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MATHEMATICS and STATISTICS RESEARCH DEPARTMENT

MASTER

Progress Report

Period Ending June 30, 1979

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MASTER

MATHEMATICS AND STATISTICS RESEARCH DEPARTMENT PROGRESS REPORT for Period Ending June 30, 1979

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Preface

The Mathematics and Statistics Research Department during the 1978–1979 reporting period continued its assistance to the DOE Applied Mathematical Sciences Program in formulating its basic research plan. Research efforts in response to the plan accelerated, and a new project in risk analysis was initiated. Some of this progress is recorded in Part A of this report.

The collaboration effort with others in the Nuclear Division continued to grow. Notable in this area was the initiation of a project in data validation, which was requested by the ORNL Energy Division and DOE's Energy Information Administration. A description of the work in data validation can be found in Part B.

Several personnel changes occurred during the report period. Victor Lowe joined the department from the Y-12 Statistical Services group and subsequently transferred to the ORNL Energy Division. Darryl Downing transferred to the Computing Applications Department of the Computer Sciences Division, and Forest Miller left to join the University of Nevada Desert Research Institute. William Thompson of the University of Missouri, Columbia, visited during the academic year to participate in the research in model evaluation and risk analysis.

Statisticians Patricia DiZillo-Benoit and Tommy Wright joined the department and immediately became involved in the data validation project. David Scott joined the Mathematics Section to work on the research in numerical linear algebra, concentrating on sparse matrix problems. The effort in numerical linear algebra was further strengthened by the arrival of Robert Funderlic, who transferred from the Computing Applications Department.

In addition, the department was pleased to welcome Vicki Hatmaker and Cynthia White to the secretarial staff.

Honors continue to accrue to the staff of the department. Kimiko Bowman was elected Ordinary Member of the International Statistical Institute and was designated by Radford College as the Outstanding Alumnus for 1978.

Summary

This is the twenty-second in the series of progress reports of the Mathematics and Statistics Research Department and its predecessor organizations.

Part A reports research progress in biomedical and environmental applications, materials science applications, model development and evaluation, moving boundary problems, multivariate multipopulation classification, numerical linear algebra, risk analysis, and complementary areas.

The results of collaboration with other researchers on problems in biology, chemistry, energy, engineering, environmental sciences, geology, health and safety research, information sciences, and material sciences are recorded in Part B.

Parts C, D, and E contain short accounts of educational activities, lists of written and oral presentations of research results, and a list of other professional activities in which the staff was engaged.

Part A. Mathematical and Statistical Research

1. Biomedical and Environmental Applications

D. G. Gosslee · J. P. O'Neill[1]
A. W. Hsie[1] · W. Y. Tan[2]
T. J. Mitchell · B. W. Turnbull[3]

ANALYSIS OF DISEASE PREVALENCE DATA FROM SURVIVAL/SACRIFICE EXPERIMENTS

In a previous report,[4] we presented a new approach to the analysis of disease prevalence data from survival experiments in which there may also be some serial sacrifice. Due to the complicated nature of the disease processes involved and the fact that the data are obtained only at the death of the animal, such data are often difficult to analyze. The statistical model that we utilized was parameterized in terms of illness-state *prevalences* and *lethalities*, and methods for estimating these from the data were discussed.

Based on expressing the prevalences and lethalities in "log-linear" form, various simplified models can now be fitted. In the case of two diseases, for example, let p_{imjk} be the prevalence of the illness state (j, k) in group i (treated or control) at the *beginning* of time interval m, where $j = 0$ (1) refers to the absence (presence) of disease A and where $k = 0$ (1) refers to the absence (presence) of disease B. The corresponding lethality q_{imjk} is defined as the probability that an animal dies in interval m, given it is in group i and illness state (j, k) at the start of the interval. Then the log-linear model expresses log p_{imjk} and logit $q_{imjk} \equiv \log[q_{imjk}/(1 - q_{imjk})]$ as a sum of main effects and interactions of the variables group, time, and disease. By imposing assumptions that certain effects and interactions are zero, a hierarchy of models can be fitted to the data and examined. The capability for fitting these "unsaturated" models enables us to simplify the model, to increase the precision of the estimates of the important parameters, and to test various simplifying assumptions, such as nonlethality of diseases. Another benefit is that the difficulties associated with the sparsity of some observed illness states are greatly alleviated.

To fit a specified model (by the maximum likelihood criterion) to a set of data, we utilize the *EM* algorithm[5] in conjunction with the well-known iterative proportional fitting algorithm. To test the goodness of fit of the model, we compute the lack-of-fit statistic $G = 2(\hat{L}^* - \hat{L})$, where $\hat{L}$ is the maximum log-likelihood for the proposed model and $\hat{L}^*$ is the maximum log-likelihood for the saturated model (all terms present). We then use, as an approximation to the null distribution of G, the chi-squared distribution with degrees of freedom ν equal to the difference between the number of terms in these two models. Approximate standard errors for specified terms in the model can also be readily computed.

We have applied these techniques, for demonstration purposes, to some of the data from a large experiment conducted at the ORNL Biology Division to examine the effects of dose, dose-rate, and type of radiation on mice. Various questions regarding disease lethality, relative risks, and independence of

1. Biology Division.
2. Memphis State University.
3. Cornell University.
4. "Analysis of Disease Data from Survival Sacrifice Experiments," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL CSD-34, pp. 17–18 (September 1978).

5. A. P. Dempster, N. M. Laird, and D. B. Rubin, "Maximum Likelihood Estimation from Incomplete Data via the *EM* Algorithm," *J. R. Stat. Soc. B* 39, 1–22 (1977).

diseases were examined for two experimental groups and four pooled disease categories.

We are currently involved in a major effort to document our computer program and make it easier for the user to specify, via a series of interactive questions and answers, the models of interest. When this is completed, the analysis should be ready for application to a wide variety of data sets.

DISTRIBUTION OF MUTANTS IN THE CHO ASSAY

The CHO/HGPRT assay technique is widely used to test the mutagenic effects of various types of chemicals or irradiation, specific to the HGPRT locus in Chinese hamster ovary (CHO) cells. The development of a valid statistical procedure for testing whether the agent in question is mutagenic is complicated by the occurrence of spontaneous mutations, the growth of the cell population during the expression period, and the need to sample the population for replating every two or three days during phenotypic expression.

Our first objective is to develop a statistical model that allows determination of the distribution of the number of mutants finally observed in this type of experiment. We have modeled the process in terms of a sequence of growth periods, interspersed by sampling and replating. We assume the following:

1. Growth of normal and mutant cells is deterministic, with exponential growth rate. For normal cells, $N_t = N_0e^{\alpha t}$, where N_t is the population size at time t; for mutant cells, $e^{\alpha'(t-z)}$ is the number of mutants at time t generated by a single mutation that occurred at time z, $z < t$. (This is more properly regarded as an approximation rather than an assumption, since the number of mutants becomes a continuous random variable.)
2. The number of induced mutations is a Poisson random variable, occurring at the time of exposure.
3. Spontaneous mutations occur randomly in the population with an intensity proportional to N_t.
4. Prior to and after each growth period, there are periods of essentially no growth, during which the mutant population remains unchanged.
5. The sampling process, which occurs during the stable period following each growth period, is such that the number of mutants that are replated is a binominal random variable.

Under these assumptions we have calculated the moment- and cumulant-generating functions for the number of mutants finally observed. These have been used to obtain straightforward (but quite lengthy) formulas for the mean and variance of this random variable. The derivation of the probability distribution itself, while theoretically possible, now appears rather formidable and may have to be computed numerically.

We have also begun to explore an alternative approach based on a branching process model; this model may be more realistic in that "partial" mutants, permitted by assumption 4 above, do not occur. Under this model, the distribution of the number of mutant "descendants" at the end of the growth period arising from a single nonmutant (or mutant) cell alive at the beginning of the period can be easily computed. The total number of mutants in the population at the end of the period is then just the sum of a set of random variables with known distributions, for given mutation rates and growth parameters. Because this formulation lends itself well to computer computation of the final distribution of mutants, we expect to calculate likelihood functions for the parameters of interest (especially the induced mutation rate) for a given set of assay data.

2. Materials Science Applications

S.-J. Chang T. Kaplan[2]
L. J. Gray P. L. Leath[3]
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C. A. Serbin

FINITE ELEMENT METHOD BASED ON THE CREEP-RECOVERY EQUATION

As reported previously,[4] the creep-recovery constitutive equation is formulated to describe the inelastic deformation of metal at elevated temperature. It has the following form:

$$\dot{\underline{\sigma}} = \underline{L}\,\dot{\underline{\epsilon}} - \underline{M} ,$$

where

$\dot{\epsilon}$ = total strain rate,

$$L_{ijkl} = 2G\left(\delta_{ik}\delta_{jl} - \frac{2G}{h+2G}\,\frac{1}{|\nabla f|^2}\,\frac{\partial f}{\partial \sigma_{ij}}\,\frac{\partial f}{\partial \sigma_{kl}}\right) ,$$

$$M_{ij} = \frac{2G}{h+2G}\,\frac{1}{|\nabla f|^2}\,\frac{\partial f}{\partial \sigma_{ij}}\left(\frac{\partial f}{\partial \sigma_{kl}}\,r_{kl} - \frac{d\kappa}{dt}\right) .$$

In this form, it is recognized as a generalization of the classical plasticity model, the difference being additional terms M_{ij} and the new internal variables α, which are governed by the equations of evolution. By implementing these additional terms at each loading step in an existing finite element code for the plasticity model, a finite element code for the creep-recovery model has been established. This program has the advantage of treating both plastic and creep deformation in a unified way.[5]

FORCES ON A DISLOCATION NEAR A CRACK TIP

Forces on an edge dislocation near a crack tip may be computed by the J-integral method. Contours of constant forces are plotted as shown in Fig. 1, where J_2, the force acting in the X_2 direction, tends to move the dislocation along its slip plane. With a strong enough J_2, dislocations are emitted from the crack tip and cause blunting and fracture. It is interesting to note that when the J-integral is expressed in its complex form, the Peach-Koehler equation for dislocations can be derived from the J-integral.

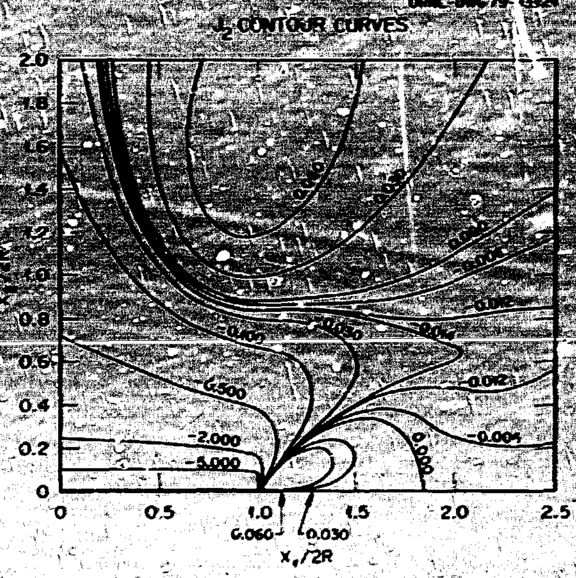

Fig. 1. Contours of constant forces in the X_2 direction on a dislocation with Burgers vector $b_x = 1$.

SELF-CONSISTENT APPROXIMATIONS FOR DISORDERED SYSTEMS

The Coherent Potential Approximation (CPA) is an excellent single-site, self-consistent approximation for disordered solids with simple diagonal disorder. Since the CPA was introduced in 1967, there has been considerable interest in finding extensions of the CPA which would properly include multisite effects and which would be valid for more general types of disorder. Virtually all of the

1. Computer Science Division.
2. Solid State Division.
3. Rutgers University.
4. "A Creep-Recovery Constitutive Equation for the Inelastic Deformation of Metals," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL CSD-34, pp. 14–15 (September 1978).
5. S.-J. Chang and S. K. Iskander, "Finite Element Method Based on the Creep-Recovery Constitutive Equation," p. 264 in *Proceedings of the Second International Conference on Computational Methods in Nonlinear Mechanics*, University of Texas, Austin, Mar. 26–29, 1979.

proposed methods have, unlike the CPA, exhibited unphysical (nonanalytic) behavior; proposed analytic methods have been severely limited in their application.[7]

R. Mills[6] has recently produced an analytic, multisite, self-consistent approximation for the diagonal disorder problem. Mills's theory is intimately related to the augmented space formalism; based on this, we have been able to generalize Mills's method to include off-diagonal disorder. By suitably modifying Mills's proof, we have been able to demonstrate that this method is analytic. Thus, for solids described by independent random variables, an extension of the CPA has been obtained. We are currently investigating the application of this method to systems with short-range order (i.e., dependent random variables).

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6. R. Mills and P. Ratanavararaksa, "Analyticity in Binary Alloys," *Phys. Rev. B* 18, 5291–308 (1978).

7. H. W. Diehl and P. L. Leath, "The Pseudo-Fermion Approach to Binary Disordered Systems," *Phys. Rev. B* 19, 587–95 (1979).

3. Model Development and Evaluation

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E. J. Gray
E. L. Miller, Jr.
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L. R. Shenton
W. A. Thompson, Jr.
V. R. R. Uppuluri
D. G. Wilson

ENERGY MODEL VALIDATION CONCEPTS

In recent years, the development of large, fast computers has made possible not only the modeling of complex physical systems but also the modeling of systems in which human behavior plays a major role. Economic energy models that attempt to forecast the future under various policy alternatives are a prime example. Principally because of the lack of experimental data with which to test their validity, these models often give conflicting results and are surrounded by controversy. The objective "validation" of such models has therefore become a topic of considerable interest.

During the past year, members of the MSRD staff have held a series of informal seminars and discussions on the concept and practice of energy model validation, particularly from a mathematical and statistical viewpoint. As a result of these discussions, a paper[3] was written, with the following objectives:

1. to give a general indication of what "model validation" meant to us, given that experimentation on the economy in the scientific sense is in most cases impossible;
2. to identify, in an organized way, a set of specific questions and activities that we felt were pertinent to model validation; and
3. to indicate the ways in which mathematicians and statisticians could contribute (*a*) in a consulting role for a particular validation study and (*b*) in a research role to develop new techniques for specific validation procedures.

We defined model validation rather broadly as "the application of any procedure designed to evaluate some aspect of the utility of a model or to detect a deficiency in it." To provide a convenient framework for discussion, we broke down the model development and modification process into various components. At the center is "the model," which includes a mental model, a mathematical model, and a set of computer programs. At each point of transition between these components, errors or approximations that affect the model's validity may be made.

For convenience, we distinguished between "passive" validation, which involves the study of the model documentation, and "active" validation, in which the model is run under the control of the validation team. It is absolutely essential for both that the model be well documented, and we listed some standards for this.

Active validation techniques, including program analysis, uncertainty analysis, response surface analysis, and stress analysis are not yet well developed. We concluded that these areas provide the most fruitful opportunities for mathematical and statistical research in model validation methodology.

APPROXIMATE PERCENTAGE POINTS FOR PEARSON DISTRIBUTIONS

The Pearson system of distributions based on the differential equation

$$\frac{1}{y}\frac{dy}{dx} = -\frac{(c+x)}{d+cx+bx^2}$$

includes many well-known densities and has had widespread application as a basis for smoothing experimental data and, perhaps more importantly, as an approximating structure for intractable theoretical distributions for which up to four moments are known.

Having chosen an acceptable approximate Pearson curve, we may like to know its percentiles, at least at a set of values likely to be of interest. In general, accurate assessments of these in standard measure are based on the skewness ($\sqrt{\beta_1}$) and kurtosis (β_2) coefficients and can be determined from

1. University of Georgia.
2. On leave from the University of Missouri.
3. T. J. Mitchell, D. G. Wilson, and others, *Energy Model Validation: Initial Perceptions of the Process*, ORNL CSD-41 (to be published).

the tabulation in Pearson and Hartley[4] or from a lengthy computer program by Amos and Daniel.[5] To avoid 16-point interpolation in the tables, approximate formulas[6,7] have been developed for the 11 commonly used percentages in terms of β_1 and β_2, in the form $\pi_1(\sqrt{\beta_1}, \beta_2)/\pi_2(\sqrt{\beta_1}, \beta_2)$, where $\pi_1(\cdot)$ and $\pi_2(\cdot)$ are bivariate polynomials of degree 3, involving 19 coefficients (the constant in π_2 being unity). The error involved over the defined domain is 0.5% or less.

The eleven levels of α formulas for the deviates of a Pearson distribution, taking into consideration the domains of validity, are much simpler to use than the programmed Amos package or the demanding two-way interpolation in the tables. Interpolation by three-point Lagrange, for a new X given three neighboring (X_α, α) points is quite safe, but the converse (i.e., interpolating for X_α given α) needs a five-point Lagrange formula for safety. The approximations and Lagrange formula may be programmed for a portable programmable computer to produce results with sufficient accuracy for most applications.

As discussed elsewhere in this section, these procedures have been applied to determine confidence intervals for predictions from a model that forecasts energy use under various conservation policies.

EVALUATION OF THE PARAMETERS OF THE JOHNSON SYSTEM OF FREQUENCY CURVES

When the distribution of a statistic is intractable, as is often the case when analyzing a computer model, it may be necessary to use an approximation. The Johnson system of frequency curves is an attractive method of approximation because the variates are transformations of the normal density. The system is defined by

$$z = \gamma + \delta f(y) , \quad z \in N(0, 1) .$$

4. E. S. Pearson and H. O. Hartley, *Biometrika Tables for Statisticians*, vol. 2, Cambridge University Press, New York, 1972.

5. D. E. Amos and S. L. Daniel, *Tables of Percentage Points of Standardized Pearson Distributions*, Report RR-71 0348, Sandia Laboratories, Albuquerque, N.M. (1971).

6. K. O. Bowman and L. R. Shenton, "Approximate Percentage Points for Pearson Distribution," *Biometrika* 66, 147–51 (1979).

7. K. O. Bowman and L. R. Shenton, "Further Approximate Pearson Percentage Points and Cornish-Fisher," *Commun. Stat., Simulation Comput.* B8(3), 231–44 (1979).

One drawback is the difficulty in finding the parameter values, but once the parameters are known, normal percentage points can be used to find the probability levels.

A rational fraction approximation for a function of one of the parameters defining Johnson's S_U system (unbounded) was developed for which the error assessment for a segment of the domain of validity showed remarkable accuracy. Furthermore, the region of validity covered far more than the previously published table.

For the S_B system (bounded) of limited range, there are no explicit solutions for the skewness and kurtosis parameters, $\sqrt{\beta_1}$ and β_2, so that it is quite difficult to calculate the parameters. We have constructed a diagram (Fig. 2) which leads to quite acceptable initial estimates of the parameters γ and δ for the range $0 \leqslant \sqrt{\beta_1} \leqslant 5$ in the S_B domain. These estimates can be improved by iteration in a computer program.

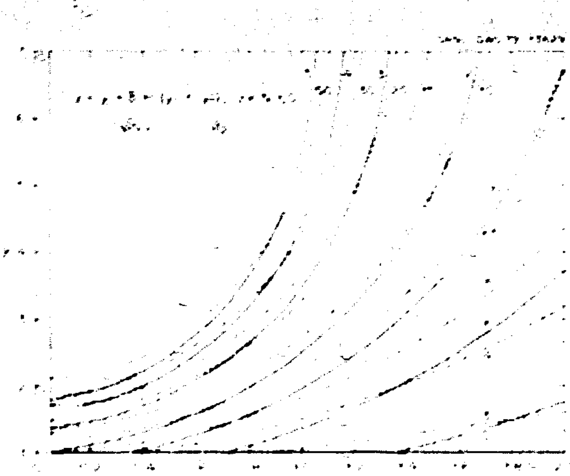

Fig. 2. S_B contour curves $\sqrt{\beta_1}$ and β_2.

CONSTRUCTING CONFIDENCE REGIONS FOR AN ENERGY MODEL

Large computational models are one set of tools used by policymakers to forecast energy use under various policy alternatives. The forecast energy values may be imprecise for various reasons, and thus we embed them in a probability structure. Monte-Carlo simulations of n realizations, based on uncertainty distributions for the model parameters, lead to the forecast energy use values $x_1(t), x_2(t), \ldots, x_n(t)$, where t represents a future time interval. From this sample the skewness b_1 and kurtosis b_2 are calculated.

For $\sqrt{\beta_1}$, β_2 (the population values) in the neighborhood of b_1, b_2, regions of specified probability content are constructed (Fig. 3) using recently developed distribution fitting and estimation procedures. By choosing points on the contour and by using the Pearson 4-moment model as the density, confidence intervals for the projected energy use are found. Finally, the extremum values are used to define an interval in which the projection is likely to fall.

For the purpose of illustration, these procedures have been applied to the construction of confidence intervals for forecasts from the *ORNL* residential energy use model.

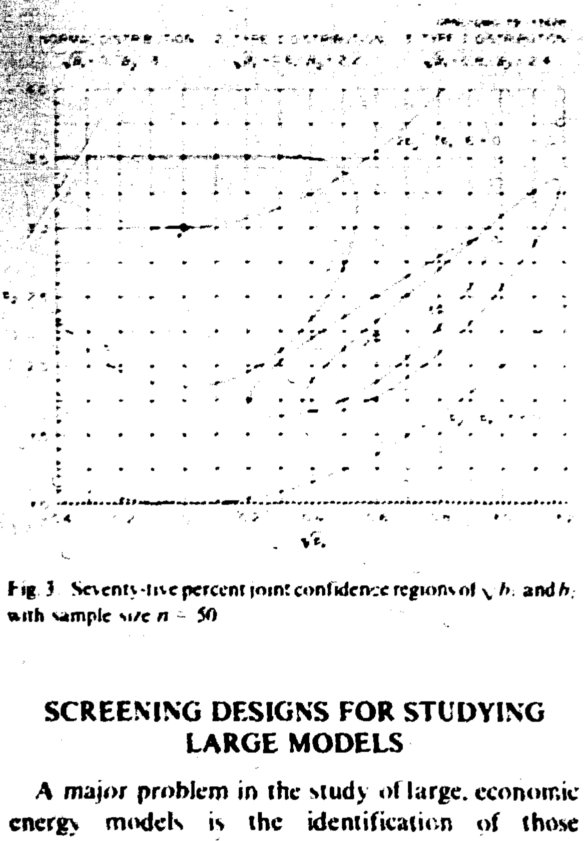

Fig. 3. Seventy-five percent joint confidence regions of $\sqrt{b_1}$ and b_2 with sample size $n = 50$.

SCREENING DESIGNS FOR STUDYING LARGE MODELS

A major problem in the study of large, economic energy models is the identification of those parameters or assumptions that have most effect on the model output. Because there may be hundreds (or even thousands) of such parameters in the model, the use of some sort of screening design is essential.

We have begun a research effort to develop a screening strategy which is more general and potentially more powerful than those now available. Our approach relates to the classical "blood-testing problem"[12] and extends the fundamental early work of Sobel and Groll[13] on this problem.

In the present context, we assume that a single experimental trial is a computer run of the energy model in which some of the variables (parameters or assumptions) in the model have been changed from a "nominal level" to a "test level." It is assumed further that the direction (i.e., positive or negative) of the effect of changing a variable is known but that its magnitude is not known. A variable is either "effective" in the sense that changing it to its test level always results in a change in the model output of at least a certain amount A or is "negligible" in the sense that no combination of changes of such variables can change the model output more than A. The problem is to correctly classify each variable as "effective" or "negligible" in as few runs as possible.

Sobel and Groll gave a recursive method for a sequential strategy that would minimize the expected number of trials to solution. They focused their attention on the special case in which the prior probability that any given variable is negligible is q for all variables. They also considered primarily a simplified class of strategies in which the unresolved variables can always be divided into two sets, exactly one of which is known to contain an "effective" variable. Only variables in one set or the other may be set at their test levels in the next trial; that is, no "mixing" of the sets is allowed.

Our extension of this work does not require q to be the same for all variables, nor does it prohibit mixing. We should therefore be able to take advantage of prior information about the model. We use an "information criterion," which was suggested by Sobel and Groll as a promising alternative to their principal strategy. The object is to minimize at each trial the "entropy" E, where $E = -\sum[p_i \log_2 p_i + (1 - p_i)\log_2(1 - p_i)]$; p_i is the current probability of the

8. K. O. Bowman and L. R. Shenton, "Notes on the Distribution of $\sqrt{b_1}$ in Sampling from Pearson Distributions," *Biometrika* **60**, 155–67 (1973).

9. K. O. Bowman, "Power of the Kurtosis Statistic (b_2) in Test of Departure from Normality," *Biometrika* **60**, 623–28 (1973).

10. L. R. Shenton and K. O. Bowman, "A Bivariate Model for the Distribution of $\sqrt{b_1}$ and b_2," *J. Am. Stat. Assoc.* **72**, 206–11 (1977).

11. E. Hirst and J. Carney, *The ORNL Engineering-Economic Model of Residential Energy Use*, ORNL/CON-24 (July 1978).

12. R. Dorfman, "The Detection of Defective Members of Large Populations," *Ann. Math. Stat.* **14**, 436–40 (1943).

13. M. Sobel and P. A. Groll, "Group Testing to Eliminate Efficiently All Defectives in a Binomial Sample," *Bell Syst. Tech. J.* **38**, 1179–252 (1959).

ith state (i.e., a particular classification of all variables as effective or not), and the summation is over all states. It is easily shown that, for a given run, this will be achieved if the current probability (based on combining the prior probability with information from runs made so far) that none of the variables set at their test levels are effective is as close as possible to 0.5.

We are currently writing a computer algorithm to implement the sequential experimental strategy based on this information criterion. We expect it to be able to handle a much larger number of variables than the methods now available. This capability will be essential for energy model applications. We are hopeful that these procedures will also prove useful for a much wider variety of experimental situations.

4. Moving Boundary Problems

C. A. Serbin   A. D. Solomon   D. C. Wilson

Research on moving boundary problems has progressed on three fronts: numerical techniques, analytical approximations, and information organization. Work on numerical techniques has centered on the development and study of numerical methods for solving moving boundary problems with other than Dirichlet boundary conditions and for solving problems in more than one space variable.

The weak solution method, involving a smudging of the moving boundary, was extended to treat a phase-change problem with a flux or convective heat input boundary condition. In the discrete version of the latter problem, the thermal energy of the system is conserved. Conditions at the boundary are determined with high accuracy by an extrapolation technique. Although a precise error analysis is lacking, results seem quite satisfactory.

For multidimensional phase-change problems, an implicit version of the weak solution method was derived and used to simulate three-dimensional processes. This work is still in a preliminary state, but preliminary results indicate that the scheme is worthy of further study.

Extending previous results, analytical expressions were obtained for the solution of the classical two-phase problem of Neumann for the semi-infinite slab[3] and for the behavior of a semi-infinite slab melting as a result of convective heat input at its fixed boundary.[4]

A selective bibliography, including a keyword index, on moving boundary problems has been assembled and will appear as a Computer Sciences Division technical report. This bibliography, which surveys literature in theory, methods, and applications, is limited mainly to references that have appeared since the publication of Rubenstein's book on the Stefan problem.[5]

1. A. Solomon, "On a Phase-Change Process with a Convective Boundary Condition," in preparation.

2. A. Solomon, "Melt Time and Heat Flux for a Simple PCM Body," *Solar Energy* 22, 251–57 (1979).

3. A. Solomon, "An Easily Computable Solution to a Two-Phase Stefan Problem," *Solar Energy*, submitted.

4. A. Solomon, "A Relation Between Surface Temperature and Time for a Phase-Change Process with a Convective Boundary Condition," *Lett. Heat Mass Transfer* 6, 192–200 (1979).

5. L. I. Rubinstein, *The Stefan Problem, Translations of Mathematical Monographs*, vol. 27, American Mathematical Society, Providence, R.I., 1971.

5. Multivariate Multipopulation Classification

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J. J. Beauchamp
J. E. Folkert[1]
K. Frankowski[2]
V. E. Kane
M. Jaeger[3]
D. S. Robson[4]
C. A. Serbin
M. Sobel[5]
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V. R. R. Uppuluri

THE EFFECT OF LOGARITHMIC TRANSFORMATION ON THE PROBABILITY OF MISCLASSIFICATION

The discriminant function has many desirable and optimal properties when it is used to classify an observation as coming from one of two underlying parent populations. However, very little work has been done to evaluate the effect of data transformation on the discriminant function. The probability of misclassifying an observation as coming from one of two populations, using the discriminant function, has been evaluated for the case when it is known that the observed random variables are lognormally distributed. The misclassification probabilities have been evaluated under the incorrect assumption that the observed random variables are normally distributed and also evaluated after applying the appropriate log transformation. The difference between the corresponding probabilities of misclassification has been used as a measure of the effectiveness of the transformation. Different combinations of the underlying population parameters have been considered to allow for comparisons in terms of population separation and relative population abundance. Figures 4 and 5 show vividly the effect of the correct transformation: $\Delta P(1|2)$ and $\Delta P(2|1)$ are the changes in the conditional probabilities of misclassification, $\Delta P(e)$ is the change in the overall probability of misclassification, Π_1 and Π_2 are the relative population abundances, and μ and σ are parameters of the underlying population distributions. We concluded that overall probability of

1. Hope College.
2. University of Minnesota.
3. University of Chicago.
4. Cornell University.
5. University of California, Santa Barbara.
6. Memphis State University.

ORNL-DWG 78-22475

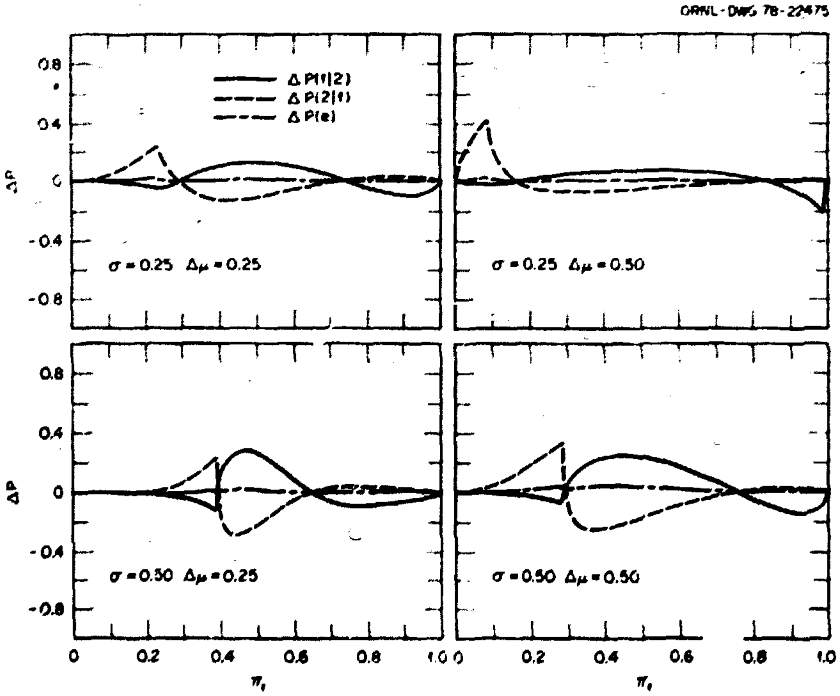

Fig. 4. $\Delta P(1|2)$, $\Delta P(2|1)$, and $\Delta P(e)$ as functions of π_1 for different values of $\Delta\mu$ and σ.

ORNL-DWG 78-22476

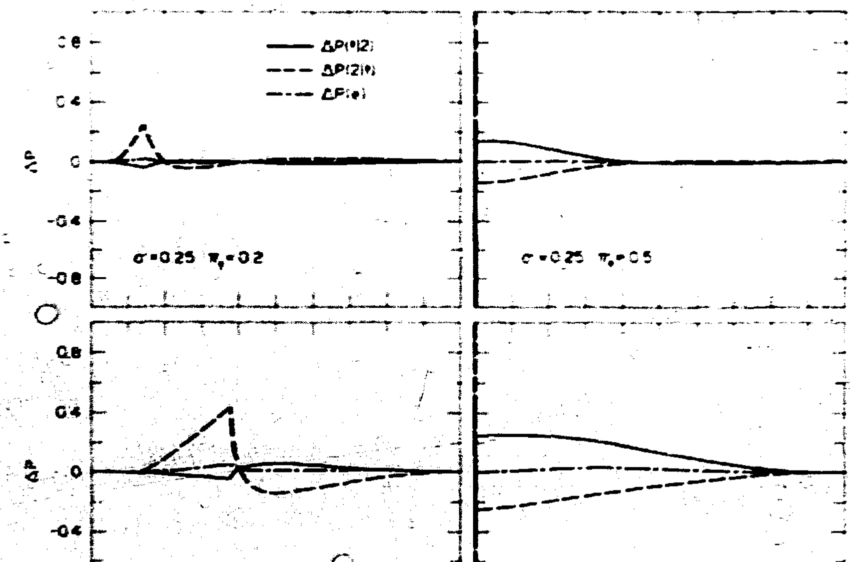

Fig. 5. $\Delta P(1|2)$, $\Delta P(2|1)$, and $\Delta P(e)$ as functions of $\Delta\mu$ for different values of π and σ

misclassification is relatively insensitive to drastic departures from optimality in the conditional probabilities of misclassification and that the overall probability of misclassification may not be an effective objective function for selecting a discrimination procedure.

APPROXIMATING MISCLASSIFICATION PROBABILITIES FOR FISHER'S QUADRATIC DISCRIMINANT FUNCTION

Fisher's quadratic discriminant function is used to discriminate between two bivariate normal populations with unequal convariance matrices. However, the theoretical misclassification probabilities are not easily obtained because knowledge of the distribution of a linear combination of noncentral chi-square random variables is required.

When the bivariate normal populations have covariance matrices that differ only by a scalar multiple, several approximations to the distribution of the sum of noncentral chi-square random variables are available. For the more general structure of the covariance matrices, it is necessary to find an approximation to the distribution of the difference of two noncentral chi-square random variables. Two methods for approximating this distribution are under investigation: (1) Pearson curves and (2) Laguerre series approximations.

The first approximation uses the skewness and kurtosis of the difference of noncentral chi-square random variables to select one of the Pearson curves as the approximating distribution. The misclassification probabilities can then be obtained from the percentage points of the approximating distribution. The second method first approximates the noncentral chi-square random variables with central chi-square random variables by matching the first two or three moments. The distribution of the difference of central chi-square random variables is then partitioned into a negative part, which can be evaluated exactly, and into a positive part, which is approximated with Laguerre polynominals.

THE THREE-PARAMETER LOGNORMAL DISTRIBUTION

The lognormal distribution is commonly encountered in applied statistics and is appropriate for data associated with many classification problems. In the three-parameter lognormal distribution, $Y = \log(x - \gamma)$ has a normal distribution with unknown mean μ and variance σ^2, where x is the observed data and γ is an unknown shift parameter. The estimation of γ by the standard maximum likelihood approach is not possible because the maximized likelihood is infinite. Computation of local maxima is the general approach, but nonstandard numerical optimization is necessary.

An alternative optimization function is the weighted order statistic

$$W(\gamma) = \frac{\left| \sum_{i=1}^{n} a_i \log(x_i - \gamma) \right|}{\sum_{i=1}^{n} \left| \log(x_i - \gamma) - n^{-1} \sum_{j=1}^{n} \log(x_j - \gamma) \right|^2} ,$$

where $x_1 \leq x_2 \leq \ldots \leq x_n$ and where the a_i's are known constants such that $a_i = -a_{n-i+1}$, $\Sigma a_i = 0$, and $\Sigma a_i^2 = 1$. The statistic $W(\gamma)$ for a fixed γ is a goodness-of-fit statistic for the normal distribution where different choices of the a_i's correspond to various tests. For example, the a_i's corresponding to the normalized expected order statistics yield a form of $W(\gamma)$ equivalent to Shapiro-Francia test for normality. The "closer" $\log(x_i - \gamma)$ is to a_i, the "closer" the x_i's are to a normal distribution.

It has been determined that $W(\gamma)$ provides estimates of γ that are similar to the local maximum likelihood estimates but are much easier to compute. Several standard methods performed poorly when compared to $W(\gamma)$. We have shown that many estimation procedures produce estimates of γ that become negatively biased as σ becomes small. Most of the estimation procedures were found to be robust with respect to heavy-tailed distributions and right-tail outliers.

LIMITING VALUES OF VARIOUS FUNCTIONS TO BE OPTIMIZED IN ACHIEVING NORMALITY

Before using many classification procedures, it is often necessary to transform the data. In an earlier report,[7] different objective functions were proposed to estimate the parameters of the power transformation, $y = (x + c)^p$. The objective functions of particular interest were (1) likelihood function, (2) weighted-order statistic function, and (3) sample skewness-kurtosis function. The optimization of these functions was iterative and presented convergence problems for some of the data sets investigated. Therefore, an analysis of the limiting values of these objective functions was performed for the two cases $c \to \infty$ and $c \to -x_{(1)}$, where $x_{(1)}$ is the first-order statistic from a sample.

Let L denote the log-likelihood function of the observed sample, assuming c and p exist such that the observed data may be transformed to approximate normality. If L_{max} is the maximum of L for a given c and p, then the limiting value of L_{max} as $c \to -x_{(1)}$ was found to range from $+\infty$ to $-\infty$ depending on the value of p, with $p = 1$ yielding the only finite limit. The limiting value of L_{max} as $c \to \infty$ was found to be finite and independent of the value of p.

Let T represent a weighted-order statistic of the form $T = N/D$, where

$$N = \left| \sum_{i=1}^{n} a_i (x_i + c)^p \right|^2 ,$$

$$D = \sum_{i=1}^{n} \left| (x_i + c)^p - n^{-1} \sum_{j=1}^{n} (x_j + c)^p \right|^2 ,$$

and the a_i's are known constants satisfying $\Sigma a_i = 0$ and $\Sigma a_i^2 = 1$. The limiting values of T as $c \to -x_{(1)}$ was found to be finite but dependent on whether $p > 0$ or $p < 0$. For $p < 0$, the limiting value was actually found to be the minimum value of T. As $c \to \infty$, the limiting value of T was found to be equivalent to the value of T with $c = 0$ and $p = 1$, that is, the value of T using the original untransformed data.

The sample skewness-kurtosis function was taken to be

$$B = \left\{ \frac{[\sqrt{b_1} - E(\sqrt{b_1})]^2}{\mathrm{Var}(\sqrt{b_1})} + \frac{[b_2 - E(b_2)]^2}{\mathrm{Var}(b_2)} \right\}^{1/2} ,$$

where $\sqrt{b_1}$ and b_2 are the sample skewness and kurtosis, respectively, of $y_i = (x_i + c)^p$. For this function

$$\lim_{c \to \infty} B = B_x ,$$

where B_x is the value of the skewness-kurtosis function defined from the untransformed ($c = 0$, $p = 1$) data. The analysis of the limit of B showed that this limit was finite if $p > 0$ but was a function of the sample size n if $p < 0$.

---

7. "Transformation to Normality," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL/CSD-34, p. 4 (September 1978).

All of these results have provided a better understanding of the difficulties inherent in estimating the parameters c and p.

INCOMPLETE DIRICHLET INTEGRALS OF TYPE II

This work is a continuation of previous work on incomplete Dirichlet integrals of type I.[8] Dirichlet distributions are multivariate distributions which have proven to be useful for several problems. For instance, incomplete Dirichlet integrals of type II arise when the problem is to find a distribution with the largest variance, given samples from k normal distributions.

These integrals occur naturally in the context of waiting time problems when sampling from multinomial distributions, and they also appear in the study of the distributional properties of the extrema of gamma-distributed random variables. Work to organize the applications and a set of tables on these integrals is in progress.

Let

$$f(x_{j+1}, \ldots, x_b) = \frac{\prod_{\alpha=j+1}^{b} x_\alpha^{r-1}\, dx_\alpha}{(1 + ja + x_{j+1} + \ldots + x_b)^{m+br}} ,$$

$$x_\alpha > 0 , \; a > 0 .$$

The generalized incomplete Dirichlet integrals of type II are defined by

$$C_a^{(b,j)}(r, m) = \frac{\Gamma(m + br)}{\Gamma(m)\Gamma^b(r)} \left(\frac{a^r}{r} \right)^j$$

$$\times \int_0^a \cdots \int_0^a f(x_{j+1}, \ldots, x_b) \prod_{\alpha=j+1}^{b} dx_\alpha ,$$

and

$$D_a^{(b,j)}(r, m) = \frac{\Gamma(m + br)}{\Gamma(m)\Gamma^b(r)} \left(\frac{a^r}{r} \right)^j$$

$$\times \int_a^\infty \cdots \int_a^\infty f(x_{j+1}, \ldots, x_b) \prod_{\alpha=j+1}^{b} dx_\alpha .$$

We are interested in $C_a^{(b)}(r, m)$ and $D_a^{(b)}(r, m)$, which are given by the above equations when $j = 0$. These integrals appear in numerous problems and may be considered as multivariate extensions of incomplete Γ-integrals. To compute these integrals, recursion formulas, together with the appropriate boundary conditions, were used.

The boundary conditions for $D_a^{(b)}(r, m)$ consisted of only positive terms, and thus the computation was straightforward. However, for $C_a^{(b)}(r, m)$, the presence of negative terms in the analogous boundary conditions was causing loss of accuracy. This problem was solved by introducing a new function $C^*_a(r, m)$, where $C^*_a(r, m) = C_a(r, m)$ and $C^*_a(r, m)$ satisfies a recurrence relation with boundary conditions involving additions of positive terms.

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8. D. B. Owen and R. E. Odeh, *Selected Tables in Mathematical Statistics*, Vol. IV, American Mathematical Society, Providence, R.I., 1977.

6. Numerical Linear Algebra

R. E. Funderlic J. E. Rall[2]
A. W. Geise[1] D. S. Scott
R. C. Ward

LANCZOS ALGORITHM SOFTWARE

Many applied problems can be reduced to finding a few eigenvalues $\{\lambda_i\}$ and corresponding eigenvectors $\{x_i\}$ of the eigenproblem

$$(\mathbf{A} - \lambda\mathbf{B})x = 0 ,$$

where both **A** and **B** are large sparse symmetric matrices and **B** is positive definite. The Lanczos algorithm is a powerful technique for solving such problems, and selective orthogonalization[3] is a viable method of maintaining stability in the algorithm.

We have developed high-quality, fully portable software which implements the block Lanczos algorithm with selective orthogonalization to solve two classes of eigenvalue problems. In one code, the user specifies the number of eigenvalues desired while in the other code the user specifies a desired interval. It is anticipated that these codes will be placed in the National Energy Software Center for general distribution as soon as testing is completed. Preliminary testing indicates that these codes offer substantial savings over currently used techniques.

We are also investigating the use of the Lanczos algorithm in conjunction with a shift and invert strategy to extract eigenvalues from a sequence of subintervals. Software development has begun, and preliminary results are quite encouraging.

THE LANCZOS ALGORITHM FOR LINEAR EQUATIONS

The conjugate gradients algorithm (*cg*) is often used to find approximate solutions to sets of linear equations

$$\mathbf{A}x = b ,$$

where **A** is a large sparse symmetric matrix. Unfortunately, *cg* is potentially unstable if **A** is indefinite (has both positive and negative eigenvalues). An alternative algorithm[4] derived from the relationship between *cg* and the Lanczos algorithm is stable for indefinite **A** but requires more storage and more arithmetic operations than does *cg*.

It is possible to use the Lanczos algorithm directly to solve symmetric sets of linear equations. This requires that a sequence of vectors be stored on disk and recalled once to form the solution vector, but otherwise it is equivalent to *cg* in both storage and work.

There are three definite advantages to the Lanczos approach:

1. **A** may be indefinite without instability.
2. The condition number of **A** can often be estimated reliably.
3. It is possible to use the stored vectors to obtain good starting approximations to other equations with the same matrix **A**.

A potential advantage of the Lanczos approach is the use of selective orthogonalization[3] to maintain orthogonality among the computed vectors.

Preliminary studies have shown that there are no difficulties in implementing the algorithm. Indeed, with clever coding it is possible to reduce the required core storage to less than that needed for *cg*. However, further study will be needed to determine whether the advantages of this approach outweigh the difficulties involved in using secondary store.

PRECONDITIONING THE GENERALIZED EIGENVALUE PROBLEM

In a previous report,[5] we have presented an outline of a three-step algorithm for preconditioning the matrices **A** and **B** to be used in conjunction with a *QZ*-type algorithm for solving the generalized eigenvalue problem $\mathbf{A}x = \lambda\mathbf{B}x$. The details of the

1. Great Lakes Colleges Association student, Lawrence University.
2. Oak Ridge Associated Universities.
3. B. N. Parlett and D. S. Scott, "The Lanczos Algorithm with Selective Orthogonalization," *Math. Comput.* **33**, 217–38 (1979).
4. C. C. Paige and M. A. Saunders, "Solution of Sparse Indefinite Systems of Linear Equations," *SIAM J. Numer. Anal.* **12**, 617–29 (1974).
5. "Scaling the Generalized Eigenvalue Problem," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL/CSD-34, pp. 7–8 (September 1978).

algorithm have been completed; a code has been developed; and many random, pathological, and pedagogical sets of matrices have been tested.

The heart of the algorithm involves scaling submatrices of **A** and **B** such that the magnitude of each of their elements is as close as possible to unity. This scaling is appropriate when the relative errors of the elements are equal in magnitude. Alternative scaling methods to equalize the magnitude of the errors should be used when this condition is not met. The scaling is accomplished by solving a consistent, singular system of linear equations by the generalized conjugate gradient method.[6] The initial guess is the solution to the system when **A** and **B** contain only nonzero elements. Unless the matrices are extremely sparse or pathological, the iterative scheme converges within three or four iterations.

The following observations can be drawn from the test results:

1. Tremendous improvement in the accuracy of the eigenvalues is possible when the eigenvalues have widely varying magnitudes or when there is a large difference between the matrix norm and the diagonal elements of the triangularized matrix resulting from the *QZ* algorithm.

2. In any of the test cases, none of the eigenvalues corresponding to the preconditioned matrices were significantly less accurate than those of the original matrices.

3. The third step of the preconditioning algorithm grades the scaled **B** submatrix; this step can markedly improve the accuracy of the eigenvalues with large magnitudes and thus should be included regardless of the scaling method employed.

4. The total number of *QZ* iterations required to converge to the eigenvalues is usually reduced. In fact, the savings in computer time executing the *QZ* algorithm will normally offset the cost of the preconditioning algorithm.

INTERACTIVE LEAST SQUARES

An interactive program INVAR has been developed for solving nonlinear least squares problems. Designed for use from a remote computer terminal, the program provides the user with on-line feedback and the opportunity to make changes or corrections during execution of the program. INVAR is especially designed for use by people with a minimal knowledge of Fortran programming.

The least squares method used is based on mathematical work of Golub and Pereyra[7] and the Stanford University computer program VARPRO. The method takes special advantage of the structure of the model equation by treating the unknown parameters as "linear" or "nonlinear," depending on how they appear in the model. Initial estimates need be provided only for the nonlinear parameters. A wide variety of statistical options and simple on-line plots are available. A user's manual is in preparation.

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6. Paul Concus, Gene H. Golub, and Dianne P. O'Leary, *A Generalized Conjugate Gradient Method for the Numerical Solution of Elliptic Partial Differential Equations*, STAN-CS-75-533, Stanford University, Stanford, Calif., 1976.

7. G. H. Golub and V. Pereyra, "The Differentiation of Pseudo-Inverses and Nonlinear Least Squares Problems Whose Variables Separate," *SIAM J. Numer. Anal.* 10, 413–32 (1973).

7. Risk Analysis

R. E. Funderlic   W. A. Thompson, Jr.[1]

COMPETING RISK PRESENTATION OF REACTOR SAFETY STUDIES

When a new, potentially dangerous technological change such as an airport, highway, or nuclear power plant is contemplated for a community, a rational approach should weigh the advantages and disadvantages before a decision is made. One of the disadvantages is that accidents may cause fatalities. How can we quantify this risk? It may be of some value to distinguish a subtopic of risk analysis which we might call safety analysis. The statistical discipline of competing risks may be a proper framework within which to analyze this subset of problems.

Competing risk theory hypothesizes a number of risks (diseases, accidents, etc.) which compete for the lives of individuals. For each individual, one of these risks will "win out," and the individual will die from that risk. The theory then attempts to predict the consequence of removing or adding a risk. For example, what would be the effect on life expectancy if a cure for smallpox were found? Similarly we might ask, what would be the effect on life expectancy if 100 atomic power plants were added to the community?

From Wash-1400, the Reactor Safety Study (1975),[2] if 100 nuclear power plants are introduced and nuclear accident is the only risk, the individual early fatality probability per year is 2×10^{-10}. Table I summarizes the competing risk presentation of the Reactor Safety Study as it concerns early fatality risk. Looking at life expectancy seems to be an effective way of quantifying this kind of risk.

1. On leave from the University of Missouri
2. U.S. Nuclear Regulatory Commission, *Reactor Safety Study. An Assessment of Accident Risks in U.S. Commercial Nuclear Power Plants*, WASH-1400 (October 1975).

A THRESHOLD DOSE-RESPONSE MODEL

Consider the following threshold model as biological motivation for the choice of a relation between dose and response:

1. An organism might or might not respond to dose x.
2. The organism has a large number of critical targets.
3. Each target has a dose threshold.
4. A single target response results in organism response.
5. Thresholds of targets are randomly chosen from some distribution.

Thus $q(x)$, the probability of organism nonresponse, is the probability that the minimum target threshold exceeds the dose, and hence a Weibull relation

$$q(x) = \begin{cases} \exp\left[-\left(\dfrac{x-\beta}{\alpha}\right)^{\gamma}\right], & x > \beta \\ 1, & x \leq \beta \end{cases}$$

is indicated. The parameters have the following interpretations: α is a scale parameter; β is an organism threshold because if dose is less than β, then response has probability 0; and γ is the "order of contact" of $p(x)$ at $x = \beta$ since

$$\lim_{x \to \beta+} p(x) \Big/ \left(\frac{x-\beta}{\alpha}\right)^{\gamma} = 1 \, .$$

The Weibull model seems to fit data equally as well as the traditional probit and logit models but no better.

Table I. Probabilities of eventual death from different competing risks

	All risks but nuclear	All risks but nuclear and motor vehicle	All risks	
			$\lambda = 2 \times 10^{-10}$	$\lambda = 10^{-6}$
Other	0.976	1.0	0.976	0.976
Motor vehicle	0.024	0.0	0.024	0.024
Nuclear	0.0	0.0	10^{-8}	7×10^{-5}
Life expectancy (years)	72.8	73.6	72.8 (−18 sec)	72.8 (−1 day)

8. Complementary Areas

S. A. Patil[1]   V. R. R. Uppuluri

SAMPLING PROPORTIONAL TO RANDOM SIZE

Let $X_1, X_2, \ldots, X_N$ be N nonnegative independent identically distributed random variables. Let $Y_1 = X_\alpha$ with probability $X_\alpha/(X_1 + \ldots + X_N)$, $\alpha = 1, 2, \ldots, N$. This is referred to as the first realization when sampling with probability proportional to size. Next, Y_1 is deleted from $X_1, X_2, \ldots, X_N$, and another observation Y_2 is made similarly. It is of interest to find the distributional properties of the sequence $Y_1, Y_2, \ldots, Y_n$ $(n \leq N)$. These properties are used by Barouch and Kaufman[2] to estimate recoverable oil resources. Such a model could also be used to predict the decline in the expected size of discovery as a resource base is depleted.

By direct methods, the distributional properties of $(Y_1, Y_2, \ldots, Y_n)$ are derived when the resource variables X_α have a gamma distribution. General results when the distribution of X_α is arbitrary were also obtained. For prediction purposes, Barouch and Kaufman utilized the formulae for the conditional expectation of Y_n given the whole past $Y_1, Y_2, \ldots, Y_{n-1}$. In the general case, we have derived the conditional Laplace Transform of Y_n given the immediate past Y_{n-1} using the joint and marginal properties of Y_n and Y_{n-1}. From this, the conditional moments of Y_n given the immediate past Y_{n-1} are obtained. In the special case of a gamma distribution for X_α, the conditional expectation of Y_n given Y_{n-1} is shown to be a ratio of two computable, one-dimensional integrals. There is a need to apply the general formulae for conditional moments when X_α has a lognormal distribution and to compare this with the work of Barouch and Kaufman. A paper containing these results is in preparation.

---

1. Tennessee Technological University.

2. E. Barouch and G. M. Kaufman, "Estimation of Undiscovered Oil and Gases," pp. 77–91 in *Mathematical Aspects of Production and Distribution of Energy*, P. D. Lax, Ed., American Mathematical Society, Providence, R.I., 1977.

Part B. Statistical and Mathematical Collaboration

The Mathematics and Statistics Research Department collaborates with many divisions of ORNL and other UCC ND and DOE installations. Triannually, the individual mathematicians and statisticians report major collaborations, which are summarized in Table 2 by division or installation for the calendar year 1978. Only a sample of these activities are included in this part of the report.

Table 2. Tabulation of major collaborations by mathematicians and statisticians during calendar year 1978

Division or installation	Total
Biology, ORNL	33
Metals and Ceramics, ORNL	22
Environmental Sciences, ORNL	20
Y-12 Plant	15
Energy, ORNL	10
Computer Sciences	8
Engineering Technology, ORNL	8
Institute for Energy Analysis, ORAU	8
Uranium Resource Evaluation Project	8
Solid State, ORNL	7
Analytical Chemistry, ORNL	5
Health and Safety Research, ORNL	5
Chemistry, ORNL	2
Chemical Technology, ORNL	2
Employee Relations	2
National Oceanic and Atmospheric Administration	2
Nuclear Regulatory Commission	2
Security	2
Department of Energy, Washington, D.C.	1
Engineering	1
Engineering Physics, ORNL	1
Gas Centrifuge Project Office	1
Oak Ridge Associated Universities	1
Paducah Gaseous Diffusion Plant	1

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9. Biology

C. K. Bayne	V. E. Kane	D. C. Topping
J. J. Beauchamp	J. P. Klein	J. S. Trent
G. A. Bingham	E. Leach	R. L. Ullrich
K. O. Bowman	T. J. Mitchell	R. A. Wallace
N. K. Clapp	P. Nettesheim	D. A. Wolf
D. G. Gosslee	J. P. O'Neill	T. Yarita
J. M. Holland	J. B. Storer	

EPIDERMAL CARCINOGENICITY OF COMPOUNDS IN MICE

The experimental program for testing the carcinogenicity of chemical compounds applied to the skin of mice is continuing in the Biology Division of ORNL. Initial statistical analyses for this assay have been reported.[3,4] New experiments, designed by utilizing statistical methods to optimally allocate mice to treatment groups, are in progress, and the development of methods of statistical analysis is continuing.

An approximation to the variance of the Weibull parameter[5] related to dose was derived. This variance was important in the optimal allocation of mice among dose groups because it is a function of the number of tumors observed and, therefore, a function of dose. Thus, it was possible to allocate animals so that the expected variance of the estimate of the response parameter was minimized.

In addition, this variance was used to obtain improved estimates of the parameters in the dose-response regressions. These parameters were estimated by weighted least squares, utilizing optimum weights that were proportional to the inverse of the respective variances.

The new experiments included additional compounds under test using an additional strain of mice and more than two dose levels of each compound. The added dose levels made it possible to introduce nonlinearity into the regression model and to test the assumption of linearity of the dose-response function.

1. Biology Division.

2. University of Missouri.

3. "Epidermal Carcinogenicity of Compounds in Mice," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL/CSD-34, p. 29 (September 1978).

4. J. M. Holland, D. G. Gosslee, and N. J. Williams, *Epidermal Carcinogenicity of Bis(2,3-epoxycyclopentyl)ether, 2,2-Bis(p-glycidyloxyphenyl)propane, and m-Phenylenediamine in C3H and C57BL/6 Inbred Male and Female Mice*, ORNL-5375 (March 1978).

5. J. M. Holland, D. G. Gosslee, and N. J. Williams, "Epidermal Carcinogenicity of Bis(2,3-epoxycyclopentyl)ether, 2,2-Bis(p-glycidyloxphenyl)propane, and m-Phenylenediamine in Male and Female C3H and C57BL/6 Mice, *Cancer Res.* **39**, 1718–25 (1979).

LOW-LEVEL RADIATION STUDY

The application of some statistical techniques to the problem of identifying suitable parametric models for the survival distributions and for the time-of-occurrence distributions for specific diseases in mice irradiated during a large multidose study was summarized in a previous report.[6] During the past year, a piecewise exponential model was considered instead, because the lack of fit associated with the common parametric models was statistically significant. This new model is much more flexible because it contains more parameters but can still be estimated with good precision.

The force of mortality in a given group was assumed to be an unknown constant μ_i for each age interval $(t_i, t_{i+1}]$, $i = 1, 2, \ldots, m$. The likelihood function for μ_i is then proportional to $\mu_i^{d_i} \exp(-\mu_i T_i)$, where d_i is the number of deaths in the interval and T_i is the number of days lived by all animals in the interval. Using a Bayesian philosophy, interferences about μ_i and functions of μ_i (e.g., the survival distribution) can be made by combining the likelihood function with a prior distribution $P(\mu_i)$ to form the posterior distribution of μ_i. The improper "noninformative" prior $P(\mu_i) = \mu_i^{-1}$ was chosen. The Bayesian analysis provided estimates for the survival function $S(t)$ = probability (lifetime exceeds t), μ_i, log μ_i, and mean survival time. Estimates of precision for these quantities were obtained from the standard deviations or from the percentiles of the corresponding posterior distribution.

This analysis was conducted for ten dose groups (0–400 rads) of RFM female mice exposed to gamma

6. "Low-Level Radiation Study," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL/CSD-34, pp. 30–31 (September 1978).

rays at 45 rads min. Age intervals of 25 days were chosen. Tables and graphs showing the force of mortality, log force of mortality, and survival probability as functions of time were constructed for each dose group, as well as the relative force of mortality compared to the control (zero-dose) group. Weighted regression analyses were also conducted to relate mean survival and force of mortality to dose.

A similar set of analyses was conducted for mortality from all causes except thymic lymphoma, and again for all causes except thymic lymphoma and ovarian tumors. These analyses were done to determine whether the observed influence of radiation dose on mortality could be accounted for by these diseases alone. For these analyses, the counting of d_i and T_i in each interval was complicated by missing data in animals that were grossly necropsied or not necropsied at all. Adjustments were made to remove this source of bias.

TEMPORAL ADVANCEMENT OF CARCINOGENESIS IN AGING MICE

Diethylnitrosamine (DEN) was administered in the drinking water of female mice of three age groups in order to examine the effect of aging on carcinogenesis.[7,8] Tumor incidence and survival were the major measurements analyzed. The incidence of tumors was analyzed by standard statistical methods based on the binomial distribution. The distributions of survival times were summarized by quartiles, and preliminary tests were made using a nonparametric test of significance for medians. To account for censoring, a nonparametric method originated by Breslow[9] was used. The Breslow statistic was computed using an algorithm described by Hoel and Walburg.[10] The test was calculated on the number of days to death following initiation of treatment for tumor-bearing animals, while the censored observation was the corresponding days to death for non-tumor-bearing animals. These analyses quantified the mortality distributions due to tumors and established the significance of the effect of DEN to induce tumors more rapidly in older mice than in younger mice.

EFFECT OF RETINOIDS ON TUMOR DEVELOPMENT IN TRACHEAS OF HAMSTERS

Previous studies have suggested (inconclusively) that vitamin A compounds (retinoids) may be able to inhibit the development of chemically induced respiratory tract cancers. An investigation of this problem was conducted recently by ORNL biologists using the tracheal tumor induction system in hamsters, with *N*-nitroso-*N*-methylurea (NMU) as carcinogen. Two different retinoids, 13-*cis*-retinoic acid and Roll-1430, were used in this study. Hamsters were intratracheally exposed either 18, 20, or 23 times to 1% NMU before the retinoids were administered in the diet. There were six different retinoid-treated groups, distinguished by different NMU exposures, types of retinoid, and concentrations of retinoid. There were also three control groups, one at each level of NMU exposure.

An odds-ratio analysis[11] was conducted to estimate the risk of death from tracheal tumors for retinoid-treated hamsters, relative to control. This approach took into account death from other causes, which would otherwise bias the results. In all four groups treated with Roll-1430, the relative risk was less than 1, although the deviation from 1.0 was not statistically significant in any of them, even at the 0.2 level of significance. This lack of significance may have been due to the modest size of the experiment and the degree of intercurrent mortality, which resulted in fairly large standard errors for the relative risks. The two groups treated with 13-*cis*-retinoic acid showed an increased relative risk, statistically significant at the 0.10 level in both cases.

Similar analyses were done excluding animals that died during the first 4, 8, or 12 weeks because of the possibility that animals dying early after the start of retinoid therapy were not treated long enough to show an effect. However, the results did not differ substantially from those of the main analysis.

An analysis of the risk of mortality from all causes (not just tracheal tumors) gave similar results; the

7. N. K. Clapp, E. H. Perkins, W. C. Klima and L. H. Cacheiro, "Temporal Advancement of Diethylnitrosamine Carcinogenesis in Aging Mice," *Biol. Div. Annu. Prog. Rep. Sept. 30, 1978*, ORNL-5496, p. 67 (February 1979).

8. N. K. Clapp, E. H. Perkins, W. C. Klima, and L. H. Cacheiro, "Temporal Advancement of Diethylnitrosamine Carcinogenesis in Aging Mice," *Cancer Res.*, submitted.

9. N. Breslow, "A Generalized Kruskal-Wallis Test for Comparing *k* Samples Subject to Unequal Patterns of Censorship," *Biometrika* **57**, 579–94 (1970).

10. D. G. Hoel and H. E. Walburg, Jr., "Statistical Analysis of Survival Experiments," *J. Natl. Cancer Inst.* **49**, 361–72 (1972).

11. "Likelihood Inference for the Log Odds Ratio in Survival Experiments," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1975*, UCCND CSD-18, pp. 1–2 (October 1975).

groups treated with Roll-1430 showed a slightly reduced but not statistically significant risk, and the groups treated with 13-*cis*-retinoic acid showed a significantly increased risk.

SURVIVAL AND DISEASE RISK IN X-IRRADIATED ATHYMIC AND NORMAL MICE

The application of statistical "odds ratio" techniques to the analysis of data from an experiment to compare mortality rate and risk for specific diseases in groups of athymic nude and normal C3H mice maintained under germfree conditions was previously reported.[12] During the past year, a similar analysis was undertaken for a corresponding set of groups that had received 300 rads of acute x rays.

The data from both experiments constituted a 2^3 fractional design with the factors phenotype (normal or athymic), radiation (irradiated or not), and sex. Main effects and interactions among these variables with respect to specific disease risks were estimated using linear combinations of the log odds ratios obtained from sets of pairwise odds-ratio comparisons.

This analysis was completed for the four principal lethal disease categories: reticular tissue neoplasms (leukemias), mesenchymal neoplasms, epithelial neoplasms, and undetermined cause of death. A similar analysis is currently being applied to the study of prevalence of several types of nonlethal solid tumors.

APPLICATION OF OCCUPANCY MODEL TO BIOLOGICAL PROBLEM

A model related to the problems of classical occupancy was considered in the study of metabolic cooperation between two kinds of cells in tissue culture. The space corresponding to the experimental dish was assumed to be divided into a large number, N, of boxes. The two kinds of cells were represented as white balls and black balls. If B black balls are randomly distributed into N boxes (each ball having an equal probability, $1/N$, of falling into a box), then the probability that there are exactly x empty boxes is well known. The probability that there were exactly y white balls occupying the boxes with no black balls present was derived. The results of the experiments were analyzed from an asymptotic point of view because very large numbers of cells were involved.

12. J. M. Holland, L. J. Mitchell, L. C. Gipson, and M. S. Whitaker, "Survival and Cause of Death in Aging Germfree Athymic Nude and Normal Inbred C3H/He Mice," *J. Natl. Cancer Inst.* **61**, 1357–61 (1978).

TIME EFFECT ON LESION COUNTS IN CARCINOGEN-EXPOSED TRACHEAS

Rat tracheas were transplanted onto the backs of host rats and were exposed to a dose of a known carcinogen for a specified time. The tracheas were then harvested at either 2, 3, 4, 8, or 12 months from cessation of exposure, approximately 45 at each time period, and the number of lesions per trachea recorded. Lesion counts at the various times after exposure were compared.

The counts at each time period were tested for agreement with a Poisson distribution and were found to exhibit a significantly larger variance than expected. The negative binomial distribution was found to fit the data quite well. The two parameters of this distribution, μ, the mean, and k, the exponent, were estimated using the method of maximum likelihood.

Comparisons of group means were made using analysis of variance and multiple comparison procedures on the transformed variable $Y = \ln(\text{count} + 1)$. Homogeneity of k was tested with a chi-square test.

The observed group mean differences were not found to be significant. However, the exponents were found to be heterogeneous. The reciprocal of k was used as a measure of "excess variance" or "clumping," that is, a measure of dispersion. At the later months more tracheas without tumors were recorded while the mean number of lesions remained relatively constant, resulting in this difference in dispersion. To improve the sensitivity of the analysis, the lesions were divided into types A, B, and C, which ranged from least to most severe. The 12-month group had significantly fewer lesions than the rest for type A, and the 4-month group had significantly more lesions than the rest for type B.

GROWTH RATE OF FROG OOCYTES

When female *Xenopus laevis* are injected with $[^3H]$vitellogenin of $[^{14}C]N$-acetyl glucosamine, most of the labeled material becomes associated three days later with oocytes having a diameter of 0.9–1.1 mm; the smaller and larger oocytes are less labeled. With time, the pattern of labeling shifts to larger oocytes, indicating that those oocytes initially labeled continue to grow.

Empirical methods were used to approximate the relationships between volume and time, taking advantage of the observed labeling shift. Two curves were recorded T days apart; each displayed counts per minute as a function of volume. Pairs of average volume and average rate of change in volume over the T days calculated at values in the range of counts approximated the true relationship. For example, at a fixed count rate C, the volumes V_1 and V_2 corresponding to C from curves 1 and 2 were used in approximating $V(t)$, volume as a function of time, and its derivative, $V'(t)$. The approximations $(V_1 + V_2)/2$ and $(V_2 - V_1)/T$ for $V(t)$ and $V'(t)$, respectively, were reasonably good because rate of change in volume was relatively constant over a short period of time. The approximate relationship between time and volume was obtained after arranging the ordered pairs by average volume from smallest to largest and applying $V'(t) = [V(t + h) - V(t)]/h$ iteratively with arbitrary starting values t_0 and $V(t_0)$.

OLD VERSUS YOUNG TISSUE SUSCEPTIBILITY TO A CARCINOGEN

The theory that young tissue is more susceptible to a carcinogen than old tissue was tested using tracheas from rats. Tracheas were removed from old and young animals and were transplanted onto the backs of host rats, an old and young pair per host. The tissue was exposed to a carcinogen, and the time until event was recorded. The event of interest was occurrence of a lesion; however, censoring due to complications arising from a lesion on the paired trachea, death from natural causes, or final sacrifice sometimes preceded lesion occurrence. Doses of 100 or 150 μg of DMBA were administered gradually over a period of time. A pellet consisting of a mixture of beeswax and the carcinogen was inserted into each trachea with a pair receiving either the 100- or 150-μg dose. A control group receiving no exposure, only beeswax pellets, developed no lesions during the experimental period.

Comparisons of the cumulative distributions of time until lesion for the old and young tracheas could not be made using the existing methods because of the dependence existing between a pair on any host. However, it was possible to approximate the distribution of $Y = T_{young} - T_{old}$, where T is the time until lesion occurrence. The method assumed that the time until lesion, or perhaps just Y, was independent of time until death. Estimates of the discrete probabilities at observed Y's were obtained using constrained maximum likelihood methods. Approximate, 95% confidence intervals for P covered 0.5 for both doses where P was defined as the probability that the lesion in a young trachea occurs first.

MOUSE STRAIN IDENTIFICATION BY MANDIBLE ANALYSIS

Response to drugs, life span, pattern of disease, and reproduction are examples of characteristics varying among strains of mice. It is of practical importance to be able to identify a mouse strain when reporting experimental results. Festing[13] has described a method of mouse strain identification based on the shape of the right mandible. Preliminary work has been started to develop a discrimination procedure based on 11 measurements suggested by Festing for (ce in identifying strains used locally.

Mandible measurements taken by two technicians for two mouse strains were available for preliminary analysis. Hotelling's T^2 test was used to assess mean differences between results of the two technicians, and these were found to be significant. Consequently, the laboratory procedure had to be reevaluated before further measurements could be taken.

As soon as the laboratory procedures have been standardized, measurements will be taken on all of the local strains. A discriminant analysis will be performed on this reference set, and the discriminant functions will be used to monitor strain purity. A series of control charts, one for each discriminant function, will be kept for each strain. Samples will be taken from a strain population periodically, and the mean discriminant function values will be calculated. If a trend appears or a mean falls outside of the control limit, the colony will be investigated further.

Other items for further consideration include reduction in the number of measurements taken with little loss in information and the effect of age on the measurements.

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13. M. F. Festing, "Mouse Strain Identification," *Nature, London* 238, 351 (1972).

10. Chemistry

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EVALUATION OF THE RESIN BEAD ISOTOPIC ANALYSIS DATA

Three spent fuel solutions were provided to test the applicability of isotopic analysis of nanogram-size samples of uranium and plutonium using the resin bead technique. Each spent fuel solution was divided into three couples of subsamples, and each couple consisted of a spiked and an unspiked aliquot. These subsamples were then prepared for resin beads either in the field by the International Atomic Energy Agency (IAEA) or in the laboratory by ORNL. The prepared resin beads were then analyzed by ORNL for the following quantities:

1. spiked plutonium: concentration (μg/g) and the ratios

$$\frac{^{238}Pu}{^{239}Pu}, \frac{^{240}Pu}{^{239}Pu}, \frac{^{241}Pu}{^{239}Pu}, \text{and } \frac{^{242}Pu}{^{239}Pu} ;$$

2. unspiked plutonium:

$$\frac{^{238}Pu}{^{239}Pu}, \frac{^{240}Pu}{^{239}Pu}, \frac{^{241}Pu}{^{239}Pu}, \text{and } \frac{^{242}Pu}{^{239}Pu} .$$

3. spiked uranium: concentration (mg/g) and the ratios

$$\frac{^{233}U}{^{238}U}, \frac{^{234}U}{^{238}U}, \frac{^{235}U}{^{238}U}, \text{and } \frac{^{236}U}{^{238}U} ;$$

4. unspiked uranium:

$$\frac{^{234}U}{^{235}U}, \frac{^{235}U}{^{238}U}, \text{and } \frac{^{236}U}{^{235}U}$$

Variation in the measured quantities due to the different subsamples, the different preparation sites, and the interaction between different subsamples and different preparation sites was examined by the method of analysis of variance. There were large statistical and practical differences between IAEA- and ORNL-prepared resin beads and among the three subsamples for each spent fuel solution in the measured quantities on the spiked plutonium samples. The large standard deviations of the measurements on IAEA-prepared resin beads indicated that the preparation of resin beads for the spiked plutonium was not sufficiently controlled to give precise measurements.

Most of the significant differences between IAEA- and ORNL-prepared resin beads and among subsamples for the measured quantities on unspiked plutonium samples, spiked uranium samples, and unspiked uranium samples were due to small biases that occurred during the resin bead preparation process. The standard deviations of the measured quantities for the three different types of solution showed consistent precision for the measurements made on IAEA-prepared resin beads and on ORNL-prepared resin beads.

STATISTICAL MODELING OF HISTOPATHOLOGICAL PROBABILITIES

In 1968, the Towards Less Hazardous Cigarette Program was initiated by the National Cancer Institute to identify cigarette characteristics that have a major influence on the carcinogenic risk of smoking. Since 1968, four series of experiments have been conducted to determine the specific carcinogenic activity of smoke condensates using the mouse skin painting method, in which smoke condensate from cigarettes is generated and painted on the backs of mice. The number of histopathologically verified tumors from these biological experiments was used to estimate the probabilities of a mouse being tumor free. These probabilities were then used as measures of the biological activity of the cigarette smoke condensates.

A corresponding sample of each of the smoke condensates was also analyzed for a number of chemical constituents in the smoke condensates. The relationship between the chemical data and the biological data sheds light on the undesirable smoke components and was used to formulate the design of more advanced or less hazardous cigarette models. This relationship was formulated as a mathematical model to predict histopathological probabilities as a function of (1) the smoke condensate concentrations applied to the mice and (2) the concentration of the chemical constituents in the smoke condensates.

1. Analytical Chemistry Division
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The prediction model for the histopathological probabilities (PF) was based on biological and chemical data from cigarettes having at least 70% tobacco content. The 196 data points used in this study consisted of a vector of the PF value, the applied smoke condensate concentration, and the concentration of nine chemical constituents of the smoke condensate measured in all four series of experiments.

The independent variables considered as terms for the prediction model were (1) concentration (mg/day), (2) nicotine (mg/g), (3) benzo[*a*]pyrene (µg/g), (4) benz[*a*]anthracene (µg/g), (5) phenol (mg/g), (6) *o*-cresol (mg/g), (7) *m&p*-cresol (mg/g), (8) pH, (9) weak acid (meq/g), and (10) very weak acid (meq/g). These ten variables are not the only variables that affect PF values but were the only ones measured on all four series of cigarettes.

The true function that related the PF values and the ten independent variables was approximated by the full second-order Taylor series of 66 terms. This was then reduced to a 17-term model by choosing 17 terms of the full quadratic on the basis of Mallows' C_p statistic and other standard tests. Each of the 17 terms in the prediction model was statistically significant at the 5% level; the prediction model, which accounted for 76.7% of the total variation, was not significantly different from the full 66-term model. The two terms that accounted for the major amount of variation in the models were (1) the square of the concentration and (2) the square of the nicotine concentration. The square of the nicotine concentration term was always a more important term than the linear term for nicotine.

PREDICTING URANIUM AND ACID CONCENTRATIONS FROM DENSITY, CONDUCTIVITY, AND TEMPERATURE MEASUREMENTS

A replicated 3^3 factorial design was used to generate data from which concentrations of uranium and acid (HNO_3) in solutions were predicted. The measured responses were conductivity and density; the design variables were uranium concentration, acid concentration, and temperature.

Two quadratic functions, estimated by least squares, were found to relate the measured values of conductivity and density to the three design variables. Although these functions gave satisfactory results for prediction purposes, they were inconvenient to apply because of the time required to interact with the computer. Therefore, a quicker second method was developed by considering measured uranium and acid concentrations made during the experimentation as dependent variables and density, conductivity, and temperature as controlled variables. Equations for uranium and acid concentrations were developed as a function of density, conductivity, and temperature using this approach. The confidence intervals on predicted values from these two equations were calculated from the estimated standard deviations of the measured uranium and acid concentrations made on each solution in the experiment.

SEPARATION OF RARE EARTHS AND ACTINIDES FROM HIGH-LEVEL NUCLEAR WASTES BY OXALATE PRECIPITATION

One method to minimize the hazard of nuclear wastes is to remove the longest-lived radioactive materials from the waste (the actinides, americium, and curium) and recycle these materials through nuclear reactors to destroy them. A series of experiments investigated one-step processes to separate these materials from high-level wastes by selective precipitation using oxalic acid. Continuous-flow systems with stirred tank reactors were used in the experiments. The experimental results were used to determine the optimal conditions for maximizing actinide and rare earth yields.

The primary independent variables under consideration included (1) time in residence, (2) power to the stirrer(s) in the tank(s), (3) oxalic acid concentration, and (4) temperature. In addition, the squares and cross products of these variables and expt-time) were considered in the regression analysis. All possible regressions of percent yield on the primary independent variables were performed. The best two sets (in the sense of largest R^2) from each subset size were retained. Coefficients were calculated for the standardized independent variables to facilitate comparisons of the coefficients in the regression function. These comparisons and conclusions were tempered by the intercorrelations and spacing of the independent variables.

The results of the regression analysis indicated that small fluctuations in temperature, which was to remain constant throughout, introduced effects in most cases greater than the effects of the other design variables, with yield decreasing with increasing temperature. Power seemed to be important only in the tank from which the yield was measured. Oxalic acid interacting with time provided the best single variable for predicting yield in all but one case.

11. Energy

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NONNEGATIVE FACTORIZATION OF POSITIVE SEMIDEFINITE, NONNEGATIVE MATRICES

There has been interest in the nonnegative factorization of positive semidefinite, nonnegative matrices in conjunction with a proposed mathematical model of energy demand for certain sectors of the U.S. economy. Let $\mathbf{A} = \{a_{ij}\}$ be an $n \times n$ positive semidefinite matrix which is also nonnegative; that is, $a_{ij} \geq 0$. The problem of factoring **A** into the form $\mathbf{A} = \mathbf{B}^T\mathbf{B}$, where **B** is also $n \times n$ and nonnegative, has been considered. In the energy model, the elements of **B** are parameters which, in addition to satisfying $\mathbf{B}^T\mathbf{B} = \mathbf{A}$, must be nonnegative because of their physical interpretation.

It has been shown that a nonnegative factorization is always possible for $n \leq 4$, and examples have been constructed to show that it is not always possible for $n > 4$. Although these results have appeared in the literature,[4,5] a more lucid account has been submitted for publication, accompanied by simple geometric proofs.

1. Computer Sciences Division
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FUSION ENERGY RESEARCH

To find the confinement time of a plasma in a tokamak, it is necessary to compute the most unstable frequency. This reduces to computing the most negative eigenvalue of the system $(\mathbf{A} - \lambda\mathbf{B})x = 0$, where **A** and **B** are large sparse symmetric matrices. To employ the power iteration method, it is necessary to factor the matrix $\mathbf{A} - \sigma\mathbf{B}$ for a given value of σ. The current computer code stores the complete half band of this matrix, but space limitations prevent the use of sufficiently large models to obtain the degree of accuracy desired.

Investigations were started to determine whether the use of fully sparse techniques together with a reordering of the variables might lead to significant savings in storage. This would allow the solution of the larger model problems.

4. P. H. Diananda, "On Non-Negative Forms in Real Variables Some or All of Which are Non-Negative," *Proc. Cambridge Philos. Soc.* **58**, 17–25 (1962).
5. M. Hall, Jr., and M. Newman, "Copositive and Completely Positive Quadratic Forms," *Proc. Cambridge Philos. Soc.* **59**, 329–39 (1963).

12. Engineering

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SENSITIVITY ANALYSIS OF ORINC

The Oak Ridge Inverse Code (ORINC)[6] is used to calculate temperature and heat flux at the surface of the electric heater rods used in the PWR-Blowdown Heat Transfer Separate Effects Program.[7] ORINC makes use of a one-dimensional, lumped parameter, implicit finite difference model of the heat conduction equation. The computer code calculates the surface temperature and heat flux as functions of time, given the heat generation rate, the geometry, thermophysical parameters, and the thermocouple temperature at an axial position of one of the heater rods in the Thermal Hydraulics Test Facility. To determine the sensitivity of ORINC's results to variations in key parameters, a computational experiment was conducted. The experimental design was a resolution IV, two-level fractional factorial design in 12 variables (parameters) and 32 computer runs. The two levels of each parameter were at one standard deviation above and below the nominal value of that parameter, where the standard deviations were based on given "uncertainty distributions."

At each time t, the sensitivity of the model "response" (flux or temperature) to parameter α_i was defined to be $S_i(t) = [h_i(t) - l_i(t)]/2$, where $h_i(t)$ was the average response at the 16 runs in which α_i was set to its high level, and $l_i(t)$ was the average response at the 16 runs in which α_i was set to its low level. It can be shown that if the response $y(t)$ is a quadratic function of the parameter vector $\boldsymbol{\alpha}$ in the neighborhood of its nominal value $\boldsymbol{\alpha}_0$, then $S_i(t)$ is the partial derivative of $y(t)$ with respect to α_i, evaluated at $\boldsymbol{\alpha}_0$. An example of this sensitivity function is shown in Fig. 6. These sensitivities were found to be relatively small (< 5%) for both flux and temperature.

The resolution IV design, together with an additional run at $\boldsymbol{\alpha} = \boldsymbol{\alpha}_0$, also provided information regarding the linearity of $y(t)$ as a function of $\boldsymbol{\alpha}$. At each t, the proportion of variation among the values of $y(t)$ attributable to a linear approximation to $y(t)$ was calculated and found to be nearly 100%. This result greatly simplified the interpretation of the sensitivities and also provided a basis for the estimation of the uncertainty distribution of $y(t)$ generated by the uncertainties in the α's.

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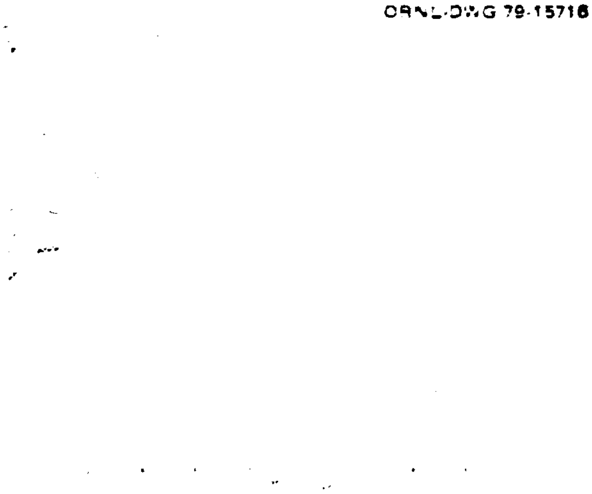

Fig. 6. Sensitivity of surface flux to input (input variable = MgO conductivity).

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2. Computing Applications Department.
3. Engineering Technology Division.
4. Separation Systems Division, Oak Ridge Gaseous Diffusion Plant.
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6. L. J. Ott and R. A. Hedrick, *ORINC — A One-Dimensional Implicit Approach to the Inverse Heat Conduction Problem*, ORNL/NUREG-23 (November 1977).
7. *Project Description ORNL-PWR Blowdown Heat Transfer Separate Effects Program — Thermal Hydraulics Test Facility (THTF)*, ORNL/NUREG/TM-2 (February 1976).

LATENT HEAT THERMAL ENERGY STORAGE

Collaboration in latent heat thermal energy storage centered on two activities: the preparation of computer programs for the modeling of phase-change phenomena[8] and the development of analytical models for phase-change processes under simple geometric and boundary conditions. Most of the work centered on models in one space dimension (valid for slab, cylindrical, or spherical symmetry) and, as yet, assumed only conduction heat transfer. The kind of results sought can be discerned from results obtained earlier for computer models and analytical approximations.[9] The work of this year may be described in the context of the classical one-phase Stefan problem, which takes the following form:

Problem: Find the temperature function $T(x, t)$ and the phase boundary

$$x = X(t)$$

obeying the conditions

$$T_t = \alpha T_{xx} \quad , \qquad 0 < x < X(t) \quad ,$$

$$T[X(t), t] = T_{cr} \quad ,$$

$$\rho H X'(t) = -kT_x[X(t), t] \quad ,$$

(where T_t, T_{xx}, and $X'(t)$ are partial or total derivatives), and in addition, satisfying one of the following boundary conditions:

$$T(0, t) = T_L > T_{cr} \qquad \text{(Dirichlet)} \quad ,$$

$$kT_x(0, t) = q_0 > 0 \qquad \text{(flux)} \quad ,$$

$$kT_x(0, t) = h[T_L - T(0, t)] \qquad \text{(convection)} \quad ,$$

$$kT_x(0, t) = \beta[T_L{}^4 - T(0, t)^4] \qquad \text{(radiation)} \quad .$$

The following notation has been used:

α – thermal diffusivity of material,

T_{cr} – melting temperature of material,

ρ – density of material,

H – latent heat of material,

k – thermal conductivity of material,

T_L – ambient temperature of heat transfer material,

q_0 – known external heat flux,

h – heat transfer coefficient,

β – physical constant.

The extension to cylindrical or spherical coordinates has been easily achieved through a slight modification of this formulation, and several results have been obtained. A relation between time and surface temperature, total heat stored, and surface heat flux has been found and studied in the case of the convection boundary condition. A number of test cases have been examined using analytical approximation techniques for the radiation boundary condition. Expansion, approximation, and numerical methods have been applied for all of these cases to a broad variety of test cases, and their results have been compared and analyzed. The application of numerical methods to these problems has been studied with particular emphasis on the convection boundary condition. Two points of particular interest have been the estimation of surface temperature as a function of time and the incorporation of density changes accompanying the phase-change process. The above results have been documented and are available.[8,9]

MODE SHAPE ANALYSIS AND CENTRIFUGE ROTOR RESPONSE TO BALANCE WEIGHTS

Understanding mode shapes of centrifuge rotors has been useful for balancing, but it has been difficult to isolate pure mode shapes experimentally. A method and computer program, MODE SHAPE,[10] have been developed for calculating the natural frequencies and mode shapes of a rotor. The governing fourth-order differential equation includes the effects of shear deformation and rotary inertia. Muller's method is used to calculate the natural frequencies and inverse iteration for the coefficients of the deflection function. A separate program that utilizes DISSPLA software has provided three-dimensional rotor deflection plots.

8. A. Solomon, *Mathematical Modeling of Phase Change Processes for Latent Heat Thermal Energy Storage*, UCCND CSD-26 (to be published).

9. A. Solomon, "On Moving Boundary Problems and Latent Heat Thermal Energy Storage," *Israel J. Chem. Eng.* (to appear).

10. R. E. Funderlic and F. H. Speckhart, *Mode Shape Analysis* (title unclassified), K/ES-3393 (SECRET) (March 1979).

A related computer program, CYLINDER,[11] has been developed over the last several years. This program predicts the response of a rotor due to balance weights and initial deflection of the rotor, and also calculates natural frequencies of a centrifuge. The response is for a steady-state circular rotor whirl. The transfer matrix method[12] is used to compute deflection, slope, moment, and shear in a rotor. A report is in progress that documents the physical assumptions, equations, methods, and all of the subroutines used in CYLINDER.

Progress is being made in making simulation calculations to calculate imperfections given deflections. This method, in contrast to CYLINDER, which calculates responses to balance weights, essentially reverses the roles in CYLINDER's equations of the unknown deflection and the known balance weights.

STUDY OF RAINFALL DISTRIBUTION

The Engineering Technology Division, as a participant in the DOE-sponsored Meteorological Effects of Thermal Energy Releases program, is conducting a rainfall study around a major power plant in northwestern Georgia. The study includes the examination of National Weather Service data and the operation of an ORNL-installed network of recording rain gauges and windsets. The search for effects of thermal energy releases from power plants is based on the understanding of rainfall distributions on a temporal and spatial sense. Distribution models have been fitted to rainfall amounts over specified periods to two sets of observations — one set used as a control and another set modified by the presence of a power station. Comparisons of the distributions of the observations from the two observation sets have been done in order to make probability statements that are useful in assessing the potential effects of thermal energy releases of power plants.

STRUCTURAL ANALYSIS

Dynamic analysis computes the response of a structure to periodic loading, such as that encountered during an earthquake. The finite element method makes it possible to reduce this problem to finding a few eigenvalues and eigenvectors of the system $(\mathbf{A} - \lambda\mathbf{M})x = 0$, where $\mathbf{A}$ and $\mathbf{M}$ are large sparse symmetric matrices. The Lanczos algorithm is ideally suited to the solution of such eigenvalue problems and offers several advantages over currently used techniques.

A computer code was written to interface existing Lanczos algorithm software with the data structures employed in the engineering codes. The results of a preliminary test showed significant improvement over the old technique. A new Lanczos code is now being written that will take advantage of the special properties of the matrices arising in vibrational analysis. The code will also be applicable to the buckling problem.

ANALYSIS OF POWER PLANT OPERATING EXPERIENCE

In a previous report,[13] several measures of power plant performance obtained from combined Edison Electric Institute (EEI) and Federal Energy Administration data bases were described. Standard data screening techniques uncovered a number of abnormalities that were reported to the EEI. Since that time the EEI has discovered discrepancies in the utilities' reporting of unit outages which biases some of the performance measures. Consequently, only capacity factor (CF) was analyzed in the current data set because CF is a measure of how well a plant performed relative to how well it could perform and is not dependent on outage.

Attempts to explain or "predict" variations in performance from year to year or from unit to unit on the basis of intrinsic unit variables like size or age were not very successful. It seems natural to expect age and increasing complexity of design to affect system performance, but other factors such as utility operating philosophy and integrated systems considerations were not considered in this study.

Nevertheless, models with size and age were fitted to the data using least squares methods. Even though the usual assumptions for regression analysis were questionable, they were entertained as approximately appropriate. Therefore, tests of significance were only approximate, and heterogeneity of variance resulted in parameter estimates that were not of

11. W. R. Hamilton, *CYLINDER, Gas Centrifuge Dynamic Model User's Guide* (title unclassified), K-TS-2677 (SECRET) (April 1977).

12. E. C. Pestel and F. A. Leckie, *Matrix Methods in Elastomechanics*, McGraw-Hill, New York, 1963.

13. "Analysis of Power Plant Operating Experience," *Math Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL/CSD-34, pp. 34–35 (September 1978).

minimum variance. The assumption of greatest concern was that of independence. The independence of action of generating units in the same utility was in doubt, and the independence of capacity factor of the same unit from year to year was of even more concern. For example, if a nuclear unit did not refuel in year k, it probably had to refuel in year $k + 1$, thus inducing serial correlation. This led to biased estimates, particularly of the age parameter.

Evaluations of the nuclear and coal power plants were made by comparing the regressions for various size and design groups. Even though the simplistic models considered in this study were not found to be of great predictive value, it was hoped that the standard statistical procedures applied here, such as testing for lack of fit, probability plotting, and residual analysis, would be incorporated into future studies of this type.

13. Environmental Sciences

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EFFECTS OF PHOSPHORUS ENRICHMENT ON ALGAL BIOMASS IN A STREAM

An experiment has been conducted in the Walker Branch, a small woodland stream, to determine if phosphorus limited the growth of algae. The study area was divided into three subareas: an upstream control area with soluble reactive phosphorus (SRP) concentrations in water of <10 μg liter, a low enrichment section with SRP concentrations of about 60 μg liter, and a high enrichment section with concentrations of about 450 μg liter. The enriched sections were fertilized continuously with phosphoric acid for 95 days. Glass slides were submerged in the three subareas of the stream to allow algal colonization and growth. Random samples of these slides were selected from each subarea; half of these slides were analyzed for concentrations of chlorophyll *a* in the algae, and the remaining slides were analyzed for total biomass. These observations were used as indicators of the growth of algae.

The purpose of the data analysis was to determine an adequate functional form to describe the behavior of the chlorophyll *a* observations from the three sampled subareas and to determine if significant differences exist among the three subareas for the chlorophyll *a* observations as well as the total biomass observations. A regression analysis led to the conclusion that the chlorophyll *a* values could be adequately described by a logarithmic function of time for each treatment. Although there was some indication of higher chlorophyll *a* values with increasing SRP concentration, no significant difference ($P > 0.10$) was detected in the rate of increase of the chlorophyll *a* concentrations among the three subareas. Nonparametric procedures were used to analyze the total biomass observations because of the failure of the distribution of the observations to satisfy the assumption of normality. From this analysis of the distribution of the biomass values, it was possible to conclude that there was a significant enrichment effect ($P \leq 0.05$) during the latter part of the experiment with the low and high enrichment areas having higher total biomass than the control area. These results were helpful in summarizing the experimental data and in indicating problems requiring additional experimentation.

ANALYSIS OF TRIHALOMETHANE PERSISTENCE DATA

Trihalomethanes have been identified as products resulting from the use of chlorine for fouling control in power plant condensor cooling systems. These compounds have potential for impacts on human health and aquatic ecosystems. Static toxicity tests were used to estimate the toxicity of trihalomethanes on hatching success of carp embryos. Total exposure was from fertilization until hatching (4 5 days), but toxicant solutions were changed every ? hr. During the period between changes, trihalomethane concentration declined continuously due to volatility and decomposition. In order to estimate the trihalomethane exposure in the toxicity experiments, the expression $y = C_0 \exp(-kt)$ has been proposed to describe the change in trihalomethane concentration over each exposure period, where y is the trihalomethane concentration at time t from the start of the exposure period, C_0 is the initial concentration, and k is a depletion constant. The nonlinear function for y has been used to estimate C_0 and k because an additive error has been shown to be appropriate. Results from the investigation of four trihalomethanes have been used to obtain estimates of C_0 and k using nonlinear least squares. The average trihalomethane concentration over the exposure period was used to estimate the dose to the embryos and was defined as

$$\frac{1}{T}\int_0^T y\,dt\,.$$

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where T is the known length of the exposure period. An asymptotic approximation was used to obtain an estimate on the standard error of the average concentration. The results were used to compare the depletion constant, k, for the different trihalomethanes. Mean values calculated for each initial concentration were then used to evaluate the impact of trihalomethanes on the hatching success of fish eggs from estimates of the trihalomethane concentration at which 50% of the animals would be dead after exposure.

A COMPARISON OF RESPONSES BETWEEN LATITUDINALLY SEPARATE POPULATIONS OF LARGEMOUTH BASS

Thermal water quality criteria are usually based on laboratory bioassays and are applied throughout the geographic range of the species. Therefore, it is important to know the influence that the origin of the test animals has on the laboratory results. Largemouth bass have been tested to determine the effect of temperature on mortality, survivorship, and growth rates. As part of this larger study, different attributes observed on the progeny of largemouth bass from different geographic areas (Louisiana, Tennessee, and Wisconsin) were compared. These attributes included (1) growth rates based on changes in length and weight, (2) change in biomass per day, (3) relative changes in biomass per day, and (4) temperature-dependent mortality. The analysis of the experimental data included an examination of the effect of test temperature on growth-related variables and the effect of acclimation temperature as well as rate of temperature change on the mortality variables. The statistical techniques of weighted regression analysis, nonparametric statistical analysis, probit analysis, and analysis of covariance have been used in the statistical evaluation of the experimental data. The results from this study will be helpful in the development and application of broad national water criteria for temperature.

CLINCH RIVER INVENTORY PROJECT

A major component of the Transuranic and Fission Products Inventory for the Clinch River is the collecting of about 250 riverbed soil core samples from the Clinch, Emory, and Tennessee rivers, each having approximately ten measurements. The major statistical activity during this reporting period has been the processing of the extensive data file to provide meaningful summaries of the multivariate data. These summaries have been done for particular elements of interest, portions of the sampled rivers, and sections of the sampled cores (i.e., top, middle, and bottom). Graphical displays including probability, frequency, and percentile plots have been provided. Tabular displays have included summary statistics for the observed variables as well as correlation matrices between the observed elemental concentrations. These summary procedures have provided concise presentations of the data, which are useful for reporting purposes and for indicating further interpretive analyses.

SAMPLING PLAN OF IMPINGED FISH

As part of an effort to quantify the number, species, and sizes of fish impinged at the Tennessee Valley Authority Kingston Steam Plant, a sampling plan was proposed to estimate the proportion of fish of a particular species impinged on a specific screen without having to count each impinged fish. This plan will be very useful during those times when there are more impinged fish than could be counted with the available manpower. The proposed sampling plan makes use of the total weight of impinged fish for a particular screen and also the most recent estimate of the average weight per fish for the same screen, so that an estimate of the total number of impinged fish on the screen under consideration can be obtained. Values of the total weight of impinged fish per screen are inexpensive to obtain. From knowledge about the most recent proportions of impinged fish on the screen being sampled for each of the species of interest and from a specification of the tolerated error in the final estimated proportion, curves have been drawn to be used in determining the required sample size for the following parameter ranges:

1. population sizes: 200 to 7700,
2. confidence levels: 0.80 (0.05) 0.95,
3. proportion composition values: 0.10 to 0.50, and
4. tolerated error values in terms of a percentage of the desired proportion: 10 to 33%.

Modifications have also been proposed to make the sampling plan sensitive to changes in the population abundance and to use subsample weight as a method of reducing the amount of time necessary to do the subsampling.

EFFECTS OF COLD STRESS ON GIZZARD AND THREADFIN SHAD

Experiments have been conducted to quantify the physiological effects of cold stress on gizzard and threadfin shad. This question is of interest because large numbers of shad are impinged annually on the intake screens of power plants in the southeastern United States. One possible cause of the large number of impinged shad is the inability of these fish to escape the rapid water current around power plant intake pipes during periods of low water temperature. The purpose of these experiments has been to determine if there have been any irreversible physiological changes on shad subjected to low temperatures and also to understand what these changes might be by comparing the blood chemistry of fish maintained at a normal water temperature (~14 C) with those fish whose environment was made colder (down to ~2 C). The experimental design randomly allocated fish to "control" or "test" tanks. The water temperature in the control tanks was maintained at a constant normal temperature (~14 C), and the water in the test tanks decreased from the normal temperature at a rate of ~1 C per day. At six predetermined temperatures in the test tank (between 14 and 2.3 C), fish were removed from a randomly selected pair of control and test tanks, and blood was taken from each fish. Concentrations of sodium, potassium, and chlorine in the blood serum were then determined. In addition, other covariate measurements length, weight, sex, and fin ray count were obtained for each sampled fish.

The statistical analysis included (1) an examination of the changes in the blood parameters as a function of the difference in water temperature between the control and test tanks, (2) an examination of the correlation between the blood parameters, and (3) an examination of the correlation between the blood parameters and the covariate observations. The results of this analysis indicated areas for which additional experimentation was needed and for which factors such as analytical techniques should be controlled to achieve more reliable results and to eliminate potential sources of bias. A second experiment has been run incorporating these suggestions. The results of this analysis will be used in determining the feasibility of using blood serum electrolytes to determine the level of physiological stress of shad in the vicinity of intake structures and in deciding on additional blood parameters that might be used.

CONFIDENCE LIMIT ON THE PROPORTION LESS THAN A SPECIFIED STANDARD

Often the assessment of compliance with environmental standards is performed using multiplicative chain models of the form $X = Z Z Z$, where X is related to the dose rate to an organ, and Z, Z, Z are related to nuclide concentrations or intake rates. The random variables Z are usually assumed to be independent, lognormally distributed random variables. Therefore, a random variable X, corresponding to the output of the multiplicative assessment model, is expressed as $X = \exp(Y + Y + Y)$, where the Y's are independent, normal random variables with mean μ and variance σ^2. A limiting value, X^*, has been given that should not be exceeded. For example, X^* might correspond to a standard set by the Environmental Protection Agency. If P = probability $\{X \leq X^*\}$, then the goal is to obtain a lower confidence limit on P. Using the concepts of Owen,[5] the problem was reduced to a problem that obtained a one-sided tolerance limit on P for the normally distributed random variable $X = \ln X = Y + Y + Y$. The following two cases were considered in the derivation: (1) $\sigma = \sigma = \sigma$ and (2) $\sigma \neq \sigma \neq \sigma$. These results were applied to data involving the ratio of the concentration of I in milk to that in air.

FACTORS AFFFCTING COAL STORAGE PILE LEACHATE QUALITY

Coal type, coal size, and coal storage technique are three factors of potential interest in determining coal storage pile leachate quality. An experiment based on a factorial design to include all combinations of these three factors, each at two levels, has been carried out under controlled laboratory conditions. Analysis of variance and regression techniques have been used to determine to what extent each factor influences leachate quality. Coal type has been found to be significant in determining concentrations of all the elements measured because this factor determines the amount of available pollutants leached from the coal. Coal size and storage technique have been found to be of little importance during the early part of the storage period, but these factors become increasingly im-

5. D. B. Owen, "Factors for One-Sided Tolerance Limits and for Variables Sampling Plans," Sandia Corp. Monograph No. SCR-607, pp. 16-17 (1963).

portant as the time of storage increases. The data indicated that some form of treatment is necessary if coal storage pile leachate is to meet certain standards that currently exist for discharges from power plants.

Electrical conductivity has been shown to be related to the concentration of important trace metals and found to be easy to observe. The following model has been proposed to describe the trace metal concentrations as a function of electrical conductivity.

$$y = \frac{\alpha}{1 + \beta e^{-\gamma x}} - \frac{\alpha}{1 + \beta},$$

where y is the trace metal concentration with an electrical conductivity value of x, and α, β, and γ are parameters to be estimated. A five-point interpolation scheme has been developed to obtain initial estimates of the unknown parameters. These initial estimates have then been used as input to a nonlinear least squares routine. This relation has already been applied to some laboratory and field data for several trace metals.

14. Geology

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URANIUM RESOURCE EVALUATION PROJECT

The Uranium Resource Evaluation (URE) project is a DOE-supported effort to estimate the uranium reserves in the United States. One portion of the project involves the collection of stream sediment and well water samples at a 10-sq mile density over most of the United States. The Oak Ridge part of the URE project is responsible for surveying the central United States by collecting over 200,000 samples. These data along with other radiometric, drilling, and geologic surveys will be coalesced and uranium reserve and resource estimates computed.

This year the Oak Ridge URE project has been in full production, releasing more than 25 reports (25,000 samples) on 1 × 2° U.S. Geological Survey quadrangles. Additionally, 13 special survey projects have been started to do detailed sampling at 1-sq mile spacings. These special projects will provide specific information on the possible locations of uranium deposits. The Mathematics and Statistics Research Department has supported the URE project since 1976 in the areas of data management, data summarization, multivariate classification, and field data quality control. Both research and consulting have been involved in these efforts.

FIELD DATA QUALITY CONTROL PROGRAM

Normally, several samplers require about two months to collect samples over a 1 × 2° U.S. Geological Survey quadrangle area. It is necessary in the interpretation of these data to combine the data collected over the entire sample collection period, introducing possible temporal variability. This variation adds to the analytical variability associated with determining the elemental concentrations of the samples. However, the most important source of variation in stream sediments is within a sampling site; this is not the case for well waters. It is desirable to quantify the relative contribution of the within-site, temporal, and laboratory variation to the total variation. Ideally, the total variation for geochemical mapping is comprised mainly of between-site variation.

An approach used by the Canadian and U.S. geological surveys has been to compute the index

$$G = \frac{\sigma^2 \text{ (between site)}}{\sigma^2 \text{ (within site)} + \sigma^2 \text{ (analytical)}} ,$$

where the values of σ^2 represent variances for the sources of variation. It has not generally been important to separate the within-site and temporal variation. Follow-up sampling has been performed to estimate the σ^2 and to enable use of an unbalanced three-level nested random effects analysis of variance model $y_{ijkl} = \mu + \alpha_i + \tau_{ij} + \gamma_{ijk} + \epsilon_{ijkl}$ with y_{ijkl} as the observed elemental concentration; μ, an overall mean effect; α_i, a site effect; τ_{ij}, a temporal effect; γ_{ijk}, an analytical measurement effect; and ϵ_{ijkl}, the random error. The sample collection design of the follow-up sampling has enabled the use of the above model, from which estimates of the components of variance in G have been obtained.

This program has monitored the quality of the data produced in the URE program. For example, in the Austin, Texas, quadrangle, estimates of G in stream sediments were 7.2 (Na), 2.6 (Li), 1.1 (As), and 0.35 (U), whereas in well waters estimates were 4.5 (Na), 16 (Li), 13 (As), and 3.0 (U). These values indicate the reproducibility of the elemental maps and the relative value of the two sample types.

CLASSIFICATION USING MEASUREMENT ERROR

The objective of the data analysis of the stream sediment and groundwater samples has been to contribute to the identification of new uranium deposits. A useful approach has been to classify the samples into groups with similar elemental concentrations. These groups have then been plotted geographically, creating patterns that can often be related to uranium mineralization. Techniques in cluster analysis have been used to classify the samples, but the measurement error has not been used in these analyses. It has been determined from the Field Data Quality Control Program that a large percentage of the variability for certain

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1. Computing Applications Department

elements can be attributed to within-site, temporal, or laboratory variation. The excess variation can cause the geochemical patterns to be masked.

One approach under development has used the measurement error in the classification procedure. Assume for each sample observation $Y_i = X_i + e_i$, where Y_i is the observed multivariate data at the ith site, X_i is the "error-free" data, and e_i is the error associated with obtaining X_i. Monte Carlo simulations have been used to create different realizations of the error e_{ij}, and $X_{ij} = Y_i - e_{ij}$ has enabled approximate classification of the X_i's. Estimates of the error distribution have been obtained from the Field Data Quality Control Program. Initial results have indicated that it is possible to both estimate the number of groups and the group membership in a manner that is superior to other methods. It should be possible to more accurately identify favorable uranium areas by improving the classification of the samples.

FACTOR ANALYSIS OF GEOCHEMICAL VARIABLES

Factor analysis is a means of summarizing the relationships among a group of variables with a reduced number of new variables, called factors, with little loss of information. If the method is successful, the set of factors will provide a description of the interrelationships among the original variables, with each factor indicating a common trait exhibited by those original variables that correlate highly with that factor. Thus, factor analysis can be an important summarization and model-building tool for the geologist faced with a typical, many-variable data set.

The variable selection process in the analysis of geochemical variables was an important first step before the factor analysis. Percentage of values above the detection limit and range of values for each variable were considered. Because a sampling area frequently consisted of several geologic units and because the relationships between variables often differed among the units, this consistency of relationships over the whole data set was checked. Only the highly correlated variables were included in the analysis.

Once the variable selection was complete, the appropriate model was chosen. Several models with varying numbers of factors were fitted and evaluated using a combination of objective and subjective criteria. How well a set of factors reproduced the observed correlation matrix and how much of the total variation in the data was accounted for by this set were two criteria easily assessed. The geochemical significance of the variables clustered in the factors was of greater importance.

Once a model was selected, factor scores (i.e., realizations of the hypothetical variables) were calculated. Contours of these factor scores, which were linear combinations of the original variables, were usually plotted so that the special characteristics of the factors could be assessed over the sampled area.

15. Health and Safety Research

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MODELS TO STUDY THE DISTRIBUTION AND EXCRETION OF CALCIUM

The purpose of this study was to apply urn model methods to study the distribution and excretion of substances like calcium in blood bone systems. These methods were generalizations of the two-compartment mamillary model considered by Sheppard and Householder.[3] The system consisted of two compartments (or urns) and the atoms (or balls) within these compartments which were exchanged between them on an "r for r" basis during constant time periods, assumed to be discrete in order to use urn model methods. Given numbers of radioactive and stable atoms (or white and black balls respectively) were introduced into each compartment (or urn) at the outset or 0th stage. The model was such that the total numbers in each urn remained fixed, only the number of each type could change, and, in fact, the expected number of the radioactive atoms in each urn was decreasing.

During each time period, the following three steps took place in order: (1) r stable atoms from outside the system were added to urn 1; (2) r atoms from urn 1 were interchanged with r atoms from urn 2 (both sets were randomly selected, and the two selections were considered to be simultaneous rather than in tandem); and (3) r atoms were removed at random from urn 1 and eliminated from the system.

These three steps constituted a single iteration. The problem was to find the first two moments of the number of radioactive atoms left in urn 1 (or in urn 2, or in both urns 1 and 2) after n iterations. The second moment gives a way of assessing the variability associated with the radioactive atoms as time progresses. The distributional properties of the number of radioactive atoms left in the system after n iterations were derived for this model and for two other modified models.

1. Health and Safety Research Division
2. University of California at Santa Barbara
3. C. Sheppard and A. S. Householder, "The Mathematical Basis of the Interpretation of Tracer Experiments in Closed Steady State Systems," *J. Appl. Phys.* 22, 510–20 (1951).

16. Information Sciences

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APPLICATION OF SAATY'S METHOD TO MANAGERIAL SELECTION

There are at least two important aspects in the problem of selecting a candidate for a managerial position from a group of candidates. One pertains to the identification of the important characteristics associated with the position, and the other is the potential performance of the candidates relative to these characteristics. In general, it is too much to expect a selector to be able to evaluate several candidates simultaneously relative to a group of characteristics and make an optimum decision. However, it is not unreasonable to assume that a selector will be reasonably good at comparing two candidates at a time on a given characteristic. Thus, if one has to choose between two candidates *A* and *B*, relative to a characteristic such as administrative skills, one may say that *A* is twice as good as *B* (or, equivalently, *B* is half as good as *A*), or that *A* is 1.5 times as good as *B*, etc. If there are four candidates *A*, *B*, *C*, and *D*, it may be difficult to assign weights to them individually relative to their administrative skills, but it may be easy to compare them two at a time.

Thomas L. Saaty[6] developed a methodology to assign weights to characteristics based on this principle and the information in the matrix of pair-wise comparisons. This method was used as an aid in the selection of an executive secretary within the Nuclear Division. In other applications of the selection of a manager, the important characteristics of a managerial position suggested by Douglas W. Bray[7] were used. A conversational mode computer program was developed as an aid for this selection process.

DATA VALIDATION PROJECT

During this reporting period, MSRD became involved in a significantly new area related to the validation of energy-related data forms. This effort, known as the Data Validation Project, was funded by the Energy Information Administration (EIA) of DOE through ORNL's Energy Division.

The initial role of MSRD was to study the validation process and to develop methodology that could be used by subcontractors actually conducting the validation studies. This role was altered when MSRD became involved in the validation study of the Federal Power Commission (FPC) Form-4, which is a form used to collect monthly data from electrical power generation facilities. Most of the methodology development work was postponed because a significant effort was required for the form validation study. However, a data editing procedure to be used to assess error rates in the data collection and storage systems was studied and developed. This effort was also directed to the validation effort of the FPC Form-4.

The general purpose of the validation study was to assess the data form's consistency and its ability to produce information that meets the legal mandate of the form as well as the needs of the users of the information. Changes in procedures were to be recommended that would make the form more realistic. Thus, much of the validation effort involved the use of survey sampling techniques to investigate the practices of the users and producers of the information. Exploratory data analysis techniques were used to assess the properties of the data produced by the form. The exploratory data analysis was generally designed to detect abnormalities in the data that would indicate possible inconsistent data reporting or collecting procedures. In addition, a general summarization of the data was provided

1. Nuclear Division Safeguards.
2. Computing Applications Department.
3. Energy Division.
4. Employee Relations Division.
5. Information Services.
6. T. L. Saaty, "A Scaling Method for Priorities in Hierarchical Structures," *J. Math. Psychol.* **15**, 234–81 (1977).
7. D. W. Bray, "The Assessment Center in the Management of Potential for Business Management," *Psychol. Monogr.* **80**, 1–27 (1966).

to obtain profiles of the reporting population (respondents).

The candidates for sampling fell into two classes—users and respondents. The user population was divided into three groups: sophisticated users, unsophisticated users, and state agency users. The identified sophisticated users formed a small group, and all were interviewed in person. The unsophisticated users tended to be associated with the federal government in the Washington, D.C., area, so the task of identifying and interviewing them was subcontracted to a consulting firm based in the same area. The survey of state agency users was designed to use telephone interviews of agencies in 15 states. The general purpose of the user surveys was to assess the degree of data quality they needed to meet their needs.

The survey of respondents was conducted in two phases. Initially, a survey plan was developed by MSRD for the in-person interviewing of 18 respondents. A second survey with national scope was designed because the results of the first survey raised several questions concerning reporting practices, geographic scope limits, and respondent's ownership. This survey accounted for the possibility that one company could control the reporting practices of several respondents in an area and other pertinent demographic factors. The general purpose of the respondent interviews was to assess reporting practices and data quality.

The results of the validation study of the FPC Form-4 monthly power plant report are currently being collated and will be available in an EIA-approved report.

AUDIT OF CLASSIFIED DOCUMENTS

A sample survey of classified documents at each of the three major Oak Ridge installations is being conducted to determine which documents, if any, are missing. Provisions were made in the procedure to increase the size of the sample if missing documents are detected.

17. Material Sciences

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KEVLAR YARN

The statistical assessment of the physical properties and life characteristics of Kevlar yarn and of products using Kevlar yarn has continued through this reporting period. An expanded review of variability patterns of denier in spools of Kevlar yarn has reaffirmed previous report results[6] that the major source of variability is the spool-to-spool variation.

Preliminary life test designs, using accelerated life test and warranty assignment methodologies, for products containing Kevlar yarn have been submitted to sponsoring agencies as input to their program plans.

PILEUP OF DISLOCATIONS

Electron microscopy of shear crack in stainless steel single crystal[7] has shown the pileup of dislocations against the crack tip. This direct observation of an elongated plastic zone showed evidence of the Bilby-Cottrell-Swinden model or the Dugdale model of fracture.

The governing equation that describes dislocations pileup and that is often used for thick specimens had to be modified to the following integral equation because of the thickness effect of the thin specimen:

$$P\int_{-a}^{a} f(x') \sum_{n=1,3,5,\ldots} \frac{1}{n} K_1\left[\frac{n\pi(x-x')}{2d}\right] dx' = \frac{G(x)}{A},$$

where P denotes the principal value of the integral. $f(x')$ is the distribution of the dislocations to be solved. K_1 is the modified Bessel function. A is a material constant, and $2d$ is the thickness of the specimen. The function $G(x)$ in this equation is defined to be

$$G(x) = \sigma \qquad |x| < c,$$

$$G(x) = (\sigma - \sigma_f) \qquad c < |x| < a,$$

where σ and σ_f are the applied stress and the friction stress, respectively, c is the half crack length, and $a - c$ is the length of the plastic zone.

It was shown that if d tended to be very large, this integral equation approached the well-known pileup equation for an infinitely thick specimen. In the present case, a numerical solution of $f(x)$ was obtained, and physical interpretation of $f(x)$ was made.

CHARACTERIZATION OF THE VOLUMETRIC METHOD AND THE GRAVIMETRIC METHOD OF DISPENSING FERTILE PARTICLES

An experiment was performed to characterize an automatic particle dispensing system using volumetric and gravimetric methods for dispensing a given weight of fertile particles. The volumetric method was calibrated to dispense 100% of the particles by volume all at once, whereas the gravimetric method discharged a fraction of the total number of particles by the volumetric method, then trickled in the remaining particles based on the

1. Metals and Ceramics Division
2. Y-12 Technical Division
3. Solid State Division.
4. Y-12 Development Division
5. Y-12 Product Engineering Division

6. "Physical Properties of Kevlar Yarn," *Math Stat Res Dep Prog Rep June 30, 1978*, ORNL CSD-34, p. 44 (September 1978).

7. S. M. Ohr and J. Narayan, "Electron Microscope Observation of Shear Cracks in Stainless Steel Single Crystals," *Philos. Mag.*, to appear.

weight required. All of the experimental runs were made in the same afternoon with the dispenser hopper level filled such that the particle level in the hopper did not change appreciably during the runs. Each experimental run consisted of dispensing fertile particles by either of the two methods to obtain a total net weight. The performance of each method was based on 20 samples run at a low net weight (4.25 g) and 20 samples run at a high net weight (7.75 g). In order to compare the data for the final net weights from the two gravimetric runs and from the two volumetric runs, the final weights were standardized as follows:

standardized final weights = final weights − mean .

These standardized final weights were plotted as box and whisker plots, which display five values of the data: the two extreme values, the upper and lower quartiles, and the median. The plot for the high-net-weight gravimetric method was quite different from that for the other three runs. The data from the high-net-weight gravimetric method had a much larger spread than any of the other runs and were skewed. The plots for the other three runs showed boxes of similar size with median values very close to zero. This observation indicated that the final weights of the three runs were symmetrically distributed about their mean values.

The weights of the particles trickled to obtain the final net weights were plotted against the desired weight in order to examine gravimetric runs in more detail. The distribution of particle weights for the gravimetric method was skewed about a point lower than the target value. The bias present in the observations from the gravimetric method was due to the inability of the trickler device to add the proper amount of particles. If the amount of particles required was between 25 and 110 mg, the trickler device added a constant amount of about 84 mg. However, the trickler device did not add any particles for an amount less than 25 mg. Therefore, the addition of the trickler device in practice did not improve on the simpler volumetric method.

LONG-TERM DRIFT EXPERIMENT FOR DISPENSING FUEL PARTICLES

An experiment was conducted to characterize the long-term behavior of volumetrically dispensed fuel particles. An automatic dispensing system was used to dispense 520 charges of each of three types of fuel material (fissile, fertile, and shim) at either a low or high net weight. The two different runs for each of the three fuel materials were replicated for a total of 12 experimental runs.

The repeatability of each of four runs on any one of the three particle types was found to be fairly constant. For example, the ranges of the standard deviations were (1) 4.01–4.81 for fissile particles, (2) 10.74–14.31 for fertile particles, and (3) 29.29–33.69 for shim particles. There were no apparent trends that the standard deviations increased or decreased from low-net-weight runs to high-net-weight runs. The standard deviations for the shim particle runs were large because 10 to 15% of the observed shim weights were abnormally large in each of the four shim runs. These large shim weights were caused by the tendency of the shim particles to clump in the dispensing nozzle. A histogram of the weight differences for each of the four shim runs was examined to eliminate those values which appeared to be outliers. The range of the standard deviations for the shim data without the outliers was reduced to 12.30–14.47.

Drifts in particle weights were examined as a function of the dispensing sequence number. Linear equations fitted to the data by the method of least squares showed a significant slope ($P < 0.05$) in 8 out of the 12 cases. If the weight differences increased as estimated by the slopes, the number of charges needed to reach 1% of the net weight from the origin was found to be a minimum of 309 charges for low-net-weight shim and a maximum of 45,588 charges for the high-net-weight fertile particles. None of the runs went beyond any practical limits until a substantial number of charges was dispersed. The actual behavior of the weight differences did not increase as a linear function of sequence number but varied in a sinusoidal manner and showed a slight increase with sequence number. The long-term drift experiment indicated that an automatic volumetric dispensing system gave repeatable results with little or no drift behavior. The drift behavior was small enough that corrections needed to be made only after a large number of particles were dispensed; this was accomplished by using moving average control chart plots. The data for shim particles showed that there was a need to modify the dispensing nozzle to prevent shim particle clumping.

VARIANCE COMPONENTS OF COATED MICROSPHERES

A number of nuclear fabrication processes require accurate dispensing of nuclear material in the form of coated particles of uranium and thorium compounds. For example, accurate amounts of uranium and thorium must be dispensed into High-Temperature Gas-Cooled Reactor (HTGR) fuel rods in the form of carbon-coated microspheres. The contribution of each component to the total variance of the microsphere weight was examined theoretically, because the coatings of the microspheres as well as the uranium and thorium kernels varied in thickness during fabrication.

The problem of finding the contribution of each component to the variance of a microsphere weight was formulated using the following assumptions:

1. The kernel and its coatings were concentric spheres.
2. The coating thicknesses were independent of each other and of the kernel diameter.
3. The density of each type of coating, the kernel density, and the percentage of uranium (thorium) weight were constants.
4. The kernel diameter and coating thicknesses were normally distributed about their respective means.

This formulation made it possible to represent the expected total weight and the variance of the total weight as a sum of the contributions from each component. The derived formulas were applied to sample data for fertile particles, which consisted of thorium kernels with inside and outside coatings. The important result of this theoretical study is that although the kernel of the fertile particle made up more than 60% of the expected weight, it contributed less than 10% of the total variance of the fertile particle. Most of the weight variation was due to the coatings. Similar results were also found for the fissile (uranium kernel) particles. This study demonstrated that a simple volumetric dispenser calibrated to weight, rather than a gravimetric dispenser, can be used to dispense fissile and fertile particles into HTGR fuel rods. Although the particle weights using the volumetric method varied more than with the gravimetric method, the two methods produced HTGR fuel rods with comparable uranium and thorium assays.

CREEP DATA FROM TESTS ON STAINLESS STEEL WELDS

The collection and analysis of creep data on stainless steel welds for the American Society of Mechanical Engineers (ASME) Joint Subgroup on Strength of Weldments have continued. The scope of the program has been narrowed to longitudinal all-weld specimens made from three filler materials (types 16-8-2, 316, and 308 stainless steel) and from two welding processes (gas tungsten arc and shielded metal arc). Also, only tests with known chemistries and known ferrite content have been considered.

The current effort has been to compare creep properties of welds, rupture life in particular, with ASME Code Case N-47 (formerly Code Case 1592) minimums for appropriate base materials. When necessary, new minimums of weld creep properties relative to those of the base material have been derived.

LIFE TESTING OF DISSIMILAR WELDS

The Dissimilar Weld Task Group of the Metal Properties Council has been exploring the causes of unexpected early failures of dissimilar welds. Dissimilar welds are welds used extensively in boiler manufacture for connecting stainless (austenitic) steels, suitable for high-temperature service, to less costly ferritic steels.

An earlier survey[8] of utility experience with dissimilar welds has motivated the development of a life-testing program to investigate five potentially improved weld joints. The Tennessee Valley Authority, a participating utility, has agreed to install spools containing dissimilar welds when reconditioning a boiler at the Kingston, Tennessee, steam plant.

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8. "Analysis of Data from Dissimilar Weld Survey," *Math. Stat. Res. Dep. Prog. Rep. June 30, 1978*, ORNL/CSD-34, p. 41 (September 1978).

STUDY OF FRACTURE TOUGHNESS OF IRRADIATED HSST-02

A proposal was prepared to study fracture toughness of irradiated specimens (1T) from a reference heat denoted HSST-02 and from other specified heats. The main purpose of this proposal was to estimate the number of specified heats that could be assigned to two of four capsules (used for irradiation) and yet provide sufficient information for studying the upper shelf region determined from fracture toughness tests. The remaining two capsules are to be used to irradiate a subset of the specified heats at a higher fluence and to irradiate specimens from reference heat HSST-02.

An equally important effort was to establish a relationship between the above 1T fracture toughness results and charpy impact results. Sixty charpy specimens accompanying each capsule are to be used to provide a one-to-one correspondence with the 1T fracture toughness specimens, with the remaining slots in the capsule for tensile specimens and precracked charpy specimens.

With 60 test specimens per capsule (~40 in the "design" fluence region, ~20 in the low fluence region), eight heats (four per capsule) will be studied. The assignment of specimens to capsule location and test temperature will be made when specific heats have been identified.

Part C. Educational Activities

The Mathematics and Statistics Research Department (MSRD) is involved in several educational activities of a professional and academic nature. This year the department was a co-sponsor of a symposium on sparse matrix computations. Members of the department presented short courses for the University of California; participated in the In-House Training Program; organized seminar series; served as part-time university lecturers, thesis advisors for doctoral candidates, and supervisors for students in the Oak Ridge Associated Universities (ORAU) Summer Student Program and the ORAU–Great Lakes Colleges Association (GLCA) Program; gave seminars under the sponsorship of the ORAU Traveling Lecture Program; and worked with visiting researchers and academicians.

SYMPOSIUM ON SPARSE MATRIX COMPUTATIONS

This symposium was held at the Hyatt Regency Hotel in Knoxville, Tennessee, November 2–3, 1978, immediately following the Society for Industrial and Applied Mathematics (SIAM) 1978 Fall Meeting. Jointly sponsored by the U.S. Army Research Office, the Office of Naval Research, SIAM, and MSRD, the meeting was organized by a committee of nine researchers, including R. C. Ward of MSRD, with D. J. Rose of Vanderbilt University as chairman. There were 190 participants, including several from outside the United States.

The purpose of the symposium was to bring together researchers in applied numerical analysis and computer science with applied scientists and engineers involved in problem formulation and modeling and to critically examine progress in sparse matrix technology relative to application areas. The program consisted of four half-day sessions, each of which began with an invited talk by a senior and experienced researcher in an application area. There were a total of 15 presentations covering such topics as medical image processing, structural engineering, operations research, chemical engineering, quantum mechanics, sparse matrix software, and multiprocessor networks of low-cost hardwire devices. Proceedings will be published by SIAM.

DEPARTMENT OPEN HOUSE

On December 6, 1978, MSRD held its second annual "Open House" to inform the Oak Ridge area technical community of our range of activities. Poster session–type displays were exhibited, and staff members were available for individual discussions. Visitors included representatives of management and staff members from the Computer Sciences Division, ORNL, the Oak Ridge Gaseous Diffusion Plant, the Oak Ridge Y-12 plant, and the University of Tennessee. Professor D. S. Robson of Cornell University was specially invited to critique the work of the MSRD staff.

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UNIVERSITY OF CALIFORNIA SHORT COURSES

T. J. Mitchell was an instructor in two short courses on "Applied Regression Analysis" sponsored by the Engineering Extension Departments of the University of California at Los Angeles and the University of California at Santa Barbara during the weeks of October 9–13, 1978, and February 26–March 2, 1979, respectively.

IN-HOUSE EDUCATION PROGRAMS

Two statistics courses were offered during this reporting period as part of the ORNL In-House Continuing Education Program. C. K. Bayne, J. J. Beauchamp, and T. J. Mitchell taught a new 11-week practical statistics course. This course, a continuation of the Practical Statistics I course, covered (1) analysis of variance, (2) regression analysis, and (3) design of experiments. The course, which was given during the fall quarter, had an enrollment of 19 students. The Practical Statistics I course, taught by J. J. Beauchamp and T. J. Mitchell, was offered in the spring quarter for the fourth time and had an enrollment of 20 students.

SEMINAR SERIES

F. E. Miller, Jr., and V. R. R. Uppuluri coordinated the continuing department seminar series. These seminars are intended to acquaint the MSRD staff with each other's work and to encourage interaction. Occasional outside speakers are also invited to inform us about research in progress at ORNL and at other facilities. The speakers' names and the titles of their talks are listed at the end of this section.

R. C. Ward of MSRD and R. J. Plemmons of the Mathematics Department of the University of Tennessee organized a weekly seminar series on matrix methods in numerical analysis. This series, held in Oak Ridge, began in January and continued into March. The speakers' names and the titles of their talks are given at the end of this section.

ORAU TRAVELING LECTURERS

Two department members, V. E. Kane and A. D. Solomon, participated in the ORAU Traveling Lecture Program this year. The titles of their talks are given at the end of this section.

VISITING RESEARCHERS

Several researchers visited the department during this reporting period.

Dr. Iain S. Duff of the Atomic Energy Research Establishment, Harwell, England, visited the department for a few days in early November. He presented two seminars on topics involving sparse matrix software and discussed potential research problems with application in the area of sparse matrices.

Professor Jay Folkert, Hope College, Holland, Michigan, visited the department during the fall and collaborated on research in the multivariate-multipopulation classification project on the effect of the logarithmic transformation on the probability of misclassification.

Professor Gene H. Golub of the Computer Science Department of Stanford University visited MSRD for several days in December 1978. He consulted with MSRD staff members on their research and with members of the Computing Applications Department, Computer Sciences Division, and ORNL's Environmental Sciences Division on their numerical problems.

Professor Ignacy I. Kotlarski of the Mathematical Sciences Department of Oklahoma State University joined the department as an ORAU faculty research participant on June 4, 1979. He worked with several staff members on problems involving probability theory and presented a series of seminars on characterization problems in probability and statistics.

Professor Beresford N. Parlett of the Mathmatics Department of the University of California at Berkeley visited the department for over a week in late July 1978. He consulted with staff members and others on numerical linear algebra problems and participated in discussions on the formulation of a department research project on sparse matrices.

Professor S. A. Patil, Mathematics Department, Tennessee Technological University, visited with V. R. R. Uppuluri periodically from October 1978 through June 1979 on an S-contract with ORAU. The two researchers worked on problems associated with the estimation of energy resources and nuclear safety.

Professor D. S. Robson, Biometrics Unit, Cornell University, visited the department twice to conduct research for the multivariate-multipopulation project.

Professor N. Shamsundar of the University of Houston was the guest of MSRD for two months and worked with A. D. Solomon and D. G. Wilson on moving boundary problems. In addition to giving several seminar talks on this topic, he took part in work on multidimensional phase-change modeling and finite element methods for heat transfer problems.

Professor L. R. Shenton of the Statistics Department of the University of Georgia visited with K. O. Bowman in March 1979. They are continuing their collaboration on problems of mathematical statistics including approximation theory, statistics in general samples, and analysis of apparently divergent series.

Professor W. Y. Tan, Director of the Statistics Division in the Department of Mathematical Sciences of Memphis State University, was an employee of the department from May 18 to August 18, 1978, and for one week in March 1979. He conducted research on the multivariate-multipopulation project and on the distribution of the number of mutants in an assay for mutagens. He began a second three months of employment with the department on May 11, 1979, and will work on similar problems. This research is summarized in Part A of this report.

Professor W. A. Thompson, Jr., Department of Statistics, University of Missouri at Columbia, was employed by the department from September 15, 1978, to May 31, 1979. He collaborated with staff members on the model validation, multivariate-multipopulation, and risk analysis research projects. His research is summarized in Part A of this report.

Professor B. W. Turnbull of Cornell University made several visits to MSRD during this reporting period in connection with his role as a consultant to MSRD staff members in the area of analysis of data from survival sacrifice experiments. The related collaborative research of Professor Turnbull with T. J. Mitchell is summarized in Part A of this report.

Professor J. A. Wenzel, Mathematics Department, Albion College, visited R. E. Funderlic during March 1979 to help complete a report[1] on the use of ordinary differential equation software. This report was taken from lectures he gave through the Technical Continuous Education Program while he was supported by ORAU GLCA.

Professor Wilhelm G. Wolfer of the Nuclear Engineering Department of the University of Wisconsin visited MSRD for a few days in April 1979. He discussed research problems with department members associated with the materials science and moving boundary research projects. In addition, he participated in discussions with staff members of both MSRD and ORNL's Solid State Division on problems of mutual interest.

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1. J. A. Wenzel and R. E. Funderlic, "Lecture Notes on Ordinary Differential Equation Software," *User's Guides for ODE, RKF45, GEAR, and EPISODE*, ORNL CSD TM-64 (June 1979).

SUPERVISION OF STUDENTS

MSRD regularly has students working with and for department members under the sponsorship of the GLCA and ORAU Student Research Participation Programs, as ORAU Graduate Fellows, and as summer employees.

Jacqueline E. A. Kent, an ORAU graduate fellow from North Carolina State University at Raleigh, completed the requirements for the Ph.D. in statistics. The MSRD members of her examination committee were F. L. Miller, Jr., and V. R. R. Uppuluri.

John P. Klein, a Ph.D. candidate at the University of Missouri, spent the summer of 1978 with MSRD continuing his work of the previous summer on the analysis of survival data from a large low-level radiation experiment.

Mark Jaeger, a graduate student in the Department of Statistics, University of Chicago, was an employee of the department during the summer of 1978, assisting with collaborative and research projects.

Michael Weinstein, a graduate student in mathematics at New York University, supported the research and consulting activities of S.-J. Chang and A. D. Solomon in phase-change modeling with applications to problems of metal castings. In addition, he participated in consulting activities for the Metals and Ceramics Division.

Ruth A. Lewis, a graduate student from the University of Tennessee, Knoxville, worked on updating the Householder KWIC Index on numerical linear algebra during the summer of 1979.

Two undergraduate students worked as ORAU student research participants during the summer of 1978. They are Donald R. Johns from Vanderbilt University, Nashville, Tennessee, and Rachel M. Harter from Wittenberg University, Springfield, Ohio. Mr. Johns supported the work of A. D. Solomon in cryosurgical modeling. His principal contribution was a literature search of thermal properties of tissues, and he also did basic work in the development of a three-dimensional cryosurgical code. Ms. Harter was involved with projects for both C. K. Bayne and V. R. R. Uppuluri. She worked on the estimation of misclassification probabilities for Fisher's quadratic discriminant function using Pearson's system of curves and also on numerical algorithms and computations involving multivariate hypergeometric and multinomial distribution.

Two more undergraduate students who worked as ORAU student research participants during the summer of 1979 are Sheryl A. Haw from Nicholls State University, Thibodaux, Louisiana, and Ronald B. Morgan from Furman University, Greenville, South Carolina. Ms. Haw worked under the direction of R. F. Fanderlic, while Mr. Morgan worked under the direction of S.-J. Chang.

Three GLCA students worked with MSRD staff members during the fall term of 1978. They are Carolyn Iwans from DePauw University, Greencastle, Indiana, who worked for V. E. Kane on the Uranium Resource Evaluation Project; A. William Geise from Lawrence College, Appleton, Wisconsin, who worked on solving sparse symmetric sets of linear equations using the Lanczos algorithm under the direction of D. S. Scott; and Cynthia Ross from Ohio Wesleyan University, Delaware, Ohio, who, continuing the work of Donald Johns under the direction of A. D. Solomon, prepared a computer program for the three-dimensional simulation of a cryosurgical procedure. The program is highly interactive and is to be developed further.

LIST OF CONSULTANTS

G. H. Golub, Stanford University
C. S. Lever, Oak Ridge, Tennessee
D. S. Robson, Cornell University
D. L. Solomon, Cornell University
B. W. Turnbull, Cornell University
W. G. Wolfer, University of Wisconsin

UT-MSRD SEMINARS ON MATRIX METHODS IN NUMERICAL ANALYSIS

M. T. Heath, Computer Sciences Division, UCC-ND, "Matrix Factorizations in Optimization," January 11, 1979

D. S. Scott, Computer Sciences Division, UCC-ND, "Survey of the Lanczos Algorithms," January 18, 1979

S. M. Serbin, Mathematics Department, UT, "Application of the Precondition Conjugate Gradient Method to Time-Stepping Procedures," January 25, 1979

D. G. Wilson, Computer Sciences Division, UCC-ND, "Nonnegative Matrix Factorization, $A = XX^t$, for Nonnegative, Symmetric, Positive Semidefinite A," February 1, 1979

R. J. Plemmons, Mathematics Department, UT, "Adjustment by Least Squares in Geodesy Using Block SOR and Chebyshev Semi-Iterative Methods," February 8, 1979

D. J. Downing, Computer Sciences Division, UCC-ND, "Kalman Filtering and Least Squares: A Comparison," February 15, 1979

R. E. Cline, Mathematics Department, UT, "Extensions of the Hurt-Waid Generalized Inverse for Integral Matrices," February 22, 1979

R. C. Ward, Computer Sciences Division, UCC-ND, "Scaling the Generalized Eigenvalue Problem," March 1, 1979

B. W. Rust, Computer Sciences Division, UCC-ND, "Solution of Ill-Conditioned Systems," March 8, 1979

W. D. Cain, Engineering Division, UCC-ND, "An Analysis of the Simplex Search Method for Local Minimization of Piece-Wise Continuous Functions of *n* Variables," March 15, 1979

ORAU TRAVELING LECTURE PRESENTATIONS

V. E. Kane, "Some Topics in Cluster Analysis," Texas A&M University, College Station, October 2, 1978

V. E. Kane, "Data Analysis in the Uranium Resources Evaluation Program," University of South Carolina, Columbia, April 26, 1979

A. D. Solomon, "Topics in Applied Mathematics," East Tennessee State University, Johnson City, November 30, 1978

A. D. Solomon, "Numerical Analysis on Your Pocket Programmable Calculator," University of Puerto Rico at Mayaguez, April 4, 1979; University of Puerto Rico at San Juan, April 4, 1979

A. D. Solomon, "On Plateau's Problem," University of Puerto Rico at San Juan, April 5, 1979

A. D. Solomon, "On Thermal Energy Storage," Institute for Energy Analysis, San Piedros, Puerto Rico, April 5, 1979

MSRD DEPARTMENT SEMINARS

N. Shamsunder, University of Houston, "Multidimensional Solidification Problems, Engineering Applications," July 12, 1978

J. Neuberger, North Texas State University, "A Numerical Technique for Nonlinear Partial Differential Equations Representing Conservation Laws," July 26, 1978

B. N. Parlett, University of California, Berkeley, "The Computation of a Few Eigenvalues of Large Sparse Symmetric Matrices or Goodbye Subspace Iteration," August 2, 1978

R. E. Funderlic, "Numerical Software and Services," August 9, 1978

M. T. Heath, Computing Applications Department, "The Core Library of Numerical Software," August 10, 1978

MSRD Summer Graduate Students (Project Reports, August 11, 1978):

- J. P. Klein, University of Missouri, "Bayesian Analysis of Survival Experiments"
- M. Jaeger, University of Chicago, "Fish and the Behrens-Fisher Problem"

ORAU Summer Research Participants (Project Reports, August 23, 1978):

- R. M. Harter, "Computer Programming of Misclassification Probabilities and the Hypergeometric Distribution"
- D. R. Johns, "Three-Dimensional Computer Modelling of the Cryosurgical Technique"

J. E. A. Kent, ORAU Fellow, "An Optimal Selection Procedure for Comparing Five Time-to-Failure Models," September 13, 1978

D. G. Gosslee, "The Art in the Art and Science of the Way in Which Statisticians and Mathematicians Consult and Collaborate with Other Scientists," September 27, 1978

E. N. Williams, Information Division, and R. D. McCulloch, Computing Applications Department, "Computerized Publications Processing at UCC-ND Present and Future," October 11, 1978

D. B. Reister, Institute for Energy Analysis, "Energy Demand Modeling," October 25, 1978

I. Duff, Atomic Energy Research Establishment, Harwell, England, "A Survey of Sparse Matrix Techniques," November 6, 1978

I. Duff, Atomic Energy Research Establishment, Harwell, England, "A Comparison of Techniques Used in the Solution of Sparse Linear Systems," November 7, 1978

R. D. Rannie, Systems and Administrative Support, "Everything You Ever Wanted to Know About Your Operating System but Were Afraid to Ask," November 8, 1978

E. C. Hise, Engineering Technology, "Magnetic Beneficiation of Dry Pulverized Coal (A Useful Black Art)," November 29, 1978

W. A. Thompson, Jr., "Reliability Models for Repairable Systems," December 13, 1978

D. G. Wilson, "Nonnegative Factorization of Symmetric, Positive Semidefinite, Nonnegative Matrices," January 10, 1979

L. J. Gray, "Nonnegative Factorization of Symmetric, Positive Semidefinite, Nonnegative Matrices: $N = 4$," January 24, 1979

C. K. Bayne, "Modeling Delayed Neutron Nondestructive Assay Techniques," February 28, 1979

V. E. Kane, "Some Statistical Considerations in Validating Data," March 21, 1979

K. O. Bowman, "Approximation of Distributions with Applications to Energy Problems," April 14, 1979

A. D. Solomon, "On the Stefan Problem with a Convection Boundary Condition," April 23, 1979

A. R. Zinsmeister, Graduate Student at Florida State University, "Markov Independent Particle Systems," May 2, 1979

W. A. Thompson, Jr., "On the Dose-Response Systems," May 16, 1979

R. E. Barlow, Florida State University, "Accelerated Life Testing and Information," May 18, 1979

I. I. Kotlarski, ORAU Faculty Research Participant, "Characterization Problems in Probability and Statistics," June 8, 15, 22, and 29, 1979

S. A. McGuire, Kansas State University, "Discrimination Using Multivariate Bernoulli Random Variables with Applications in Physical Anthropology," June 11, 1979

G. E. Liepins, Energy Division, "The Fields to Impute Problem of Automated Data Editing," June 20, 1979

Part D. Presentations of Research Results

Publications

BOOKS AND PROCEEDINGS

C. K. Bayne, J. J. Beauchamp, C. L. Begovich,[1] and V. E. Kane, "Monte Carlo Comparisons of Selected Clustering Procedures," pp. 297–301 in *Proceedings of the Statistical Computing Section*, American Statistical Association, Washington, D.C., 1978.

K. O. Bowman, Hing-Kam Ceva Lam,[2] and L. R. Shenton,[3] "Characteristics of Moment Series for Student's *t* and Other Statistics in Nonnormal Sampling," pp. 206–11 in *Proceedings of the Statistical Computing Section*, American Statistical Association, Washington, D.C., 1978.

K. O. Bowman and L. R. Shenton,[3] "Coefficient of Variation on Sampling from a Gamma Universe," pp. D1-19–D1-24 in *Proceedings of the International Conference on Quality Control*, Union of Japanese Scientists and Engineers, Tokyo, Japan, 1978.

K. O. Bowman and L. R. Shenton,[3] "Approximation to Distributions," contribution to *Encyclopedia of Statistical Sciences*, ed. by S. Kotz and N. L. Johnson, John Wiley & Sons, Inc., to be published.

S.-J. Chang, "A Creep-Recovery Constitutive Equation and its Time-Independent Limit," pp. 497–508 in *Developments in Theoretical and Applied Mechanics*, vol. 9, ed. by R. M. Hackett, Vanderbilt University, Nashville, Tenn., 1978.

S.-J. Chang and S. K. Iskander,[1] "Finite Element Method Based on the Creep-Recovery Constitutive Equation," p. 264 in *Proceedings of the Second International Conference on Computational Methods in Nonlinear Mechanics*, University of Texas, Austin, Tex., 1979.

W. M. Generoso,[4] K. T. Cain,[4] S. W. Huff,[4] and D. G. Gosslee, "Heritable Translocation Test in Mice," Chap. 3 in *Chemical Mutagens – Principles and Methods for Their Detection*, vol. V., ed. by A. Hollaender and F. J. deSerres, Plenum Press, New York, 1978.

W. M. Generoso,[4] K. T. Cain,[4] S. W. Huff,[4] and D. G. Gosslee, "Inducibility by Chemical Mutagens of Heritable Translocations in Male and Female Germ Cells of Mice," Chap. 6 in *Advances in Modern Toxicology*, vol. V., ed. by W. G. Flamm and M. A. Mehlman, Hemisphere Publishing Corp., Washington, D.C., 1978.

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1. Computing Applications Department.
2. Fordham University.
3. University of Georgia.
4. Biology Division.

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M. Sobel,[7] V. R. R. Uppuluri, and K. Frankowski,[8] *Incomplete Dirichlet Integrals - Type II (Selected Tables in Mathematical Statistics)*, to be submitted.

A. D. Solomon, "Heat Transfer in a PCM-Filled Wall," *Proceedings of the Conference on Systems Simulation and Economic Analysis for Solar Heating and Cooling*, San Diego, Calif., 1978.

A. D. Solomon, "On Modeling for Moving Boundary Problems," *Workshop on Solar Energy Storage*, Department of Chemical Engineering, Panjab University, Chandigarh, India, to be published.

JOURNAL ARTICLES

K. M. Anderson,[9] M. Sobel, and V. R. R. Uppuluri, "Hypergeometric and Multinomial Waiting Times," *Can. J. Stat.*, to be submitted.

C. K. Bayne, J. J. Beauchamp, C. L. Begovich,[1] and V. E. Kane, "Monte Carlo Comparison of Selected Clustering Procedures," *Pattern Recognition*, submitted.

J. J. Beauchamp, J. E. Folkert,[10] and D. S. Robson,[11] "A Note on the Effect of Logarithmic Transformation on the Probability of Misclassification," *Commun. Stat., Theory Methods*, submitted.

J. J. Beauchamp, C. S. Gehrs,[12] and D. A. Wolf, "Statistical Evaluation of Factors Affecting Reproduction Within a Calanoid Copepod Population," *Ecology*, submitted.

A. Berman,[13] R. S. Varga,[14] and R. C. Ward, "ALPS: Matrices with Nonpositive Off-Diagonal Entries," *J. Linear Algebra Its Appl.* 21, 233-44 (1978).

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K. O. Bowman, "Statistical Research in Japan," *ONR Tokyo Sci. Bull.* 3, 63-74 (1978).

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K. O. Bowman and L. R. Shenton,[3] "Approximate Percentage Points for Pearson Distribution," *Biometrika* 66, 147-51 (1979).

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5. Institute for Energy Analysis, Oak Ridge Associated Universities.
6. University of Missouri at Columbia.
7. University of California at Santa Barbara.
8. University of Minnesota.
9. Stanford University.
10. Hope College.
11. Cornell University.
12. Environmental Sciences Division.
13. Technion-Israel Institute of Technology, Israel.
14. Kent State University.

K. O. Bowman and L. R. Shenton, "Evaluation of the Parameters of S_U by Rational Fractions," *Commun. Stat., Simulation Comput.*, to be published.

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16. University of Tennessee.
17. University of Washington.
18. Solid State Division.
19. Chemistry Division.
20. National Institute of Environmental Health Sciences, Research Triangle Park, N.C.
21. Y-12 Product Certification Division.
22. Princeton Applied Research Corporation.
23. Los Alamos Scientific Laboratory.

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25. Purdue University.
26. Nuclear Division General Staff.
27. University of California at Berkeley.
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34. Albion College.

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A. D. Solomon. "Mathematical Aspects of Latent Heat Thermal Energy Storage," presented at the Institute for Energy Conversion, University of Delaware, Newark, Del., Nov. 8, 1978.

A. D. Solomon. "Topics in Applied Mathematics," presented at East Tennessee State University, Johnson City, Tenn., Jan. 17, 1979.

A. D. Solomon, "Numerical Methods on Your Pocket Programmable Calculator," presented at the University of Tennessee, Chattanooga, Tenn., Apr. 17, 1979.

A. D. Solomon, "Heat Transfer in a PCM-Filled Wall," presented at the Conference on System Simulation and Economic Analysis for Solar Heat and Cooling, San Diego, Calif., June 28, 1979.

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35. Tennessee Technological University.

Part E. Professional Activities

Members of the Mathematics and Statistics Research Department participate in several activities in support of their professions. Some of their contributions are outlined below.

C. K. Bayne

Member:	*Technometrics* Prize Committee
Instructor:	In-Hours Continuing Education Program

J. J. Beauchamp

Instructor:	Division of Mathematics and Science, Roane State Community College
Coordinator and Instructor:	In-Hours Continuing Education Program
Representative:	ORNL Professional Education Resource Committee

K. O. Bowman

Member:	International Editorial Board, *Communications in Statistics: Part B, Simulation and Computation*
Associate Editor:	*Journal of Statistical Computation and Simulation*
Reviewer:	National Science Foundation
Chairman:	Technical Session, Application of Statistical Methods, International Conference on Quality Control
Organizer:	Invited Paper Session, Annual Joint Meeting of the American Statistical Association, the Biometric Society, and the Institute of Mathematical Statistics
Contributing Editor:	*Current Index to Statistics*
Member:	Local Arrangements Committee, 1979 DOE Statistical Symposium

S.-J. Chang

Reviewer:	*Applied Mechanics Review*

R. E. Funderlic

Lecturer:	Department of Mathematics, University of Tennessee
	Traveling Lecture Program, Oak Ridge Associated Universities

Chairman:	Contributed Papers Session, 1978 SIAM Fall National Meeting
D. A. Gardiner	
Professor:	Department of Mathematics, University of Tennessee
Chairman:	Management Committee, *Current Index to Statistics*
	Steering Committee, 1979 DOE Statistical Symposium
Member:	Nominations Committee, Oak Ridge Chapter of Sigma Xi
	International Editorial Board, *Communications in Statistics Theory and Methods*
	Editorial Board, *Journal of Statistical Computation and Simulation*
	Steering Committee, 1978 DOE Statistical Symposium
	Program Committee, Fifth Symposium on Statistics and the Environment
D. G. Gosslee	
Lecturer:	The University of Tennessee Oak Ridge Graduate School of Biomedical Sciences
Representative:	Council of the American Statistical Association representing the Biometrics Section
L. J. Gray	
Lecturer:	Department of Mathematics, University of Tennessee
T. L. Hebble	
Member:	Local Arrangements Committee, 1979 DOE Statistical Symposium
V. E. Kane	
Lecturer:	Traveling Lecture Program, Oak Ridge Associated Universities
Member:	Program Committee, 1979 DOE Statistical Symposium
W. E. Lever	
Member:	*Technometrics* Prize Committee
	Committee to Review International Standards in Statistics, American Statistical Association
V. W. Lowe, Jr.	
Member:	Institute of Nuclear Materials Management (INMM) Subcommittee, INMM-3

T. J. Mitchell

Lecturer:	**The University of Tennessee Oak Ridge Graduate School of Biomedical Sciences**
Associate Editor:	***Technometrics***
Instructor:	**In-Hours Continuing Education Program**
	Continuing Education in Engineering and Mathematics, University Extension, UCLA

D. S. Scott

Lecturer:	**Department of Mathematics, University of Tennessee**

A. D. Solomon

Lecturer:	**Traveling Lecture Program, Oak Ridge Associated Universities**
	SIAM 1978–79 Visiting Lectureship Program

W. A. Thompson, Jr.

Associate Editor:	***Journal of the American Statistical Association***

V. R. R. Uppuluri

Lecturer:	**Visiting Lecturer Program, Mathematical Association of America**

R. C. Ward

Co-Chairman:	**Organization Committee, 1978 SIAM Fall National Meeting**
Lecturer:	**Department of Mathematics, University of Tennessee**
	SIAM 1978–79 Visiting Lectureship Program
Coordinator:	**University Relations Program Computer Sciences Division, Oak Ridge Associated Universities**
Reviewer:	***Computing Reviews***
Member:	**Organization Committee, 1978 Sparse Matrix Symposium**
	ORNL Graduate Fellowship Selection Panel

D. G. Wilson

Chairman:	**Contributed Papers Session, 1978 SIAM Fall National Meeting**
Editor:	***Oak Ridge Computer Association Newsletter***

Articles Reviewed or Refereed for Periodicals

Reviewer or referee	*Am. Math. Soc. Proc.*	*Ann. Stat.*	*Appl. Mech. Rev.*	*Commun. Stat.*	*Comput. Rev.*	*IEEE Trans. Autom. Control*	*J. Am. Stat. Assoc.*	*J. Econometrics*	*J. Heat Transfer*	*J. R. Stat. Soc., Ser. B*	*J. Stat. Planning Inference*	*Linear Algebra Its Appl.*	*Math. Rev.*	*Numer. Math.*	*Nucl. Sci. Eng.*	*Nucl. Technol.*	*SIAM J. Numer. Anal.*	*J. Stat. Comput. Simulation*	*Technometrics*	Proposals	Books	Total
	Number of articles reviewed or refereed for indicated periodical																					
Beauchamp, J. J.							2															2
Bowman, K. O.				5			2											1	2	1		11
Chang, S.-J.			2																			2
DiZillo-Benoit, P. M.							1															1
Funderlic, R. E.														1	1							2
Gray, L. J.	1																					1
Kane, V. E.				1			1															2
Lever, W. E.																					1	1
Lowe, V. W., Jr.							1											1				2
Mitchell, T. J.								1		1	1								3	3		9
Scott, D. S.												1										1
Solomon, A. D.									4				6			1						11
Thompson, W. A., Jr.				1																		1
Uppuluri, V. R. R.		1		1											1			1				4
Ward, R. C.					1	1						1					1					4
Total	1	1	2	8	1	1	7	1	4	1	1	2	6	1	2	1	1	3	5	4	1	54