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MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

FOR

PERIOD ENDING JUNE 30, 1954

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MATHEMATICS PANEL

SEMIANNUAL PROGRESS REPORT

for

Period Ending June 30 1954

A S Householder Chief

W C Sangren Editor

DATE ISSUED

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MATHEMATICS PANEL SEMIANNUAL PROGRESS REPORT

INTRODUCTION

THE ORACLE

On February 4 1954 the initial test program was completed and the ORACLE was put into useful service performing calculations Through May a total of 473 hr of com puter time was used by programmers in debugging (eliminating coding errors) and running problems Since the demand for ORACLE time is constantly increasing a regular evening shift is being scheduled The evening shift will be used mainly for production problems which can be run by the evening operator During the past two months the computer has been operating on a nonscheduled basis an average of three evenings per week

Engineering time is regularly scheduled for 4 hr each morning A maintenance program has been adopted whereby all tubes in the computer will be removed and checked in an orderly sequence Tube replacement and testing records are kept to help establish criteria for the selection of new tubes and to collect data concerning tube life In addition to preventive maintenance it is planned that much of the installation of auxiliary equipment will be done during engineering time thus holding shutdown time to a minimum

Room preparation for the installation of the Magnetic Tape Memory is now under way The tape unit proper has recently arrived from the Argonne National Laboratory The control circuitry has been designed by ORNL staff members and is now being constructed

The input output system presently used on the ORACLE has long been considered inadequate Consequently much thought has gone into the consideration of improved systems As a result of these studies a complete input output system has been planned which will provide all the flexibility needed to prepare computed results in final edited form Completion of the entire system is expected to take two years but some auxiliary equipment will be ready at an earlier date

LECTURES

ORINS Lectures Under the Traveling Lecture Program the following ORINS lectures were given

A W Kimball *Factorial Experiments* Vanderbilt University March 15 1954 *Micro biological Assay with Non Parallel Response Curves* Vanderbilt University March 15 1954 *Misfits in Modeling* North Carolina State College April 8 1954

W C Sangren *High Speed Calculation of Eigenvalues* University of Alabama Feb 17 1954 *Differential Equations with Discontinuous Coefficients* Duke University March 23 1954 *The ORACLE* University of Maryland March 25 1954

J Z Hearon *Kinetics of Linear Systems and Biological and Chemical Periodicities* University of Maryland Feb 17 1954 Georgia Institute of Technology May 18 1954

[redacted]

Alabama Polytechnic Institute May 19 1954 University of Georgia May 21 1954 *Kinetics and Thermodynamics of Steady State Systems* Oklahoma A & M College March 15 1954 University of Texas March 16 1954 Louisiana State University March 17 1954 University of Louisville April 20 1954 University of Kentucky April 21 1954 Georgia Institute of Technology May 17 1954

A S Householder *Generation of Errors in Digital Computations and the Structure of an Automatic Digital Computer* University of Miami March 12 1954 *Solution of Algebraic and Transcendental Equations* Florida State University March 18 1954 *Generation of Error in Digital Computations* U S Naval Proving Ground April 21 1954 University of Maryland April 22 1954

A C Downing *On Surface Waves Generated by Travelling Disturbances with Circular Symmetry* Alabama Polytechnic Institute April 26 1954

Other Lectures Other lectures given during the report period are as follows

W C Sangren *High Speed Calculation of Eigenvalues* Computer Conference Louisiana State University Jan 29 1954

A S Householder *A Functional Description of an Automatic Digital Computer* Computer Conference Louisiana State University Jan 29 1954 *The Effect of Computers on the Training of Applied Mathematicians and Scientists* Conference on Training Personnel for the Computing Machine Field Wayne University June 23 1954

N M Dismuke *Monte Carlo Calculations* Symposium on Monte Carlo Methods Gainesville Florida March 16 1954

J Z Hearon *Kinetics of Linear Systems* Mathematics Colloquim University of Tennessee Feb 24 1954 *Temperature Dependence of Reaction Rates* Chemistry Seminar Oak Ridge National Laboratory March 3 1954

S G Campbell *Some Generalizations of Some Minimal Surface Equations* Mathematics Colloquium University of Tennessee May 19 1954 *On a Class of Non Linear Partial Differential Equations* Mathematics Colloquium Syracuse University May 22 1954

S E Atta *Calculations of Generalized Hypergeometric Series* Associations for Computing Machinery Meeting Ann Arbor Michigan June 24–25 1954

C P Hubbard *Test Routines for the ORACLE* Associations for Computing Machinery Meeting Ann Arbor Michigan June 24–25 1954

W C Sangren *High Speed Reactor Calculations* Associations for Computing Machinery Meeting Ann Arbor Michigan June 24–25 1954

LIST OF PUBLICATIONS

W C Sangren and C W Sheppard A Mathematical Derivation of the Exchange of a Labeled Substance Between a Liquid Flowing in a Vessel and an External Compartment *Bull Math Biophys* **15** 387 (1953)

A Simon J H Vander Sluis and L C Biedenharn *Tables of the Racah Coefficients* ORNL 1679 March 26 1954

The following chapters of the ORACLE Manual, CF-53 12 2, have appeared for distribution Use and Construction of Subroutines by M R Arnette Coding a Complete Routine by N. M Dismuke

EMPLOYEE CHANGES

Jack Moshman terminated during this period E C Long transferred to the Panel in May R A Willoughby research participant has completed his work with the Panel and has returned to Georgia Institute of Technology Joining the Panel as research participants are N Macon from Alabama Polytechnic Institute N Heerema from Florida State University and W R Mann from the University of North Carolina B J Fisher and C D Griffies joined the Panel as operators for the ORACLE

MEETINGS

A Symposium on Nonlinear Problems was sponsored by the Mathematics Panel on May 3 and 4 On May 5 the AEC Computer Council held its meeting in the Research Building of ORNL A S Householder was the host at this meeting

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UNCLASSIFIED PROJECTS

PROGRESS OF THE ORACLE SUBROUTINE LIBRARY

Participating Members of Panel M R Arnette S E Atta S G Campbell A C Downing C L Gerberich C P Hubbard R C Weaver R A Willoughby

References Mathematics Panel Quarterly Progress Reports ORNL 1498 1435
Mathematics Panel Semiannual Progress Reports ORNL 1588 1662

Background and Status The subroutines which were checked on the ORACLE while it was at Argonne and recoded relative to cell No 000 have now been rechecked on the ORACLE here and copies of most of them have been made for the file

The library is steadily increasing there are now 70 or more different subroutines in the library although not all of these are completely checked out

Some of the additions which have not been mentioned in previous progress reports are as follows

A subroutine to compute the following six functions has been written and checked out $2^{-3} \sin 2^k x$ $2^{-3} \cos 2^k x$ $2^{-3} \sinh 2^k x$ $2^{-3} \cosh 2^k x$ $2^{-3} e^{2kx}$ $2^{-3} e^{-2kx}$ where k is a nonnegative integer and $-1 \leqq x < 1$ This subroutine uses fixed point operations

A least squares curve fitting subroutine has been coded and used This routine will take any amount of input information and will fit up to and including a 10th degree polynomial

The routine which evaluates the polynomial is soon to be made a subroutine

A subroutine which computes $u^{1/n}$ is being checked out

A subroutine for calculating the generalized hypergeometric series has been written and checked out This routine has a built in floating point and scaling combination for the parameters and argument Many elementary and nonelementary special functions are easily expressed in the generalized hypergeometric function notation

Two subroutines have been coded and checked out for numerical integration The two methods are Simpson s and Gauss s Simpson s code is shorter and the two codes take approximately the same computing time however Gauss s method is more stable than Simpson s

A subroutine has been written to get differences when the main routine supplies it with the number of terms to be differenced the number of differences wanted and hexadecimal input numbers

In addition to the square root to be used with floating point operations (3 1 b) there are now subroutines for getting sin cos sinh cosh and Legendre polynomials Also to be used with 3 1 b are some double-precision operations

A floating decimal point subroutine has been written and used in a problem but has not yet been added to the library

A linear equation solver subroutine has been written and checked out It will solve any number of equations up to 29 One version of this subroutine takes only one system and solves it Another version will take m systems of n equations solve them and print out the error

The subroutine for matrix multiplication by precision scaling has been checked out

There are now various versions of the routine to get the characteristic values of symmetric matrices

The subroutine to get the eigenvectors is in the process of being checked It is written up separately

Another floating point subroutine has been written and used in problems It is to be added to the library This subroutine is described in the section Floating-Point System for the ORACLE

In addition to these larger subroutines many smaller ones have also been added These include varieties of tape comparisons tape checks sum checks tape correctors etc One small subroutine shifts all numbers in certain locations to the right one place – a form of scaling when overflow occurs

A few more versions of conversion subroutines have been added in the last six months

Also a sin cos subroutine has been checked in it obtains the sines and cosines of any set of equally spaced arguments whether in degrees or radians

Likewise for equal arguments there is a subroutine which computes the probability function for any range

TEST ROUTINES FOR THE ORACLE

Participating Members of Panel C L Gerberich C P Hubbard

Reference Mathematics Panel Semiannual Progress Report ORNL 1662

Status The initial test program referred to in the last report was completed in February Therefore future work will be devoted to only the improvement of and additions to the operating test routines

An acceptance test used to test all components of the machine prior to the beginning of calculations has been written The use of this test has indicated the desirability of certain features which will be incorporated in a newer version

The installation of the Ferranti photoelectric reader made it advisable to program four new test routines for checking the input output system

Several new type read around tests were written during a basic investigation of the electrostatic memory This investigation resulted in a slightly different pattern configuration on the cathode ray tubes which improved the read around ratio These new tests are being reviewed and a permanent test routine will be designed from them

THE DEVELOPMENT OF OPTIMAL SUBROUTINES

Participating Members of Panel M R Arnette A S Householder

Background and Status In the construction of a routine for a special purpose a very rough estimate will often suffice to show that the generated errors (due to rounding) cannot exceed permissible limits of tolerance However with subroutines and standard service routines which are used many times and for a variety of purposes it is important that the error be analyzed as precisely as possible and that the routine be devised so that the maximum error is as small as possible Special effort has been made to develop efficiently some of the standard subroutines in the library and to make the error estimates precise

For the square root using Newton s method calculated in a special way it is possible to obtain a digital number x satisfying

$$(x^2)^* - a = 0 \qquad a \leqq 2^{-1}$$

$$|(x^2)^* - a| \leqq 2\epsilon \qquad a > 2^{-1}$$

where a is understood to be digital the asterisk designates the machine pseudo operation and $\epsilon = 2^{-40}$ Moreover

$$(a + \epsilon^2)^{1/2} - \epsilon \leqq x < (a + \epsilon^2)^{1/2} + \epsilon$$

and in fact whenever $a^{1/2}$ is digital then $x = a^{1/2}$ exactly Even a slight (although

mathematically legitimate) deviation from the prescribed sequence will invalidate these estimates and give results that are less precise

It appears to be not possible to obtain a cube root (a fortiori one of higher index) with the same degree of accuracy although an x can be obtained which satisfies

$$-2\epsilon(1 + 2\epsilon/x) < x - a/x^2 \leqq 4\epsilon$$

and up to terms in ϵ^2 this is equivalent to

$$\alpha - 2\epsilon/3 - 2\epsilon^2/\alpha < x < \alpha + 4\epsilon/3 + 2\epsilon^2/\alpha \qquad \alpha = a^{1/3}$$

In evaluating a power series

$$y = a_0 + a_1 x + a_2 x^2 +$$

the maximal error is in general much less when a reverse recursion of the form

$$y_{i-1} = y_i x + a_{i-1} \qquad y_0 = y$$

is used than when the series is evaluated term by term and summed For $\exp(-x)$ $\sin x$ and $\cos x$ it is a simple matter to determine the maximal number of terms needed and it turns out that the generated error is essentially independent of the number of terms utilized If the uncertainty is defined as the length of the interval about the computed value upon which the true value might lie then the uncertainty for each of these functions can be reduced to $2\epsilon e^{+x}$

The functions $\log(1 + x)$ $\arctan x$ and $\tanh x$ have been programmed with continued fractions For the first function the error analysis presupposes a digital $x \geqq -2^{-1}$ It is important that the continued fraction be written in such a form that the terms (numerator and denominator) of the successive approximations do not build up fast enough to complicate the scaling nor decrease fast enough to cause the relative errors to grow too rapidly It is possible to hold the absolute value of each term below the sum of the two preceding terms Finally since the errors build up rather rapidly at best the approximation at which the residual and generated errors are approximately equal should be accepted This being done the uncertainty for each of these three computations is approximately 2^{-35}

FLOATING POINT SYSTEM FOR THE ORACLE

Participating Member of Panel A C Downing

Background and Status In order to facilitate the coding of floating point problems for the ORACLE a self imitative floating point code has been written that is an interpretative code which permits floating point computations to be coded in precisely the same manner as fixed point computations Thus a person who is acquainted with the ORACLE code of commands is automatically acquainted with the floating point commands

So far the floating point system includes subroutines for computing exponentials of floating point numbers square roots of floating point numbers and input and output conversion routines These conversion routines transform input data in the form of decimal

magnitudes with a power of 10 into the floating binary point form used for computation and perform the analogous conversion for the output answers

The first version of this floating point system was written by using two memory locations to describe each number – one for the magnitude and one for the exponent In the very near future a second version will be written which will use just one memory location to describe both the magnitude and the exponent of the number

To date four problems have been coded with the use of the first version of the floating point system

ALGEBRAIC CODING FOR THE ORACLE

Origin Mathematics Panel

Participating Member of Panel A C Downing

Background and Status The ultimate goal in automatizing problem preparation for a high speed computer is the direct insertion into the machine of the problem described as a system of mathematical equations and relations The art of automatic programming is still far from this goal

However a preliminary investigation into the feasibility of writing for the ORACLE an executive routine which would come close to this goal has been completed and a report is now in preparation

INVERTING MATRICES OF HIGH ORDER

Participating Member of Panel V C Klema

Reference Mathematics Panel Semiannual Progress Report ORNL 1662

Status The general purpose routine for inverting matrices of high order which uses the method reported by von Neumann and Goldstine [1] was coded for the ORACLE by using floating point operations Machine checking of the code reveals that floating point operations do not give sufficient accuracy in the inverse matrix except for cases with very special conditions These conditions are that the original matrix be positive definite symmetric and have diagonal elements positioned in decreasing size with the largest element in the upper left hand corner

An entirely new method for inverting matrices is now under consideration by the Panel

NUMERICAL COMPUTATION OF CHARACTERISTIC VALUES AND VECTORS OF A REAL SYMMETRIC MATRIX

Participating Members of Panel W Givens V C Klema

References Mathematics Panel Quarterly Progress Reports ORNL 1498 1574
Mathematics Panel Semiannual Progress Reports ORNL 1588 1662

Status Codes for reducing a symmetric matrix to Jacobi form and subsequently determining the characteristic values of a matrix of order up to 30 have been placed in the

[1] J von Neuman and H H Goldstine *Bull Am Math Soc* 53 1021 (1947)

ORACLE Subroutine Library These codes make use of the internal memory capacity of the ORACLE and with the coming of external storage equipment the order of the matrix can be increased

An addition to these codes is the finding of the characteristic vectors of a symmetric matrix This code makes use of the Jacobi form and the characteristic values previously calculated The code is now being machine checked It is anticipated that the maximum order handled in the internal memory will be 30

CALCULATION OF THE GENERALIZED HYPERGEOMETRIC SERIES

Origin W C Sangren Mathematics Panel

Participating Members of Panel S E Atta W C Sangren

Background It is believed that a routine on hypergeometric functions will be able to calculate most of the special functions of mathematical physics A hypergeometric function W can be defined by the following

$$W \equiv Z^{\rho}\ {}_pF_q(a_1 + \rho \quad a_2 + \rho \qquad a_p + \rho \quad b_1 + \rho \qquad b_q + \rho \quad Z)$$

$$\equiv Z^{\rho}\ {}_pF_q(a_i + \rho \quad b_j + \rho \quad Z) = \sum_{n=0}^{\infty} \frac{(a_1 + \rho)_n \qquad (a_p + \rho)_n}{(b_1 + \rho)_n \qquad (b_q + \rho)_n} \frac{Z^{n+\rho}}{(\rho + 1)_n}$$

where

$$(\alpha)_n = \frac{\Gamma(\alpha + n)}{\Gamma(\alpha)} = \alpha(\alpha + 1) \qquad (\alpha + n - 1)$$

and $(\alpha)_0 = 1$

Many elementary and nonelementary functions are easily expressed in the notation of hypergeometric functions

Status A simple program has been written as a subroutine for the ORACLE The routine is arranged so that by feeding in the real parameters and the argument of the function ${}_pF_q$ can be calculated for p s and q s up to size 10 Both scaling and a built in floating point were used in this routine

FERMI AGE CALCULATIONS

Origin R A Charpie Research Director s Division

Participating Member of Panel C L Gerberich

Reference Mathematics Panel Semiannual Progress Report ORNL 1662

Status Since the original code for calculating Fermi age was found to be extremely slow the problem has been recoded for the ORACLE in a slightly different form Six seconds were used for the average neutron case history in water Since best results can be obtained only with a large number of such case histories it was decided that the original code should be completely streamlined The biggest change was that of the geometry of

the system The first code used a Cartesian coordinate system which was extremely bulky However since the medium was of infinite extent it was decided that a spherical system would simplify the equations Another change was made in the method of selecting the cross sections This selection was the biggest consumer of time in the original code It is believed that these and other smaller changes may cut the time needed for a calculation At the present time the new code is being tested on the ORACLE The time needed to run the new code is not yet known

FISSION PRODUCT PROBLEM

Origin R A Charpie Research Director s Division

Participating Members of Panel A C Downing S G Campbell R C Weaver

Background and Status The purpose of thefission product problem is to have available an ORACLE code for computing those properties of the fission product mixtures which are needed in design of off gas shielding chemical processing waste disposal and other facilities of a power reactor system It is necessary that the concentration of each fission product be computed as a function of the parameters flux ϕ irradiation time τ and cooling time t

The atomic concentration of each species in each fission product chain must also be computed From the definition of a typical chain nine differential equations are ob tained A modified Euler method has been used to integrate the nine differential equations The code allows for an increase or decrease in interval size depending on the percentage difference from values of concentrations obtained by two different formulas Given a flux a numerical integration is carried out to the desired irradiation time The flux is then set equal to zero and another numerical integration is carried out to the desired cooling time Ten different values of each one of the set (ϕ τ t) can be used in a calculation At each set (ϕ τ t) the concentrations are printed out

The problem has been debugged to the point that computation on 88 chains can now proceed When the magnetic tape units are installed the desired functions of the concen trations (and their sums over the whole fission spectrum) will be calculated

PENETRATION OF GAMMA RAYS THROUGH LAMINATED SLAB SHIELDS

Origin R A Charpie Research Director s Division C D Zerby Physics Division

Background and Status The energy spectrum of the photons penetrating laminated slab shields of various thicknesses is to be computed as a function of the incident energy and angle of the photons The Monte Carlo method was adopted for solution of this shielding problem and it was coded for computation on the ORACLE

Portions of the problem are being periodically calculated on the ORACLE and several cases with various initial conditions are already complete

BIOASSAY CALCULATIONS FOR THYROID STIMULATING HORMONE IN MOUSE TUMORS

Origin W T Burnett Biology Division

Participating Members of Panel A W Kimball G J Atta

Background and Status In the study of tumor induction in mice the presence or absence of thyroid stimulating hormone (TSH) furnishes useful information with regard to morphogenesis No satisfactory chemical methods for the determination of TSH are available but reasonably reliable estimates of TSH concentration can be obtained from bioassays

In these experiments both young mice and day old chicks were tried as test animals Measured amounts of TSH standards and tumor extracts were administered to test animals and these were followed by injections of I^{131} The I^{131} uptake at 24 and 48 hr after injection was determined for both the thyroid and the total body Reasonably accurate estimates of TSH concentration were calculated by using the slope ratio method for continuous responses although in some cases it was found that better results could be obtained by expressing the thyroid uptake as a percentage of the total body uptake and applying the bioassay technique for quantal responses based on the logistic function [2] The mouse as a test animal provided slightly more consistent results than the chick but because the chick assay is considerably cheaper to run it was used for most of the determinations

EVALUATION OF MITOTIC INHIBITION STUDIES WITH BETA AND X RAYS IN NEUROBLASTS OF *CHORTOPHAGA VIRIDIFASCIATA* EMBRYOS

Origin M E Gaulden Biology Division

Participating Members of Panel A W Kimball G J Atta

Background and Status Previous studies with neuroblasts of the grasshopper embryo have demonstrated the inhibitory effect of beta and x radiation on the mitotic cycle In some cases slight differences between the two types of radiation were noted but could not be considered significant Other evidence had indicated that cells in certain phases of mitosis are more sensitive to radiation than others but this point had never been studied exhaustively It was to correlate these two results that the present intensive experiment was planned and carried out

Embryos from each of several egg cases were divided into three groups one of which served as controls The other two groups received equivalent doses of beta and x radiation After irradiation the embryos were mounted and about 24 cells from each embryo were chosen for examination The mitotic phase of each cell was recorded immediately after irradiation and at regular intervals thereafter for a total period of about 400 min

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[2] J Berkson *J Am Stat Assoc* 48 565 599 (1953)

The major purpose of the investigation was to study mitotic rates with respect to phases of mitosis and type of radiation and for this it was necessary to find some manner of reducing the data to a quantitative basis The mitotic cycle was divided into 14 phases the lengths of which were established in a separate investigation several years ago The phases of each cell were then coded in proportion to the phase lengths of normal cells in such a way that the coded values when plotted against time after irradiation should have yielded a slope of 2 0 for the control group (With a few exceptions most of the plots were reasonably linear even in the irradiated groups) Instead the control slopes varied from 1 4 to 1 6 This discrepancy was attributed to the fact that the cells were metabolizing under somewhat artificial conditions and hence probably at a slower rate than normal It is also possible that some errors in the original measurements of phase lengths could have occurred

Accordingly the cells from different experiments were reclassified into groups homogeneous with respect to the phase of the cell at the time of irradiation or in the case of controls at the time of mounting Slopes for the control beta and x ray groups were computed for each initial phase and then plotted against the coded phase values The statistical analysis revealed maximum sensitivity in middle prophase and very little effect in the mid mitotic phases In addition x radiation was found to depress mitotic activity slightly more than beta radiation in all phases except mid mitosis

FIRST ORDER RATE CONSTANT FOR SUBSTRATE CONSUMPTION BY INTACT CELLS

Origin R F Kimball Biology Division

Participating Member of Panel J Z Hearon

Background and Status As a matter of some general interest and in particular for use in studies designed to elucidate the so called oxygen effect in irradiation damage it is necessary to know the time course of substrate concentration in free floating cells and to be able to evaluate from relatively simple experiments the parameters involved An approximate version of the diffusion equation is

$$\frac{dS}{dt} = -kS + \lambda(C - S) \tag{1}$$

where S is the mean cellular concentration C is the concentration in the medium k is the rate constant and λ is a constant determined by the geometry permeability and diffusion coefficients The total amount of substrate in the system is

$$\sigma(t) = VC + nvS \tag{2}$$

and clearly

$$\frac{d\sigma}{dt} = -nvkS \tag{3}$$

The solution of Eqs 1 to 3 for $\sigma(t)$, subject to $S(0) = 0$ $C(0) = C_0 = \sigma(0)/V$ is

$$\sigma(t) = \frac{\sigma(0)}{\beta_2 - \beta_1}\left(\beta_2 e^{\beta_1 t} - \beta_1 e^{\beta_2 t}\right) \tag{4}$$

where

$$\begin{cases} 2\beta_1 = -(k + \lambda) + [(k + \lambda)^2 - 4\epsilon k\lambda]^{1/2} \\ \beta_1 + \beta_2 = -(k + \lambda) \\ \epsilon = \dfrac{nv}{V} \end{cases} \tag{5}$$

If $\epsilon \leqq 10^{-2}$ then with a maximum error of 1 in 500

$$\begin{aligned} \beta_1 &= \frac{\epsilon k\lambda}{k + \lambda} \\ \beta_2 &= k + \lambda \end{aligned} \tag{6}$$

Further $\beta_2/(\beta_2 - \beta_1)$ is at most 1 0025 and β_1/β_2 is at most $2\ 5 \times 10^{-3}$ With a maximum error of 2 5 in 10^3 Eq 4 can be written as

$$\sigma(t) = \sigma(0)e^{\beta_1 t} \tag{7}$$

and a semilog plot of Eq 6 determines β_1 as given by Eq 6 For certain purposes it is enough to know β_1 but by standard chemical methods k can be determined and from β_1 and k λ is estimated

PRODUCTION OF H_2O_2 IN FREE FLOATING CELLS BY X RAYS

Origin R F Kimball Biology Division

Participating Member of Panel J Z Hearon

Background and Status Consider a mixed population of cells which are irradiated for a time τ The concentration of H_2O_2 in the cells at time τ and the time course of this concentration for $t > \tau$ are to be determined Let

S_i = concentration of H_2O_2 in type i cells

λ_i = diffusion parameter for type i cells

k_i = rate constant for type i cells

v_i = cell volume for type i cells

n_i = cell number for type i cells

V = volume of the medium

R = volume rate of production of H_2O_2 by x rays

σ = total amount of H_2O_2 in cells and medium

$\epsilon_i = n_i v_i/V$

Then the equations are

$$\frac{dS_i}{dt} = R - k_i S_i + \lambda_i(C - S_i), \tag{1}$$

(2) $$\sigma = V\left(C + \sum_i \epsilon_i S_i\right)$$

(3) $$\frac{d\sigma}{dt} = V\left[\left(1 + \sum_i \epsilon_i\right) R + \sum_i \epsilon_i k_i S_i\right]$$

The results of the preceding report show that after a time of the order of $1/(k_i + \lambda_i)$ the S_i are given by

(4) $$S \cong \frac{R + \lambda_i C}{k_i + \lambda_i}$$

By using Eqs 2 to 4

(5) $$\frac{dC}{dt} = R - \beta C$$

where

(6) $$\beta = \frac{\sum_i \epsilon k_i \lambda_i/(k_i + \lambda_i)}{1 + \sum_i \epsilon_i \lambda_i/(k_i + \lambda_i)}$$

If $\sum_i \epsilon_i << 1$ then β is a sum of terms of the type β_1 of the preceding report and each term may be evaluated from studies on unmixed cells as outlined there From Eq 5 and $C(0) = 0$

(7) $$C(t) = \frac{R}{\beta}\left(1 - e^{-\beta t}\right)$$

and substituting Eq 7 into Eq 4 gives the $S_i(t)$ After the cessation of irradiation

(8) $$C = Ae^{-\beta t}$$

(9) $$S_i = \frac{C\lambda_i}{k_i + \lambda_i}$$

where $A = C(\tau)$ from Eq 7 For $\tau \geqq 15$ sec the error in $C(\tau)$ from Eq 7 and $S(\tau)$ from Eq 4 is $\leqq 10\%$ For $t \geqq 15$ sec the error in Eq 9 is negligible The error involved in extrapolating Eq 9 to $t = 0$ is $R/(k + \lambda)$ which is the order of 5% at most

TESTS FOR OSCILLATORY BEHAVIOR OF DIVISION RATES IN PARAMECIA

Origin R F Kimball Biology Division

Participating Members of Panel A W Kimball G J Atta

Background and Status Paramecia are taken from autogamy and mounted in individual depression slides Each 24 hr the number of daughter animals is counted and one animal is transferred to another depression and allowed to divide for another 24-hr period When this procedure is repeated for several days and each line of descent is maintained intact the division rate decreases linearly from about 5 divisions per day to 2 or 3 divisions per day in about 40 to 50 days

In one experiment about 48 lines of descent were followed for 44 days One half the original animals had been treated with x rays and one half were controls No difference between the two groups could be found but both groups exhibited what appeared to be a regular oscillatory behavior about the linear downward trend A test for the significance of this behavior was desired

The first step was to remove the linear trend Then by using the residuals serial correlation coefficients of order up to 22 were computed and the resulting correlograms were plotted Except for one or two cases none of the correlation coefficients differed significantly from zero Furthermore the correlograms did not give a typical picture for any of the standard models of oscillatory behavior and none could be found which would adequately describe the data Finally several auxiliary tests based on frequencies of peaks and troughs failed to detect any departure from the kind of behavior which would be expected in a purely random series Thus in spite of the apparent significance of this oscillatory movement no evidence could be found to establish any departure from randomness

EFFECT OF X RADIATION ON SPERMATOGONIA IN MICE

Origin E F Oakberg Biology Division

Participating Members of Panel A W Kimball G J Atta

Background and Status Two male mice in each of nine groups were exposed to x radiation in doses from 0 to 200 r Either two or three sections were prepared from the testes of each mouse and the number of normal spermatogonia was counted in each of several tubules from each section

The data were analyzed first for variance components and it was found that the component among sections of the testes from one mouse was significantly less than the component among mice within the same dose group Accordingly it was recommended that in future experiments one section per mouse and more mice per dose group be used in order to provide smaller error estimates

The second part of the analysis consisted in fitting a survival curve to the data by a method described elsewhere [3] The numbers of normal spermatogonia at each dose were expressed as a percentage of the control and the resulting quantities (y) were related to dose (x) according to the multihit survival curve $y = (1 - e^{-kx})^n$ The parameter n was estimated as 1.44

[3] A W Kimball *Biometrics* 9 201 211 (1953)

THE FITTING OF DOSE RESPONSE CURVES FOR EXCHANGE ABERRATIONS IN *TRADESCANTIA*

Origin Drew Schwartz Biology Division

Participating Members of Panel A W Kimball G J Atta

Background and Status Chromosomal aberrations in *Tradescantia* occur when the cells are exposed to x radiation In one type of aberration referred to as an exchange one hit causes a break in each of two sister strands and opposite ends rejoin If the material is exposed to various doses of radiation (x) and the average number of exchanges per cell (y) is plotted against dose the relation $y = ax^b$ is adequate to describe the effect In many experiments the cells are exposed to radiation under different conditions and accurate estimates of the parameters a and b are needed if environmental factors are to be evaluated properly

For a given dose the random variable y has a Poisson distribution with $E(y) = m$ and $\mathrm{Var}(y) = m/n$ where m is the expected number of exchanges per cell at that dose and n is the number of cells scored The variance of log y is given approximately by

$$\mathrm{Var}(\log y) \sim \frac{1}{[E(y)]^2}\mathrm{Var}(y) = \frac{1}{mn}$$

In estimating a and b from the regression of log y on x each observation must be weighted by the inverse of its variance or in this case by mn the total number of exchanges

Weighted least squares fits of this nature have been completed in connection with several experiments designed to study the oxygen effect in *Tradescantia*

ANALYSIS OF LEUKEMIA INCIDENCE IN AN X RAY EXPERIMENT

Origin A C Upton Biology Division

Participating Member of Panel A W Kimball

Background and Status In this experiment five groups each of male and female mice were exposed to various treatments and after several months examined for the occurrence of four different types of leukemia The results are shown in Table 1

Before analysis the data were transformed to a uniform variance scale by means of the relation $y = \sin^{-1}\sqrt{P}$ where P = percentage incidence The analysis of variance shown in Table 2 was based on the transformed variables and the means in Table 1 were converted back from the $\sin^{-1}$ units In addition to the analysis shown in Table 2 separate analyses were made for each type of leukemia

From the complete analysis the differences among treatments (T) among types (P) and the $T \times P$ interaction were found to be significant at the 1% level All three irradiated groups manifested a higher incidence than either the control or the cortisone groups and cortisone had little or no effect in altering leukemia incidence in either the control or irradiated groups Of the four types thymic leukemia was found in greatest numbers with myeloid nonthymic and reticulum leukemia ranking next in that order The significant

TABLE 1 PERCENTAGE INCIDENCE OF LEUKEMIA

Treatment	Sex	Type of Leukemia				Mea s	
		Myeloid	Thymic	Nonthymic	Reticulum		
Control	M	1 4	4 2	9 9	2 8	4 1	4 8
	F	0	19 0	7 6	5 1	5 6	
Cortisone	M	0	8 1	12 9	8 1	5 4	6 7
	F	4 1	11 0	11 0	6 8	8 0	
X ray	M	29 2	18 5	4 6	6 2	13 1	13 6
	F	18 3	33 3	11 7	1 7	14 0	
Cort sone before x r y	M	28 3	26 7	15 0	0	13 4	11 8
	F	11 4	31 4	5 7	1 4	10 2	
Cort sone after x ray	M	30 4	8 7	7 2	1 4	9 9	11 5
	F	21 0	29 0	4 8	4 8	13 2	
Means		10 5	17 8	8 7	3 2	9 4	

TABLE 2 ANALYSIS OF VARIANCE

Source of Variat on	Degrees of Freedom	Mean Squ re	F Rat o
Among treatments (T)	4	116 11	4 25
Between sexes (S)	1	13 92	0 51
$T \times S$ nteraction	4	11 94	0 44
Among types (P)	3	364 29	13 32
$T \times P$ interaction	12	122 65	4 48
$S \times P$ nte a t on	3	82 02	3 00
$T \times S \times P$ nteract an	12	27 35	
Total	39		

$T \times P$ interaction is a reflection of the fact that treatment differences were actually found only in the myeloid and thymic groups and not in the nonthymic and reticulum groups This result was supported by the separate analyses of each type In general the effects of the leukemias were the same for both sexes except for thymic leukemia which was shown by individual analyses to occur with definitely greater incidence among females

On the basis of the transformation the theoretical variance was 12 24 but since this differed significantly from the three factor interaction mean square the latter was used in all tests of significance

PREDICTION OF AIR CONTAMINATION IN CERTAIN PROCESS AREAS IN Y 12

Origin W H Baumann Health Physics Division Y 12

Participating Members of Panel A W Kimball G J Atta

Background and Status In certain process areas at Y 12 production varies considerably and air contamination in general depends on production rate Thus it is important to be able to estimate the average amount of contamination for a given amount of production so that proper health safeguards may be imposed

For one area during a calendar year production indexes based on different criteria were computed and air samples for the corresponding periods were taken The regression of air contamination on each of the several production indexes was computed and one index was found to provide significantly better estimates than any other On the basis of this index confidence intervals for the average air contamination were calculated for the range of production encountered and for reasonable distances outside this interval As more production and air sample data are accumulated the calculation will be repeated to improve the predictive value of the regression function over a wider range

DENSITY EFFECT ON SLOWLY MOVING IONS

Origin J Neufeld Health Physics Division

Participating Member of Panel M F Todd

Background and Status A number of formulas supplied by J Neufeld were computed with the use of a desk calculator

DAMAGE TO TISSUE FROM NEUTRON BEAMS

Origin W S Snyder Health Physics Division

Participating Member of Panel N M Dismuke

References Mathematics Panel Quarterly Progress Reports ORNL 345 through ORNL 1435

Background During the period 1949–1952 the maximum permissible neutron flux was determined for neutron beams of energy 0 025 ev and 0 005 0 5 2 5 5 and 10 Mev For the thermal beam and for the thermal component of the other beams flux determinations were made by solving an integral equation [4] For the components above thermal the flux determinations were Monte Carlo estimates [5]

The problem has been programmed for the ORACLE in order to obtain additional values of the maximum permissible neutron flux for beams of 0 0001 0 02 0 1 and 0 3 Mev The computations for the 0 005 and 0 5-Mev beams will be repeated with the use of the ORACLE program

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[4] W S Snyder *Nucleonics* 6 No 2 46 (1950)

[5] W S Snyder *Calculated Depth Dose Curves in Tissue for Broad Beams of Fast Neutrons* (to be published) W S Snyde and J Ne feld *Maximum Permissible Neutron Flux for Fast and Thermal Neut ons* WASH 95 Sympos m on the Biophysical nd B ologic l Effe ts of Ne t ons Ma ch 17–18 1952

Status The Monte Carlo estimates for the components above thermal have been computed The thermal component determinations are in progress

DAMAGE TO TISSUE FROM NEUTRONS WITH MAXIMUM ENERGIES RANGING FROM 1 TO 300 kev

Origin W S Snyder Health Physics Division

References Mathematics Panel Semiannual Reports ORNL 1662 1588 Mathematics Panel Quarterly Progress Report ORNL 1435

Participating Member of Panel N M Dismuke

Status It was decided that energy loss due to the various processes should be tabulated separately rather than that the damage from all processes be tabulated collectively Since this decision implies increased output requirements further work will be delayed until faster ORACLE output is available

DISORDERING OF SOLIDS BY NEUTRON RADIATION

Origin W S Snyder Health Physics Division

Participating Members of Panel S G Campbell M F Todd

Background and Status The rather complex analysis involved in the paper *Disordering of Solids by Neutron Radiation* (to be published) which was prepared under the joint authorship of J Neufeld and W S Snyder of the Health Physics Division was checked in detail Some of the numerical calculations involved were recalculated and checked

SCATTERING CALCULATIONS FOR 3 × 3 AND 1 5 × 1 5 CRYSTALS

Origin P R Bell Physics Division

Participating Members of Panel S G Campbell C P Hubbard M F Todd

Background and Status It is necessary to use numerical integration in order to evaluate the integral

$$T(\tau) = \frac{1}{2} \int_{a}^{\alpha_2} \sin \alpha [1 - e^{-\tau x(\alpha)}] \, d\alpha$$

where

$$x = t \sec \alpha \quad \text{for} \quad 0 \leqq \alpha \leqq \alpha_1 = \tan^{-1} \frac{r}{\mu + t}$$

$$x = r \csc \alpha - \mu \sec \alpha \quad \text{for} \quad \alpha_1 \leqq \alpha \leqq \alpha_2 = \tan^{-1} \frac{r}{\mu}$$

t and r are the length and the radius of the crystal respectively τ is the absorption coefficient and μ is the distance from the crystal to the source Calculations were made for 14 different τ s ranging from 0 123 to ∞ and for 31 different μ s ranging from 0 to 70 cm Since the limits of the integration vary from case to case Simpson s rule was used in a program which allowed the limits and the mesh size to be varied The convergence of the integration process was checked to at least five significant decimal digits

A similar but much more complicated calculation is now being programmed for a 3 × 3 in crystal with a ½ in bevel removed from the edge of the forward face Gaussian integration is being used in the current program in place of Simpson s rule

ANGULAR CORRELATION FUNCTIONS OF MIXED PURE GAMMA GAMMA CASCADES

Origin E D Klema and F K McGowan Physics Division

Participating Member of Panel V C Klema

Status The angular distribution functions $W(\theta)$ for gamma gamma cascades in which one gamma ray is pure and the other is mixed electric and magnetic multipole radiation are calculated as a function of the mixing ratio δ These calculations are programmed for the ORACLE by using floating point operations

ENTROPY OF PARAMAGNETIC SALTS IN MAGNETIC FIELDS AT LOW TEMPERATURES

Origin L D Roberts and J W T Dabbs Physics Division

Participating Member of Panel M F Todd

Reference Physics Division Semiannual Progress Report ORNL 1705

Background and Status The following formulas were computed

$$\frac{S}{R} = -\ln Z - \theta\left(\frac{\partial \ln Z}{\partial \theta}\right)$$

$$Z = \sum_{m=-s}^{s} e^{-m^2/\theta}\left(1 + \frac{1}{2}\frac{m^2 h_3^2}{\theta^2}\right) + \frac{1}{2}(h_1^2 + h_2^2)\left\{\left[s(s+1) + \frac{1}{4}\right]\frac{e^{-1/4\theta}}{2\theta^2}\right.$$

$$\left. + \sum_{m \neq -\frac{1}{2}} [s(s+1) - m(m+1)]\frac{e^{-m^2/\theta}}{2m+1}\left(\frac{1}{\theta} + \frac{e^{-(2m+1)/\theta} - 2}{2m+1}\right)\right\}$$

$$0 \leqq h \leqq 0\ 30$$

$$0\ 25 \leqq \theta \leqq 2$$

$$s = \tfrac{3}{2} \quad \tfrac{5}{2}$$

The computations were performed on a desk calculator and the answers were returned to the originators

CALCULATION OF INTERNAL CONVERSION COEFFICIENTS WITH SCREENING

Origin M E Rose Physics Division

Participating Member of Panel M F Todd

Reference Mathematics Panel Semiannual Progress Report ORNL 1662

Background and Status Answers obtained from the SEAC of the National Bureau of Standards in Washington have been plotted and the graphs have been returned to M E Rose Some hand computations were done to aid in the plotting

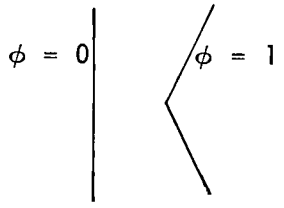
Since the SEAC calculations have proved to be adequate no further examination of this problem is being considered for the ORACLE

MAGNETIC FIELD

Origin J E Sherwood Physics Division

Participating Members of Panel S E Atta W C Sangren

Background and Status The mathematical problem consists in solving $\phi_{xx} + \phi_{yy} = 0$ subject to the boundary conditions shown in the following diagram



Numerically this means that a set of rectangular mesh points were chosen and that the difference equations equivalent to the differential equation must be solved on the mesh The problem has been programmed for the ORACLE to take any size angle on the boundary $\phi = 1$ and with any number of points up to the capacity of the memory of the ORACLE Three cases have been run on the ORACLE

TABULATION OF ANGULAR MOMENTUM FUNCTIONS

Origin A Simon Physics Division

Participating Member of Panel J H Vander Sluis

Background A method of computing tables of the Racah function $W(a\ b\ c\ d\ e\ f)$ and the Clebsch Gordan coefficient $C^{abc}_{\alpha\beta\gamma}$ was coded for the UNIVAC The Racah function is given by the formula

$$W(\ b\quad d\quad f) = \Delta(\ b\ )\ \Delta(\ d\ )\ \Delta(\quad f)\ \Delta(b\ d\ f)\ \sum(-1)$$

$$\times \frac{(\ +b+\ \ +d+1-\ )!}{(a+b-\ \ -\ )!\,(\ +d-\ \ -\ )!\,(\ +\ \ -f-z)!\,(b+d-f-\ )!\,z!\,(\ +f-a-d+\ )!\,(\ +f-b-\ \ +z)!}$$

where

$$\Delta(a\ b\ e) \equiv \left[\frac{(a+b-e)!\ (a-b+e)!\ (-a+b+e)!}{(a+b+e+1)!}\right]^{1/2}$$

The Racah functions were calculated to 10 decimal places with the range of arguments as follows

$a\ c$ =	0	½	1	15/2
$b\ d$ =	0	½	1	9/2
e =	0	½	1	3
f =	0	1	2	8

The Clebsch Gordan coefficient is given by the formula

$$C^{b}_{\alpha\beta\gamma} = \delta_{\alpha+\beta\ \gamma} \sqrt{2c+1} \sqrt{\frac{(a+b-c)!\,(a-b+c)!\,(-a+b+c)!}{(a+b+c+1)!}}$$

$$\times \sqrt{(a+\alpha)!\,(a-\alpha)!\,(b+\beta)!\,(b-\beta)!\,(c+\gamma)!\,(c-\gamma)!}$$

$$\times \sum_{z} \frac{(-1)^{z}}{z!(a+b-c-z)!\,(a-\alpha-z)!\,[(a+\alpha)-(a+b-c)+z]!\,[(b+\beta-z)!\,(b-\beta)-(a+b-c)+z]!}$$

The Clebsch Gordan coefficients were also computed to 10 decimal places All those are given which have no argument greater than $9/2$

In the case of both functions it was necessary for all allowable arguments to satisfy both integral and triad conditions [6] When these conditions were satisfied the functions were then calculated in a straightforward manner Since it was noticed that only 25 factorials in all were needed for both calculations a table of these factorials was stored in the memory The tables of the Racah function and Clebsch Gordan coefficient were printed out by the UNIVAC in completely edited form and needed only to be photographically reproaduced for final distribution

Status The Racah functions were distributed in one report[6] and the Clebsch Gordan coefficients in a second report [7]

DATA ANALYSIS OF Xe^{135} MEASUREMENTS

Origin E C Smith Physics Division R A Charpie Research Director s Division

Participating Member of Panel S E Atta

Background The following definitions were agreed upon

τ = clock time (min) ($\tau = 0$ when sample holder was loaded)

C_0 = open beam count

t_0 = measured time (min) for count C_0

C_1 = sample in place count

t_1 = measured time (min) for count C_1

C_2 = background count (average of 83 channels all in Cd region)

t_2 = measured time (min) for count C_2

$$K = \frac{\text{background rate with sample holder in}}{\text{background rate with sample holder out}}$$

T_0 = measured transmission of sample holder

It was desired that an appropriately averaged cross section for each channel be computed For this purpose the variance of each previously computed σ was needed in order

[6] A Simon J H V nder Sluis and L C B edenharn *Tables of the Racah Coefficients* ORNL 1679 Ma ch 26 1954

[7] A S mo *Numerical Table of the Cleb ch Go dan Coeff cients* ORNL 1718 J e 21 1954

to get a good set of weighting factors for use in obtaining an average

$$\sigma = - \frac{\left[(1/T_0) \dfrac{(C_1/t_1) - K(C_2/t_2)}{(C_0/t_0) - (C_2/t_2)} \right]}{N_0 e^{-\lambda\tau}}$$

The variance of σ to a high order of accuracy can be approximated by

$$V(\sigma) = C_0 \left(\frac{\partial\sigma}{\partial C_0}\right)^2 + C_1 \left(\frac{\partial\sigma}{\partial C_1}\right)^2 + C_2 \left(\frac{\partial\sigma}{\partial C_2}\right)^2$$

or

$$V(\sigma) = \left(\frac{1}{N_0 e^{-\lambda\tau}}\right)^2 \frac{1}{8} \left[\left(\frac{C_0/t_0}{(C_0/t_0) - (C_2/t_2)}\right)^2 \right.$$

$$\left. + \frac{1}{C_1}\left(\frac{C_1/t_1}{(C_1/t_1) - K(C_2/t_2)}\right)^2 + \frac{40}{C_2}\left(\frac{K(C_2/t_2)}{(C_1/t_1) - K(C_2/t_2)} - \frac{C_2/t_2}{(C_0/t_0) - (C_2/t_2)}\right)^2 \right]$$

If the nth measurement of σ in a given channel is denoted by σ_n and its variance by V_n define $\bar{\sigma}$ as

$$\bar{\sigma} = \frac{\sum_n \sigma_n/V_n}{\sum_n 1/V_n}$$

Status The problem has been programmed for the ORACLE There are 498 average cross sections to be computed In all there are about 4000 cases to be analyzed or about eight samples in each average For each case there are 10 data items which have to be punched on paper tape before the problem is run

TRANSITION PROBABILITIES AND CRYSTAL REFLECTED NEUTRON BEAM INTENSITIES

Origin C P Stanford Physics Division

Participating Members of Panel M R Arnette M F Todd

Background and Status In order to help carry out a demonstration of neutron spin from the magnetic resonance experiment [8] it was necessary to compute the following

[8] C P Stanford T E Stephenson and S Bernstein *Phys Semiann Prog Rep March 10 1954* ORNL 1705 p 50

formulas

$$P(S, M\ M\ ) = (S + M)!\,(S - M)!\,(S + M\ )!\,(S - M\ )!\left(\sin\frac{\alpha}{2}\right)^{4S}$$

$$\times\left[\sum_{\rho=0}^{2S}(-1)^{\rho}\frac{(\cot\alpha/2)^{M+M\ +2\rho}}{(M + M\ + \rho)!\,(S - M\ - \rho)!\,(S - M - \rho)!\,\rho!}\right]^2$$

$$I(S_j\ M_n) = (7\ 65 - 31\ 05\ SM)^2$$

$$I\ (S_j\ M_n) = \sum_{i=-S}^{S} I(S_j\ M_n)\,P(S_j\ M_i\ M_n)$$

$$N\left(\frac{\alpha}{2}\right) = \sum_{n=-S}^{S} I_n(S_j\ M_n)\,I_n(S_j\ M_n)$$

for $S = 1/2\ 1\ 3/2\ 2\ 5/2$

$-S \leqq M \leqq S$ at intervals of 1

$-S \leqq M \leqq S$ at intervals of 1

$0 \leqq \alpha/2 \leqq 90°$

These formulas were calculated on the ORACLE and 8190 P s and 455 N s were given to C P Stanford

COULOMB WAVE FUNCTIONS

Origin T A Welton Physics Division

Participating Members of Panel S E Atta W C Sangren

Background and Status The regular Coulomb wave function is given in terms of a confluent hypergeometric function by

$$L(l\ \eta\ x) = e^{(-1/2)\pi\eta}\ \frac{|\Gamma(l + 1 + i\eta)|}{2\Gamma(2l + 2)}\ (2x)^{l+1}\ e^{ix}\ {}_1F_1(l + 1 + i\eta\ \ 2l + 2\ -2ix)$$

where

$l = 0\ 1\ 2\ 3\ 4\ 5$

$$x = \sqrt{E}\ \frac{\sqrt{1840}}{137}\sqrt{\frac{A_1A_2}{A_1 + A_2}}\left(A_1^{1/3} + A_2^{1/3}\right)$$

$$\eta = \frac{Zz}{2 \times 137}\ \frac{\sqrt{1840[(A_1A_2)/(A_1 + A_2)]}}{E}$$

This problem has been programmed and checked out on the ORACLE No tables of functions have been prepared however since the National Bureau of Standards has prepared fairly extensive tables

EFFECT OF DEVIATIONS FROM A COULOMB POTENTIAL FOR SCATTERING OF CHARGED PARTICLES

Origin T A Welton Physics Division

Participating Member of Panel M F Todd

Background and Status Numerical integrations were carried out by using Simpson s Rule The problem has been completed and the results have been given to T A Welton

ORACLE CODE FOR TWO GROUP TWO REGION SPHERICAL REACTOR CALCULATION

Origin M C Edlund T B Fowler L C Noderer Reactor Experimental Engineering Division

Participating Members of Panel M R Arnette R A Willoughby

Background and Status The problem considers a spherical homogeneous reactor composed of a core shell and multiplying reflector The variable parameters are (1) core radius (2) shell thickness (3) reflector thickness (4) extrapolation distance (5) Fermi age for core and reflector (6) fast and slow diffusion coefficients for core and reflector (7) average number of fast fission neutrons emitted per thermal neutron captured in fuel for core and reflector (8) resonance escape probability for core and reflector (9) macroscopic absorption cross section of everything but fuel for the core (10) total macroscopic absorption cross section for the reflector (11) macroscopic ab sorption cross section for the fuel in the reflector (12) macroscopic absorption cross section for the shell and (13) diffusion coefficient for the shell The critical equation is represented by a fourth order determinant whose value is zero for criticality For a particular set of input data the critical determinant is made zero by varying indirectly the concentration of fuel in the core For the correct fuel concentration the total macro scopic absorption cross section for the core is obtained and the absorptions in core and reflector and the leakages are computed as output data In addition flux samples are computed if specified at various distances from the center for the core and re flector

The code first computes the elements of the critical determinant that depend upon the reflector parameters and functions The elements of the critical determinant that depend upon the core parameters and functions are then computed by assuming a value of the core concentration and the determinant is evaluated If the value of the de terminant is not less than a number ϵ another value for the core concentration is used those elements affected are recomputed and the critical determinant is again evaluated

When the determinant value becomes less than ϵ the total macroscopic cross section for the core and the absorptions and leakages are computed With each set of input data there is assigned a key word of 10 digits When this key word begins with zero only the above data are punched out If the key word begins with an eight the flux samples as well as the above answers are computed and punched out

SAFETY CALCULATIONS FOR THE HRT

Origin P R Kasten Reactor Experimental Engineering Division

Participating Member of Panel C P Hubbard

Background and Status The kinetic conditions for the HRT have been represented by a system of four first order differential equations and one linear algebraic equation The purpose of the calculations is to determine maximum power and maximum pressure within the reactor for various values of the controllable parameters

The equations were solved by the modified Euler method with the use of a floating decimal point routine coded for this problem

Over 40 cases have been run to date on the ORACLE and additional cases will be run as soon as computer time is available

DISTRIBUTION OF FISSION PRODUCTS IN THE HRE

Origin D O Campbell Chemical Technology Division

Participating Member of Panel S G Campbell

Background and Status In order to interpret the results of the decontamination of the HRE with respect to the distribution of fission products between the reactor fuel solution and any state insoluble in the fuel an estimate of the fission products the reactor had produced at the times of the various radiochemical analyses was necessary The estimate was also required in order to determine the ease of removal of the fission products from the reactor system Because of the intermittent operation of the HRE such a calculation would be formidable The reactor operation was divided into 10 periods each consisting of several consecutive days and the assumption was made that all power produced during the period was produced at the median time of the period On this basis the problem was coded for the ORACLE The code required about 20 min to calculate the activity contributed by 20 fission products of reasonably long half life for 15 different times and to punch the results It is anticipated that the same tapes will be used for future calculations of the same type

A HEAT PROBLEM CONNECTED WITH WASTE DISPOSAL

Origin S H Jury Chemical Technology Division

Participating Members of Panel C L Gerberich J Z Hearon W C Sangren

Background and Status It was necessary to know the temperature distribution in the soil surrounding a large disposal pit containing hot solution In particular the

flux through the bottom of the pit had to be determined so that the boiling rate and hence safety precautions could be established The radius R of the pit is of the order of 250 ft and the depth of the order of 20 ft The pit was idealized as a flat plate in the $Z = 0$ plane It was assumed that the temperature in the pit remained at the boiling point τ_2 of the solution The steady state problem is then

$$\frac{\partial^2 T}{\partial Z^2} + \frac{1}{R^2}\left(\frac{1}{\xi}\frac{\partial T}{\partial \xi} + \frac{\partial^2 T}{\partial \xi^2}\right) = 0$$

$$T(\xi\ 0) = 1 \qquad 0 \leqq \xi \leqq 1$$

$$k\left(\frac{\partial T}{\partial Z}\right)_{Z=0} = hT(\xi\ 0) \qquad \xi > 1$$

where

$T(\xi\ Z) = (\tau - \tau_1)/(\tau_2 - \tau_1)$

τ = temperature at any point

τ_1 = temperature of atmosphere

$\xi = r/R$

$r\ Z$ = cylindrical coordinates

k = thermal conductivity of soil

h = transfer coefficient for soil air interface

The above equations were replaced by appropriate difference equations and after assigning $T(5\ Z) = T(\xi\ 5R) = 0$ and $\partial T(\xi\ Z)/\partial r = 0$ at $\xi = 0$ (by symmetry) a network of 625 points was iterated until the change per iteration was $\leqq 1/10\%$ The problem was completed and the results were returned to S H Jury

APPROXIMATE ENERGY EQUATION FOR THE CYCLONE SEPARATOR

Origin M Whatley Chemical Technology Division

Participating Member of Panel J Z Hearon

Background and Status It is desired to have an equation giving the kinetic energy E of a fluid particle as a function of the distance r from the axis of rotation The dissipation equation is

$$\frac{dE}{dr} = \mu\left(r\frac{d\omega}{dr}\right)^2$$

the energy equation is by *assumption*

$$E = \frac{\rho}{2}(r\omega)^2$$

and the radial velocity of a fluid particle is

$$r = \frac{-Q}{2\pi r}$$

where μ Q and ρ (constant and known) are the viscosity volume flow and density respectively and ω is the angular velocity These equations lead to the equation

$$(1) \qquad E - \left(2K + \frac{1}{r}\right) E + \frac{2KE}{r} + \frac{Kr}{2E} (E)^2 = 0$$

where $K - 2\pi\mu/Q\rho$ If the nonlinear term is neglected it is easily verified that $1 + 2Kr$ and $\exp(1 + 2Kr)$ are particular solutions of the resulting equation If E^* is the E value at $r = r^*$ the maximum value of r and if it is assumed that ω is bounded at the origin so that $E = 0$ at $r = 0$ then

$$(2) \qquad \frac{E}{E^*} = \frac{e^{\beta x} - (1 + \beta x)}{e^{\beta} - (1 + \beta)}$$

where $x = r/r^*$ and $\beta = 2Kr^*$ An improvement of the approximation by expressing the nonlinear term in Eq 1 in terms of the solution (Eq 2) is planned

MODIFIED LEAST SQUARES CURVE FIT

Origin A R Brosi Chemistry Division

Participating Member of Panel C L Gerberich

Background and Status A fit was needed for six sets of experimental information Each of the sets was to be fitted separately by a polynomial of the following type

$$N_t = B + f(w)(a_0 + a_1 w + a_2 w^2)$$

where N_t $f(w)$ and w are values given by the experimental information and B a_0 a_1 a_2 are the constants to be calculated by the modified least squares At the present time the least squares subroutine has been modified to handle such a case but it has not been run on the ORACLE

THERMOCOUPLE CURVE FIT

Origin D J Sasmor Chemistry Division

Participating Member of Panel C L Gerberich

Background and Status This problem was a least squares fit of three sets of experimental information by two polynomials The first was a polynomial of degree 6 and the second of degree 8 The input information was taken from thermocouple experiments and listed millivolts vs temperature The desired polynomials gave millivolts as a function of temperature As a check the polynomials were evaluated from 0 degrees to 1200 degrees at 1 degree intervals As was to be expected the 8 degree polynomial had a better fit in general than the 6 degree polynomial

NEUTRON AND GAMMA SPECTRA INVESTIGATIONS

Origin J B Trice Solid State Division

Participating Member of Panel A C Downing

Background and Status Routine computation for determining the activity of foils irradiated in the Brookhaven Reactor has been coded for the ORACLE The raw data for about 4000 foils have been punched on paper tape and are ready to be fed into the ORACLE when computation schedules permit

CALCULATION OF ENERGY LEVEL VALUES

Origin Henry Morgan Stable Isotope Research and Production Division

Participating Member of Panel M R Arnette

Background and Status The energy of a rotational level may be expressed by

$$E_{j\ k-1\ k+1}(a\ b\ c) = \frac{a+c}{2}[j(j+1)] + \frac{a-c}{2}E_{j\ k-1\ k+1}(\delta)$$

The term $E_{j\ k-1\ k+1}(\delta)$ is defined by

$$E_{j\ k-1\ k+1}(\delta) = w\delta^0 + x\delta^1 + y\delta^2 + z\delta^3$$

Here a b c are rotation constants expressed in megacycles The constants w x y z were determined by the energy level and were supplied

δ is a function of a b c and is defined by

$$\delta = \frac{b-c}{a-c}$$

The parameters (a c δ) were supplied for seven sets The calculation has been done on the ORACLE for the seven sets by taking the value of j from 1 through 12 There were 168 answers for each of the seven sets and an identification word for each answer making a total of 2352 words of printout

EIGENVALUES FROM SYMMETRIC MATRICES

Origin Henry Morgan Stable Isotope Research and Production Division

Participating Members of Panel M R Arnette V C Klema

Background and Status Characteristic values have been obtained for seven real symmetric matrices of order 5

M LINE CHARACTERISTICS – MATRIX SOLUTION

Origin Tennessee Valley Authority

Participating Members of Panel M R Arnette W C Sangren R A Willoughby

Background and Status The first part of this problem is to determine a nonsymmetrical real matrix z which is divided into four submatrices a 42 by 42 42 by 40 40 by 42 and 40 by 40 For simplicity in computing z is broken down into smaller matrices so

that z can be represented by [redacted]

$$z = z_1 - AF^{-1}B - DG^{-1}H$$

where z_1 is a 42 by 42 A is a 42 by 28 D is a 42 by 12 B is a 28 by 42 F is a 28 by 28 H is a 12 by 42 and G is a 12 by 12

So far the inverse of the G^{-1} and part of the inverse of F^{-1} have been obtained

A BATCH MIX MODEL FOR Ca UPTAKE IN BONE

Origin C L Comar UT AEC Agricultural Research Program

Participating Member of Panel J Z Hearon

Background and Status It is desired to have an order of magnitude estimate for the time at which the specific activity of radiocalcium Ca* in bone will be a prescribed fraction of that in the blood stream The model is this To an amount A of calcium is added an amount a of tagged Ca The specific activity of the added sample is x_0 and that of the resultant mixture C_1 From the mixture is removed a sample of amount a and to what remains is added a sample of amount a specific activity x_0 This process is repeated The value of C_n the specific activity of the mixture after n repetitions is to be determined

After the ith repetition the specific activity C_i is given by

$$C_i = \frac{ax_0}{\beta} + \frac{AC_{i-1}}{\beta} \tag{1}$$

where $\beta = A + a$ But $C_0 = 0$ and the recursion (Eq 1) gives

$$\frac{C_n}{x_0} = \frac{a}{\beta} \sum_{k=0}^{n-1} \left(\frac{A}{\beta}\right)^k$$

$$= \frac{a}{\beta} \frac{(A/\beta)^n - 1}{(A/\beta) - 1} = 1 - \left(\frac{A}{\beta}\right)^n$$

When C_n/x_0 is prescribed n may be computed for any A and a and the time for the prescribed value is $n\tau$ where τ is the time per repetition When the crude model has been evaluated the continuous case will be considered with complications such as shunting etc

[redacted] PROJECTS

CAPTURE CROSS SECTION OF Np^{239}

Origin R A Charpie Research Director s Division

Participating Member of Panel A C Downing

Background and Status Observed values for the ratio Pu^{240}/Pu^{239} suggest that the capture cross section of Np^{239} may be very large If this is the case it could radically affect future developments in chemical processing An attempt has therefore been made to deduce this capture cross section from these observed ratios

The production of Pu^{240} from U^{238} is described by the fission chain

$$\begin{tikzcd}
U^{238} \arrow[r, "n"] & U^{239} \arrow[d, "\beta^-"] & \\
& Np^{239} \arrow[r, "n"] \arrow[d, "\beta^-"] & Np^{240} \arrow[d, "\beta^-"] \\
& Pu^{239} \arrow[r, "n"] & Pu^{240} \arrow[r, "n"] & {}
\end{tikzcd}$$

The system of six differential equations describing this system may be solved by Laplace transform methods and an analytical solution obtained Calculations of the ratio of the concentration of Pu^{240}/Pu^{239} were therefore carried out for a parameter study ranging over a number of values for the flux and irradiation time and the capture cross section of Np^{239} The computation has been coded for the ORACLE and the initial parameter study is now being evaluated

MULTIGROUP REACTOR CALCULATIONS

Origin R A Charpie Research Director s Division

Participating Members of Panel N M Dismuke N D Given W C Sangren

References Mathematics Panel Semiannual Progress Reports ORNL 1588 1662

Background and Status The fourth complete multigroup multiregion code has been put in a production status on the UNIVAC This code supersedes the other three In the previous reports a two region code a five region code and a nine region code known as Medusa have been mentioned The latest and fourth code is known as Eye wash Eyewash like Medusa allows as many as nine regions and as many as 60 space points The number of groups for Eyewash can still be as many as 30 although in this code the thermal group can be chosen arbitrarily after the first eight fast groups Eyewash was written to take into account hydrogen scattering The method used is generally referred to as the Goertzel Selengut method A number of package-reactor and criticality experiment calculations have been run off with the use of this code The time for the customary reactor calculation is now about 15 min for two regions and 25 min for nine regions

ESTIMATION OF DOSE INSIDE CREW SHIELD

Origin F C Maienschein Aircraft Nuclear Propulsion Division

Participating Members of Panel S E Atta M F Todd

References Mathematics Panel Semiannual Progress Reports ORNL 1662 1588

Status The computations on the estimation of dose inside the crew shield for radial beam skew beam and direct beam were completed by the use of desk calculators Values of Φ_{kmn} and β_{kmn} from previous UNIVAC calculations were used

EFFECT OF TEMPERATURE ON FLUX DISTRIBUTIONS IN REACTORS

Origin R K Osborn and W K Ergen Aircraft Nuclear Propulsion Division

Participating Member of Panel J H Vander Sluis

Background The effect of temperature upon the energy distribution of neutrons slowing down in an infinite homogeneous absorbing medium is being investigated numerically The transport equation is being integrated directly on the assumptions that the scattering and absorbing atoms are in a Maxwell Boltzmann energy distribution and that the microscopic scattering cross section is energy independent in the center of mass system Solutions are anticipated for several different scattering masses as well as for both $(1/v)$ and resonance absorption

The equation to be solved is $f(x) = \sum_n f_n(x)$ where

$$f_n(x) = \frac{[(A + 1)^2/4A] \int_0^\infty K(x \quad x\ ) f_{n-1}(x\ )\, dx}{xD + (1/\sqrt{\pi})\, e^{-x^2} + [x + (1/2x)]\, \mathrm{erf}(x)}$$

$$A = \text{mass}$$

$$D = \begin{cases} \dfrac{\sum_a}{\sum_s} \dfrac{1}{v} & \text{absorption} \\[2ex] \dfrac{\sum_a}{\sum_s} Q_a(x) & \text{resonance absorption}^{1} \end{cases}$$

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[1] R K Osborn *The Temperature Dependence of a Cross Section Exhibiting a Resonance* Y F10 112 Nov 17 1952

and where

$$K(x\ x\ ) = e^{(1/2A)(x\ ^2 - x^2)} \left\{ e^{(1/2A)|x^2 - x\ ^2|} \left[\operatorname{erf}\left(\frac{|x - x\ |}{2} + \frac{x + x}{2A} \right) - \operatorname{erf}\left(\frac{|x - x\ |}{2A} + \frac{x + x}{2} \right) \right] + e^{-(1/2A)|x^2 - x\ ^2|} \left[\operatorname{erf}\left(- \frac{|x - x\ |}{2A} + \frac{x + x}{2} \right) - \operatorname{erf}\left(\frac{|x - x\ |}{2} - \frac{x + x}{2A} \right) \right] \right\}$$

The use of Hasting s approximation for the error function introduced some scaling difficulties which necessitated the regrouping of the separate terms in the kernel The integration variable was transformed to

$$z = \frac{x}{x_T} = \frac{v}{v_T}$$

where v_T is the speed of the neutrons in thermal equilibrium With this new variable the interval of integration was chosen to be 1/20 and it was discovered that integration from 0 to 200 would be sufficient Because of the large number of kernels required for each calculation the kernels are calculated when needed rather than being calculated once and stored

Status This problem has been checked on the ORACLE through the first iteration It is expected that it will soon be ready to run

MINIMUM COST CALCULATIONS FOR A NUCLEAR REACTOR

Origin H F McDuffie Chemistry Division

Participating Members of Panel A W Kimball G J Atta

Background and Status In the planning and construction of large reactors calculations relating to efficiency of operation are detailed and costly If the services of a high speed digital computer such as the ORACLE are available the speed and economy with which such calculations can be performed are increased manifold but situations will arise in which data of sufficient accuracy can be obtained even though the amount of work is reduced An example of this type of situation occurs in the determination of factor levels at which a reactor may operate with minimum cost

Let the cost of power (y) produced from a nuclear reactor depend on the core diameter (x_1) the fuel concentration (x_2) and the flux (x_3) In a space of four dimensions the function $y = f(x_1\ x_2\ x_3)$ can be visualized as describing a surface which has a minimum at some optimum combination of levels of the three factors To find this optimum one obvious procedure is to compute y for every reasonable combination of factor levels spaced at small intervals Essentially this would amount to constructing the surface

and the number of calculations could easily run into thousands An alternative procedure would make use of some recent work by G E P Box[2] in the exploration and exploitation of response surfaces The method amounts to a stepwise approach to the vicinity of the minimum by the principle of steepest descent and the subsequent fitting of a second or third degree equation in that vicinity The minimum cost combination is then estimated from the fitted equation The number of calculations required depends on the nearness of the original guess to the actual minimum and on the skill and experience of the computer In the present example an experienced computer should be able to find the minimum with not more than 30 calculations and even less if the initial guess is good

The fitting procedure has been applied to some data already available for a one region U^{233} breeder and has been written up in CF 54 3 126

DESIGN PARAMETERS OF THE K 49 REACTOR

Origin J C Bresee and W Stewart M I T Engineering Practice School

Participating Member of Panel A C Downing

Background and Status In designing a reactor to produce Pu^{239} it is desired that the ratio of the production of this isotope to the production of Pu^{240} be maximized A study for the K 49 reactor of the effects of several design parameters upon this ratio was coded for the ORACLE The parameters involved were the rate of the bleed-off stream the reaction rate for the production of plutonium dioxide the ratio of the blanket volume to the total volume and several estimates for the capture cross section of Np^{239} This computation was carried out for two different values of the uranium concentration and associated flux

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[2] G E P Box *Biometrics* 10 16 60 (1954)