at other installations. Members of the system programming group have maintained this liaison through attendance and participation at meetings of computer users and in particular at the large computer users' group, SHARE. Innovations now in use at ORNL that were obtained from other installations range from simple one-instruction changes to entire teleprocessing programs. Installations which provided system modifications that were adapted for use on the IBM 360 computers during the year included the Stanford Linear Accelerator Center, McGill University, NASA-Goddard, UCLA, University of Waterloo, Miter Corporation, the National Institutes of Health, and the Applied Physics Laboratory of Johns Hopkins University.

Notices of the development of system modifications carried out at ORNL have been carried in newsletters of computer user groups. Distributions of several copies of these modifications have been made to various installations.

Current System Projects

Generation, modification, and installation of the HASP input-output system on the ORNL IBM 360 computers will be a continuing project. The HASP system is expected to provide a much greater overall reliability, and an increase in system efficiency is also to be expected. The HASP system should facilitate the change to release 19.6 of the operating system. Generation of portions of this release of the system is now in progress, and the system is expected to be in use early next year. The ability to monitor the activity of the system will be enhanced due to new features of this release.

Preparations for the addition of several remote connections to the System/360 computers are under way.

There will also be an interconnection between the IBM 360/91 and the IBM 360/75 computers with the installation of two channel switches that will allow a number of direct access devices to be dynamically shared between the computers. The IBM 2914 switching unit will also allow device switching but not on a dynamic basis. These features are presently under consideration as a part of the upcoming system generation activities.

IMMEDIATE ANALYSIS AND COORDINATING COMPUTER (IACC)

C. E. Hammons D. R. Winkler

Since awarding the contract for the IACC to Digital Equipment Corporation (DEC), close check has been maintained on the progress and workability of the PDP-10 system which is scheduled to be delivered in March 1971. Through mutual cooperation several errors were detected and corrected in special (nonstandard) devices. The massive direct-access storage device (4×10^8 characters) specified in the contract proved to be an unreliable device in DEC's tests, and a mutually satisfactory replacement was accepted. Briefly the equipment will consist of a 36-bit-word PDP-10 computer with $80K$ ($K = 1024$) of 1-μsec memory, 14 removable disk pack drives, a high-speed swapping disk, 4 phone-link display stations, a communications multiplexer, and several standard pieces of peripheral equipment.

ORELA

Nancy A. Betz J. C. Craven D. R. Winkler

Phase I. Data Acquisition

The major programming effort for the ORELA phase I data acquisition computer system[8] has been successfully completed. We have designed and developed all of the software used in phase I except for a

8. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 36.

manufacturer-supplied assembler and paper tape loader which have been greatly modified. It has taken approximately three years to complete the system. Due to the uniqueness of the method of data acquisition and the specially designed disks which are used for channel storage, a patent[9] on the system was issued May 26, 1970.

The executive system, ODAC, and the following routines which operate under it have been provided: the data acquisition program for multiple experiments, ODAR-IV; routines to operate all of the peripherals including the computer links; an accelerator inventory program; and a variety of utility routines including those which read paper tapes generated by other equipment used for ORELA experiments and plot, list, or transfer the data to magnetic tape.

ODAR-IV is a system of routines which accepts data from the experiments, passes each event to its proper CRUNCH[10] routine, and updates the channels on the disk. Each experiment has its own CRUNCH routine which processes the events produced by the associated experimental equipment. This allows the experimenter to uniquely define the method in which his data are to be acquired even though other experimenters are acquiring different data by other methods at the same time on the same DAC. As many as four experiments can simultaneously use each of the two data acquisition computers.

Although the intensive development of phase I has been completed, it will require continuous support. Plans are already being made to change the scaler interfaces so the experimenters can make more use of them, to interface an existing PDP-9 to DAC-2, and to purchase more data acquisition equipment under phase III. We have also started analyzing the core and time requirements to accomplish the various functions of ODAR-IV as a first step in attempting to improve it. Presently ODAR-IV can update 3000 to 5000 events per second depending upon the CRUNCH routines involved.

Phase II. Data Analysis

The process of reducing raw experimental data to publishable cross sections requires a considerable amount of interaction between the experimenter and computers. Bias introduced by the experimental equipment and the background must be removed from the data. Then the data must be analyzed to extract the cross sections which are compared with both theory and previously published data. Each of these steps requires the judgment and interpretation of the experimenter. The magnitude of the problem involved in analyzing the data becomes even more apparent when one realizes that the minimum number of data points currently being acquired per experimental run at ORELA is 64,000, with the average being between 200,000 and 300,000.

Even though the data are compacted in the analysis process, the data sets are always so large that they must be available to the experimenter in graphical form if he is to be able to extract any meaning from them. An interactive, time-sharing, display-oriented system which will provide the facilities required by the experimenters to analyze their raw data for publication is being developed as ORELA phase II. Figure 24 shows the computers involved in this system. The unshaded equipment is the Immediate Analysis and Coordinating Computer,[11] IACC, which will provide for the immediate analysis portion of ORELA phase II and act as a coordinating computer for the Mathematics Division. The IACC is a PDP-10 from Digital Equipment Corporation which is due for delivery in the first quarter of 1971. We expect that the extensive acceptance tests will be completed in July 1971.

---

9. N. A. Betz et al., *Totalizing Memory for Multichannel Analyzers with Increased Capacity*, Patent No. 3,514,763 (May 26, 1970).

10. *Phys. Div. Ann. Progr. Rept. Dec. 31, 1969*, ORNL-4513, p. 105.

11. *Neutron Phys. Div. Ann. Progr. Rept. May 31, 1970*, ORNL-4592, p. 27.

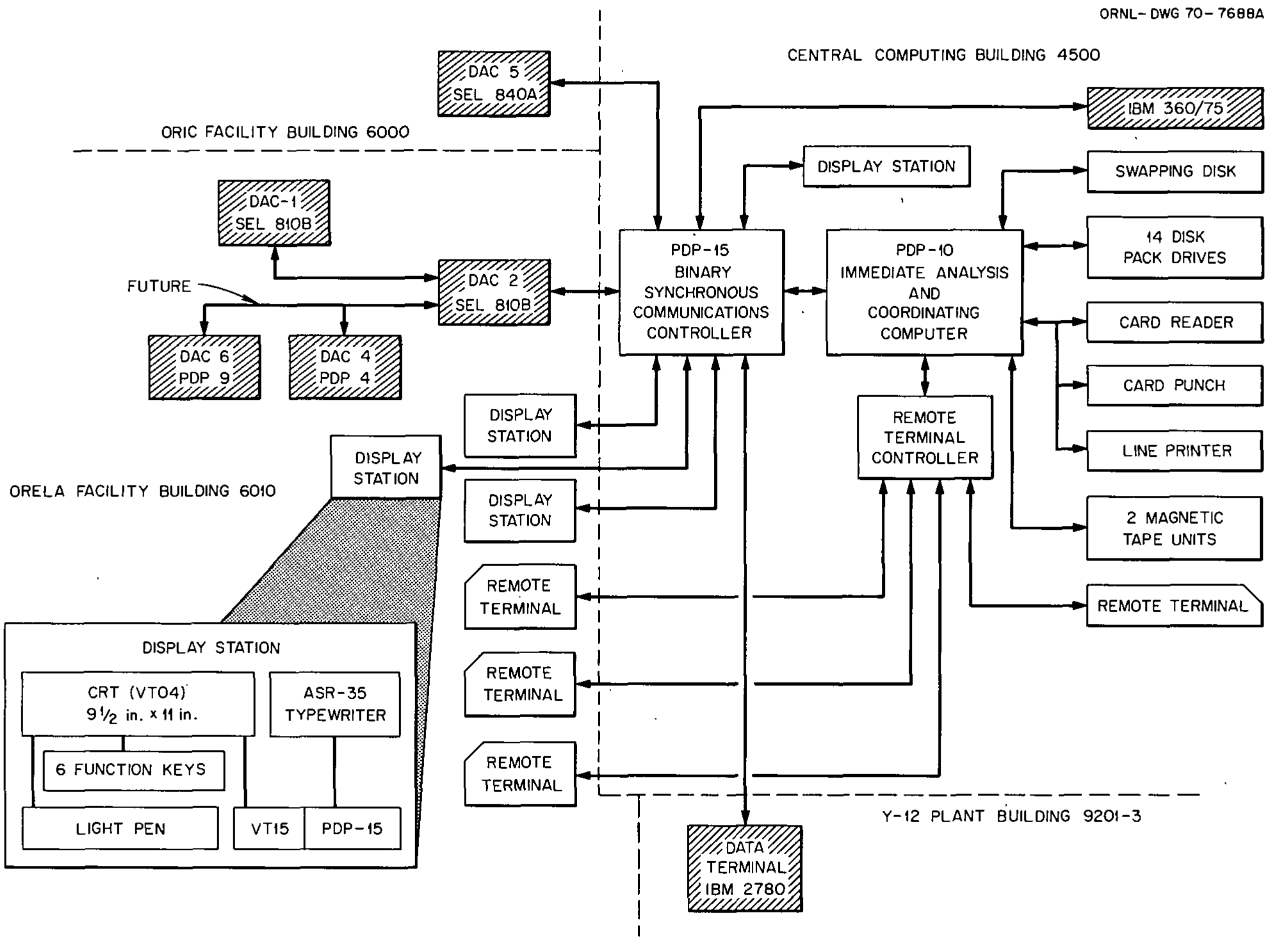

Fig. 24. ORELA phase II computer system.

Although we plan to have a useful display system available for the experimenters within six months after the acceptance tests for the IACC have been completed, it will take approximately two and a half years to develop the software for the full system.

CONVERSATIONAL REMOTE BATCH ENTRY SYSTEM (CRBE)

Carla L. Armstrong R. P. Leinius

The ORNL CRBE system allows users at remote typewriter terminals to create and manipulate files and submit jobs for execution on the 360/75. The system is intended primarily as a method for low-speed transmission of programs to the computer. It provides on-line debugging assistance, faster job turnaround, and eliminates card-handling problems. Communication with the 360/75 is accomplished through dial-up telephone lines.

The IBM version of this teleprocessing system was installed in November 1969. During the first six months of operation, the CRBE system was regarded as an experimental program, and access to it was limited. Several significant improvements were incorporated into the system before it was released for general use as a production system; these include an expanded set of file searching and file editing commands, data file reformatting to improve response time, more efficient procedures for the movement of files, and elimination of errors in the system's FORTRAN language syntax scanner. Many minor design deficiencies were corrected, an accounting system was developed, and an extensive library of commonly used files and programs was created.

In May 1970 the ORNL version of CRBE was released for general use. The system is currently supporting 14 IBM 2741 typewriter terminals, with 95 persons in 11 different divisions or projects enrolled as CRBE users. The number of jobs submitted from remote CRBE terminals for execution on the 360/75 averages approximately 1500 per month. Additional programming and hardware acquisition to allow the use of teletypewriter terminals is nearly complete and will permit low-cost remote access to the computer.

PROGRAMMING ASSISTANCE

Linda P. Helton J. D. McDowell Delores Paulk

This group is available to all programmers to assist with debugging problems encountered on the IBM 360 computers. The group determines whether errors are the result of hardware or systems malfunctions. Any errors found are documented when necessary and reported to the appropriate party for rectification. Particular attention is devoted to the IBM FORTRAN IV Compiler and use of the Calcomp plotters. On a typical day approximately 25 phone calls and 30 personal visits are handled. Divisions make use of this service in about the same degree as they use the computers. A good portion of their time is devoted to running problem programs to discover if errors are responsible in order to facilitate pinpointing hardware errors.

BASIC COMPILER

J. G. Sullivan

Many of the commercial computer time-sharing services feature a problem-oriented language named BASIC. As users became used to the language and developed a number of production-type programs, there developed a need to have this language available on the IBM System/360 computers. This was due to the long running time of some of the programs and the consequent expense in both commercial computer time and the telephone line charges. The Metals and Ceramics Division requested that we develop the BASIC language for the ORNL computers. This has been accomplished, and the report (ORNL-TM-3042) is now available. One comparative example is a program which required 45 min of computer time on the commercial system and 19 sec on the 360/75. Programs written in the BASIC language can be run either as batch jobs or from one of the typewriter terminals under user control; both ways are now in use.

Computer Services

P. N. Coffey L. G. Hodge
L. S. Finch J. E. Parham
R. L. Finch S. O. Smith
T. A. Gardner, Jr. C. S. Williams

THE IBM COMPUTERS

The IBM 360/91 computer system installed last year and described in the previous report[1] continues to operate 24 hr a day, five days a week. In addition, the system operates on weekends whenever required by contractual commitments with the Naval Research Laboratory in Washington, D.C. So powerful a processor is it that the majority of the batch processing work submitted to the Computing Center is run on this system, particularly during the prime (day) shift. This in turn has permitted some dedication of the IBM 360/75 computer system to the servicing of remote terminals, as will be described later.

Some modifications were made to the 360/91 configuration described in the previous report. The 2501-B2 card reader and 2520-B2 card punch were shifted to the 360/75 computer system, and the 2540-1 card read/punch was brought from the 360/75 and installed on the 360/91. This move was made in order to put the higher card volume devices onto the 360/91 system. In December 1970 a 2914 switching unit was installed to permit the (manual) switching of peripheral devices from one computer system to another. Thus, in the event the 360/75 system fails, some of its peripheral devices, notably the teleprocessing units, can be switched to the 360/91 system. Successful testing of this device was concluded as the report period ended.

Two two-channel switches have also been ordered for installation on a 2314 direct-access storage facility and on a 2841-1 data cell and disk control unit, both of which are currently part of the 360/75. With the installation of the two-channel switches, however, both computer systems will be able to access these storage devices electronically, without the necessity of physically switching the units. This capability will eliminate some of the duplication of disk packs currently required and should make more storage space available to users. As of the end of the report period, the two-channel switches had not been delivered; therefore, experience with them will be described in the next report.

During this report period, the 360/75 computer system was used to an ever-increasing degree in the support of various remote terminal systems (see also the section on Systems Programming). The CRBE and RJE software systems previously reported[2] proved to operate satisfactorily, and users at the Laboratory

1. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 55.
2. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, pp. 53, 55.

were introduced to these systems. By the end of the period, 14 IBM 2741 terminals (Selectric typewriter terminals) were in use throughout the Laboratory, as well as the Reactor Division's 2780 remote terminal (card reader, card punch, and printer) and the ORIC terminal mentioned in the previous report.[2]

In order to fulfill agreements made with the Naval Research Laboratory (mentioned earlier), one IBM 2701-1 data adapter was installed on the 360/91 system and a second unit on the 360/75. These devices will permit the submission of work from NRL's remote terminals via private leased telephone lines. Installation and check-out of these two devices were not quite complete by the end of the period and will be reported later.

Two other special-purpose remote terminal systems were ordered during the year. The first was an information storage and retrieval system called RECON and was installed under the sponsorship of the Division of Technical Information Extension of the AEC. This system services five terminals via a party-line-type private telephone line. Each remote terminal consists of a keyboard, a cathode ray tube display, and a teletypewriter together with necessary control units. One terminal is located at DTIE and another here at ORNL. The others are located at AEC facilities in Washington, D.C., West Mifflin, Pennsylvania, and Berkeley, California. Installation of the system was completed in December, and routine operation began the first of the year.

The second special remote terminal is a Culler-Fried algebraic terminal system developed initially at UCLA and installed at ORNL under the auspices of the Thermonuclear Division. Two terminals are to be installed (one at Thermonuclear and the other at the ORNL Computing Center) and will connect to the 360/75 via telephone lines. The equipment involved was being delivered as the report period ended and has not yet been installed. (Further descriptions of the RECON and Culler-Fried systems may be found in the section on Systems Programming.)

During the year, an IBM 2321-1 data cell drive was procured in order to provide a very large capacity storage device on the 360/75. The storage requirement was brought about by the installation and expansion of the various remote terminal systems already described. The 2321-1 data cell has a storage capacity of 400 million bytes spread over ten removable subcells and has an access time ranging from 175 to 600 msec. The device was installed in August 1970, passed acceptance without incident, and has operated satisfactorily since that time.

THE CDC COMPUTERS

The CDC 1604-A, as announced in the previous report, was retired effective January 1, 1970, and appropriate announcement of its availability was made via GSA Excess Property Bulletins. During the first part of the year, some of the magnetic tape drives were transferred to other uses in the Laboratory; two were attached to our own 160-A computer system, two were transferred to the 160-A system at the High Voltage Laboratory, and two (along with a tape control unit) were transferred to the Instrumentation and Controls Division where they were integrated into their hybrid computer system.

In July the remainder of the 1604-A system was picked up by the South Dakota School of Mining and Technology, and was shipped to their weather research facility outside Rapid City, South Dakota.

The CDC 160-A computer system continues to be operated in a peripheral capacity, performing the various tasks associated with any computing center, for example, tape-to-printer operations, card listing and duplication, paper tape processing, etc.

WORK LOAD AND PERFORMANCE

The figures which follow give some indication of equipment performance and utilization for the report period. Figures 25 and 26 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 27 and 28 indicate the use of the 360/91 and 360/75, respectively, by the various divisions during 1970. Figure 29 indicates the work load at the ORNL Computing Center as measured by the number of jobs received per scheduled working day; use of the three Calcomp plotter systems is shown in Fig. 30.

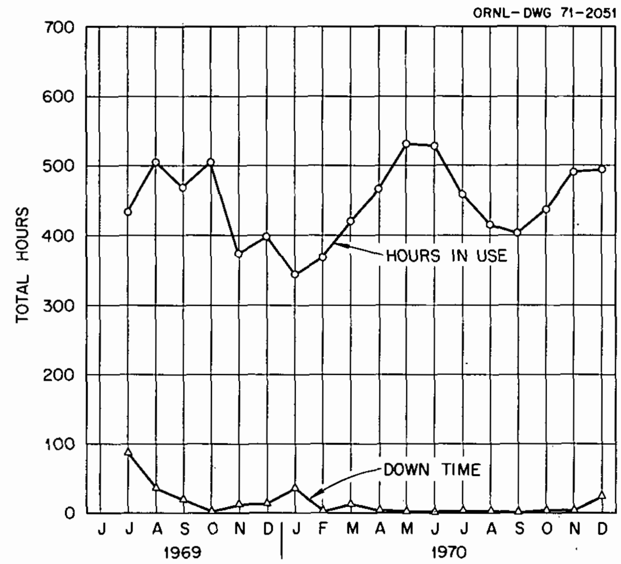

Fig. 25. Hours in use and downtime for the IBM 360/91.

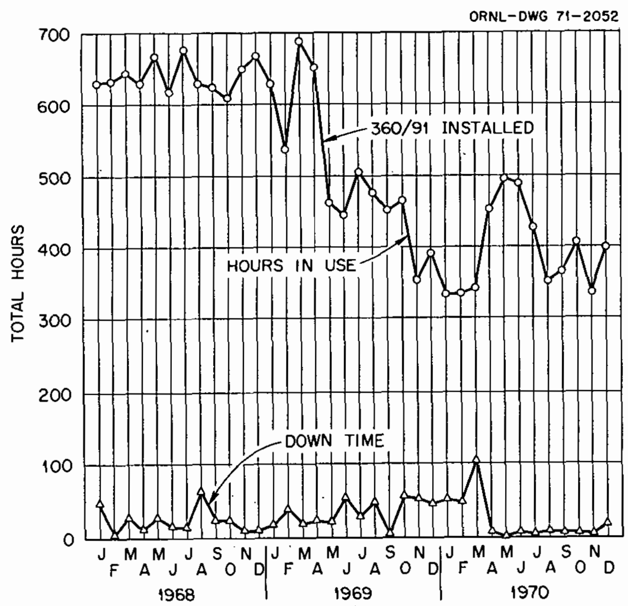

Fig. 26. Hours in use and downtime for the IBM 360/75.

Throughout the report period, both computer systems were operated under release 17 of Operating System/360 as supplied by IBM and modified by ORNL. Performance was smooth and efficient as indicated by the fact that over 140,000 jobs were processed by both systems during the year. This represents an increase of over 10,000 jobs from the number of jobs run on these computers last year. Toward the end of the period, operating system performance was further enhanced by the introduction of the HASP (Houston Automatic Spooling Program) system, which not only handles all input/output operations in a more efficient manner, but requires less storage space to do so. (See the section on Systems Programming for additional information.)

Toward the end of the report period, the work load at the center was such that the computer operator staff was reorganized once again into three full shifts, although with a fewer number of men per shift than

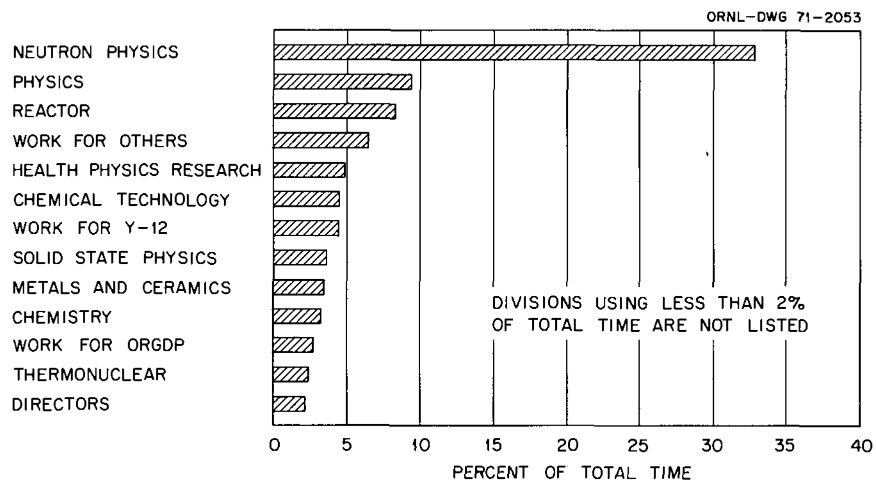

Fig. 27. Divisional use of the IBM 360/91.

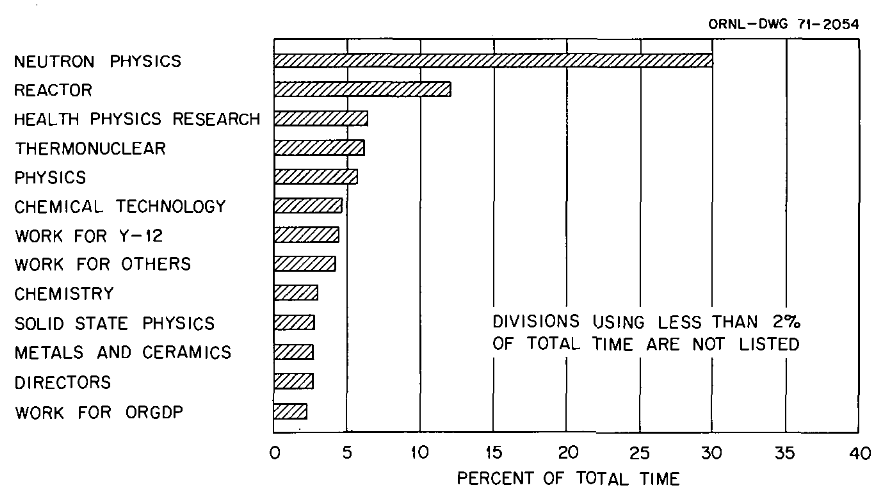

Fig. 28. Divisional use of the IBM 360/75.

was possible in mid-1969. This step has resulted in improved performance in the Computing Center and was accomplished with the addition of just one computer operator. The remainder of the Computer Services staff remains at about the level described in the last report.[3] Their functions have been described in earlier reports.

3. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 58.

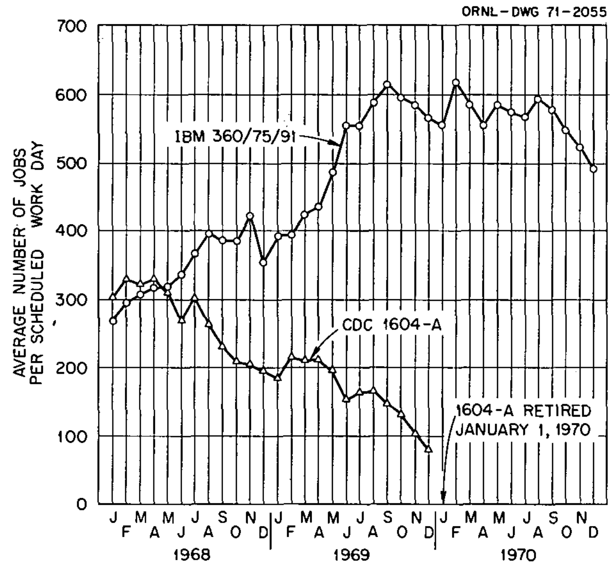

Fig. 29. Work load at the ORNL Computing Center.

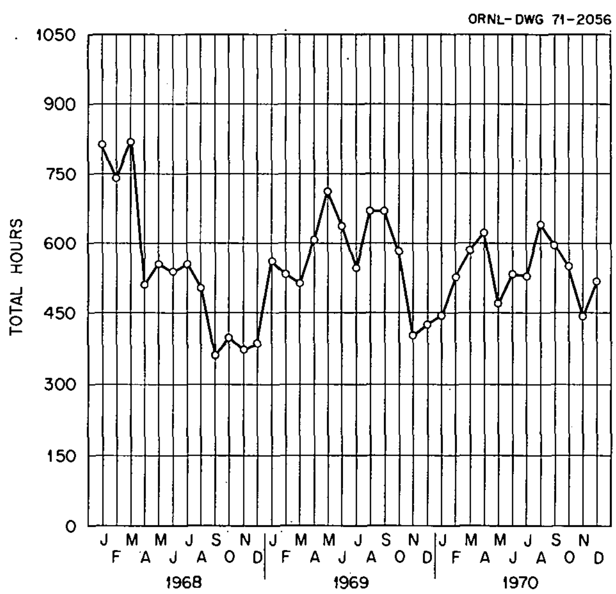

Fig. 30. Use of Calcomp plotter systems.

Mathematical Statistics

INTRODUCTION

D. A. Gardiner

The Statistics Department of the Mathematics Division continues to be engaged in statistical research and consulting in the Oak Ridge area. ORNL statisticians now occupy on a part-time regular basis an office in the Biology Division five mornings per week, another office in the Ecology Division three mornings per week, and a third office in the Y-12 Technical Department five mornings per week. For several months during 1970 an ORNL statistician had been housed with the Y-12 Development Division on a similar basis. This activity is in addition to the more or less casual schedule of consulting which takes place with other units and divisions in Oak Ridge. Some of this work is reported in the following pages in the section on Statistical Applications.

The department "graduated" another statistician during 1970 when one of its ORAU Fellows was granted a Ph.D. degree from Virginia Polytechnic Institute and State University. A summary of his research is contained in the Statistical Research section which follows. Because of budget restrictions the Statistics Department was not fortunate to have a research participant assigned during the summer nor was it able to employ a young graduate student as a temporary summer employee. This kind of association with members of the academic community has been a source of stimulation and enjoyment in previous years. Hopefully, it will be possible to continue the association in the years to come.

An IBM 2741 terminal connected to the ORNL IBM 360/75 computer was installed in the spaces of the Statistics Department during the year. Together with the commercial time-sharing terminal these devices have allowed the statisticians to accomplish numerical calculations in a much shorter period of time. A résumé of this activity is contained in the section on Statistical Programming.

The Department augmented its educational activities by including in the program of lectures for the MIT School of Engineering Practice sessions of statistical consulting wherein the students' experimental programs were planned according to statistical principles. In a program of self-education the Department conducted a series of Statistical Seminars which are listed in this report. Currently a series of educational sessions on Experiment Design is being planned for the Laboratory.

STATISTICAL RESEARCH

Use of "Design Repair" to Construct Designs for Special Linear Models

T. J. Mitchell F. L. Miller, Jr.

A technique for augmenting existing data with additional runs has been described in two previous reports.[1,2] This method was called "design repair" because of its applicability to situations in which the original experiment had been poorly planned or executed. The procedure is simply to choose each new experimental design point at the point in the experimental region at which the variance of the fitted response is the largest. It has been shown in various examples that the precision of the fitted response over the region of interest can be improved substantially in this way.

This method has been modified to develop an algorithm to construct a complete design in n points for a given model. The steps are as follows:

1. Assign the n points randomly in the region of experimentation.
2. Use the design repair technique to augment this n-point design with a single point, namely, that point in the experimental region at which the variance of the fitted response is *largest.*
3. Remove from the collection of $n + 1$ points that point at which the variance of the fitted response is *smallest.*
4. Go to step 2 and continue.

At each stage, we improve the design by adding the point which will do the "most good" and discarding the point which will do the "least harm." The process is continued until no further improvement can be made.

Although this approach is still intuitive and the method is not yet well developed, we have applied it to the following problem: Consider the model

$$y = \beta_0 + \beta_1 x_1{}^2 x_2{}^2 + \beta_2 x_1{}^2 x_2{}^4 + \beta_3 x_1{}^3 x_2{}^4 + \beta_4 x_1{}^4 x_2{}^2 \ ,$$

where the region of interest is $-1 \leqslant x_1 \leqslant 1, -1 \leqslant x_2 \leqslant 1$. What ten-point design is best for this situation?

The method described above did not converge to a specific design for two reasons:

1. The search technique used to add the 11th point at each stage was a random one, in which a preassigned number of randomly selected points were tested for the variance of the fitted response at that point. The point at which the maximum variance was found was then chosen as the 11th point.
2. Because of the symmetry of the model, there are a number of "optimal" designs. For example, changing any design point from (x_1, x_2) to $(x_1, -x_2)$ will not alter the model. We found the method to oscillate from one approximately optimal design to another.

Our results did suggest, however, that the optimal ten-point design for this model belongs to the class shown in Table 7, where individual members of the class are identified by a particular value of c and a particular choice of plus and minus signs in the last four runs. The *estimation matrix* X is the matrix of coefficients of the β's in the model. In the last four runs, the final choice of signs and the magnitude of c

1. *Math. Div. Ann. Progr. Rept. Dec. 31, 1967,* ORNL-4236, pp. 43–46.
2. *Math. Div. Ann. Progr. Rept. Dec. 31, 1968,* ORNL-4385, pp. 57–60.

Table 7. Representation of the class of "optimal" ten-point designs for the given type of response function

Design matrix x_1	x_2	Estimation matrix 1	$x_1^2x_2^2$	$x_1^2x_2^4$	$x_1^3x_2^4$	$x_1^4x_2^4$
−1	−1	1	1	1	−1	1
1	−1	1	1	1	1	1
−1	1	1	1	1	−1	1
1	1	1	1	1	1	1
0	0	1	0	0	0	0
0	0	1	0	0	0	0
$\pm c$	± 1	1	c^2	c^2	$\pm c^3$	c^4
$\pm c$	± 1	1	c^2	c^2	$\pm c^3$	c^4
± 1	$\pm c$	1	c^2	c^4	$\pm c^4$	c^4
± 1	$\pm c$	1	c^2	c^4	$\pm c^4$	c^4

were made so as to maximize $|X'X|$. (This is a popular design criterion, which can be derived from several approaches.[3]) The result specified the last four runs to be:

x_1	x_2
$-\sqrt{2}$	1
$-\sqrt{2}$	−1
1	$\sqrt{2}$
1	$-\sqrt{2}$

We are currently planning to refine this approach to designing experiments and to test it for a wide variety of models.

Design Repair with Several Criteria

T. J. Mitchell   T. L. Hebble

In two previous reports,[1,2] a design repair technique was proposed to choose further experimental points, given an initially run experiment. This method was based on a single design criterion, which was shown to be the same as the stepwise minimization of the generalized variance of the coefficient estimates, or equivalently, the stepwise maximization of $|X'X|$. Here, **X** is the matrix which arises in the formulation of the linear model $y = \mathbf{X}\boldsymbol{\beta} + \epsilon$, where y is the vector of observations, ϵ is the vector of "errors," and $\boldsymbol{\beta}$ is the vector of coefficients to be estimated from the data.

Although the maximization of $|X'X|$ seems to be the most popular formal design criterion, there are others which have been suggested. We have now extended the design repair technique to include the simultaneous consideration of three criteria:

1. the minimization of $c_1 = |X'X|^{-1}$ (i.e., the maximization of $|X'X|$),
2. the minimization of c_2 = trace of $(X'X)^{-1}$,
3. the minimization of c_3 = average variance of the fitted response ($\hat{y}$) over the region of interest.

---

3. M. J. Box and N. R. Draper, *Univ. of Wis. Dept. of Stat. Tech. Rept. No. 207,* 1969.

Although either c_2 or c_3 could be used as an alternative to c_1, we are currently considering all three. This approach is intended for the experimenter who does not wish to commit himself to a single criterion, and who prefers that the computer *suggest* further points for his consideration rather than *determine,* arbitrarily, the next experimental point.

Given **X** for the original design, it is necessary to be able to calculate the change effected in c_1, c_2, and c_3 through the addition of a single design point p. If p were included in the design, **X** would be augmented by a single row, which we call **a**$'$, where **a**$'$ depends on p and on the form of the model. We denote the augmented **X** matrix by $\widetilde{\mathbf{X}}$, and let $\mathbf{H} = (\mathbf{X}'\mathbf{X})^{-1}$ and $\widetilde{\mathbf{H}} = (\widetilde{\mathbf{X}}'\widetilde{\mathbf{X}})^{-1}$. Then it can be shown that

$$
\begin{aligned}
&|\widetilde{\mathbf{H}}| = |\mathbf{H}|/(1 + \mathbf{a}'\mathbf{H}\mathbf{a}) \,, \\
&\mathrm{tr}(\widetilde{\mathbf{H}}) = \mathrm{tr}(\mathbf{H}) - [\mathbf{a}'\mathbf{H}^2\mathbf{a}/(1 + \mathbf{a}'\mathbf{H}\mathbf{a})] \,, \qquad (1) \\
&\text{“new” av } V(\hat{y}) = \text{“old” av } V(y) - \left\{ [(\boldsymbol{\xi}'\mathbf{H}\mathbf{a})^2 + \mathbf{a}'\mathbf{H}\mathbf{V}\mathbf{H}\mathbf{a}]/(1 + \mathbf{a}'\mathbf{H}\mathbf{a}) \right\} ,
\end{aligned}
$$

where $\boldsymbol{\xi}$ and **V** are the mean vector and covariance matrix, respectively, of **a**, assuming p has a uniform distribution over the region of interest. For simple types of region, for example, cubic, exact values of $\boldsymbol{\xi}$ and **V** can be calculated. In more complicated cases, $\boldsymbol{\xi}$ and **V** can be estimated by repeated sampling.

A computer program has been written to apply the method. Starting with the initial **X** matrix, a predetermined number of candidates for the next design point is selected at random from the region of interest. The effects of the inclusion of each candidate can be calculated using (1). For each criterion, the ten best candidates found by this search are printed out. After viewing the results, the experimenter is then required to use his judgment to select the next design point. In general, it is good practice to select a point which appears on all three "top ten" lists, even though it may not be in first place on any of them. Preliminary examples have indicated that there are generally several such points.

Once the next design point has been selected, the procedure can be repeated and a set of new points can be built up stepwise, just as was done previously for the single criterion.

Tables of Rank Order Probabilities: One-Sample Shift Alternatives

Claudia S. Lever

Of considerable interest in the area of statistical tests of hypotheses are tests based on the rank order of the observations as opposed to the values of the observations themselves. Examples of such tests are the sign test, the Wilcoxon signed rank test, the Fraser test, and more recently the sequential one-sample grouped rank test developed by Bradley and Weed.[4] What has been lacking in this area is a knowledge of the behavior of the tests when the hypotheses tested are false and when the samples are of small or moderate size. Such knowledge is important for planning experiments, especially for determining sample size. What is required are tables of rank order probabilities when alternative hypotheses are true.

To this end, a set of tables has been computed for the case where the population sampled has a normal distribution with mean of θ and variance 1. Denote the density function of this distribution by $f(x, \theta)$. Let $x_1, x_2, \ldots, x_N$ represent the observations from a sample of size N from this distribution and let $y_1, y_2, \ldots,$ y_N represent the absolute values of these numbers arranged from smallest to largest. Then define $z = (z_1,$

---

4. R. A. Bradley and H. D. Weed, Jr., *Bull. International Statistical Institute* (in press 1969).

z_2, ..., z_N) to be the observed rank order, where $z_i = 1$ if y_i is the absolute value of a positive number and $z_i = 0$ if y_i is the absolute value of a negative number. If Z represents the random vector corresponding to an observed vector z, then $P(Z = z|\theta)$, the probability of the rank order z, given that the mean of the normal distribution is θ, is given by

$$P(Z = z|\theta) = N! \int_{0<u_1<\ldots<u_N<\infty} \int \prod_{i=1}^{N} f[u_i - (2z_i - 1)\theta]\ du_i\ .$$

This function has been tabled to nine decimal places for all the 2^N possible realizations of the vector Z for $N = 1, 2, \ldots, 12$ and for values of θ equal to 0, 0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.5, 2.0, and 3.0.

The integrals were evaluated by a composite midpoint quadrature formula modified to take into account the nonrectangular region of integration. Because of the factorability of the integrand, it was possible to use an efficient algorithm which required only $N^2 \times M$ arithmetic operations instead of M^N operations, where M is the number of subintervals into which the interval was divided.[5] A sequence of approximations was calculated, doubling the number of subintervals each time. Then the accuracy of the approximations was improved by "extrapolation to the limit" according to the Romberg scheme.

The tables have been used to calculate the small sample power of the Wilcoxon test, the Fraser test, and the sign test against normal shift alternatives. The power of these one-sample tests has been compared with the power of the one-sample t test.

Bradley and Weed developed a sequential one-sample group rank test for Lehman-type alternatives. Tables of the distribution of the Wilcoxon signed rank statistic have been prepared from the basic tables to aid in performing a sequential grouped rank test for normal shift alternatives. The null hypothesis to be tested is that of symmetry about the origin, $H_0: F(x) + F(-x) = 1$, where $F(x)$ is the normal cdf. The tables give the probabilities of the different values of the Wilcoxon statistic W under the null hypothesis $P_0(W|0)$ and the probabilities under the alternative hypothesis $P_1(W|\theta_1)$ for $\theta_1 = 0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.5, 2.0$, and 3.0. Tables of the log of the sequential probability ratio log $[P_1(W|\theta_1)/P_0(W|0)]$ were also computed, since the logs are more convenient to use in combining the calculations for different groups. The average sample number (ASN) was calculated for groups of size $N = 2, \ldots, 12$ for $\alpha = 0.01$ and 0.05. The functions needed to calculate the ASN for other values of α were also tabulated for the different group sizes.

Canonical Analysis

J. J. Beauchamp D. G. Hoel[6]

Multivariate experimental situations arise in which one has a set of observation vectors on a collection of similar experimental units which have been classified into a number of different experimental groups. Canonical analysis is a multivariate statistical technique which may be used to determine what differences exist among the groups. Seal[7] gives a detailed discussion of canonical analysis. During this year, simulation work investigating the multivariate technique of canonical analysis which was mentioned in an earlier report[8] was completed.

---

5. The algorithm was developed by R. C. Milton (*Rank Order Probabilities Two-Sample Normal Shift Alternatives,* Wiley, New York, 1970) to evaluate rank order probabilities for two samples, but it was applicable to the one-sample case with only a few modifications.

6. On leave of absence.

7. H. Seal, *Multivariate Statistical Analysis for Biologists,* pp. 123–52, Methuen, London, 1968.

8. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 71.

A computer program was written to generate, from a specified group of multivariate normal distributions, sets of observation vectors of the form displayed in Table 8. The program calculated and plotted the first two canonical variates. This plot may be used as a graphical means of differentiating between various groups. For all of the simulation work presented here $h = 3, N_1 = N_2 = N_3 = 50$, and $\mu^{(1)}$ is a $p \times 1$ vector of zeros, where $\mu^{(1)}$ is the mean vector of the multivariate normal distribution, $N(\mu^{(1)}, \Sigma)$, for the first group. Two basic forms of the $p \times p$ variance-covariance matrix, Σ, were used for the simulation work. The first form, referred to as the "adjacent" model, is given by

$$\Sigma = \begin{pmatrix} 1 & \rho & 0 & \dots & 0 \\ \rho & 1 & \rho & \dots & 0 \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ 0 & 0 & 0 & \dots \rho & 1 \end{pmatrix}.$$

The second form, referred to as the "power" model, is given by

$$\Sigma = \begin{pmatrix} 1 & \rho & \rho^2 & \dots \rho^{p-1} \\ \rho & 1 & \rho & \dots \rho^{p-2} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \rho^{p-1} & \rho^{p-2} & \rho^{p-3} & \dots 1 \end{pmatrix}.$$

The form of the model when $\rho = 0$ is referred to as the "independent" model.

In Table 9 the different models used in the simulation work are given. For all of the models the difference between any two of the mean vectors was equal to a constant, that is, $\mu_j^{(i)} - \mu_j^{(i')}$ is independent of j, where $\mu_j^{(i)}$ is the jth element of the mean vector of the ith group for $i = 1, 2, 3$ and $j = 1, 2, \dots, p$. Let $\Delta_i = \mu_j^{(i+1)} - \mu_j^{(1)} = \mu_j^{(i+1)}$, since $\mu_j^{(1)} = 0$.

The following are a few conclusions observed from this simulation study:

1. The range of the second canonical variate does not change significantly for either the "adjacent" or "power" model. For both models the negative values of ρ appear to give better separation of the groups.

Table 8. General example of data

Variate or characteristic observed	Group 1				Group i				Group h			
	Observation vector No.				Observation vector No.				Observation vector No.			
	1	2		N_1	1	2		N_i	1	2		N_h
1	x_{111}	x_{112}	...	x_{11N_1}	x_{i11}	x_{i12}	...	x_{i1N_i}	x_{h11}	x_{h12}	...	x_{h1N_h}
2	x_{121}	x_{122}	...	x_{12N_1}	x_{i21}	x_{i22}	...	x_{i2N_i}	x_{h21}	x_{h22}	...	x_{h2N_h}
.	.	.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.
p	x_{1p1}	x_{1p2}	...	x_{1pN_1}	$x_{i:1}$	x_{ip2}	...	x_{ipN_i}	x_{hp1}	x_{hp2}	...	x_{hpN_h}

Table 9. Simulation models

Case	Model type	ρ	p	Δ_1	Δ_2
1	Adjacent	−0.95	10	1	2
2	Adjacent	−0.50	4	1	2
3	Adjacent	−0.50	6	1	2
4	Adjacent	−0.50	10	1	2
5	Adjacent	−0.50	10	0	1
6	Adjacent	0.50	10	1	2
7	Adjacent	0.95	10	1	2
8	Independent	0	10	1	2
9	Power	−0.95	10	1	2
10	Power	−0.50	4	1	2
11	Power	−0.50	6	1	2
12	Power	−0.50	10	1	2
13	Power	0.50	10	1	2
14	Power	0.95	10	1	2

2. For the "adjacent" model and a fixed value of ρ, the range of the second canonical variate does not change significantly as p changes. There was a discernible separation of the first two canonical variates into three distinct groups for the values of p considered, and this separation was more evident for the large values of p than it was for the small values.

3. For the "power" model and a fixed value of ρ, the range of the second canonical variate does not appear to change significantly as p changes. For all the values of p considered, there was a discernible separation of the first two canonical variates into three distinct groups, and this separation appeared to improve as p increased.

4. The "adjacent" model appears to separate the first two canonical variates better than the "power" model. In addition, there appears to be a value of ρ which optimizes the separation of the groups under consideration, and this value is not necessarily the same for the two models investigated.

5. The first two canonical variates also do a good job of separating the groups for the case when the p variates observed are all independent, that is, $\rho = 0$.

6. For the particular case when the observation vectors for the first two groups come from the same distribution and the third group come from a different distribution, the first two canonical variates from the first two groups fell in the same general region, indicating no separation of these groups, which is desirable, and, for the third group, the canonical variates fell in an entirely disjoint region, showing very good separation.

7. The first canonical variate is performing most of the separation of the groups, and it is doubtful any of the canonical variates beyond the first two will add to the separation of the various groups.

The computer program has the additional option that one may calculate and plot the first two canonical variates for the case when the data are already available in the form given in Table 8. As an indication of the uncertainty of the location of the various groups, "circles of uncertainty" may also be included as an option of this program. For the ith group the circle of uncertainty has its center at the point (m_1, m_2) and radius r_i. The values of m_1 and m_2 are, respectively, the first and second canonical variates of the $p \times 1$ vector $\hat{\mu}^{(i)}$, whose jth element is given by

$$\sum_{k=1}^{N_i} x_{ijk}/N_i \, ,$$

where $i = 1, 2, ..., h$ and $j = 1, 2, ..., p$. The radius r_i is equal to $t/\sqrt{N_i}$, where t is the appropriate Student's t statistic with

$$\sum_{i=1}^{h} (N_i - 1)$$

degrees of freedom. In Figs. 31 and 32 plots of the first two canonical variates for cases 5 and 12 from Table 9 are shown. In Fig. 33 an example of the circles of uncertainty is shown using the data from an article by Horton et al.[9] A report compiling the results from this simulation study is in preparation.

Multiple Range Test for Slopes of Regression Lines

J. J. Beauchamp

An extension of Duncan's multiple range test will be given which may be applied to the comparison of estimates of slopes of regression lines. A brief description of Duncan's multiple range test applied to the comparison of means from samples of equal size is given by Li,[10] and an extension of this test to the case of unequal sample sizes is given in an article by Kramer.[11] The ideas from Kramer's article will be used extensively in the following discussion.

Assume that we have k linear regression equations specified by

$$y_{ij} = \alpha_i + \beta_i x_j + \epsilon_{ij} ,$$

where $i = 1, 2, ..., k$; $j = 1, 2, ..., n_i$. y_i and ϵ_{ij} are normally distributed random variables with means $\alpha_i + \beta_i x_j$ and 0, respectively, and the variance of y_{ij} = variance of $\epsilon_{ij} = \sigma^2$. Note that σ^2 is assumed to be independent of i and j. From the observed values of the random variable y_{ij} estimates of the parameters $\beta_1, ..., \beta_k$ are available which are also normally distributed. The present aim is to propose a multiple range test of the estimates of $\beta_1, ..., \beta_k$ that will test which of these parameters differ significantly from each other.

Let $\hat{\beta}_1, ..., \hat{\beta}_k$ be the estimates of the parameters of interest. From each of the k regression equations an estimate of σ^2 is obtained and denoted by

$$s_i^2 = \frac{\sum_{j=1}^{n_i} (\text{obs}\, y_{ij} - \text{pred}\, y_{ij})^2}{n_i - 2}$$

= error mean square from the regression analysis for the ith regression equation.

It is known that $(n_i - 2)s_i^2/\sigma^2$ has a χ^2 distribution with $n_i - 2$ degrees of freedom. A pooled estimate of σ^2 is obtained by using

$$s^2 = \frac{\sum_{i=1}^{k} (n_i - 2)s_i^2}{\sum_{i=1}^{k} (n_i - 2)} .$$

9. I. F. Horton, J. S. Russell, and A. W. Moore, *Biometrics* **24**, 858 (1968).
10. J. C. R. Li, *Introduction to Statistical Inference*, pp. 529–30, Edwards Brothers, 1957.
11. C. Y. Kramer, *Biometrics* **12**, 307–10 (1956).

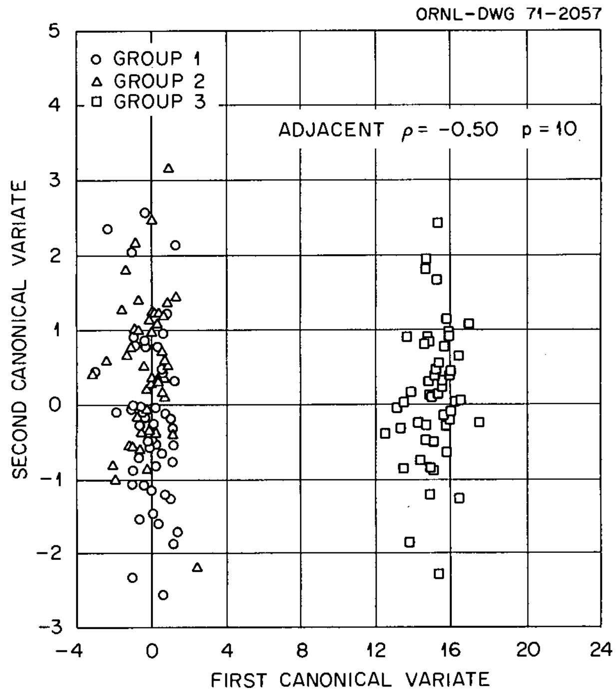

Fig. 31. First two canonical variates for case 5.

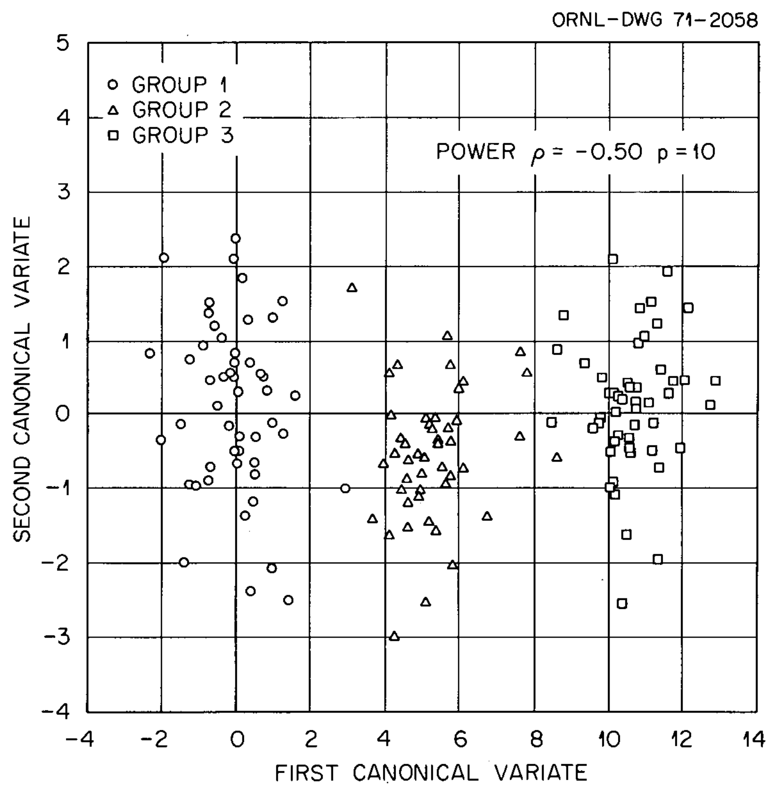

Fig. 32. First two canonical variates for case 12.

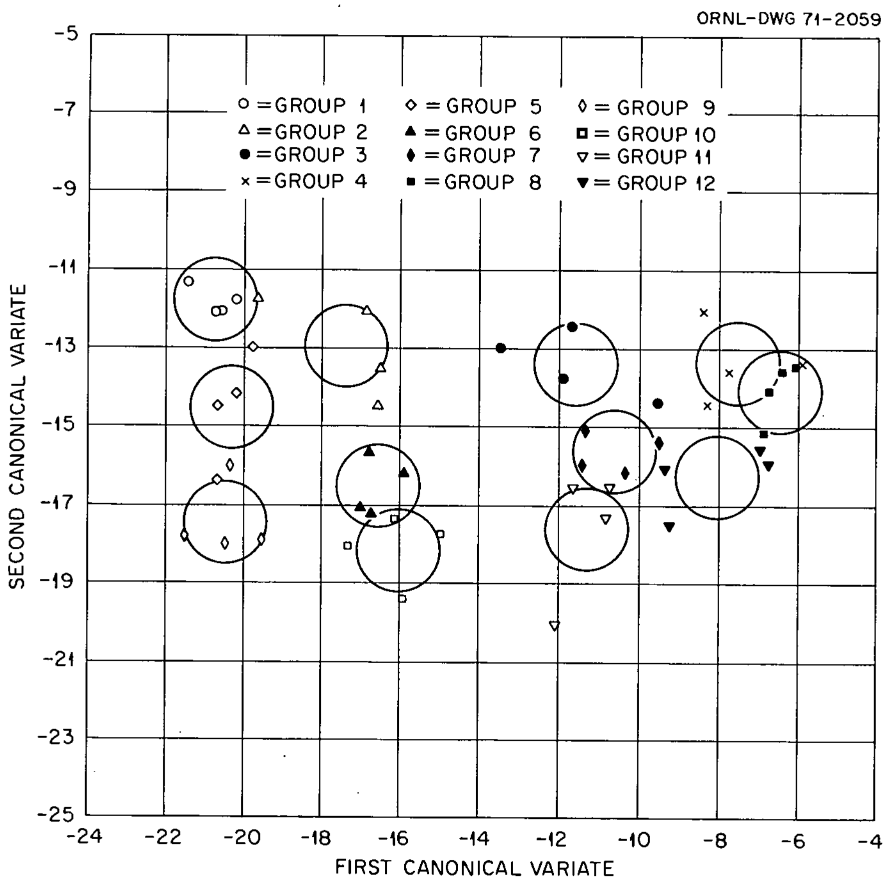

Fig. 33. Example of 95% circles of uncertainty with h = 12, p = 9, $N_1 = N_2 = \ldots = N_{12} = 4$.

The statistic

$$\sum_{i=1}^{k} (n_i - 2)s^2/\sigma^2$$

has a χ^2 distribution with

$$\sum_{i=1}^{k} (n_i - 2)$$

degrees of freedom. On ranking the estimates of the regression coefficients from low to high, suppose the ranking becomes

$$\hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_k \; .$$

In order for β_l and $\beta_{l'}$ to be judged significantly different,

$$\frac{\hat{\beta}_l - \hat{\beta}_{l'}}{\sqrt{\mathrm{var}(\beta_l) + \mathrm{var}(\beta_{l'})}}$$

must exceed some value denoted by $r_{p,\nu}$, where p is the number of regression coefficients involved in the comparison and ν is the number of degrees of freedom associated with the estimate of σ^2.

From the assumptions mentioned earlier, it is known that var($\hat{\beta}_i$) is proportional to σ^2. Therefore let the estimate of var(β_i), $i = 1, 2, ..., k$, be given by $s^2\ g_i(x)$. Hence in order for β_l and $\beta_{l'}$ to be judged significantly different, the following inequality should be satisfied:

$$\hat{\beta}_l - \hat{\beta}_{l'} > \frac{[g_l(x) + g_{l'}(x)]\, s^2}{2}\, z_{p,\nu} ,$$

where $z_{p,\nu} = \sqrt{2}\, r_{p,\nu}$ is the value appearing in the tabled values of Duncan's significant Studentized ranges.

Bibliography of Mixture Designs

T. L. Hebble

There have been recent advances in statistical techniques for studying mixtures in which it is desirable to find the optimum combination of components. Most statistically designed experiments require that the controllable variables be independent of one another. This is not possible in the case of mixtures since the component fractions must add up to unity.

To meet the increasing need for statistical design and analysis of mixtures, a bibliography on the subject of mixture designs has been compiled. A report listing the sources and a short text is being prepared, and efforts will be made to maintain a copy of each reference.

Probability that a Nucleus Will Be Detected in a Tissue Section

W. E. Lever V. R. R. Uppuluri

It is of interest to estimate the number of nuclei that are cut and exposed on any one surface of a tissue section. In order to do this, all the nuclei are assumed to be spherical, to have the same diameter $2R$, and to be homogeneously spread on the tissue. Let w denote the thickness of the section. A typical configuration of nuclei on a tissue section is shown in Fig. 34.

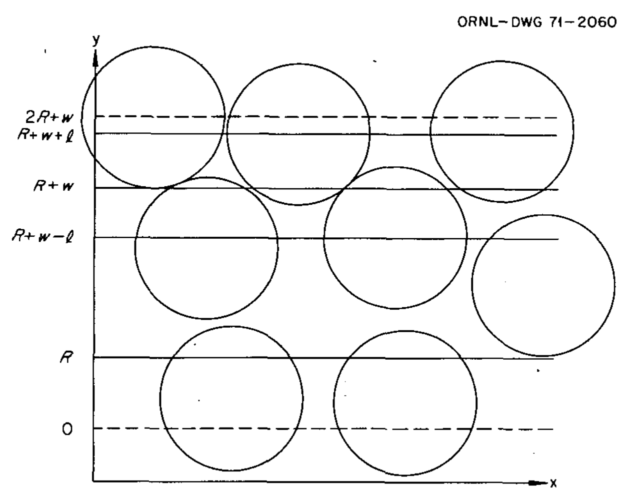

Fig. 34. Typical configurations of nuclei on a tissue section. Circles denote nuclei; the area between the solid black lines ($R \leqslant y \leqslant R + w$) denotes the section.

Then it is of interest to estimate the number of nuclei which can be detected, that is, nuclei that are cut only by the upper side of the section. The problem is considered in the following general way. If a portion of the nucleus is in the section, it can only be detected if the nucleus is cut by the upper side in such a way that the distance between this side and the center of the nucleus is at most l.

If a nucleus intersects the section in some way, the y coordinate of the center of the circle must vary between 0 and $2R + w$. However, if the nucleus is to be detected, the y coordinate must vary between $R + w - l$ and $R + w + l$. Now, if the nuclei are randomly distributed throughout the tissue, the probability distribution of the center of a nucleus Y is a uniform distribution with density function

$$f(y) = \frac{1}{2R + w}, \quad 0 \leqslant y \leqslant 2R + w\,.$$

The probability that a nucleus may be detected is given by

$$\text{Prob }[R + w - l < y < R + w + l] = \int_{R+w-l}^{R+w+l} \frac{1}{2R + w}\, dt = \frac{l/R}{1 + w/2R}\,.$$

In the special case $l = R$, all nuclei that touch the upper boundary of the section will be detected. In this case, the probability of detecting a cell is given by

$$\frac{1}{1 + w/2R} = \frac{2R}{2R + w} = 1 - \frac{w}{2R + w} = 1 - \frac{1}{1 + s}\,,$$

where $s = 2R/w$ = nuclear diameter/section thickness.

A short table giving the expected percentages of nuclei that may be detected is given as Table 10 for the special case $l = R$ and for the case $l = \frac{1}{2}R$. For the case $l = R$, the detection of a nucleus when two or three types of nuclei are in the section was also considered.

Two kinds of nuclei. Suppose there are two kinds of nuclei, one type of radius R and the other of radius θR $(0 \leqslant \theta \leqslant 1)$. Let them be mixed homogeneously in the proportion $\alpha{:}1 - \alpha$ on the tissue $(0 \leqslant \alpha \leqslant 1)$.

Table 10. Expected percentages of nuclei that may be detected

s = nuclear diameter/section thickness

s	$l = R$	$l = \frac{1}{2}R$
$\frac{1}{4}$	20.00	10.00
$\frac{1}{3}$	25.00	12.50
$\frac{1}{2}$	33.33	16.67
1	50.00	25.00
2	66.67	33.33
3	75.00	37.50
4	80.00	40.00
5	83.33	41.67
6	85.71	42.86
7	87.50	43.75
8	88.89	44.44
9	90.00	45.00
10	90.91	45.45

Given that a nucleus is in the section, the probability of detecting it can be shown to be

$$P(\alpha, \theta, s) = 1 - \frac{\alpha}{1+s} - \frac{(1-\alpha)}{1+\theta s},$$

where $0 < s = 2R/w$, $0 \leqslant \theta \leqslant 1$, $0 \leqslant \alpha \leqslant 1$.

For a given (α, θ, s), $100\,P(\alpha, \theta, s)$ gives the expected percent of nuclei *detected.*

Three kinds of nuclei. Suppose there are three kinds of nuclei: one type of radius R, another type of radius $\theta_2 R$, and the third type of radius $\theta_3 R$. Let them be mixed homogeneously on the tissue in the proportion $\alpha_1 : \alpha_2 : 1 - \alpha_1 - \alpha_2$.

Given that a nucleus is in the section, the probability of detecting it can be shown to be

$$P(\alpha_1, \alpha_2, \theta_2, \theta_3, s) = 1 - \frac{\alpha_1}{1+s} - \frac{\alpha_2}{1+\theta_2 s} - \frac{1-\alpha_1-\alpha_2}{1+\theta_3 s},$$

where $0 < s = 2R/w$, $0 \leqslant \theta_2, \theta_3 \leqslant 1$, $0 \leqslant \alpha_1, \alpha_2 \leqslant 1$.

For a given $(\alpha_1, \alpha_2, \theta_2, \theta_3, s)$, $100\,P(\alpha_1, \alpha_2, \theta_1, \theta_2, s)$ gives the expected percent of nuclei detected.

Sample Size Requirements

D. G. Hoel[6]   Kim O. Bowman

An experimenter who is interested in determining sample sizes necessary for testing hypotheses about the equality of several Gaussian means in a one-way analysis of variance can refer to one or several of the existing articles on this subject in the statistical literature. Many of the tables which accompany these articles are limited in scope, thereby restricting their applicability. As a result, the experimenter has been obliged to operate within a narrow range of tabulated values, or to evaluate the appropriate mathematical function for each specific set of conditions. Both situations are constraining, and neither has encouraged a wider use of correct techniques for determining adequate sample sizes by the very people who are performing experiments.

As far as the statistician is concerned, answers to questions concerning adequate sample size in an analysis of variance situation depend on such things as the number of categories to be compared, the levels of risk the experimenter is willing to assume, and some knowledge of the noncentrality parameter. The experimenter, on the other hand, can deal better intuitively with an estimate of the standardized range of the means than with the noncentrality parameter. Tables[12] have been developed which are oriented toward the experimenter, and present maximum values of the standardized range τ when the means of k groups each containing N observations are being compared at α and β levels of risk, where

1. τ is the difference between the largest and the smallest of the k means, divided by the standard deviation;
2. α is the probability of a "type I error," or the risk an experimenter is willing to take in rejecting the null hypothesis when it is true;
3. β is the probability of a "type II error," or the risk an experimenter is willing to take in accepting the null hypothesis when it is false. The quantity $1 - \beta$ is the "power" of the test, or the probability of detecting a prescribed difference.

---

12. M. A. Kastenbaum, D. G. Hoel, and K. O. Bowman, *Sample Size Requirements: Tests of Equality of Several Gaussian Means,* ORNL-4468 (1969).

If $X_{i1}, X_{i2}, ..., X_{in}$ $(i = 1, ..., k)$ are n independent normally distributed random variables each having mean μ_i and variance σ^2, then the usual test for

$$\mu_1 = \mu_2 = ... = \mu_k$$

is based upon the F statistic. Defining

$$\bar{\mu} = \sum_{i=1}^{k} \mu_i/k$$

and

$$\delta_i = \mu_i - \bar{\mu} ,$$

it follows that the F statistic is distributed as a noncentral F distribution with $f_1 = k - 1$ and $f_2 = k(n - 1)$ degrees of freedom and noncentrality parameter

$$\lambda = n \sum_{i=1}^{k} \delta_i^2/2\sigma^2 .$$

Various tables have been produced which give either the power of the F test or the noncentrality parameter for a fixed type II error β. In experimental situations, however, one has a better "feel" for the standardized maximum difference between any two means,

$$\tau = (\mu_{max} - \mu_{min})/\sigma ,$$

than for the noncentrality parameter λ. Therefore, the preference is for tables of τ. Although the power is not a function of τ it can easily be shown that

$$\tau \leqslant 2\sqrt{\lambda/n} = \phi\sqrt{2k/n}$$

with equality if and only if

$$\mu_i = (\mu_{max} + \mu_{min})/2$$

for all μ_i other than μ_{max} and μ_{min}. Therefore, values of $2\sqrt{\lambda/n}$, which give the maximum possible difference between any two standardized means, appear in the tables.[13] These values of τ are given for:

$\alpha = 0.01, 0.05, 0.1, 0.2$

$\beta = 0.005, 0.01, 0.025, 0.05, 0.1, 0.2, 0.3, 0.4$

$k = 2$ (1) 6

$N = 2$ (1) 30 (5) 50 (10) 100 (50) 200 (100) 500 (500) 1000

An additional set of tables has been developed for testing treatment effects in a randomized block design. Maximum values of the standardized range of the treatment means are tabulated for $k = 2$ (1) 6 treatments; $b = 2$ (1) 5 blocks; $N = 1$ (1) 30 (2) 50 (5) 100 observations per cell; and $\alpha = 0.01, 0.05$ and $\beta =$ 0.005, 0.01, 0.025, 0.05, 0.1, 0.2, 0.3, 0.4 levels of risk.

---

13. M. A. Kastenbaum, D. G. Hoel, and K. O. Bowman, *Adequate Sample Sizes for Randomized Block Designs*, ORNL-4527 (1970).

Some Modifications of Play-the-Winner Sampling for Selecting the Better of Two Binominal Populations

D. G. Hoel[6]

For selecting the better of two binomial populations with play-the-winner sampling, Sobel and Weiss[14] have considered the following procedure.

"Let S_A and S_B be the number of A successes and B successes, respectively, let $\Delta = p - p' \geqslant 0$, and let P^* and Δ^* be probabilities specified by the experimenter. The procedure R_S declares treatment i to be the better one when $S_i - S_j = r$ (where j is the other treatment). The integer r is chosen to be the smallest such that

$$P(CS) \geqslant P^* \text{ whenever } \Delta \geqslant \Delta^* \text{."} \tag{1}$$

We consider the following modification of R_S. Treatment i is declared the better when $R_{ij} = S_i + F_j - (S_j + F_i) = r$. Since play-the-winner sampling is used, we have $|F_i - F_j| \leqslant 1$, and thus the modified procedure will not differ much from R_S.

The same analysis as Sobel and Weiss employed can be easily applied to the procedure. To begin, let

$$\begin{aligned} P_n &= \text{Prob}\left\{A \text{ is selected} \mid R_{AB} = n, NT = A\right\}, \\ Q_n &= \text{Prob}\left\{A \text{ is selected} \mid R_{AB} = n, NT = B\right\}, \end{aligned} \tag{2}$$

where $NT = A$ means the next trial is from population A. From the definition of the procedure it can be shown that

$$\begin{aligned} P_n &= pP_{n+1} + qQ_{n-1}, \\ Q_n &= q'P_{n+1} + p'Q_{n-1}, \end{aligned} \tag{3}$$

where p (p') is the probability of success from population A (B). Using the boundary conditions $P_r = 1$, $Q_{-r} = 0$ the solution of (3) is

$$\begin{aligned} P_n &= \frac{p'q' - pq\lambda^{r+n}}{p'q' - pq\lambda^{2r}}, \\ Q_n &= \frac{p'q' - p'q'\lambda^{r+n}}{p'q' - pq\lambda^{2r}}, \end{aligned} \tag{4}$$

where $\lambda = p'/p$. The error requirement (1) is equivalent to

$$(P_0 + Q_0)/2 \geqslant P^* \text{ whenever } p - p' \geqslant \Delta^*. \tag{5}$$

---

14. M. Sobel and G. H. Weiss, *Play-the-Winner Sampling for Selecting the Better of Two Binomial Populations*, Technical Report No. 123, Department of Statistics, University of Minnesota (1969).

Now

$$(P_0 + Q_0)/2 = \frac{p'q' - \tfrac{1}{2}(pq + p'q')\lambda^r}{p'q' - pq\lambda^{2r}}$$

is an increasing function of r (note: $\lambda < 1, r \geqslant 1$) and is equal to 1 as $r \to \infty$. Thus there exists a unique smallest integer r such that (5) is satisfied. The required value of r is therefore the smallest integer greater than or equal to the r found from

$$\lambda^r = \left\{\tfrac{1}{2}(pq + p'q') - [(pq + p'q')^2/4 - 4\,pq\,p'q'\,P^*(1 - P^*)]^{1/2}\right\} \Big/ 2pqP^* . \tag{6}$$

Next, the right-hand side of (6) is an increasing function of Δ ($\Delta \geqslant 0$), where $p = p_0 + \Delta/2, p' = p_0 - \Delta/2$, and λ is a decreasing function of Δ. Therefore r is a decreasing function of Δ. Thus for $\Delta \geqslant \Delta^*$, $P(CS)$ is minimized at $\Delta = \Delta^*$. However, it is not clear what value of p_0 minimizes $P(CS)$. Some sample values are given in Table 11.

Continuing with the Sobel and Weiss argument, (6) may be written as

$$\lambda^r = \frac{2}{1 + pq/p'q'}\;(1 - P^*) + O[(1 - P^*)^2] .$$

Thus we find as an approximation to r (P^* close to 1)

$$r \doteqdot \log\,[2(1 - p^*)/\log\,(1 - \Delta^*) , \tag{7}$$

which is the same value as Sobel and Weiss found for the procedure R_S. Table 12 gives a comparison of (7) with the correct value of r for the least favorable configuration (i.e., Table 11).

To obtain expressions for the expected number of observations from each population, we define

$$\begin{aligned} U_n &= E\left\{N_B | R_{AB} = n,\, NT = A\right\} , \\ V_n &= E\left\{N_B | R_{AB} = n,\, NT = B\right\} . \end{aligned} \tag{8}$$

Following the Sobel and Weiss analysis we have

$$\begin{aligned} U_n &= pU_{n+1} + qV_{n-1} , \\ V_n &= p'V_{n-1} + q'U_{n+1} + 1 , \\ V_{-r} &= U_r = 0 , \end{aligned} \tag{9}$$

which yield the solution

$$U_n = \frac{q(r-n)}{p-p'} + \frac{(\lambda^r - \lambda^n)q\,[q(2r-1) + p]\,\lambda^{r-1}}{(1 - p\lambda - q\lambda^{2r-1})(p - p')} . \tag{10}$$

Table 11. Values of p_0 which minimize $P(CS)$

Δ^*	$P^* = 0.75$	$P^* = 0.90$	$P^* = 0.95$	$P^* = 0.99$
0.1	0.830	0.874	0.890	0.914
0.2	0.777	0.829	0.850	0.881

Table 12. Values of r required to satisfy the error requirement

P^*	$\Delta^* = 0.1$		$\Delta^* = 0.2$	
	Exact	Approx	Exact	Approx
0.75	7.6	6.6	3.3	3.1
0.90	16.7	15.3	7.5	7.2
0.95	23.2	21.9	10.6	10.3
0.99	38.0	37.1	17.6	17.5

The risk as defined by Sobel and Weiss is then

$$L = \frac{1}{2}(p - p')(U_0 + V_0) .$$

Noticing that $V_0 = U_0/q - pU_1/q$, we find that

$$L = \frac{1}{2(1 - p\lambda - q\lambda^{2r-1})} \Big\{(2qr + p)(1 - p\lambda - q\lambda^{2r-1}) + (2qr + p - q)[2q\lambda^{2r-1} + p\lambda^r - (1 + q)\lambda^{r-1}]\Big\}. \quad (11)$$

To obtain $E(N_A)$ we switch p and p' (also q and q') in the expression for $E(N_B) = ½\,(U_0 + V_0)$. Then the total expected number of observations $E(N)$ is equal to $E(N_A) + E(N_B)$. Performing this we find

$$E(N) = \frac{1}{2p(1 - \lambda)(1 - p\lambda - q\lambda^{2r-1})} \Big\{-(1 - p\lambda - q\lambda^{2r-1})\,[p(1 - \lambda)(2r - 1)] + [2r - 2\lambda p(r - 1) - 1]\,[2(1 - \lambda p) + \lambda^r(p - 2 + \lambda p)] + [2q(r - 1) + 1]\,[2q\lambda^{2r-1} + p\lambda^r - (1 + q)\lambda^{r-1}]\Big\} .$$

A Nonparametric Model for Competing Risks

D. G. Hoel[6] H. E. Walburg[15]

In a previous report[16] cohort mortality data were represented by a probabilistic combination of competing risks (diseases). Each risk S_i was described by an age-at-death distribution F_i and a net probability of occurrences p_i ($i = 1, \ldots, k$). In the report it was assumed that the age-at-death distribution

15. Biology Division.
16. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, pp. 78–80.

had a known parametric form. A representation of the data may also be made without this parametric assumption as follows.

Suppose the ages at death are ordered as $0 \leqslant t_1 \leqslant t_2 \leqslant \ldots \leqslant t_n$, and let $G_i(t)$ be the distribution function of the cause S_i. The $\{t_i\}$ are then made up of ages associated with S_i and ages of death due to the other causes. Thus we can consider the data to be a set of randomly censored observations. Kaplan and Meier[17] have given a nonparametric maximum likelihood estimate of $G_i(t)$ which they call the *product-limit estimate.* This estimate is given by

$$\hat{G}_i(t) = 1 - \prod_{r_i} [(n - r_i)/(n - r_i + 1)] \ , \tag{1}$$

where r_i assumes values for which $t_{r_i} \leqslant t$ and t_{r_i} is an age associated with cause S_i. They have further shown that if the number of deaths at ages greater than or equal to t tends to infinity as n tends to infinity, then $\hat{G}_i(t)$ converges in probability to $G_i(t)$.

Since the model identifies $G_i(t)$ with $p_i F_i(t)$, we estimate the net probability p_i by

$$\hat{p}_i = \hat{G}_i(\infty) \tag{2}$$

and the age-at-death distribution F_i by

$$\hat{F}_i(t) = \hat{G}_i(t)/\hat{p}_i \ . \tag{3}$$

Combining these estimates we find

$$\hat{F}(t) = 1 - \prod_{i=0}^{k} [1 - \hat{p}_i \hat{F}_i(t)]$$

$$= 1 - \prod_{i=0}^{k} \prod_{r_i} [(n - r_i)/(n - r_i + 1)] = r/n \ ,$$

where r is the largest integer s such that $t_s \leqslant t$. In other words, $\hat{F}(t)$ is the empirical distribution function for the complete set of age-at-death data.

The calculation of the nonparametric estimates (2) and (3) is straightforward in comparison with the difficulties in obtaining the parameter estimates for a given functional form of $F_i(t)$. An alternative method for finding these parametric estimates is to construct a sample based upon the nonparametric estimate $\hat{F}_i$ of F_i. To do this, suppose $x_1, x_2, \ldots, x_m$ denote the points of increase of $\hat{F}_i$ with jumps of size $j_1, j_2, \ldots, j_m$ [i.e., $\hat{F}(x_i) - \hat{F}(x_i-) = j_i$]. Since each j_i is a rational we let $j_i = h_i/d_i$ integers $(i = 1, \ldots, m)$ and define $d = \prod_{i=1}^{m} d_i$. Then a sample with $j_i d$ observations equal to x_i $(i = 1, \ldots, m)$ will have $\hat{F}_i$ as its empirical distribution function. We then propose estimating the parameters of F_i by finding their maximum likelihood estimates based upon the constructed sample. The likelihood function for the sample is

$$L = \prod_{i=1}^{m} f(x_i)^{j_i d} \ ,$$

17. E. L. Kaplan and P. Meier, *J. Am. Statist. Assoc.* **53,** 457–81 (1958).

and thus it is required to maximize

$$\prod_{i=1}^{m} f(x_i)^{j_i} .$$

Estimates determined in this manner will naturally differ from the maximum likelihood extimates. However, they are generally easier to find.

Finally, there is a relationship between the product-limit estimate (1) and the usual actuarial-interval estimates. To obtain the interval estimates, divide the time axis into m intervals I_i ($i = 1 \ldots, m$), and let n_i denote the number of animals alive at the start of interval I_i. The net probability of death due to risk S_i in interval I_j is defined as (see Chiang)[18]

$q_{ij} = Pr$ {an animal alive at the start of I_j will die in I_j if
S_i is the only risk acting on the population}.

From these net interval probabilities we can form a cumulative mortality due to risk S_i from the relation

$$F_{ij} = F_{i,j-1} + (1 - F_{i,j-1})\, q_{ij} \tag{4}$$

($F_{i_0} = 0$), where F_{ij} is the probability of death due to S_i up to and including interval I_j when S_i is the only risk acting on the population.

Now, assume the intervals are sufficiently small so that at most one death occurs in each interval. Most estimates of q_{ij}, including Chiang's, are then of the form

$$\hat{q}_{ij} = \begin{matrix} 1/n_j \text{ if a death due to } S_i \text{ occurs in } I_j \text{ ,} \\ 0 \text{ otherwise.} \end{matrix}$$

Let $x_1 < x_2 < \ldots < x_r$ represent the observed deaths due to risk S_i, and define s_i to be the number of animals alive before the death at x_i. Now, in the limit as the interval lengths tend to zero, the cumulative mortality function (4) has jumps only at the observed deaths x_i. The value of the estimated cumulative mortality function at x_i is then

$$\hat{F}(x_i) = \hat{F}(x_{i-1}) + [1 - F(x_{i-1})]\,/s_i \,, \tag{5}$$

with $\hat{F}(x_0) = 0$. Solving (5) we find

$$\hat{F}(x_i) = 1 - \prod_{j=1}^{i} (1 - 1/s_j) \,, \tag{6}$$

which can be shown to be equal to the product-limit estimate (1).

---

18. C. L. Chiang, *Introduction to Stochastic Processes in Biostatistics,* Wiley, New York, 1968.

Chance Mechanisms Associated with Dirichlet Type II Distributions

V. R. R. Uppuluri Milton Sobel[19]

Definition. The multivariate probability density function

$$f(x_1, \ldots, x_r) = \frac{\Gamma(M + N_1 \ldots + N_r)}{\Gamma(M)\,\Gamma(N_1) \ldots \Gamma(N_r)} \; \frac{x_1^{N_1 - 1} \ldots x_r^{N_r - 1}}{(1 + x_1 + \ldots + x_r)^{M + N_1 + \ldots + N_r}},$$

where $0 < x_i < \infty; M, N_1, \ldots, N_r > 0$ is called the type II Dirichlet distribution.

This is related to the negative multinomial distribution when $N_1, \ldots N_r$ are integers.[20] A special case of this gives the multivariate t distribution defined by Dunnett and Sobel.[21] The lower and upper tails of this distribution appear in the study of the distribution of the largest and smallest Studentized chi-square statistics.[22] These cumulative integrals also appear in the context of the selection of a subset containing the "best" of several type III distributions,[23] and the problem of ranking variances,[24] and in the inverse sampling procedure for selecting the most probable event in a multionomial distribution.[25]

A study of cumulative integrals associated with this distribution will be useful for computational purposes and for the limiting behavior as some of the parameters tend to infinity. We will illustrate below some recursive relations obtained in the case of upper tails. Define

$$D_r^{(j)}(M; N; a) = \frac{(1 + ja)^M\, \Gamma(M + rN)}{\Gamma(M)\, \Gamma^r(N)} \int_a^\infty \ldots \int_a^\infty \frac{\prod_{i=1}^{r} (y_i^{N-1}\, dy_i)}{\left(1 + ja + \sum_{i=1}^{r} y_i\right)^{M + rN}} \tag{1}$$

for $M \geq 1$ with integers j, $r \geq 0$, $N \geq 1$, and $a \geq 0$.

For $M > 1$ and $r > 0$, we get the recursion

$$D_r^{(j)}(M; N; a) = D_r^{(j)}(M - 1; N; a)$$

$$- r \binom{M + N - 2}{M - 1} \frac{a^N (1 + ja)^{M-1}}{[1 + (j + 1)a]^{M+N-1}}\, D_{r-1}^{(j+1)}(M + N - 1; N; a). \tag{2}$$

19. Consultant.

20. I. Olkin and M. Sobel, *Biometrika* **52**, 167–79 (1965).

21. C. W. Dunnett and M. Sobel, *Biometrika* **41**, 153–69 (1954).

22. J. V. Armitage and P. R. Krishnaiah, *Tables for the Studentized Largest and Smallest Chi-Square Distribution and Their Applications,* ARL-64-188 and ARL-218 (1964).

23. S. S. Gupta, *Ann. Inst. Statist. Math.* **14**, 199–216 (1963).

24. R. E. Bechhofer and M. Sobel, *Ann. Math. Statist.* **25**, 273–89 (1954).

25. T. Cacoullos and M. Sobel, "An Inverse-Sampling Procedure for Selecting the Most Probable Event in a Multinomial Distribution," *Multi-Variate Analysis I* (ed. by P. R. Krishnaiah), pp. 423–55, Academic, New York, 1966.

It is easily seen that

$$D_0^{(j)}\,(M;N;a) = 1 \qquad \text{for all } M, N, a, \text{ and } j\,, \tag{3}$$

$$D_r^{(j)}\,(M;N;0) = 1 \qquad \text{for all } M, N, r, \text{ and } j\,, \tag{4}$$

$$D_r^{(j)}\,(M;N;\infty) = 0 \qquad \text{for all } M, N, r, \text{ and } j\,. \tag{5}$$

The boundary conditions for computations are (3) and

$$D_r^{(j)}\,(1;N;a) = 1 - r\left(\frac{\bar{c}}{1+j\bar{c}}\right)^N D_{r-1}^{(j)}\,(N;N;\bar{c})\,, \tag{6}$$

where $\bar{c} = a/(1+a)$. These generalize the results given by Cacoullos and Sobel.[25] Similar results are available in the case of lower tails.

On Centro-Hermitian and Centroskew-Hermitian Matrices

V. R. R. Uppuluri J. A. Carpenter

In 1962, Collar[26] discussed some useful methods for the determination of eigenvalues and eigenvectors of centrosymmetric and centroskew matrices. These were used by Doner and Uppuluri.[27] We now extend the results of Collar to matrices with complex elements.

Let C be an $n \times n$ matrix whose elements may be complex numbers. We let $C = P + iQ$, where P and Q are $n \times n$ real matrices. It can be shown[28] that Γ_1 is similar to Γ_2 where

$$\Gamma_1 = \begin{bmatrix} P & -Q \\ Q & P \end{bmatrix}$$

and

$$\Gamma_2 = \begin{bmatrix} P - iQ & 0 \\ 0 & P + iQ \end{bmatrix} = \begin{bmatrix} \bar{C} & 0 \\ 0 & C \end{bmatrix}.$$

As pointed out by Householder,[28] the results due to Muller and mentioned by Bodewig[29] about the eigenvalues and eigenvectors of C can be deduced from this.

Definition. C is said to be centro-Hermitian if and only if $c_{ij} = \bar{c}_{n+1-i,\,n+1-j}$, $1 \leqslant i, j \leqslant n$, where $\bar{c}_{ij}$ is the complex conjugate of c_{ij}.

We immediately see that C is centro-Hermitian implies P is centrosymmetric and Q is centroskew as defined by Collar. Thus we have

$$J = JPJ \text{ and } Q = -JQJ\,,$$

26. A. R. Collar, *Quart. J. Mech. Appl. Math.* **15**, 265–81 (1962).
27. J. R. Doner and V. R. R. Uppuluri, *SIAM J. Appl. Math.* 18, 191–209 (1970).
28. A. S. Householder, "Compound Matrices and Characteristic Roots of a Complex Matrix," unpublished (1963).
29. E. Bodewig, *Matrix Calculus*, Interscience, New York, 1959.

where J is the $n \times n$ matrix with units in the secondary (counter) diagonal and zeros elsewhere. In fact we have the following:

Theorem 1. The following statements are equivalent.

1. $C = P + iQ$ is centro-Hermitian.
2. $P = JPJ$ (or P is centrosymmetric) and $Q = -JQJ$ (or Q is centroskew).
3. $C = J\bar{C}J$.

Using the similarity of Γ_1 and Γ_2, one can reduce the problem of finding the roots of an $n \times n$ complex matrix to that of finding the roots of a $2n \times 2n$ real matrix. But as Householder[28] said: "As a practical matter, whether the advantage of dealing with a real matrix than a complex one offsets the disadvantage of the doubled order is open to question." We will show in the next theorem that if we know a priori that C is a centro-Hermitian matrix, then the eigenvalue problem of C is equivalent to finding the eigenvalues of an $n \times n$ real matrix.

Theorem 2. If C is a centro-Hermitian matrix, then

1. Γ_1 is a centrosymmetric matrix.
2. Γ_1 can be written in the form

$$\Gamma_1 = \begin{bmatrix} A & BJ \\ JB & JAJ \end{bmatrix},$$

where $A = P$ and $B = JQ$.

3. Γ_1 is similar to

$$\begin{bmatrix} P + JQ & 0 \\ 0 & P - JQ \end{bmatrix}.$$

Thus, we have $\bar{C}$ is similar to $P + JQ$ and C is similar to $P - JQ$. We next define a centroskew-Hermitian matrix and show that the eigenvalue problem depends only on an $n \times n$ real matrix.

Definition. C is said to be centroskew-Hermitian if and only if $c_{ij} = -\bar{c}_{n+1-i,\, n+1-j}$, $1 \leqslant i, j \leqslant n$, where $\bar{c}_{ij}$ is the complex conjugate of c_{ij}.

Theorem 3. The following statements are equivalent:

1. $C = P + iQ$ is centroskew-Hermitian.
2. $P = -JPJ$ (or P is centroskew) and $Q = JQJ$ (or Q is centrosymmetric).
3. $C = -J\bar{C}J$.
4. iC is centro-Hermitian.

From theorems 3(4) and 2(3) it follows that $Q - iP$ is similar to $Q + JP$. Thus, to find the eigenvalues of a centroskew-Hermitian matrix $C = P + iQ$, one needs to find the eigenvalues of an $n \times n$ real matrix $Q + JP$ and multiply each of them by i.

On Wigner's Conjecture about the Asymptotic Distribution of Eigenvalues

V. R. R. Uppuluri

The study of the properties of the eigenvalues of random matrices as related to the energy levels was initiated by Wigner and pursued vigorously by a number of physicists.[30] In high-energy regions it is

30. C. E. Porter (ed.), *Statistical Theories of Spectra*, Academic, New York, 1965.

impossible in practice to determine exactly all the energy levels; thus one is interested only in the statistical properties of the energy levels in these regions.

In 1955, Wigner[31] showed that the asymptotic distribution of the eigenvalues of a symmetric random matrix whose elements take the values +1 and −1 with probabilities ½ and ½ and whose diagonal elements are identically equal to zero is a semicircle distribution. In a recent report[32] we proved a conjecture made by Wigner[33] indicating the validity of the semicircle limit distribution for more general ensembles. In fact we proved the following theorem.

Let $X = (X_{ij})_{i,j=1}^{n}$ be a random matrix such that:

1. $X_{ij} = X_{ji}$, almost surely (a.s.);
2. $\{X_{ij}, i \leqslant j\}$ is independent.
3. $E(X_{ij}) = 0$.
4. $E(X_{ij}^2) = \sigma^2, i \neq j$.
5. $E|X_{ij}^k| \leqslant C_k < \infty, k = 1, 2, \ldots$.

Denote by $W_n(x)$ the empirical distribution function of the eigenvalues of $X/2\sigma\sqrt{n}$.

Theorem. $W_n(x) \to W(x)$ a.s., as $n \to \infty$, where $W(x)$ is the absolutely continuous distribution function with semicircle density

$$w(x) = \begin{cases} \frac{2}{\pi}(1 - x^2)^{1/2}, & |x| \leqslant 1 \\ 0 \quad , & |x| > 1 . \end{cases}$$

This result is stronger than (1) Wigner's conjecture,[33] (2) Grenander's result,[34] and (3) may be compared with the result of Arnold.[35]

STATISTICAL APPLICATIONS

Analytical Chemistry

Optimizing specific transfer ribonucleic acid assay conditions (T. J. Mitchell and I. B. Rubin[36]). Response surface optimization techniques have been used to establish optimum reaction conditions for the assay of arginine-, glutamic acid-, and lysine-accepting transfer ribonucleic acids. A list of the 11 variables (factors) involved and an outline of the experimental program which was developed to determine an optimum combination of these variables are given in a previous report.[37]

This program has been modified slightly during the past year. The sequence of designs now used is as follows:

1. A 16-run fraction of a 4 × 2^9 factorial design, in which the four-level factor represents four different buffers. Previously, the initial design included a two-level buffer factor and a two-level time of

31. E. P. Wigner, *Ann. Math.* **62**, 548–64 (1955).
32. W. H. Olson and V. R. R. Uppuluri, *Asymptotic Distribution of Eigenvalues of Random Matrices,* ORNL-4603 (1970). Also to appear in the *Proceedings of the Sixth Berkeley Symposium,* University of California Press, Berkeley (1971).
33. E. P. Wigner, *Ann. Math.* **67**, 323–26 (1958).
34. U. Grenander, *Probabilities on Algebraic Structures,* Wiley, New York, 1963.
35. L. Arnold, *J. Math. Anal. Appl.* **20**, 262–68 (1967).
36. Analytical Chemistry Division.
37. *Math. Div. Ann. Progr. Rept. Dec. 31, 1968,* ORNL-4385, pp. 83–84.

incubation factor (now held at one level). The current design permits the estimation of the main effects of all ten variables as well as the pH × buffer interaction, assuming all other interactions negligible.

2. A 16-run fraction of a 2^5 factorial design. This plan permits the estimation of all main effects and two-factor interactions of five selected variables, chosen to be those whose effects are still in doubt or which were shown to be important in the previous design.
3. A 20-run central composite design in three variables, used to fit a quadratic surface to the three most important variables. The fitted equation is then used to estimate the location of the maximum.

In addition, a separate factorial design in the factors "pH" and "buffer" is run about halfway through the program to make a final decision on the buffer to be used.

In each of the above experiments, every point is replicated. Moreover, it is usually necessary to perform several experiments of each type, using the results of each to move to a more favorable region in the factor space. As a result, 360 to 540 trials were required for each optimization performed during the past year. This is less than half the number required prior to the introduction of the statistically designed experimental program. However, it is still rather large, and we have identified several areas in which further reductions can be made.

Biology

Effect of diets on spontaneous mutations (T. J. Mitchell and H. V. Malling[15]). An experiment has been performed to determine the frequency of spontaneous mutations in conidia (Neurospora) injected into rats which have been fed various diets. The seven diets (treatments) are

1. normal food,
2. fresh strawberries, unirradiated,
3. fresh strawberries, irradiated at 150 kR,
4. fresh strawberries, irradiated at 300 kR,
5. dried strawberries, unirradiated,
6. dried strawberries, irradiated at 150 kR,
7. dried strawberries, irradiated at 300 kR.

To perform the experiment, five suspensions of conidia are prepared. From each suspension, samples are taken and injected into rats from each of the seven diets. In this experiment, there was one rat per treatment-suspension combination. Thirty-six hours after injection, the rats are sacrificed and the conidia harvested. After harvesting, it is necessary to let the conidia grow in specially prepared jugs (two per rat) so that the colonies of mutated cells will be large enough to observe. Then the mutations are counted and the mutation rate calculated.

The data were analyzed as a "randomized block" experiment, with the four suspensions as blocks. One suspension was omitted because it has been applied to rats representing only a few of the diets. The initial analysis indicated no significant differences among treatments. However, a study of the residuals indicated three suspiciously low mutation rates, all of which were zero. The investigator found that the jugs associated with these extreme data points were all contaminated and should not be included in the analysis. All jugs were then examined for contamination under the same criterion to avoid bias.

With "missing data" caused by the contaminated jugs, the analysis is not straightforward. Two approaches were taken:

1. Estimate the missing data using good data, and perform a standard analysis, in which treatment differences may be compared by means of Duncan's multiple range test, for example.
2. Fit a "simple acceptable model" to the data, and attempt to draw inferences from it.

Both approaches indicated that the irradiated fresh strawberry diets as well as all three dried strawberry diets gave a higher mutation rate than the normal food or the unirradiated fresh strawberry diets. A second experiment gave the same result, with the puzzling exception that the normal food diet ended up in the higher mutation rate group.

Later experiments have shown that the frequency of *ad-3* mutations among the Neurospora conidia incubated for 36 hr in the rats increased from 20 to 60 times above the in vitro control. To avoid this increase in the spontaneous mutation frequency the conidia were incubated only 18 hr in the rats in the two next experiments with strawberry-mixed diet. The results of these two additional experiments need to be analyzed in detail before final conclusions can be made.

Chromosome classification (Claudia S. Lever and Norma C. Hull). The analysis of the human karyotype has been discussed in a previous report.[38] As a part of this study, the measurements of the chromosomes of 723 cells from 100 humans (50 males and 50 females) were analyzed to develop an objective means of chromosome classification. Mean long and short arm lengths and their respective dispersions were estimated for each chromosome. The mean vectors and disperson matrices were used in a program CHROME which classifies chromosome measurements and determines a karyotype of the cell. This set of measurements is also useful as a source of test data for evaluating various classification procedures. All the cells had already been karyotyped by a skilled cytogeneticist, and her classification was the standard used for comparison.

Minkler, Gofman, and Tandy[39] have developed a "cutting line" diagram to classify the chromosomes in a cell into different groups (A1, A2, A3, B, C + X, D, E16, E(17 + 18), F, G + Y) according to the Denver system. The classification is determined by the total arm length of a chromosome normalized by the total length of all the chromosomes in the cell and by the centromeric index, which is the ratio of the short arm length to the total arm length of a chromosome. Figure 35 shows the "cutting line" diagram with the boundaries for the different classes. The chromosomes whose measurements fall outside these boundaries are defined as marker chromosomes.

All the measurements of the chromosome 16 (that is, the chromosomes classified as 16 by the cytogeneticist) from the 723 cells were plotted on the cutting line diagram to see how many points fall in the E16 box. Other chromosome measurements were plotted the same way. Figure 36 shows the E16 chromosomes and Al chromosomes on the same plot. The E16 chromosome is of particular interest because the abnormal cells studied by Minkler et al. consistently showed an excess of E16 chromosomes. The Al chromosome measurements were plotted for comparison purposes because the abnormal cells showed the greatest imbalance between the number of E16 chromosomes and the number of Al chromosomes. The lengths were scaled to put the maximum number of E16 points in the E16 box. This scale shifted many of the Al points out of the Al box (Fig. 36). The mean centromeric index of chromosome 16 for the 723 cells is 0.367, which is below the boundary for E16, 0.395. This accounts for the large percentage of the 16's falling outside the E16 area. This plot does suggest that the imbalance between the number of chromosome 16's and the number of chromosome 1's could be caused by the choice of scaling factor. When the scale factor was chosen to put the maximum number of Al chromosomes in the Al box, most of the E16 chromosomes fell in the F area.

There may be some disagreement among cytogeneticists about the classification of particular chromosomes, but there is general agreement on the correct number of chromosomes in each group. For each of 723 cells, the number of chromosomes in each of the areas of the "cutting line" diagram was

---

38. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 123.
39. J. L. Minkler, J. W. Gofman, and R. L. Tandy, UCRL-72191 (1969).

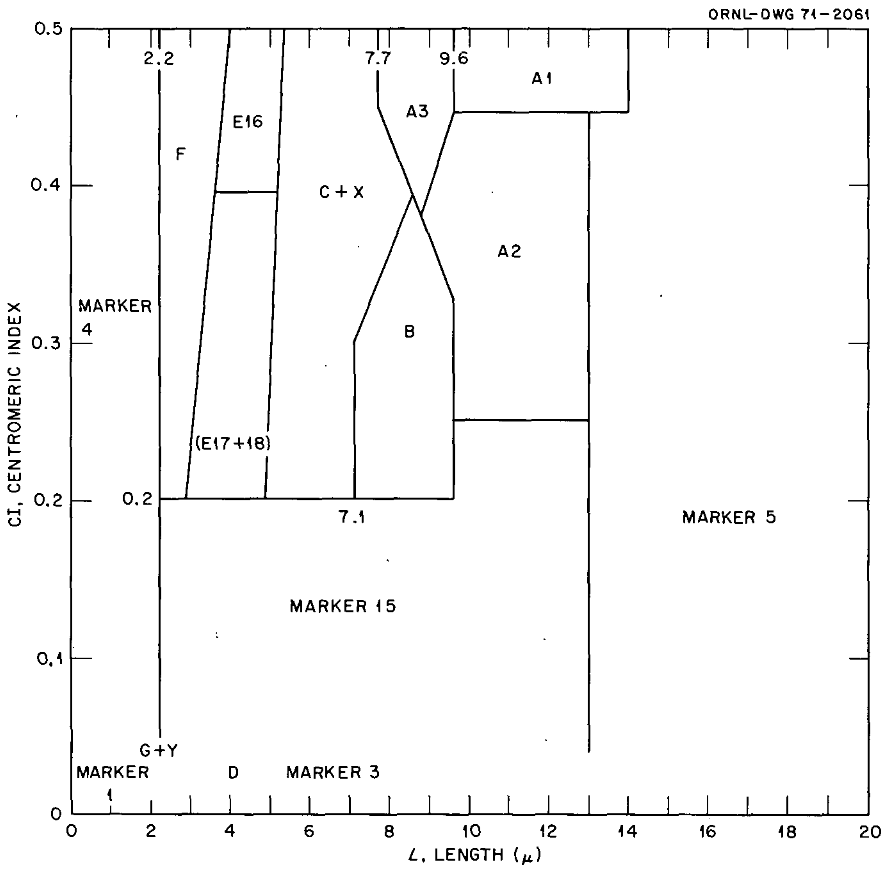

Fig. 35. Cutting line diagram.

counted. Tables 13 and 14 give, for males and females respectively, the expected mean number in each group, the actual mean number in each group, and the standard error of the mean.

In these tables, the data were scaled only by the total chromosome length. Different scale factors were used to shift the data to the right or left on the "cutting line" diagram, but no factor was found which accurately classified most of the cells. The variation in this set of normal cells is too large for the "cutting line" diagram to be successful for classification.

Detection of chemically induced mutation in mice (D. G. Hoel[6] and D. G. Gosslee). Alkylating compounds are being extensively investigated for genetic effects in mice. Mutagenic effect of compounds, such as ethyl methanesulfonate (EMS), can be investigated through their ability to induce heritable translocations – a direct measure of chromosome breakage. These chemically induced translocations cause sterility and semisterility. The current procedure used for measurement of translocation induction is to test F_1 male progeny of treated parents for sterility or semisterility by mating each one to three or more different females. Each female is opened prior to giving birth, and the number of implants and the number of live embryos are counted. Detection of sterile translocations is straightforward, but, because of (1) the natural variation in the fertility of background females and (2) chance variations in the type of sperm used in fertilization, detection of semisterile males is more difficult. From the fertility data on three or more females, a semisterile male is expected to sire half as many live embryos as a normal male. This procedure for detecting translocation males is obviously expensive and requires a good deal of animal handling and record keeping. The procedure described below reduces the time and cost of testing for semisterility considerably, hence it is more suitable for widescale screening.

Each F_1 male to be tested is caged with a female of the (SEC X C57Bl)F_1 strain, and the young produced are counted and discarded immediately. If the size of the first litter is large enough, the F_1 male is declared fertile and removed from the experiment. If the first litter is not large enough, a second litter from the same mating is observed with the same rule applying. Detailed study is then made on the remaining F_1 males. It should be noted that no mouse is declared semisterile on the basis of these first two litter sizes. However, it is expected that the majority of the fertile animals will be eliminated from the

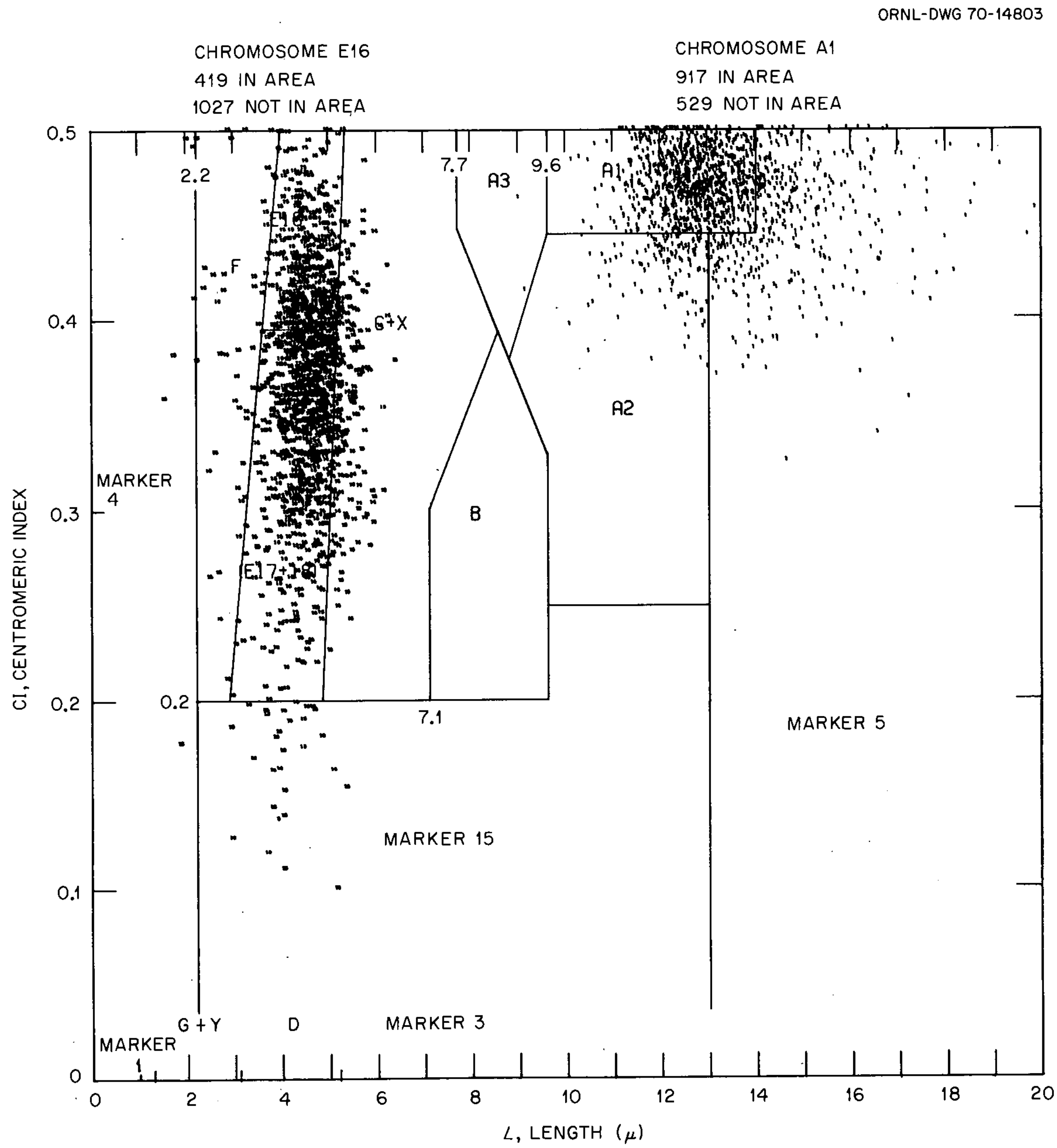

Fig. 36. Plot of chromosomes 1 and 16 from 723 cells.

Table 13. Classification of 362 normal male cells

Group	Expected number per cell	Mean number per cell	Standard error of mean
A1	2.00	1.754	0.042
A2	2.00	2.702	0.054
A3	2.00	1.345	0.042
B	4.00	4.738	0.065
C + X	15.00	12.135	0.132
D	6.00	5.425	0.042
E16	2.00	0.453	0.036
E(17 + 18)	4.00	3.102	0.084
F	4.00	4.508	0.093
G + Y	5.00	4.351	0.066
Marker 1	0.0	0.644	0.071
Marker 3	0.0	0.580	0.036
Marker 4	0.0	1.729	0.097
Marker 5	0.0	0.425	0.050
Marker 15	0.0	2.108	0.135

Table 14. Classification of 361 normal female cells

Group	Expected number per cell	Mean number per cell	Standard error of mean
A1	2.00	1.701	0.042
A2	2.00	2.634	0.051
A3	2.00	1.399	0.044
B	4.00	4.651	0.065
C + X	16.00	13.288	0.125
D	6.00	5.440	0.040
E16	2.00	0.432	0.035
E (17 + 18)	4.00	3.330	0.085
F	4.00	4.693	0.098
G + Y	4.00	3.532	0.055
Marker 1	0.0	0.526	0.059
Marker 3	0.0	0.501	0.036
Marker 4	0.0	1.709	0.097
Marker 5	0.0	0.330	0.041
Marker 15	0.0	1.834	0.132

experiment on the basis of the two litter sizes. This procedure is possible only because of the extremely good reproductive performance of the (SEC × C57Bl)F_1 females.

To obtain information on litter sizes for the particular strain of animals being considered, the litter sizes for matings with 899 fertile male mice were found for the first two litters. From these data estimates were made of the probability f_{ij} that a fertile male would have a litter of size j on its ith litter ($i = 1, 2; j = 1, 2, \ldots$). Let p denote the probability that a fertilization produces a newborn mouse with a semisterile father when it would have done so with a fertile father. Then the probability that a semisterile male has an ith litter size of s is equal to

$$\sum_{n=s}^{\infty} f_{in} \binom{n}{s} p^s (1-p)^{n-s} ,$$

which is denoted $h_i(s)$, $i = 1, 2$; $s = 0, 1, 2, \ldots$. Since a litter size of zero is not observed the estimated conditional probability that the ith litter of a semisterile mouse is of size s is

$$h_i(s)/[1 - h_i(0)] \; .$$

The estimates of the litter sizes of semisterile mice obtained from the large sample of fertile mice were checked by comparison with litter sizes from a limited number of actual semisterile mice. The estimated sizes agree well enough to be used until more litters from semisterile mice can be obtained. These estimated litter sizes can be used to construct the screening procedure as described in the next paragraph.

If the first litter is of size n_1 or larger, declare the mouse fertile; otherwise the second litter is produced. If the second litter is of size n_2 or larger, declare the mouse fertile. Now, n_1 and n_2 are chosen to maximize the number of fertile mice eliminated while keeping the probability of declaring a semisterile mouse to be fertile below a preassigned level. For example, for two sets of n's, estimates of the percentage of males declared fertile (%F) and the risk of declaring a semisterile mouse fertile (%R) are given in the following table.

n_1	n_2	%F	%R
9	10	96.1	1.1
10	11	86.1	0.2

Thus, a large percentage of the males can be declared fertile by the simple procedure of counting the number of live births in at most two litters with a small risk of declaring a semisterile male as fertile. The overall objective is to be able to make a decision on the fertility of each F_1 male as early as possible. Since (SEC × C57Bl)F_1 females normally produce 12 good litters, it is now possible to test several F_1 males per female instead of sacrificing three or more females per F_1 male as in the old procedure.

Sample size determination (J. J. Beauchamp and Paul Nettesheim[15]). It is important in planning an investigation to estimate the sample size required to have a reasonable chance of correctly declaring positive results. In Table 15, ratios of the percentage incidence of people in two communities, C1 and C2, classified according to the criteria of interest are recorded. For example, the ratio 89/77 means 89% of the people in Cl and 77% of the people in C2 are classified as "normal nonsmokers." For each cell in this table it is desired to determine what sample size should be taken from each community in order to state that the percentages from the two communities are significantly different.

The method applied to determine the sample size made use of the normal approximation to the binomial distribution. For any arbitrary but fixed cell let

p_1 = probability of falling in this cell for community C1,

p_2 = probability of falling in this cell for community C2,

Table 15. Ratios of percentage incidence for two communities

	All normal	Abnormal			All abnormal
		I	II	III	
Nonsmokers	89/77	10/20	1/2	0/1	11/23
Smokers, <10 per day	75/50	20/40	4/8	1/2	25/50
Smokers, >10 per day	75/50	20/40	4/8	1/2	25/50

$\Delta = p_1 - p_2$,

Z_α = abscissa of standard normal density cutting off a portion equal to $\alpha/2$ in each tail of the distribution.

With these definitions the sample size from each community needed to declare with a reasonable chance the observed proportions as significantly different at the α level of significance is given by

$$n = \frac{Z_\alpha{}^2}{\Delta^2} [p_1(1 - p_1) + p_2(1 - p_2)] \ . \qquad (1)$$

In Table 16 the values of n for the different cells of Table 15 are given for various values of α. All of the values given in this table were found by Eq. (1), except the entries in the "abnormal III nonsmokers" cell. In this cell the normal approximation was not used since $p_1 = 0$. Therefore the exact probability for this cell was determined for various sample sizes under the null hypothesis of no difference between C1 and C2. When this probability bounded the level of significance, α, for two successive sample sizes these were recorded in Table 16.

Probabilistic modeling of pathology data (D. G. Hoel[6] and H. E. Walburg[15]). The nonparametric approach summarized in the research section of this report[40] describing the age-at-death distributions for pathology data has been applied to laboratory animal experiments. It was found that this method agreed with the classical actuarial interval estimates as the intervals were made arbitrarily small. For purposes of comparing treated groups with controls the estimated mean and standard error of the age-at-death distributions proved to be useful in suggesting statistical differences. The results agreed well with the experimenter's evaluation of the effect of a treatment on a particular disease mechanism.

Survival distributions (W. E. Lever and T. Makinodan[15]). In order to investigate the possible effect of living conditions on the survival of mice, 797 mice were allowed to complete their normal life-spans and die of natural causes. All of the mice spent the first six weeks of their life on a conventional farm. After this period 403 of the mice were moved to a dirty farm.

To ensure that a seasonal bias did not occur, mice born in each of the four seasons were used in the experiment. However, since a significant seasonal pattern did not appear in the survival times, the seasonal birth classification was not considered further.

To illustrate the survival distributions of the mice, abridged cohort life tables were constructed for both male and female mice for each of the farms. The tables were calculated utilizing information only from the cohort in question and were abridged to 50-day intervals.

The life tables were constructed using the methods given by Chiang.[41] For each time interval the following estimates or data were presented:

1. The estimated probability Q that an animal will die in a particular interval if it is alive at the beginning of the interval.

2. The standard error of Q.

3. The estimated additional life E of an animal if it is alive at the beginning of a time interval.

4. The standard error of E.

---

40. D. G. Hoel and H. E. Walburg, *"A Nonparametric Model for Competing Risks,"* this report.
41. C. L. Chiang, *Introduction to Stochastic Processes in Biostatistics*, pp. 189–241, Wiley, New York, 1968.

Table 16. Sample sizes needed to have a reasonable chance of declaring observed proportions as significantly different

	Level of significance	All normal	Abnormal I	Abnormal II	Abnormal III	All abnormal
Nonsmokers	0.05	74	97	1134	500–600	74
	0.01	127	166	1958	700–800	127
	0.005	151	198	2330	800–900	151
	0.002	183	239	2817	900–1000	183
Smokers, <10 per day	0.05	27	39	269	1134	27
	0.01	47	67	465	1958	47
	0.005	56	79	553	2330	56
	0.002	67	96	669	2817	67
Smokers, >10 per day	0.05	27	39	269	1134	27
	0.01	47	67	465	1958	47
	0.005	56	79	553	2330	56
	0.002	67	96	669	2817	67

Table 17. Life table for males raised on the dirty farm

Interval	*Q*	*S*(*Q*)	*E*	*S*(*E*)	*D*	*L*
0–599	0	0	958.4	10.3	0	199
600–649	0.02	0.01	358.4	10.3	4	199
650–699	0.041	0.014	315.1	9.9	8	195
700–749	0.027	0.012	277.1	9.4	5	187
750–799	0.082	0.02	233.9	9.2	15	182
800–849	0.048	0.017	202.9	8.6	8	167
850–899	0.182	0.031	162	8.4	29	159
900–949	0.231	0.037	142.4	8.1	30	130
950–999	0.18	0.038	127.9	7.5	18	100
1000–1049	0.293	0.05	100.5	7.1	24	82
1050–1099	0.379	0.064	82.1	6.4	22	58
1100–1149	0.472	0.083	63.3	5.9	17	36
1150–1199	0.579	0.113	44	4.3	11	19
1200–1249	1	0	16	0	8	8

5. The number of animals *D* which died in a particular time interval.
6. The number of animals *L* which were alive at the beginning of a time interval.

The life table for the cohort "males raised in the dirty farm" is listed as an example (see Table 17). To illustrate how this life table is read, consider the interval 900 to 949 days. There were 130 mice alive at the end of 899 days, and they lived an average of 142.4 additional days. During the interval 900 to 949 days 30 (23.1%) of the 130 mice died.

In this life table the time intervals between 0 and 600 days are combined, since none of the members of the cohort died before 600 days. Also, the estimated additional life given for the 0-to-600-day interval can be interpreted as the mean life-span of the animals in this cohort.

In addition to describing the survival characteristics of the cohorts, the information given in the four life tables was used to compare the survival characteristics of the four cohorts. These comparisons were based on the fact that the number of animals which died in an interval is a multinomial random variable.

The comparisons yield the following information: The survival distributions for males raised on the dirty farm and males raised on the clean farm were not significantly different. A similar result held for females. However, while the survival distributions of males and females raised on the clean farm were not significantly different, the males raised on the dirty farm lived significantly longer than the females raised on the dirty farm.

The results of these comparisons are illustrated in Fig. 37, which shows the estimated additional life curves for each of the four cohorts.

Additional survival studies are being planned where the mice will be subjected to some external stimuli. The survival distributions generated by these experiments will then be compared with the survival distributions reported here to see if the stimuli produced significant changes in the survival characteristics of the mice.

Tentative design for a proposed dose–dose-rate experiment (T. J. Mitchell, F. L. Miller, Jr., and M. A. Kastenbaum[42]). An experimental design has been proposed as the basis for a study of the effect of dose rate and total dose on the life expectancy in irradiated LAF_1 male mice. The design is laid out below with X denoting 200 mice and Y denoting 100 mice.

Total Dose (rads)						
400		X		X		X
200	X	Y	Y	Y	Y	X
100		Y		Y		X
50	X	Y	Y	Y	Y	X
25		X		X		X
Dose Rate (rads/day)	1	5	25	125	625	3125

The sample sizes are tentative, and only those at dose rates 5 and 125 rads/day have been based directly on statistical considerations. These considerations are:

1. It is assumed that a quadratic model for life expectancy as a function of total dose will give an adequate fit to the data at each dose rate.
2. It is assumed that the standard deviation of the lifetime is 20% of the expected lifetime, so that the standard deviation of the log lifetime is approximately 0.2.

Under the above assumptions, the fitted curve will be sufficiently precise that, over the dose range considered (25 to 400 rads), the standard error of any estimated life expectancy will be less than 1.3% of the true life expectancy at that dose. Before the experiment is begun, however, it will be necessary to revise the sample size estimates to allow for the grouping of mice into cages and the variation in response from cage to cage.

In the plan shown here, there are 3200 irradiated animals, and it is proposed that there be 800 controls. These 4000 mice are to be entered into the experiment in ten "cycles" at the rate of 400 mice per cycle, where each cycle is to contain one-tenth of the controls and one-tenth of the mice at each of the experimental points. In this way, variation in overall response from one cycle to another will not affect the precision of the fitted response surface.

Secondary disease (heterologous): Design VIII (T. J. Mitchell, C. C. Congdon,[15] R. E. Toya,[15] M. A. Kastenbaum,[42] and D. A. Gardiner). A series of experiments has been designed in an attempt to determine conditions which minimize mortality due to secondary disease in mice which have been lethally irradiated and then injected with rat bone marrow. The plan for Design VIII, which is the latest in this series, was described in a previous report.[43] This experiment was recently completed, and a preliminary analysis of the

42. Director's Division.
43. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 103.

90-day mortality data has been made on the main part of the design. This covers four levels of the age of donor (15, 30, 45, and 60 days) and six levels of cell dose (25.6, 32, 40, 62.5, 78.1, and 97.7 million cells). The experiment was restricted to males kept in an unlimited filter-top environment, and the day of injection was held at one day after irradiation. Previous experiments in this series had indicated that lowest mortality could be achieved at these conditions.

The design was constructed to permit a precise fit of a quadratic response function in the variables "age of donor" and "log cell dose." The statistical analysis indicated, however, that a model which represented the 90-day mortality as a simple linear function of log dose was suitable over the range of the two factors considered. Under this model, the 90-day mortality decreases with increasing cell dose, implying that it will be necessary to extend the range of dose still further before we are able to identify an optimum.

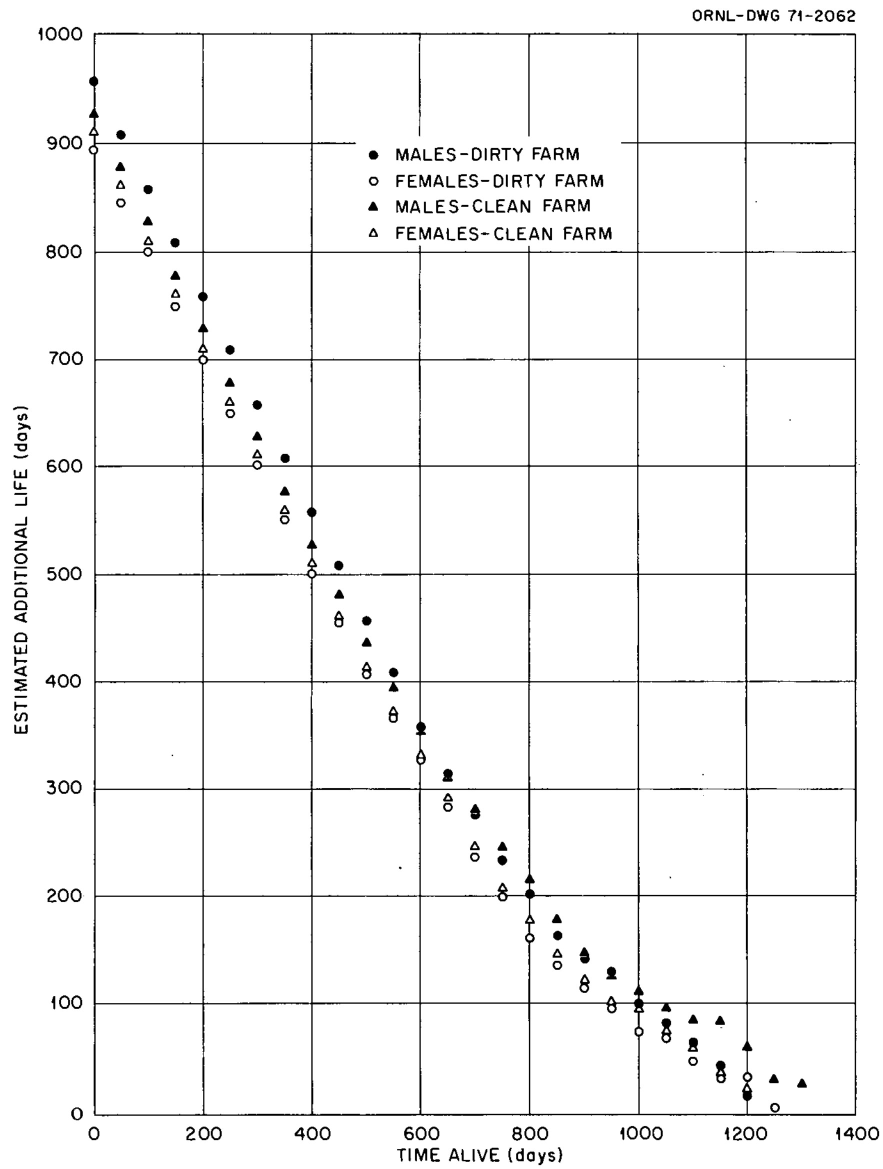

Fig. 37. Estimated additional life curves.

Linear and quadratic terms in age of donor were statistically significant in one replicate of the experiment, but not in the other, nor were they significant when the two replicates were considered together. The age factor remains extremely difficult to pin down. Each marrow pool is necessarily associated with only one age of donor, and the variation in response from one pool of donor marrow to another is quite large, thus tending to mask the true nature of the age effect.

The possibility of a change in the dose effect from one age to another has also been investigated. The statistical significance was borderline (significant at the 0.10 level) and appeared to result from the difference between a very weak dose effect at the two intermediate donor ages (30 and 45 days) and a strong dose effect at ages 15 and 60 days.

Although there are still some unresolved questions, one of the goals of this study, which was to achieve a relatively low mortality, has been attained. At the two highest levels of cell dose, for example, only 22.5% (18 out of 80) of the mice were dead at 90 days. This compares favorably with 90-day mortalities of 65 to 90% in earlier work with rat marrow transplants.

Analysis of factors which may relate to tumor occurrence in mice (W. E. Lever and T. Makinodan[15]). Analysis of factors possibly relating to tumor occurrence in mice was continued. In addition to those factors reported before[44] (body weight, spleen weight, and the number of plaque-forming cells per spleen), hemagglutinin titer, hemolysin titer, and serum protein concentration levels were analyzed in relation to living conditions, sex, and tumor occurrence for 30-month-old mice.

The same set of factors was also analyzed for three-month-old mice in relation to living conditions, sex, and tumor occurrence.

With the exception of body weight and spleen weight, the factors were compared between age groups to indicate changes in immunization in relation to age.

Reanalysis of irradiated guinea pig data (T. J. Mitchell and C. C. Congdon[15]). Data from an experiment on irradiated guinea pigs, conducted over 20 years ago by Lorenz and his associates,[45] are now being reanalyzed. The primary reason for reconsidering these data is to study the induction of leukemia by the irradiation, which was overlooked in the original investigation. At the same time, we are reanalyzing the life-span data using linear regression methods.

The analysis of life expectancy of the unlimited exposure groups, in which radiation exposure was maintained until death, has now been completed. The variables considered were:

1. strain of guinea pig,
2. sex,
3. age at start of irradiation,
4. exposure rate.

Using the OMNITAB programming system, various empirical models were fitted to the data, and statistical tests were made to determine the most suitable representation of the response in terms of the experimental variables.

At the highest dose rate (8.8 rads/day) it was found that, in order to eliminate the effect of "age at start," it was necessary to consider the response as life after start of irradiation rather than the life-span itself. Confidence intervals were calculated for the mean life after start of irradiation for all three strains.

44. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 101.

45. E. Lorenz et al., "Effects of Long-Continued Total-Body Gamma Irradiation on Mice, Guinea Pigs, and Rabbits," *Biological Effects of External X and Gamma Radiation,* vol. 22B, part I. National Nuclear Energy Series, Manhattan Project Technical Section. Division IV – Plutonium Project Record (R. E. Zirkle, ed.). McGraw-Hill, New York, 1954.

At the remaining exposure rates (1.1, 2.2, and 4.4 rads/day) there was no detectable effect of age at start on the life-span. These groups, together with the control group (unirradiated), were analyzed using a regression model which expressed the life-span as a function of exposure rate. For each strain, it was found that a straight line response function gave a good fit over the range 0 to 4.4 rads/day. Because the variance was not constant from one dose rate to another, a weighted least squares criterion was used to determine the fitted lines. With each regression line, an "upper bound" curve and a "lower bound" curve were calculated to display the 95% confidence limits for life expectancy over the range of dose rates.

The log transformation of the response was considered as well as the untransformed response. Although this transformation did remove the dependence of the variance on the mean response, it did not result in a better straight line fit. It also had the undesirable effect of skewing the distributions of the low-exposure-rate groups rather severely to the left. Therefore the results of the experiment were presented in terms of the untransformed data.

We are currently analyzing the life-span data for the limited exposure groups, which contain those animals which were withdrawn from the irradiation exposure prior to death.

Analysis of counts of cell colonies (D. G. Gosslee). Treatment with radioprotective chemicals and bone marrow transplants each offers means of reducing the effects of radiation damage in mice. The comparison of responses from treated and untreated mice gives an estimate of the degree of protection. Measured responses include the average age at death, the dose required to result in 50% mortality at a given number of days after exposure, and a measure of repopulation of hemopoietic tissue.

A lethal dose of radiation essentially kills all of the hemopoietic cells, and repopulation can be accomplished by injection of bone marrow. The repopulation of hemopoietic tissue can be observed in the spleen of mice. Counts of colonies of cells, each colony assumed to arise from a single hemopoietic stem cell, give a measure of the amount of repopulation. The standard methods of analyzing these counts are based on an exponential increase in damage with increasing radiation dose.

A simple and commonly used method is to fit a straight line to the logarithms of the means of the counts for the animals in each dose group. This method, in its simplest form, ignores the variation among animals, and the resulting statistical tests are inefficient. Since the parameters are estimated from the logarithms of the means, the variation among counts cannot be used to perform tests of significance and place confidence limits on estimates of parameters by known statistical methods.

In order to fit a straight line to the logarithms of the counts a method must be used to replace the zero counts with a number larger than zero. A commonly used method is to add one to each count before taking the logarithm. However, this caused an overcorrection and a masking of treatment effects.

A new method was developed to estimate a value to substitute for each zero based on an assumption that the counts have a log normal distribution. The variation among animals is compounded with the Poisson variation assumed for individual counts and is assumed to explain the approximately log normal distribution observed in groups of 20 animals each. A normal distribution is fitted to the logarithms of the counts which are greater than zero using standard methods for censored distributions. Then a substitute value for the one or more zeros in each group is estimated under the assumption of normality.

The possibility of replacing a zero count with the average number of colonies per spleen from control animals is being investigated. These counts are theoretically zero but in fact average 0.067.

Ecological Sciences

Irradiation of seeds (J. J. Beauchamp and R. C. Dahlman[46]). Little information is available with regard to the effect of chronic irradiation on the reproductive phase of plant activity. Attempts were made to determine effects of chronic irradiation on production and germination of tall fescue (*Festuca arundinacea*) seeds which were collected from eight 100-m^2 plots at the 0800 area of ORNL. The local fallout simulant was synthesized and applied to four of the eight plots during the summer of 1968. The four contaminated plots received 2.2 curies of ^{137}Cs radioactivity, and the four uncontaminated plots served as controls. The selection of plots for contamination was made in a "pseudorandom" manner because physical limitations made it impossible for some plots to be irradiated. An additional factor was taken into consideration for the analysis because of the introduction of herbivorous animals used in another study. Four cotton rats were released in each of four plots, of which two were contaminated and two were not. By taking this factor into account in the analysis, it was possible to detect some significant differences between the control and irradiated plots.

Standing panicles were collected from each plot during the summers of 1969 and 1970. Germination tests were conducted after the seeds from the panicles were cured at room temperature for 30 days, and the following quantities for each panicle were observed at 25 days after the curing of the seeds: (1) total number of seeds produced; (2) number of germinated seeds; and (3) number of empty seeds (1970 study only).

The data from the 1970 study were analyzed to determine which factors had a significant effect upon the total seed production. Since the counts of total seed production were assumed to follow a Poisson distribution, the square root transformation was used. From the analysis it was evident that the most significant factor upon total seed production was the grazing of the cotton rats. A significant effect was detected from the irradiation as well as a significant interaction between the factors of irradiation and grazing.

In addition to the analysis of the total seed production, the proportion of empty seeds for the 1970 study was also analyzed. The transformation arc sine $\sqrt{p}$ for the proportion of empty seeds, p, was used. From the analysis it was obvious again that the grazing was the most significant factor, but it was not possible to detect a significant irradiation effect for the empty seeds even with the grazing factor taken into account. The total seed production for the 1969 study resulted in similar conclusions, except for the grazing × irradiation interaction. A rank correlation coefficient was calculated to determine if similar plot-to-plot patterns were present in the 1969 and 1970 studies, but the results were inconclusive. Additional analyses will be carried out during the coming year on the germination data for both the 1969 and 1970 studies.

Snail radiation sensitivity (F. L. Miller, Jr.). In an experiment reported last year[47] freshwater snails were chronically irradiated with 0, 1, 10, or 25 rads/hr of gamma irradiation. The effects of radiation on egg production were reported then. Some of the eggs laid were polyvitelline, that is, the eggs each contained more than one vitelline space. Chi-square tests were performed to test the hypothesis that radiation did not affect the frequency of laying of polyvitelline eggs. The data are as follows:

Rads/hr	0	1	10
Number of eggs laid	79,079	74,229	6,365
Number of polyvitelline eggs	298	202	486
Percentage of polyvitelline eggs	0.377	0.272	7.64

46. Ecological Sciences Division.

47. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 106.

The percentage of polyvitelline eggs at the 10-rad/hr dose is significantly larger while the percentage is significantly smaller at the 1-rad/hr dose, both at the 0.0005 level of significance, than the controls. No viable eggs were laid by the snails given 25 rads/hr.

Element content of a forest understory (F. L. Miller, Jr.). An experiment was designed to estimate the element content of four species of the understory of the *Liriodendron* forest. Dogwood and wild hydrangea will be sampled from the shrub layer, while ground peanut and Christmas fern will be sampled from the herbaceous layer. Each species will be sampled during seven phenophases (bud swelling, vegetative growth, flowering, etc.) in order to estimate the amounts of 15 elements present throughout the year. For each phenophase of each species, replicated samples will be taken of the various compartments (roots, trunk, leaves, etc.). The amounts of the 15 elements tied up in areas of similar forest at various times of the year will be estimated from the sample information.

Analysis of wind velocity data for a radioactive material disposal site (J. J. Beauchamp and Y. Tanaka[46]). The increasing volumes of radioactive waste products from nuclear reactors, radiological research, and radioactive materials used in medical treatments are creating a critical disposal problem. Suitable burial grounds for these materials are essential in order to maintain a quality environment. An analysis has been carried out on available wind velocity data from six stations surrounding the disposal site at Lyons, Kansas, which was recently selected by the AEC. The analysis of wind conditions is of particular interest in this project because direction and velocity of wind determine the extent of contaminated areas in case any radioactive materials are released into the atmosphere. Since no wind data were available at the site in question, it was decided to use the data from nearby meteorological stations, from which the wind conditions at Lyons might be inferred. However, as a preliminary analysis, the data from the nearby stations were analyzed to determine if there is a detectable difference among stations.

At each of the six stations the average wind velocity, averaged over extended periods of time, for each month was available. In addition, the average velocities were also available for the 16 directions N, NNE, NE, etc. It was evident that the analysis of these data should take account of the cyclic relation among the 12 months as well as the cyclic relation among the 16 directions.

The first step in the analysis of the data was to propose a tentative model to describe the observations and perform a regression analysis using this model. Let

$$y_{ijk} = \text{observed average wind velocity at station } i\text{, from direction } j\text{, and in month } k\,,$$

where $i = 1, 2, \ldots, 6; j = 1, 2, \ldots, 16$: and $k = 1, 2, \ldots, 12$. The additive model used to explain each y_{ijk} was assumed to have contributions from the following components: (1) an overall mean; (2) station-to-station effect; (3) direction-to-direction effect; (4) month-to-month effect; and (5) unexplained variability designated as error; that is,

$$y_{ijk} = \text{overall mean} + \text{station effect} + \text{direction effect} + \text{month effect} + \text{error}\,.$$

In order to include in the model the cyclic nature of the direction effect, the 16 directions were considered as points equally spaced around the circumference of a circle. For the jth direction, $2\pi j/16$ was the associated angle, and the direction effect was assumed to be given by a sine-cosine curve represented by

$$\gamma_1 \sin\left(j\,\frac{2\pi}{16}\right) + \gamma_2 \cos\left(j\,\frac{2\pi}{16}\right)\,.$$

Similarly, for the month effect the circumference of a circle was divided into 12 equal parts, and from the associated angles the month effect was given by

$$\gamma_3 \sin\left(k\frac{2\pi}{12}\right) + \gamma_4 \cos\left(k\frac{2\pi}{12}\right).$$

Assuming a simple additive station effect the final complete model used in the subsequent analysis was given by

$$y_{ijk} = \beta_0 + \beta_i + \gamma_1 \sin\left(j\frac{2\pi}{16}\right) + \gamma_2 \cos\left(j\frac{2\pi}{16}\right) + \gamma_3 \sin\left(k\frac{2\pi}{12}\right) + \gamma_4 \cos\left(k\frac{2\pi}{12}\right) + \epsilon_{ijk}\,, \tag{1}$$

where β_0 represents the overall mean effect, β_i represents the station effect from the ith station, and ϵ_{ijk} represents the remaining unexplained variation not taken into consideration by the model.

With the model specified by Eq. (1), the computer program GENLIN was used to perform an analysis of variance on the data. The proportion of the total variability explained by the model given in Eq. (1) was 96%. The proportion of the variability explained by the model after correcting it for the mean, β_0, was equal to 26%. From the analysis of variance it was seen that the station, direction, and month effects were significant, with the month effect being the most significant. Therefore, it will be necessary to continue the investigation of the available weather data before making inferences about the conditions at Lyons.

Instrumentation and Controls

An idealized probabilistic model for the collapse of field elements (V. R. R. Uppuluri and Claudia S. Lever). Let n events occur in a time interval $[0, T = l, \Delta t]$. Let us assume that an event can occur in any of the l time intervals with the same probability, and the events occur independently. If more than B events occur in any interval, we say that a disaster befalls. We are interested in the probability of a disaster and the expected number of the largest realized events.

This can be identified as a box and urn problem where n balls are dropped independently in l urns. Let N_i denote the number of balls in the ith urn and $N_{\max} = \max(N_1, ..., N_l)$. For small values of n and l, the distribution and the moments of $N_{\max}$ are tabulated by Steck.[48] For large values of n, Owen and Steck[49] suggest the following expressions for the asymptotic mean and variance:

$$E[N_{\max}] \cong \frac{n}{l} + \left(\frac{n}{l}\right)^{1/2} E[X_{n,n}]\,,$$

$$\mathrm{Var}[N_{\max}] \cong \frac{n}{l}\left\{\mathrm{Var}[X_{n,n}] - \frac{1}{l}\right\}\,,$$

where $E[X_{n,n}]$ and $\mathrm{Var}[X_{n,n}]$ are the mean and variance, respectively, of the largest of a set of n independent standard Gaussian variates. These results with appropriate computations answered some of the questions raised by the investigator.

---

48. G. P. Steck, *Table of the Distribution of r Jointly Distributed Multinomially Distributed Variables with All Cell Probabilities Equal, r = 2 (1) 50, N = 1 (1) 50*, unpublished.

49. D. B. Owen and G. P. Steck, *Ann. Math. Statist.* **33**, 1286–91 (1962).

Metals and Ceramics

Augmenting a 6 X 6 Latin square design (T. L. Hebble and W. J. Lackey[50]). Greco-Latin square designs are valuable in arranging combinations of levels of treatments and controlled variables in statistically planned experiments. The 6 X 6 Greco-Latin square is an impossible configuration. That is, it is not possible to assign six different Greek letters to a 6 X 6 Latin square so that each Greek letter appears once and only once in each row, and in each column, and with each Latin letter. However, it is possible to distribute three pairs of Greek letters symmetrically over a 6 X 6 Latin square.

The problem arose when a 6 X 6 Latin square experiment design was applied to the making of fuel pellets. From each of six sintering runs, three pairs of fuel pellets were prepared for a total of 36 pellets. In a given run, each pair represents a particular location in the sintering oven. Each set of six pellets is then placed in an analysis oven. Since the analysis oven can only hold six pellets, six analysis runs must be made. Oxygen-to-metal ratio is the response and is a function of the weight gain (or loss) during the analysis run.

The problem is to assign the pellets from the sintering oven runs to the proper locations in the analysis oven so that the effect due to positions can be separated from treatment effects and tested in a valid statistical analysis of the data. This is not possible if the three pairs associated with oven position represent six distinct locations.

Consider a 6 X 6 Latin square in which the rows are analysis run positions and the columns are the analysis runs (or days). The treatments (capital Latin letters) are sintering oven runs. Let α, β, and γ be the three different positions in the original oven runs. These Greek letters may be distributed over the 6 X 6 Latin square in the following manner:

		Analysis days					
		1	2	3	4	5	6
Analysis positions	1	A_{α}	B_{β}	C_{γ}	D_{α}	E_{β}	F_{γ}
	2	B_{α}	C_{β}	D_{γ}	E_{α}	F_{β}	A_{γ}
	3	C_{β}	D_{γ}	E_{α}	F_{β}	A_{γ}	B_{α}
	4	D_{β}	E_{γ}	F_{α}	A_{β}	B_{γ}	C_{α}
	5	E_{γ}	F_{α}	A_{β}	B_{γ}	C_{α}	D_{β}
	6	F_{γ}	A_{α}	B_{β}	C_{γ}	D_{α}	E_{β}

Each Greek letter occurs twice in each row, twice in each column, and twice with each treatment (Latin letter). Circled entries in the above array demonstrate this for the α position. In the application of this design, the square is to be properly randomized. The data analysis for this design is an extension of the

50. Metals and Ceramics Division.

Latin square analysis. The analysis of variance table showing the partition of the degrees of freedom is as follows:

Analysis of variance

Source	Degrees of freedom
Analysis days	5
Analysis positions	5
Sintering oven runs	5
Oven positions	2
Residual (error)	18
Total	35

The sum of squares for oven positions is computed from the total of the 12 observations for each position.

Stainless steel irradiation experiment (T. L. Hebble, G. M. Goodwin,[50] and Nancy C. Cole[50]). Tensile specimens from 13 different weldments were subjected to four heat treatments and then inserted in the Idaho EBR-2 reactor as part of an irradiation experiment. A base metal of type 304 stainless steel was joined by either the shielded metal arc or sub-arc welding process using a filler metal of type 308 stainless steel. The major differences between weldments were differences in flux composition. A study of the tensile properties of the specimens cut from different positions in the weld was of primary importance.

Reactor locations allotted to the irradiation program were specified in advance so that the greatest amount of information could be obtained by the proper assignment of specimens. To achieve this, a two-level factorial design was employed. Since it was not possible to consider all possible combinations of variable levels, eight of the more important weldments were considered. For each of the eight welds, a full two-level factorial design in four variables (heat treatment, position of specimen in weld, fluence, and irradiation temperature) was selected. Provision for estimating experimental error was made by repeating 16 specimens. The statistical design utilized 168 of 256 assigned locations. The remaining locations were designated by the experimenter to study specific combinations of weld, heat treatment, and weld location for metallographic analyses.

Four pin locations were assigned. Each pin contained 64 specimen locations and was divided into two sections which, when inserted into the reactor, were symmetric about the core. Thus, each section received the same total fluence but different irradiation temperatures. Eight specimens were contained in each of four rows within a given section. Although each row within the section receives a different total fluence, the eight specimens in each row receive the same fluence and irradiation temperature. Each row in one section has a counterpart in the other section of the same pin.

Three pins were placed in the EBR-2 reactor in October 1970. The remaining pin will replace one of the inserted pins after about 213 days. This replacement pin and one other will be removed approximately 426 days after the October 1970 insertion date. The last pin will not be removed until about 852 days. The experiment design was so constructed that statistical analysis can be performed on data from the first pin to be removed. At this time, estimates can be made of the effects of temperature and heat treatments on eight weldments.

Nuclear Safety

Reproducibility of Nuclear Safety Pilot Plant runs (T. L. Hebble, L. F. Parsly,[51] and T. H. Row[51]). As part of the spray technology program to study the specific removal of elemental iodine, a measure of the

51. Reactor Division.

reproducibility of Nuclear Safety Pilot Plant runs was obtained. Because of mechanical difficulties and other factors, only three of the five originally planned experiments were carried out. Thus, the estimate of variance has only two degrees of freedom with which to perform statistical tests. The three pilot plant runs[52] (74, 76, and 77) employed a base borate spray solution (13.7 g/liter H_3BO_3 and 3.4 g/liter NaOH) under simulated accident conditions. The containment vessel atmosphere was brought to 130°F and 45 psig with the addition of steam.

The variability of important responses is listed below.

	Mean	Range	Variance (2 d.f.)	Std. error of mean
Dose reduction factor				
After 60 min	40.9	6.5	13.5	2.12
After 240 min	87.3	28.6	213.2	8.43
Decontamination factor	140.3	54	849.3	16.80

The variance of the dose reduction factor at 240 min is significantly greater than the variance at 60 min, indicating that reproducibility decreases sharply with increased time.

ORAU Medical Division

Model for the kinetics of white blood cell and platelet concentration in patients with chronic granulocytic leukemia (J. J. Beauchamp and Helen Vodopick[53]). In normal healthy individuals there is a spontaneous oscillation of the white blood cell and platelet concentration, due to the activity of a mechanism controlling granulopoiesis. This same effect has been observed in patients with chronic granulocytic leukemia (CGL). However, the relative stability observed in the oscillations of a normal healthy individual appears to be absent in the patients with CGL. In Fig. 38 a representative set of data is displayed for a patient with CGL showing the white blood cell concentration (Y_1) and platelet concentration (Y_2) at various times t, where t is measured in days. A model has been derived to describe these relations.

It is assumed that the same functional relation may be used to describe the relation between Y_1 and t as well as between Y_2 and t. However, the values of the parameters in the model are not assumed to be the same for Y_1 as they are for Y_2. From Fig. 38 the following characteristics are observed: (1) over the range of t investigated, periodic oscillations are present in the white blood cell and platelet concentration; (2) as t increases the amplitude of the periodic response increases; and (3) as t increases the average value, about which the response cycles, tends to increase linearly.

Some results from the physics of vibrations were used in the derivation of a model describing the phenomenon under consideration. Many periodic phenomena are described by means of differential equations of the form:

$$\frac{d^2 Y_1}{dt^2} + 2k \frac{dY_1}{dt} + n^2 Y_1 = f(t) , \qquad (1)$$

52. W. B. Cottrell, *ORNL Nuclear Safety Research and Development Program Bimonthly Report for January–February 1970,* ORNL-TM-2919 (May 1970).

53. ORAU Medical Division.

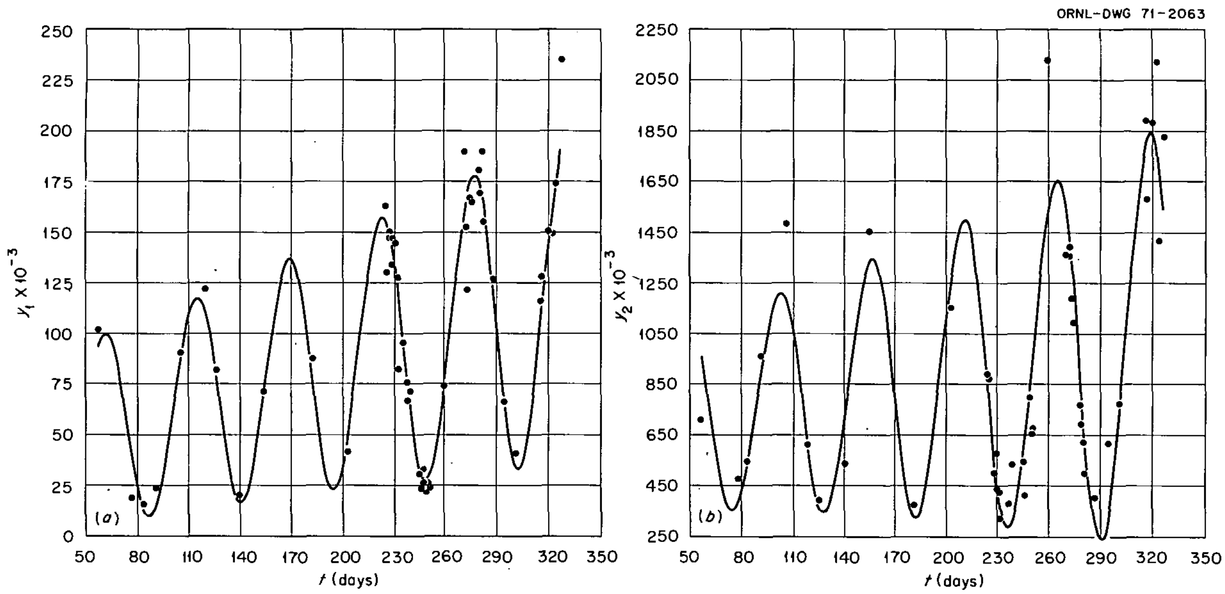

Fig. 38. ***(a)*** **Observed (*) and calculated white blood cell concentration;** ***(b)*** **observed (*) and calculated platelet concentration.**

where $2k$ is related to the force of friction acting on the system, n is related to the period of the response if no friction and no forcing are present, and $f(t)$ is the force function. Since friction usually tends to damp out the oscillations, there must be some type of "negative" friction present in the system under consideration from characteristic (2) stated above. In addition, the forcing function appears to be linearly related to t from characteristic (3) above. From these considerations the following second-order differential equation is used to describe the relation between Y_1 and t:

$$\frac{d^2 Y_1(t)}{dt} - 2k \frac{dY_1(t)}{dt} + n^2 \; Y_1(t) = \alpha_0 + \alpha_1 t \, . \qquad (2)$$

The general solution of Eq. (2) is given by a sum of the general solution of the reduced equation

$$\frac{d^2 U(t)}{dt^2} - 2k \frac{dU(t)}{dt} + n^2 \; U(t) = 0 \qquad (3)$$

and a particular solution $V(t)$ of the complete equation (2); that is,

$$Y_1(t) = U(t) + V(t) \, . \qquad (4)$$

It can be shown that the general solution of Eq. (3) is given by

$$U(t) = Ae^{kt} \sin{(\omega t + B)} \, , \qquad (5)$$

where $\omega = n^2 - k^2$ and A and B are initial condition constants introduced by the solving of Eq. (3). Let

$$V(t) = \beta_0 + \beta_1 t \qquad (6)$$

be a particular solution of Eq. (2). By substitution it can be shown that

$$\beta_0 = \frac{\alpha_0}{n^2} + \frac{2k\alpha_1}{n^4}$$

and (7)

$$\beta_1 = \frac{\alpha_1}{n^2} \; .$$

From Eqs. (4)–(7) the general solution of Eq. (2) is given by

$$Y_1(t) = Ae^{kt} \sin(\omega t + B) + \frac{\alpha_0}{n^2} + \frac{2k\alpha_1}{n^4} + \frac{\alpha_1}{n^2} t$$

$$= \theta_0 + \theta_1 t + Ae^{kt} \sin(\omega t + B) \; , \tag{8}$$

where $\theta_0 = \alpha_0/n^2 + 2k\alpha_1/n^4$; $\theta_1 = \alpha_1/n^2$; $-k$ is related to the force of friction acting on the system; and A, ω, and B are related to the amplitude, period, and phase shift, respectively, of the periodic component of the response. The line denoted by $\theta_0 + \theta_1 t$ represents the average or mean value about which the response cycles. The functions denoted by $\theta_0 + \theta_1 t + Ae^{kt}$ and $\theta_0 + \theta_1 t - Ae^{kt}$ represent the upper and lower envelopes, respectively, of the response. From the basic assumptions, the relation for the platelet counts, $Y_2(t)$, is given by

$$Y_2(t) = \theta'_0 + \theta'_1 t + A'e^{k't} \sin(\omega' t + B') \; . \tag{9}$$

In the table below the least squares estimates of the parameters in Eqs. (8) and (9) are given for the data in Fig. 38. Plots of the fitted curves are also shown in Fig. 38 for Y_1 and Y_2.

$\theta_0 \times 10^{-3}$	$\theta_1 \times 10^{-3}$	$A \times 10^{3}$	k	ω	B
37.87	0.25	41.19	0.002	0.117	0.709
$\theta'_0 \times 10^{-3}$	$\theta'_1 \times 10^{-3}$	$A' \times 10^{-3}$	k'	ω'	B'
666.22	1.13	318.28	0.003	0.117	4.16

University of Tennessee Memorial Research Center

Effects of testosterone and erythropoietin on rabbit bone marrow cells (T. J. Mitchell and T. McDonald[54]). An experiment was performed to determine how ^{59}Fe incorporation (iron uptake) is affected by the addition of various combinations of erythropoietin (ESF) and testosterone to rabbit bone marrow cultures. The nucleus of the experiment was a 3 X 2 X 6 factorial design with three rabbits, two levels of erythropoietin (0.0 and 1.0 unit per culture), and six levels of testosterone (0.0, 0.0078, 0.03125, 0.0625, 0.125, and 0.25 mg per culture). The response at each combination of factor levels was taken to be the average of the square roots of the percent iron uptakes of three to four cultures. The object of the square root transformation was to stabilize the variance, which appeared to depend on the mean uptake.

54. University of Tennessee Memorial Research Center.

An analysis of variance was applied to the data, using a mixed model[55] with ESF and testosterone as fixed effects and rabbits as a random effect. The purpose of viewing rabbits as a random effect was to enable us to draw inferences which would apply to a larger population of rabbits than the three actually used in the experiment. Although this "larger population" is a nebulous concept, the main benefit of this approach is that it takes account of the variability of the experimental results from one rabbit to another.

It was found that the effect of erythropoietin, which increased the iron uptake, was statistically significant at the 0.025 level. The main effect of testosterone and the testosterone × ESF interaction were not sufficiently strong to be conclusive, yielding significance at the 0.25 and 0.10 levels respectively. To examine the possibility of interaction further, the difference between the response at 0.0 unit and at 1.0 unit of ESF was considered at each level of testosterone. It appeared that the stimulatory effect of ESF on iron uptake was depressed over the testosterone dose range of 0.0078 to 0.0625 mg per culture. However, the number of rabbits considered here was insufficient for a firm conclusion.

Y-12

Procedure for estimating plant laboratory efficiencies (W. E. Lever and Norma C. Hull). The procedure for estimating efficiencies of analysis times in the Y-12 Chemical Laboratories[56] has been adapted to estimate efficiencies of test times in the Y-12 Physical Testing Laboratory and of inspection times in the Y-12 Dimensional Inspection Laboratory.

The procedures are at present using three-month moving averages of times as bases. However, a new procedure is being evaluated, which will use standard times as bases.

Insulation material development (D. G. Gosslee). A thermal insulation material, named Palarite, composed of carbon-bonded silica fibers was developed for aerospace applications.[57] The fabrication process entails vacuum forming, from a dilute water slurry containing silica fibers and starch, a fibrous molding on a mandrel of the desired shape. The molding then is processed through a curing, drying, and furnace-heating operation to obtain a rigid carbon-bonded fibrous structure.

Data were taken on the density of the product from the production process. The variations in processing conditions and raw material variability could not be controlled in a balanced design in the fabrication process, nor was it feasible to run pilot plant experiments. Even though these limitations presented difficulties in the statistical analysis and interpretation of the data, the results were valuable in making process adjustment to improve product yield.

The statistical analyses consisted of a variance components analysis, a multiple regression analysis, and a summary of the means and standard errors in each cell of the multiple classified density measurements. The component of variance due to each identifiable source of variation in the procurement of fibers was estimated. The regression analyses yielded estimates of the effects on density of variables which can be controlled. The estimates from both types of analyses were used to improve the production process.

Estimate of variance of total job load (J. J. Beauchamp and R. P. Lucke[58]). In the area of production the aspect of time estimation is of great interest. With each special production job the estimate of the time needed to complete the job and the actual time required to complete the job are recorded. From data of estimated and actual times for a number of jobs, a straight line was fitted to a log-log plot of the data. The

---

55. H. Scheffe, *The Analysis of Variance*, Wiley, New York, 1959.
56. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969*, ORNL-4514, p. 123.
57. C. D. Reynolds and Z. L. Ardary, *Palarite Thermal Insulation*, Y-1716 (April 1970).
58. Y-12 Statistical Services.

log-log transformation was used since the variability at various estimated times increased with increasing actual times. In particular, let

$\ln Y_j$ = natural logarithm of the jth actual job time in hours

and

$\ln X_j$ = natural logarithm of the jth estimated job time in hours;

then the following straight line was fitted to the data:

$$\ln Y_j = \alpha + \beta \ln X_j + (\text{error})_j$$

for $j = 1, 2, \ldots, n$. From the n data points $(\ln X_j, \ln Y_j)$ estimates of α and β are obtained and denoted by a and b respectively.

Assume there are N additional new jobs each with an estimated time $X_i, i = 1, 2, \ldots, N$. Since there are no actual job times available, the predicted actual job times, $\hat{Y}_i$, from the earlier n data points are used; that is,

$$\hat{Y}_i = \exp(\widehat{\ln Y_i}) = \exp(a + b \ln X_i)$$

for $i = 1, 2, \ldots, N$. The total job load is defined as

$$\text{TJL} = \sum_{i=1}^{N} \exp(\ln Y_i) = \sum_{i=1}^{N} Y_i .$$

However, since the Y_i's are unknown, the TJL is predicted by

$$\widehat{\text{TJL}} = \sum_{i=1}^{N} \exp(\widehat{\ln Y_i}) = \sum_{i=1}^{N} \exp(a + b \ln X_i) .$$

The actual observed value of $\ln Y$ varies about its mean value with a variance σ^2; therefore, the predicted value $\exp(\widehat{\ln Y_i})$ has a variance given by

$$\sigma^2 + \text{Var}\,[\exp(a + b \ln X_i)] .$$

An approximation to the variance of $\widehat{\text{TJL}}$ is given by

$$\sigma^2 \sum_{i=1}^{N} \exp[2(\alpha + \beta \ln X_i)]$$

$$+ e^{2\alpha} \left\{ \left[\sum_{i=1}^{N} \exp(\beta \ln X_i) \right]^2 \text{Var}(a) + \left[\sum_{i=1}^{N} \ln X_i \exp(\beta \ln X_i) \right]^2 \text{Var}(b) \right.$$

$$\left. + 2 \left[\sum_{i=1}^{N} \exp(\beta \ln X_i) \right] \left[\sum_{i=1}^{N} \ln X_i \exp(\beta \ln X_i) \right] \text{Cov}(a, b) \right\} .$$

In order to obtain an estimate of the above variance, estimates of Var (a), Var (b), Cov (a, b), α, β, and σ^2 obtained from the earlier regression analysis are substituted into the above expression.

From the usual normality and independence assumptions

$$Z = \frac{\sum_{i=1}^{N} (\ln Y_i) - \sum_{i=1}^{N} (a + b \ln X_i)}{\sqrt{\text{Var}\left(\sum_{i=1}^{N} \ln Y_i\right) + \text{Var}\left[\sum_{i=1}^{N} (a + b \ln X_i)\right]}}$$

has an $N(0, 1)$ distribution. By using the estimates of

$$\nu_1 = \text{Var}\left(\sum_{i=1}^{N} \ln Y_i\right)$$

and

$$\nu_2 = \text{Var}\left[\sum_{i=1}^{N} (a + b \ln X_i)\right]$$

in the expression for Z, a confidence interval may be put on

$$\sum_{i=1}^{N} (\ln Y_i) .$$

The limits of this interval are given by

$$\sum_{i=1}^{N} (a + b \ln X_i) \pm t \sqrt{\hat{\nu}_1 + \hat{\nu}_2} , \tag{1}$$

where t is the appropriate Student's t statistic with $n - 2$ degrees of freedom. It may be shown that

$$N \left[\prod_{i=1}^{N} \exp (\ln Y_i) \right]^{1/N} \leqslant \sum_{i=1}^{N} \exp (\ln Y_i) = \text{TJL} . \tag{2}$$

From Eq. (1) the confidence limits on

$$N \exp \left(\frac{1}{N} \sum_{i=1}^{N} \ln Y_i \right) = N \prod_{i=1}^{N} [\exp (\ln Y_i)]^{1/N}$$

are given by

$$N \exp\left(a + b \frac{\sum_{i=1}^{N} \ln X_i}{N} \pm \frac{t}{N} \sqrt{\hat{\nu}_1 + \hat{\nu}_2} \right) . \qquad (3)$$

From the inequality in (2) the upper confidence limit on TJL is greater than (3) with the plus sign.

STATISTICAL PROGRAMMING

The Time-Sharing Computer Terminal

E. Leach

The Statistics Department of the Mathematics Division has been using the time-sharing service of the Data Network Corporation, now known as Megasystems, Incorporated, for the past year.

The time-sharing service used is obtainable through a local multiplexer which allows immediate access from our remote location to a computer situated at New York. The General Electric 400 series computer is used for our time-sharing computer applications. The remote terminal installed on-site consists of one standard model 33 100-word/min Teletype machine. The programs used through the time-sharing service are either FORTRAN or BASIC.

Figure 39 shows the use of the time-sharing facility by month from November 1, 1969, through October 31, 1970. The time-share use for this period is less than 40% of the time-share use for the preceding period from November 1, 1968, through October 31, 1969.

Conversational Remote Batch Entry Terminal

E. Leach

In August 1970, the Statistics Department had an IBM 2741 communications terminal installed. It is a remote conversational terminal that provides direct access to the IBM System/360 model 75 computer at the Oak Ridge National Laboratory Computing Center. The 2741 terminal is connected to the computer by use of a Bell DATA•phone data set and a standard telephone.

Several members of the Statistics Department have experienced great success in using the terminal for submitting programs written in FORTRAN IV, OMNITAB, and BASIC. Through the use of the terminal a program may be submitted several times in one day, whereas if the program is submitted through the courier service, it may not be returned on the same day it is submitted.

Of the original 16 potential CRBE users in the Statistics Department, eight have already gained considerable experience using the terminal since it has been installed. As the use of the CRBE terminal increases, the use of the time-sharing terminal connected with the Megasystems, Incorporated, computer is expected to drop. Figure 40 shows the use of the CRBE terminal by month since it has been installed. As the system improves, more potential users are expected to start using the CRBE terminal.

Biology Programming

Mouse body weight analysis (E. Leach). Two programs for analyzing the body weights of mice have been written for a member of the Biology Division. From the time of weaning, the weight of each mouse in a cage of eight mice is recorded weekly for several weeks. Each cage is assigned a cage number, and mice of the same sex with the same litter order, the same group number, and the same birth date are caged together.

The cage number, litter order, group number, sex code, birth date, weighing date, and the weight of each mouse in the cage at the weighing dates are used as input data for a program that creates a master file on magnetic tape. In addition to the above information, the age at weighing for the mice in each cage is computed and written on the master file.

Another program uses the master file as input and permits the user to specify the group number, the litter order, and the sex code for the cages of mice to be used in each analysis. The program searches the master file for the cages with the given specifications and computes for each cage with the specifications the number of mice weighed at each of eight age intervals and the average weight and the standard deviation of the weights for the mice at each age interval. A similar analysis is done over all cages with the specifications.

Histology studies (Norma C. Hull). Two programs have been written for the Biology Division to produce printed forms to be used for keeping records on histology studies. One program produces pages of experiment numbers listed consecutively with space after each number for the necessary recordings to be made by the biologist. The biologist furnishes the first and the last experiment number as input to the program. Usually several hundred pages of the experiment numbers are produced that make up a log book for histology studies.

A second program produces the same experiment numbers in duplicate as requested by the biologist. These pages of duplicate experiment numbers are treated with a coating substance, and then each number is

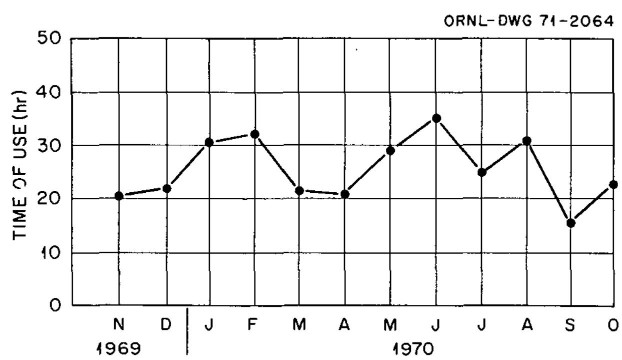

Fig. 39. Use of onsite computing service.

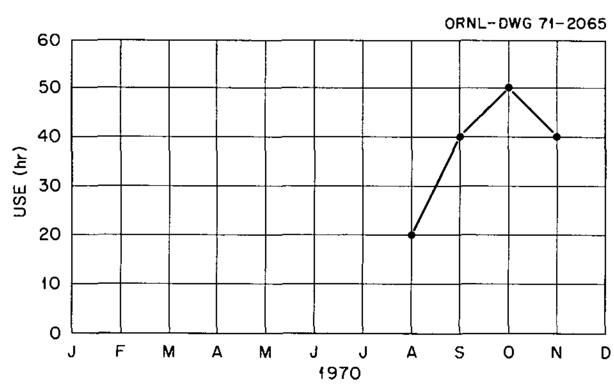

Fig. 40. Use of CRBE terminal.

sliced off the page and used as an identification tag for tissue undergoing examination within that experiment.

Address labels (E. Leach). Several members of the Biology Division at ORNL expressed the need for programs that would list selected addresses on gummed address labels. Programs were written to meet these needs. Each address was coded by using one alphameric character for the classification and a four-digit number for the identification.

A program was written to produce a master file on a magnetic tape that included the address, classification, and identification number for each individual included in the project. A second program was written that allowed the user to specify the code for the classification of the individuals for which address labels were wanted. The program searched the master file for the addresses requested and wrote them on a magnetic tape that was used later for listing the addresses on gummed labels. The program also prints a list of the addresses that are selected by classification.

Statistical Programs

General purpose programs on disk (Norma C. Hull). Several general purpose statistical programs have been placed on disk at the ORNL Computer Center. They are BMD08V, an analysis of variance program for any hierarchal design; NESTED, an analysis of variance program for four-fold or less hierarchal designs; and CONTOUR3, a contour plotting program.

STATPAK (Norma C. Hull). The programs contained in STATPAK,[59] with the exception of the programs written in ALGOL language, have been modified for the IBM 360 computer system. Many of the programs have been put on disk at the ORNL Computer Center and are accessible either through control cards sent to the computing center or through a Conversational Remote Batch Entry (CRBE) terminal.

Ecological sciences (F. L. Miller, Jr.). The average number of eggs laid per capsule is important in studying the freshwater snail *Physa heterostropha.* Since the distributional form of eggs per capsule is unknown, a program was written in ORDEAL to examine the distribution empirically. The program will compute summary statistics, tally the number of egg capsules of various size ranges, and plot the counts.

Select subroutines (Norma C. Hull). The Statistics Department has obtained a package of subroutines, SELECT,[60] to add to its regression programs. The routines will find the best (the minimum residual sum of squares) p-subset regression from a "pool" of $k > p$ predictor variables. The routines will also provide the user with nearly as good alternatives to the best p-subset regression.

The user must supply a calling or driver program. Sample calling programs have been written to allow the user to either input original data or the matrix of simple correlations between the predictor variables and the vector of simple correlations between the predictor variables and Y which have been obtained from some other regression program.

Programs for estimating plant laboratory efficiency[61] (Norma C. Hull). The procedure for estimating plant laboratory efficiency is being used on a monthly basis to evaluate several different types of analyses.[62] Programs are now being written to provide standards to use in the calculations of these evaluations rather than having averages computed from the monthly data being analyzed.

---

59. *Math. Div. Ann. Progr. Rept. Dec. 31, 1967,* ORNL-4236, p. 96.

60. SELECT was written at Texas A and M University by L. R. LaMotte following an algorithm of R. R. Hocking and LaMotte.

61. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 123.

62. W. E. Lever and Norma C. Hull, "Procedure for Estimating Plant Laboratory Efficiencies," this report.

Data Processing

Pathology data control: cumulative mortality and diagnosis lists (E. Leach). The revised version of the program LISTAUT[63] was developed for the purpose of listing the autopsy records for the various diagnoses within an experiment, and to determine the number of animals with neoplasms, without neoplasms, with leukemia, and with abscesses. A further revision was requested which presently gives in addition to the above the number of animals with amyloid, edema, hemorrhage, other leukemia, and lung tumors.

Programming is now being done which will produce a listing of 45 different diagnoses or combinations of diagnoses and the number of animals with each of the diagnoses. The program will also give for each diagnosis the percent incidence, the mean age at death, and the standard error of the mean age at death for the males and females within each group in the experiment.

PITFALL I (Norma C. Hull). PITFALL I[64] is a series of programs that are being used to analyze data obtained in environmental monitoring. The programs in the series are stored on a disk at the ORNL Computing Center, with the exception of the program that compiles information that is stored on magnetic tape. These programs can be accessed by submitting control cards to the computing center or through a Conversational Remote Batch Entry (CRBE) terminal.

It is believed that the PITFALL I package is flexible enough to be of use in analyzing data from other sources. The results obtained from these programs have been good.

STATISTICAL SEMINARS

Beauchamp, John J. (Mathematics Division, ORNL), "Variables Sampling Inspection Plan," April 15, 1970.

Gardner, William B. (IBM Corporation), "APL, a Programming Language," September 24, 1970.

Gosslee, David G. (Mathematics Division, ORNL), "Generalized Inverses of Matrices Used in Statistics," February 11, 1970.

Gosslee, David G. (Mathematics Division, ORNL), "Testing Normality by Graphical Methods," April 22, 1970.

Guinn, Sandra J. (ORAU Summer Student Trainee), "The Weibull Distribution," August 26, 1970.

Hebble, Thomas L. (Mathematics Division, ORNL), "Design Problem Concerning Nuclear Reactors," May 21, 1970.

Hoel, David G. (Mathematics Division, ORNL), "Probabilistic Model for Mortality Data," April 8, 1970.

Kastenbaum, Marvin A. (Director's Division, ORNL), "Lecture Series on Contingency Tables, Lecture I: Review," February 12, 1970.

Kastenbaum, Marvin A. (Director's Division, ORNL), "Lecture Series on Contingency Tables, Lecture II," February 19, 1970.

Kastenbaum, Marvin A. (Director's Division, ORNL), "Lecture Series on Contingency Tables, Lecture III," March 5, 1970.

Kastenbaum, Marvin A. (Director's Division, ORNL), "Lecture Series on Contingency Tables, Lecture IV," March 12, 1970.

Kastenbaum, Marvin A. (Director's Division, ORNL), "Lecture Series on Contingency Tables, Lecture V," April 3, 1970.

---

63. *Math. Div. Ann. Progr. Rept. Dec. 31, 1969,* ORNL-4514, p. 125.

64. N. C. Hull, J. J. Beauchamp, and D. E. Reichle, *PITFALL I,* ORNL-IBP-70-2 (1970).

Kastenbaum, Marvin A. (Director's Division, ORNL), "Lecture Series on Contingency Tables, Lecture VI," April 9, 1970.

Kastenbaum, Marvin A. (Director's Division, ORNL), "Lecture Series on Contingency Tables, Lecture VII," April 16, 1970.

Leinius, Ronald P. (Mathematics Division, ORNL), "The Uses of CRBE: Applications and Demonstration," September 10, 1970.

Lever, Claudia S. (Mathematics Division, ORNL), "Analysis of the Human Karyotype," April 29, 1970.

Lever, William E. (Mathematics Division, ORNL), "The Evaluation of Preventative Maintenance Systems," May 27, 1970.

Miller, Forest L. (Mathematics Division, ORNL), "Fabrication of Uranium Nitride Fuel Pellets," April 1, 1970.

Mitchell, Toby J. (Mathematics Division, ORNL), "Effect of Diets on Spontaneous Mutations," May 13, 1970.

Mitchell, Toby J. (Mathematics Division, ORNL), "Report on University of Wisconsin Model Building Conference," June 10, 1970.

Paulson, Albert S. (University of Tennessee), "Some Probabilistic Models for Pollution Phenomena," November 19, 1970.

Ramakrishnan, Alladi (Institute of Mathematical Sciences, Madras, India), "Inverse Probability in Stochastic Processes," June 5, 1970.

Tefler, John (Y-12), "Estimation of Potency in a Parallel Line Assay with Heterogeneity of Variance," November 12, 1970.

Professional Activities

Beauchamp, John J., Reviewer, *Journal of the American Statistical Association* and *Microvascular Research.*

Bowman, Kim O., Referee, *Technometrics* and *Biometrics.*

Brooks, A. A., Member, ACM SIGPLAN Committee for Symposium on Data Structures in Programming Languages.

Crowell, J. S., Co-Chairman of Program Evaluation Committee of the Numerical Analysis and Statistical Methodology Project.

Funderlic, R. E., Referee, Society for Industrial and Applied Mathematics.

Gardiner, D. A., Chairman of Programs, 1970, Section on Physical and Engineering Sciences, American Statistical Association.

Gardiner, D. A., Member, 1970 Joint Program Committee, American Statistical Association.

Gardiner, D. A., Reviewer, *Science.*

Gardiner, D. A., Consultant, Office of Director of Regulation, U.S. Atomic Energy Commission.

Gosslee, D. G., Secretary and Treasurer of the Eastern North American Region of the Biometric Society.

Gosslee, D. G., Reviewer, *I.E.E.E. Transactions on Reliability.*

Hebble, T. L., Member, Advisory Board to Section on Physical and Engineering Sciences of the American Statistical Association.

Hebble, T. L., Reviewer, *Technometrics* and *Nuclear Applications and Technology.*

Hoel, D. G., Reviewer, *Journal of the American Statistical Association, Biometrics, Technometrics,* and *I.E.E.E. Transactions on Reliability.*

Hoel, D. G., Consultant, Office of Director of Regulation, U.S. Atomic Energy Commission.

McCulloch, R. D., Chairman, Mid-Southeast Chapter, Association for Computing Machinery, 1969–1970.

Mynatt, F. R., Member, Program Committee for American Nuclear Society, Mathematics and Computations Division Topical Meeting.

Nelson, Paul, Referee, *Nuclear Science and Engineering.*

Nelson, Paul, Reviewer, *Computing Reviews.*

Nestor, C. W., Reviewer, *Computing Reviews* and *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.*

Tucker, T. C., Reviewer, *Computing Reviews.*

Uppuluri, V. R. R., Reviewer, *Journal of the American Statistical Association, Journal of the Association for Computing Machinery,* and *Biometrics.*

Westley, G. W., Co-Chairman of Program Evaluation Committee of the Numerical Analysis and Statistical Methodology Project.

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 Calculational Methods for Nuclear Criticality Safety, American Nuclear Society.

Mathematics Division Publications

Anderson, V. E. (with R. H. Ritchie), "The Penetration of Low-Energy Electrons in Matter," *Bull. Amer. Phys. Soc.* **15**(11), 1338 (1970).

Barish, J. (with T. W. Armstrong), "Reduction of the Residual Photon Dose Rate around High-Energy Proton Accelerators," *Nucl. Sci. Eng.* **40**(1) (April 1970).

Barish, J. (with T. W. Armstrong), *Calculated Activation of Copper and Iron by 3-GeV Protons,* ORNL-TM-2902 (February 1970).

Barish, J. (with T. A. Gabriel and R. G. Alsmiller, Jr.), *Calculation of the Long-Lived Induced Activity in the Soil around High-Energy Accelerator Target Areas – II,* ORNL-4599 (October 1970).

Barish, J. (with R. G. Alsmiller, Jr.), "High-Energy (<18 GeV) Muon Transport Calculations and Comparisons with Experiment, II," *Nucl. Instrum. Methods* **75** (1969).

Bartine, D. E. (with R. G. Alsmiller, Jr., F. R. Mynatt, W. W. Engle, Jr., and J. Barish), *Electron Transport with the Method of Discrete Ordinates,* ORNL-4592 (September 1970).

Baxley, John V., "Eigenvalues of Singular Differential Operators by Finite Difference Methods, I and II," *J. Math. Anal. Appl.* (in press).

Beauchamp, J. J. (with E. B. Darden, Jr., K. W. Christenberry, R. S. Bender, M. C. Jernigan, J. W. Conklin, and A. C. Upton), "Comparison of 60-MeV Protons and 300 kVp X-Rays for Induction of Lens Opacities in RF Mice," *Radiat. Res.* **43**, 598–612 (1970).

Bowman, Kim O. (with M. A. Kastenbaum), "Tables for Determining the Statistical Significance of Mutation Frequencies," *Mutat. Res.* **9** (May 1970).

Bowman, Kim O. (with L. R. Shenton), "Properties of the Maximum Likelihood Estimator for the Parameter of the Logarithmic Series Distribution," *Volume on Random Counts in Scientific Work*, Pennsylvania State University Press, May 1970.

Bowman, Kim O. (with L. R. Shenton), *Small Sample Properties of Estimator for the Gamma Distribution,* CTC-28 (June 1970).

Bowman, Kim O. (with K. Hutcheson, E. P. Odum, and L. R. Shenton), "Comments on the Distribution of Indices of Diversity," *Population Dynamics and Many Species Population,* Pennsylvania State University Press, December 1970.

Bowman, Kim O. (with L. R. Shenton), "Maximum Likelihood Estimator Moments for the 2-Parameter Gamma Distribution," *SANKHYA* 31 (1970).

Bowman, Kim O. (with L. R. Shenton), "Remarks on Thom's Estimators for the Gamma Distribution," *Mon. Weather Rev.* **98**(2) (1970).

Brooks, A. A. (with A. Hume and B. J. Handley), *RESAP Program for Least Squares Analysis of Gamma Spectra Involving Intermixed Standard Samples,* CTC-25 (March 1970).

Brooks, A. A., and F. D. Hammerling, *An Analysis of an (r, θ, φ) Inspection Machine,* CTC-38 (July 1970).

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

Chang, S. J., "Elastic-Viscoplastic Torsion for a Sokolovsky's Oval Section," *Acta Mech.* **9**, 264 (1970).

Chang, S. J., "Thermomechanical Coupling Problem for an Axially Symmetric Region of a Viscoelastic Medium," *J. Appl. Mech. (Trans. ASME)* 37, 1195–98 (December 1970).

Chang, S. J., "Diffraction of Plane Dilatational Waves by a Finite Crack," *Quart. J. Mech. Appl. Math.* (in press).

Chang, S. J. (with C. E. Pugh and S. E. Moore), "Viscoelastic Analysis of Graphite under Neutron Irradiation," *Proceedings of the Fifth Southeastern Conference on Theoretical and Applied Mechanics* (in press).

Cramer, S. N. (with M. L. Tobias, R. S. Carlsmith, G. W. Perry, O. W. Hermann, J. L. Lucius, and G. W. Morrison), *Application of the ESP Code to Two Neutron Distribution Problems, a Review of the Monte Carlo Method for Radiation Transport,* ORNL-RSIC-29 (1970).

Dolan, J. M., "On the Oscillatory Behavior of the Nonhomogeneous Second-Order Differential Equation $(ry')' + gy = f$," *J. Differential Equations* 7(2), 367–88 (March 1970).

Durfee, R. C., *FORTRAN Dynamic Storage Allocation,* ORNL-CF-70-8-59 (August 1970).

Emmett, Margaret B. (with E. A. Straker and M. L. Gritzner), *Neutron and Secondary Gamma-Ray Induced Heat in the Ground Due to Point 12.2-to-15-MeV and Fission Sources at an Altitude of 50 Feet,* ORNL-4626 (November 1970).

Engle, W. W., Jr. (with C. E. Burgart), "Time-Dependent Coupled Neutron-Gamma Calculations in Polyethylene," *American Nuclear Society* (November 1970).

Feliciano, M., Jr., *Geometric Properties of Solutions of the Differential System $x' = Ax$,* University of Tennessee dissertation (1970).

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

Ford, W. E., III (with D. H. Wallace), *The Use and "Testing" of Al, Fe, Ni, Cu, and Pb Secondary Gamma-Ray Production Data Sets from the POPOP4 Library,* CTC-20 (July 1970).

Fowler, R. H., "Investigation of Point-Charge Models for the H_2O Molecule," *Bull. Amer. Phys. Soc.* **15**, 164 (1970).

Funderlic, R. E., "A Theorem on Rank and a Related Characterization of Semi-Inverses," *American Mathematical Society* **17**(1), 126 (1970).

Funderlic, R. E., *Norms and Semi-Inverses,* CTC-35 (July 6, 1970).

Greene, N. M. (with W. R. Cobb), "A Calculational Sensitivity Study for a Selected LMFBR Using S_n Theory," *American Nuclear Society* (June 1970).

Greene, N. M. (with R. Q. Wright and J. H. Marable), "Musings on a Theme by L. W. Nordheim," *American Nuclear Society* (November 1970).

Greene, N. M. (with J. L. Lucius and C. W. Craven, Jr.), *An Evaluation and Compilation of the Fission and Capture Cross Sections of ^{239}Pu in the Energy Range 25 kev–15 MeV,* ORNL-TM-2797 (ENDF-131) (January 1970).

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

Haeuslein, G. K., "On the Algebraic Independence of Symmetric Functions," *Proc. Amer. Math. Soc.* **25**, 179–82 (1970).

Haeuslein, G. K., "On the Invariants of Finite Groups Having an Abelian Normal Subgroup of Prime Index," *J. London Math. Soc.* (in press).

Heath, M. T. (with A. J. Miller, H. R. Payne, M. E. Lackey, G. Samuels, E. W. Hagen, and A. W. Savolainen), *Use of Steam Electric Power Plants to Provide Low-Cost Thermal Energy to Urban Areas,* ORNL-HUD-14 (in press).

Hermann, O. W. (with R. G. Alsmiller, Jr.), "Calculation of the Neutron Spectra from Proton-Nucleus Nonelastic Collisions in the Energy Range 15 to 18 MeV and Comparison with Experiment," *Nucl. Sci. Eng.* **40**, 254–61 (1970).

Hoel, David G., "On the Monotonicity of the OC of an SPRT," *Ann. Math. Statist.* **41**, 310–14 (1970).

Hoel, David G. (with M. A. Kastenbaum and K. O. Bowman), "Sample Size Requirements: One-Way Analysis of Variance," *Biometrika* **57**, 421–30 (1970).

Hoel, David G., "Some Modifications and Applications of Wald's OC Formula," *Ann. Inst. Statist. Math.* **22**, 65–75 (1970).

Hoel, David G. (with D. P. Gaver, Jr.), "Comparison of Certain Small-Sample Poisson Probability Estimates," *Technometrics* **12**, 835–50 (1970).

Hoel, David G. (with M. A. Kastenbaum and K. O. Bowman), "Sample Size Requirements: Randomized Block Designs," *Biometrika* (December 1970).

Hoel, David G. (with K. S. Crump), "Some Applications of Renewal Theory on the Whole Line," *J. Appl. Prob.* (December 1970).

Hoel, David G. (with M. A. Kastenbaum and K. O. Bowman), *Adequate Sample Sizes for Randomized Block Designs,* ORNL-4527 (February 1970).

Hoel, David G. "A Simple Two-Compartmental Model Applicable to Enzyme Regulation," *J. Biol. Chem.* (in press).

Hoel, David G., and T. J. Mitchell, *The Simulation, Fitting and Testing of a Stochastic Cellular Proliferation Model,* ORNL-TM-2811 (1970).

Hoel, David G., and Toby J. Mitchell, "The Simulation, Fitting and Testing of a Stochastic Cellular Proliferation Model," *Biometrics* (in press).

Hoel, David G., *A Selection Procedure Based upon Wald's Double Dichotomy Test,* ORNL-TM-3237 (Jan. 29, 1971).

Householder, A. S., "Bezoutiants, Elimination and Localization," *SIAM Rev.* **12**, 73–78 (1970).

Householder, A. S., "Generalizations of an Algorithm of Sebastiao e Silva," *Numer. Math.* **16** (1970).

Householder, A. S., "On the Penultimate Remainder Algorithm and the Catalytic Multiplier," *SIAM J. Appl. Math.* **19**, 668–71 (1970).

Householder, A. S., *The Numerical Treatment of a Single Nonlinear Equation,* McGraw-Hill, 1970.

Householder, A. S. (with R. S. Varga and J. H. Wilkinson), "A Note on Gerschgorin's Inclusion Theorem for Eigenvalues of Matrices," *Numer. Math.* **16**, 141–44 (1970).

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

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

Hull, Norma C., and J. J. Beauchamp (with D. E. Reichle), *Pitfall 1: A General Purpose Data Processing Program for Environmental Data,* ORNL-IBP-70-2 (February 1970).

Kastenbaum, M. A., and Toby J. Mitchell, "Studies in Inhalation Carcinogenesis: A Critique," *Inhalation Carcinogenesis,* AEC Symposium Series No. 18 (Conf-691001), M. G. Hanna, Jr., P. Nettesheim, and J. R. Gilbert, eds., 1970.

Leinius, R. P., *Error Detection and Recovery for Syntax Directed Compiler Systems,* University of Wisconsin dissertation (1970).

Lu, C. C. (with R. D. Present), "Nuclear Quadrupole Coupling in the LiH Molecules," *Phys. Rev.* **B1**, 2025 (1970).

Lu, C. C. (with C. V. Dodd), *Non-Destructive Test for Measuring the State of Heat Treatment in Closure Welds,* ORNL-TM-3024 (July 1970).

Mankin, J. B., *A Study of Control Sensitivity,* University of Tennessee dissertation, CTC-21 (January 1970).

McCulloch, R. D. (with J. W. Moulder, N. E. Garrett, L. M. Tucker, W. M. Bugg, G. T. Condo, and H. O. Cohn), "K^- Meson Absorption in Neon," *Nucl. Phys.* (July 1970).

McCulloch, R. D., and H. W. Graben (with S. T. Thornton and H. B. Willard), "TENMO – General Tensor Moment Polarization Computer Program," *Nucl. Instrum. Methods* **78**, 328–30 (1970).

McCulloch, R. E. (with W. M. Bugg, G. T. Condo, N. E. Garrett, J. W. Moulder, and H. O. Cohn), "Hyperfragment Production Following Slow Σ^- Capture in Liquid Neon," *Phys. Lett.* **31B**(9) (April 1970).

McCulloch, R. D. (with H. O. Cohn, W. M. Bugg, and G. T. Condo), "Inelastic PN Interactions at 3.7 GeV/*c*," *Nucl. Phys.* **B21**, 505–14 (1970).

McCulloch, R. D. (with N. E. Garrett, W. M. Bugg, G. T. Condo, J. W. Moulder, and H. O. Cohn), "Excitation of Nuclear Fragments Following K^- Absorption by Neon," *Nucl. Phys.* (in press).

McNeilly, G. S., *Reaction Mechanism Studies of Single and Double Differential Cross Sections from the Reaction* $^{24}Mg(\alpha;\alpha',\gamma)^{24}Mg$, Florida State University dissertation, CTC-43 (July 1970).

McNeilly, G. S. (with W. I. van Rij), "A DWBA plus Hauser-Feshbach Analysis of Single and Double Differential Cross Sections for the Reaction $^{24}\mathrm{Mg}(\alpha,\alpha'\gamma)^{24}\mathrm{Mg}$," *Bull. Amer. Phys. Soc. II* **15**(4), 544 (1970).

McNeilly, G. S., "A Comparison of DWBA plus Hauser-Feshbach and Coupled Channels plus Hauser-Feshbach Analyses of Single and Double Differential Cross Sections for the Reaction $^{24}Mg(\alpha,\alpha'\gamma)^{24}Mg$," *Bull. Amer. Phys. Soc. II* **15**(11), 1330 (1970).

Miller, Forest L., Jr. (with M. R. Patterson and E. C. Long), *Digital Filtering and Spectral Comparison Using the Fast Fourier Transform,* CTC-44 (September 22, 1970).

Mitchell, Toby J. (with C. C. Congdon, D. A. Gardiner, M. A. Kastenbaum, and R. E. Toya), "Secondary Disease Mortality in Rat-Mouse Radiation Chimeras," *J. Nat. Cancer Inst.* (November 1970).

Mitchell, Toby J. (with N. R. Draper), "Construction of a Set of 512-Run Designs of Resolution $\geqslant 5$ and a Set of Even 1024-Run Designs of Resolution $\geqslant 6$," *Ann. Math. Statist.* **41**, 876–87 (1970).

Mitchell, Toby J. (with E. P. McDonald and R. D. Lange), "Effect of Testosterone and Erythropoietin on Rabbit Bone Marrow Cells," *Proceedings of Tel Aviv Symposium of Erythropoiesis,* Y. Matoth, ed., Academic (in press).

Morrison, G. W. (with T. G. Miller and F. P. Gibson), "A Monte Carlo Technique for Correcting Experimental Fast-Neutron Polarization Data," *Nucl. Instrum. Methods* **80**, 325–32 (1970).

Morrison, G. W. (with T. G. Miller and F. P. Gibson), *PMS1 – a FORTRAN Monte Carlo Code for Producing Experimental Left-Right Ratios in Fast Neutron Polarization Experiments,* CTC-9 (1970).

Morrison, G. W. (with D. C. Irving), *PICTURE: An Aid in Debugging Input Data,* ORNL-TM-2892 (1970).

Morrison, G. W. (with T. G. Miller and G. W. Westley), "Study of the $Be^9(d,n)B^{10}$ and $B^{11}(d,n)C^{12}$ Reactions Using Distorted Wave Born Approximation," *Bull. Amer. Phys. Soc.* **15**, 1315 (1970).

Morrison, G. W. (with R. F. Haglund, Jr., C. A. Pearson, and G. W. Westley), "Study of the $^{12}C(d,p)^{13}C$ Reaction from 7 to 10 MeV Using the WBP Model," *Bull. Amer. Phys. Soc.* **15**, 1316 (1970).

Mynatt, F. R., "Neutron Transport in Iron," *Amer. Nucl. Soc.* 13(1) (1970).

Mynatt, F. R. (with C. E. Clifford and H. C. Claiborne), *LMFBR Shielding Program Interim Report, Preliminary Evaluation of Techniques for Predicting the Spectra of Neutrons Transmitted by Grid Plate Shields,* ORNL-TM-2896 (Mar. 2, 1970).

Mynatt, F. R. (with R. G. Alsmiller, M. L. Gritzner, J. V. Pace, and J. Barish), *The Lateral Spread of High-Energy ($\leqslant$400 MeV) Neutron Beams and Earthshine,* ORNL-TM-3025 (1970).

Mynatt, F. R. (with C. E. Clifford and H. C. Claiborne), *Preliminary Evaluation of Techniques for Predicting the Spectra of Neutrons Transmitted by Grid Plate Shields,* ORNL-TM-2896 (July 31, 1970).

Mynatt, F. R., *An Analysis of the Effect of Streaming Paths on the Radiation Shielding Capability of a Missile Silo Cover Shield,* ORNL-TM-2824 (Jan. 13, 1970) (classified).

Nelson, Paul, "Application of Invariant Imbedding to the Solution of Partial Differential Equations by the Continuous-Space Discrete-Time Method," *Proc. 1970 SJCC,* AFIPS **36**, 397–402, AFIPS Press, 1970.

Nelson, Paul (with T. S. Kress), "Theory and Iterative Solution of a Model for Fission-Product Deposition," *SIAM J.* **19**, 60–74 (1970).

Nestor, C. W., Jr. (with T. A. Carlson, N. Wasserman, and J. D. McDowell), *Comprehensive Calculation of Ionization Potentials and Binding Energies for Multiply Charged Ions,* ORNL-4562 (July 1970).

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

Nestor, C. W. (with T. A. Carlson, C. C. Lu, T. C. Tucker, and F. B. Malik), *Eigenvalues, Radial Expectation Values, and Potentials for Free Atoms from $Z = 2$ to 126 as Calculated from Relativistic Hartree-Fock-Slater Atomic Wave Functions,* ORNL-4614 (December 1970).

Nestor, C. W., *Calculation of Characteristic X-Ray Energies from Relativistic Hartree-Fock-Slater Electron Binding Energies,* ORNL-CF-70-3-20 (Mar. 30, 1970).

Nestor, C. W., *A Hartree-Fock Program with Configuration Mixing,* ORNL-CF-70-11-31 (Nov. 10, 1970).

Nestor, C. W. (with J. D. McDowell), *Investigation of Compound Superconductors,* ORNL-CF-70-1-14 (Apr. 17, 1970).

Patterson, M. R. (with E. C. Long and F. L. Miller), *Digital Filtering and Spectral Comparison Using the Fast Fourier Transform,* CTC-44 (August 1970).

Patterson, M. R. (with G. W. Westley, J. A. Watts, and P. R. Coleman), *Vibration Analysis of a Floor Structure,* CTC-30 (June 1970).

Patterson, M. R. (with R. L. Becker), "Splitting of Single Hole Strength and Fine Structure in $(p,2p)$ Spectra," *Bull. Amer. Phys. Soc. II* **15**(11), 1315 (1970).

Penny, S. K., "Calculations of Cross Sections for Gamma-Ray Production via Neutron Inelastic Scattering in ^{56}Fe," *Trans. Amer. Nucl. Soc.* **13**(1), 396 (1970).

Reeves, Mark, III, *A Microscopic Analysis for Elastic Scattering of Deuterons and Alpha Particles,* University of Tennessee dissertation, CTC-32 (July 1970).

Reeves, Mark, III (with C. M. Jones, J. L. C. Ford, Jr., and F. E. Obenshain), "Search for Parity Nonconservation in the Force between Nucleons," *Phys. Rev.* (in press).

Stallmann, F. W., and Sandra H. Merriman, *A Computer Program for the Inversion of the Laplace Transform,* ORNL-4604 (1970).

Sullivan, J. G. (with J. R. Stockton), *ORNL Basic Compiler,* ORNL-TM-3042 (1970).

Thompson, C. L. (with I. J. Brown and R. W. Roussin), *Users Manual for Programs to Edit and Combine DLC-5/Hallmark Calculational Results of Neutron and Secondary Gamma-Ray Transport in Air-over-Ground Geometry,* ORNL-TM-3129 (September 1970).

Thompson, C. L., *Calculated Neutron Flux Distribution Resulting from a Fission Source Located at the Center of a 10-Meter-Diameter Sphere of Sodium,* ORNL-TM-3156 (Oct. 27, 1970).

Thompson, C. L., *A FORTRAN-360 Subroutine Package for Producing Printed Linear, Semilogarithmic or Logarithmic Graphs,* ORNL-TM-3079 (Aug. 6, 1970).

Tucker, T. C., *Two Subroutines Which Can Reduce Storage Space for Floating-Point Data,* ORNL-CF-70-8-40 (August 1970).

Turner, W. D. (with M. Siman-Tov), *HEATING3 – an IBM 360 Heat Conduction Code,* ORNL-TM-3208 (1970).

Tyrrell, T. J., *TDUMP – a Translation Routine for Dumping Arrays,* ORNL-CF-70-7-8 (July 1970).

Uppuluri, V. R. R. (with K. Nagabhushanam), "Representation of a Stochastic Process Based on Its Mean Value" (abstract), *Notices Amer. Math. Soc.* **17**(119), 264 (1970).

Uppuluri, V. R. R. (with W. H. Olson), "Characterization of the Distribution of a Random Matrix by Rotational Invariance" (abstract), *Ann. Math. Statist.* **41**, 1144 (1970).

Uppuluri, V. R. R., and John A. Carpenter, "A Generalization of the Classical Occupancy Problem," *J. Math. Anal. Appl.* (in press).

Uppuluri, V. R. R. (with W. H. Olson), *Asymptotic Distribution of Eigenvalues of Random Matrices,* ORNL-4603 (September 1970).

Westley, G. W. (with J. A. Watts), *Computing Technology Center Numerical Analysis Library,* CTC-39 (1970).

Westley, G. W., *A Linearly Constrained Nonlinear Programming Algorithm,* ORNL-4644 (1970).

Whitesides, G. E., "The Monte Carlo Method as Applied to Nuclear Criticality Safety Calculations," *Amer. Nucl. Soc.* (June 1970).

Wright, R. Q. (with 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).

Wright, R. Q. (with P. R. Kasten and C. W. Craven, Jr.), *Cross-Section and Nuclear-Constant Data for Heavy Metal Nuclides (Fuels),* ORNL-TM-2851 (revised) (Feb. 12, 1970).

Mathematics Division Lectures and Papers

Bowman, Kim O. (with L. R. Shenton), "Small Sample Properties of Estimator for the Gamma Distribution," Annual Meeting of the Institute of Mathematical Statistics, Laramie, Wyoming, August 27, 1970.

Brooks, A. A., "Retrieval and Analysis of Mixed Alphanumeric and Digital Data," University of Florida, Gainesville, October 1970.

Carter, H. P., "Large Scientific Computers," University of Tennessee Mathematics Club, April 1970.

Carter, H. P., and C. S. Williams, "The ORNL Large Scientific Computer – a Description of the IBM System/360 Model 91," Mid-Southeast Chapter Meeting, Association for Computing Machinery, Gatlinburg, Tennessee, March 20, 1970.

Chang, S. J., "A Crack Problem in Viscoelastic Medium," Applied Mathematics Division, National Bureau of Standards, Washington, D.C., February 1970.

Chang, S. J., "Viscoelastic Analysis of Graphite under Neutron Irradiation," Fifth Southeastern Conference on Theoretical and Applied Mechanics, North Carolina State University, Raleigh, April 16–17, 1970.

Chang, S. J., "Thermomechanical Coupling Problem for an Axially Symmetric Region of a Viscoelastic Medium," Sixth U.S. National Congress for Applied Mechanics, Harvard University, Cambridge, Massachusetts, June 15–19, 1970.

Chang, S. J., "A Viscoelastic Representation of the Behavior of Graphite under the Influence of Neutron Irradiation," Conference on Continuum Aspects of Graphite Design, Gatlinburg, Tennessee, November 9–12, 1970.

Fowler, R. H. (with R. A. Dory), "MHD Equilibria in Tokamaks and Doublets," Sherwood Meeting, Princeton Plasma Physics Laboratory, Princeton, New Jersey, April 1970.

Funderlic, R. E., "A Theorem on Rank and a Related Characterization of Semi-Inverses," Annual Meeting of the American Mathematical Society, San Antonio, Texas, January 1970.

Funderlic, R. E., "Characterization of Some Classes of Norms," Annual Meeting of the Society for Industrial and Applied Mathematics, University of Denver, June 1970.

Gardiner, D. A., "Elements of Probability Plotting," Memphis State University, Memphis, Tennessee, March 12, 1970; Concord College, Concord, West Virginia, May 6, 1970.

Gardiner, D. A., "Statistical Consulting at a Large Research Laboratory," Memphis State University, Memphis, Tennessee, March 13, 1970; Concord College, Concord, West Virginia, May 6, 1970.

Gosslee, D. G., "Design and Analysis of Experiments," Georgia Institute of Technology, Atlanta, July 24, 1970.

Hoel, D. G., "Some Sequential Selection Procedures," Carnegie-Mellon University, Pittsburgh, Pennsylvania, January 21, 1970.

Hoel, D. G., "A Class of Selection Procedures," University of California at Los Angeles, February 20, 1970.

Joseph, A. F., "A Linear Programming Application to Spectrum Analysis," Fourteenth Annual Conference on Analytical Chemistry in Nuclear Technology, Gatlinburg, Tennessee, October 13–15, 1970.

Lever, Claudia S., "Nonparametric Tests of Independence in Time Series," Meeting of the Florida Chapter of the American Statistical Association, Tallahassee, Florida, March 6, 1970.

McCulloch, R. D., "PL/1 Revisited," Association for Computing Machinery, Mid-Southeast Chapter, Chattanooga, Tennessee, October 16, 1970.

McNeilly, G. S., and W. J. van Rij, "A DWBA plus Hauser-Feshbach Analysis of Single and Double Differential Cross Sections for the Reaction $^{24}Mg(\alpha,\alpha'\gamma)^{24}Mg$," American Physical Society Meeting, Washington, D.C., April 25, 1970.

McNeilly, G. S., "A Comparison of DWBA plus Hauser-Feshbach and Coupled Channels plus Hauser-Feshbach Analyses of Single and Double Differential Cross Sections for the Reaction $^{24}Mg(\alpha,\alpha'\gamma)^{24}Mg$," American Physical Society Meeting, New Orleans, Louisiana, November 1970.

Nelson, Paul, "Positive Solutions of Positive Operator Equations," University of Tennessee Mathematics Department Colloquium, May 1970.

Nelson, Paul, and Carla L. Armstrong, "Application of Invariant Imbedding to the Determination of Stresses in Long Shells," 1970 SIAM National Meeting, Denver, Colorado, July 1970.

Nelson, Paul, and Carla L. Armstrong, "Accurate Analysis of Two-Point Boundary-Value Problems by Invariant Imbedding," Mid-Southeast Chapter Meeting of the Association for Computing Machinery, Chattanooga, Tennessee, October 1970.

Patterson, M. R. (with R. L. Becker), "Empirical Validity of Renormalized Finite Nuclear Brueckner-Hartree-Fock Theory," APS Division of Nuclear Physics Meeting, Houston, Texas, October 15, 1970.

Rannie, R. P., "MVT Operating System on the IBM System/360 Computers at ORNL," Association for Computing Machinery Mid-Southeast Chapter Meeting, Chattanooga, Tennessee, October 16, 1970.

Uppuluri, V. R. R. (with K. Nagabhushanam), "Representation of a Stochastic Process Based on Its Mean Value," Annual Meeting of the American Mathematical Society, San Antonio, Texas, January 23, 1970.

Uppuluri, V. R. R. (with John A. Carpenter), "A Generalization of the Classical Occupancy Problem," Annual Meeting of the Southeastern Section of the Mathematical Association of America, Clemson, South Carolina, March 20–21, 1970.

Uppuluri, V. R. R., "Representation of a Stochastic Process Based on Its Mean Value," Mathematics Colloquium, University of Tennessee, April 22, 1970.

Uppuluri, V. R. R. (with W. H. Olson), "Characterization of the Distribution of a Random Matrix by Rotational Invariance," Meetings of the Institute of Mathematical Statistics, Chapel Hill, North Carolina, May 5–7, 1970.

Uppuluri, V. R. R. (with W. H. Olson), "Asymptotic Density of Eigenvalues of Random Matrices," Invited Paper, Sixth Berkeley Symposium on Mathematical Statistics and Probability, Berkeley, California, July 13, 1970.

Uppuluri, V. R. R., "Theory and Applications of Markov Chains," Six-Week Course, University of Sao Paulo, Brazil, September 14–October 23, 1970.

Uppuluri, V. R. R., "Random Difference Equations," Mathematics Colloquium, Fayetteville State University, Fayetteville, North Carolina, December 10, 1970.

Warner, G. G. (with W. S. Snyder), "Estimation of Dose and Dose Commitment to Bladder Wall from a Radionuclide Present in Urine," Health Physics Society Meeting, Chicago, Illinois, June 28 –July 2, 1970.

Warner, G. G. (with W. S. Snyder and Mary R. Ford), "Estimation of Dose to Gonads from Gamma Emitters Present in Body," Second IRPA Congress, Brighton, England, May 3–8, 1970.

Whitesides, G. E., "The Monte Carlo Method as Applied to Nuclear Criticality Safety Calculations," American Nuclear Society Meeting, Los Angeles, California, July 1970; University of Cincinnati, December 1970.

ORNL-4661
UC-32 – Mathematics and Computers

INTERNAL DISTRIBUTION

1. H. I. Adler
2. C. L. Allen
3. R. G. Alsmiller
4. D. W. Altom
5. E. C. Anderson
6. N. G. Anderson
7. V. E. Anderson
8. D. E. Arnurius
9. S. I. Auerbach
10. J. Barish
11. D. E. Bartine
12. S. E. Beall
13. J. J. Beauchamp
14. M. Bender
15. N. A. Betz
16. D. S. Billington
17. C. J. Borkowski
18. K. O. Bowman
19. G. E. Boyd
20. J. C. Bresee
21. A. A. Brooks
22. F. R. Bruce
23. N. A. Buhl
24. T. D. Calton
25. J. A. Carpenter
26. S. F. Carson
27. G. W. Chandler
28. K. C. Chandler
29. S. J. Chang
30. R. L. Childs
31. P. R. Coleman
32. W. C. Colwell
33. J. A. Cox
34. S. N. Cramer
35. N. F. Cross
36. J. S. Crowell
37. A. H. Culkowski
38. F. L. Culler
39. G. W. Cunningham
40. C. S. Day
41. J. M. Dolan
42. R. A. Dory
43. R. C. Durfee
44. M. B. Emmett
45. W. W. Engle
46. M. Feliciano
47. D. E. Ferguson
48. W. E. Ford
49. J. L. Fowler
50. P. G. Fowler
51. R. H. Fowler
52. J. H. Frye
53. R. E. Funderlic
54–58. D. A. Gardiner
59. J. H. Gibbons
60. C. A. Giles
61. J. S. Gillen
62. J. H. Gillette
63. L. W. Gilley
64. D. G. Gosslee
65. N. B. Gove
66. N. M. Greene
67. W. R. Grimes
68. M. L. Gritzner
69. G. E. Guest
70. G. K. Haeuslein
71. F. D. Hammerling
72. C. E. Hammons
73. G. R. Handley
74. M. T. Heath
75. T. L. Hebble
76. L. P. Helton
77. O. W. Hermann
78. R. F. Hibbs
79. R. J. Hinton
80. R. B. Hofstra
81. C. W. Holland
82. D. J. Horen
83. A. S. Householder
84. N. C. Hull
85. W. H. Jordan
86. A. F. Joseph
87. M. T. Kelley
88. W. E. Kinney
89. J. R. Knight
90. E. Leach
91. R. P. Leinius
92. C. S. Lever
93. W. E. Lever
94. J. L. Liverman
95. R. S. Livingston
96. C. C. Lu
97. J. L. Lucius
98. H. G. MacPherson
99. F. C. Maienschein
100. J. B. Mankin
101. J. J. Manning
102. R. D. McCulloch
103. J. D. McDowell
104. G. S. McNeilly
105. S. H. Merriman
106. F. L. Miller, Jr.
107. T. J. Mitchell
108. K. Z. Morgan
109. G. W. Morrison
110. F. R. Mynatt
111. D. B. Nelson
112. Paul Nelson, Jr.
113. C. W. Nestor, Jr.
114. J. V. Pace
115. J. E. Parham
116–117. R. B. Parker
118. M. R. Patterson
119. C. D. Paulk
120. S. K. Penny
121. F. Perey
122. L. M. Petrie
123. H. Postma
124. R. P. Rannie
125. J. P. Reavis
126. Mark Reeves
127. D. J. Rose
128. O. W. Russ
129. H. E. Seagren
130. V. A. Singletary
131. M. J. Skinner
132. A. H. Snell
133. W. S. Snyder
134. E. A. Straker
135. J. G. Sullivan
136. D. A. Sundberg
137. E. H. Taylor
138. C. L. Thompson
139. M. L. Tobias
140. D. B. Trauger
141. T. C. Tucker
142. W. D. Turner
143. T. J. Tyrrell

144. G. Ulrikson
145. V. R. R. Uppuluri
146. C. P. Walker
147. G. G. Warner
148. C. C. Webster
149. A. M. Weinberg
150. T. A. Welton
151. G. W. Westley
152. J. E. White
153. G. E. Whitesides
154. C. S. Williams
155. L. R. Williams
156. R. O. Williams
157. D. L. Wilson
158. D. R. Winkler
159. R. Q. Wright
160. W. J. Yaggi
161. Gale Young
162. Biology Library
163–165. Central Research Library
166. ORNL – Y-12 Technical Library Document Reference Section
167–191. Mathematics Division Library
192–211. Laboratory Records Department
212. Laboratory Records, ORNL R.C.

EXTERNAL DISTRIBUTION

213. C. O. Alford, Oak Ridge Associated Universities, Oak Ridge, Tennessee
214. Richard L. Anderson, Dept. of Statistics, University of Kentucky, Lexington, Kentucky
215. John V. Baxley, Dept. of Mathematics, Wake Forest University, Winston-Salem, North Carolina
216. Bruce M. Beardsley, Computer Sciences Branch, Idaho Nuclear Corp., Idaho Falls, Idaho
217. Gilbert W. Beebe, Follow-Up Agency, National Academy of Sciences, Washington, D.C.
218. Ralph A. Bradley, Dept. of Statistics, Florida State University, Tallahassee, Florida
219. Joseph M. Cameron, National Bureau of Standards, Washington, D.C.
220. T. A. DeRouen, Dept. of Statistics, University of Tennessee, Knoxville, Tennessee
221. Norman R. Draper, Dept. of Statistics, University of Wisconsin, Madison, Wisconsin
222. C. L. Dunham, Division of Medical Sciences, National Academy of Sciences, Washington, D.C.
223. C. W. Edington, U.S. Atomic Energy Commission, Washington, D.C.
224. Sidney Fernbach, Computation Division, Lawrence Radiation Laboratory, Livermore, California
225. Wallace Givens, Argonne National Laboratory, Argonne, Illinois
226. Joseph D. Goldstein, U.S. Atomic Energy Commission, Washington, D.C.
227. W. W. Grigorieff, Oak Ridge Associated Universities, Oak Ridge, Tennessee
228. Sandra J. Guinn, Route 1, Lenoir City, Tennessee
229. John J. Harley, Health and Safety Laboratory, U.S. Atomic Energy Commission, New York, New York
230. Boyd Harshbarger, Dept. of Statistics, Virginia Polytechnic Institute, Blacksburg, Virginia
231. David G. Hoel, National Institute of Environmental Health Sciences, P.O. Box 12233, Research Triangle Park, North Carolina
232. International Computation Centre, Casella postale no. 10053, Zona dell'E.U.R., Rome, Italy
233. John L. Jaech, Battelle Northwest, Richland, Washington
234. Leon Jacobs, Health, Education and Welfare, Washington, D.C.
235. M. A. Kastenbaum, The Tobacco Institute, 1776 K Street, NW, Washington, D.C.
236. J. S. Kirby-Smith, U.S. Atomic Energy Commission, Washington, D.C.
237. Roger B. Lazarus, Los Alamos Scientific Laboratory, Los Alamos, New Mexico
238. David D. Mason, Dept. of Experimental Statistics, North Carolina State University, Raleigh, North Carolina
239. T. Matthews, Dept. of Mathematics, University of Tennessee, Knoxville, Tennessee
240. Paul D. Minton, Dept. of Statistics, Southern Methodist University, Dallas, Texas
241. Lincoln E. Moses, Stanford University, Stanford, California
242. W. H. Olson, Dept. of Mathematics, McGill University, Montreal 110, Canada
243. John R. Pasta, Dept of Computer Science, University of Illinois, Urbana, Illinois
244. A. S. Paulson, Dept. of Statistics, University of Tennessee, Knoxville, Tennessee
245. Harry Polachek, U.S. Atomic Energy Commission, Washington, D.C.
246. Umberto Saffiotti, National Cancer Institute, Bethesda, Maryland
247. Marvin A. Schneiderman, National Cancer Institute, Bethesda, Maryland
248. Yoshio Shimamoto, Brookhaven National Laboratory, Upton, Long Island, New York
249. C. V. L. Smith, U.S. Atomic Energy Commission, Washington, D.C.
250. Milton Sobel, Dept. of Statistics, Stanford University, Stanford, California

251. F. W. Stallmann, Dept. of Mathematics, University of Tennessee, Knoxville, Tennessee
252. Julius Smith, Dept. of Mathematics, University of Tennessee, Knoxville, Tennessee
253. Eva Sobocinski, Document Room, Computing Center, University of Notre Dame, Notre Dame, Indiana
254. J. A. Swartout, Union Carbide Corporation, New York, New York
255. John R. Totter, U.S. Atomic Energy Commission, Washington, D.C.
256. R. W. Touchberry, U.S. Atomic Energy Commission, Washington, D.C.
257. N. Scott Urquhart, New Mexico State University, P.O. Box 3130, Las Cruces, New Mexico
258. Jack Vanderryn, U.S. Atomic Energy Commission, Washington, D.C.
259. W. W. Wade, Dept. of Mathematics, University of Tennessee, Knoxville, Tennessee
260. J. W. Wilkinson, Rensselaer Polytechnic Institute, School of Management, Troy, New York
261. A. H. Wolff, Consumer Protection and Environmental Health Service, Health, Education and Welfare, Washington, D.C.
262. Laboratory and University Division, AEC, ORO
263. Patent Office, AEC, ORO

264–477. Given distribution as shown in TID-4500 under Mathematics and Computers category (25 copies – NTIS)