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PROTEUS
A COMPUTER CODE TO EXTEND THE BURNUP
DATA FROM A POINT BURNUP CODE

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JUNE 1968

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PROTEUS -
A COMPUTER CODE TO EXTEND THE BURNUP DATA
FROM A POINT BURNUP CODE

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ABSTRACT

A computer code named PROTEUS has been developed to modify and extend data produced by the reactor fuel burnup code ALTHAEA in its zero dimensional mode. PROTEUS simulates either batch or graded fueling, prepares a table of maximum-to-minimum ratios of fuel specific power at constant flux, and calculates analytical curve fits of isotopic concentrations versus burnup.

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P R O T E U S -
A COMPUTER CODE TO EXTEND THE BURNUP DATA
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INTRODUCTION

Analyzing thermal reactor fuel cycles to select likely optimum conditions for a given set of economic circumstances is an extremely complicated process. It requires sifting or surveying a very large number of possible fueling schemes at an even larger number of specific enrichment levels.

In initial surveys of this multitude of possibilities, simplified reactor and economic models are used. Even so, it is necessary to make reasonably good preliminary estimates of the relative concentrations of successively formed isotopes, and this calls for considerable sophistication in reactor physics. Fortunately, in initial surveys, the variations in fuel burnup throughout a reactor need not be known for each fueling scheme investigated. The surveys can be made by considering fuel to be burned in the central region of the reactor wherein the neutron flux does not vary rapidly. Thus the fuel burnup is considered at a point, or in "zero dimension."

If the burnup is calculated using a zero-dimensional code the ability to estimate the reactivity of a reactor in which fuel is moved about during the fuel cycle is limited. This limitation has created a need for a new code. Such a code has been developed and is named PROTEUS. It modifies and extends the zero-dimensional burnup data of the ALTHAEA⁽¹⁾ code. Although the ALTHAEA-PROTEUS combination cannot achieve the detail and accuracy of existing multiple-dimensional burnup codes, it does give, for the time invested (20 seconds per burnup on a 7090 computer), very useful data for analyzing a thermal reactor fuel cycle.

SUMMARY

A new computer code called PROTEUS significantly increases the amount of data obtainable from a single run of the ALTHAEA fuel burnup code in its zero-dimensional mode. The new code converts batch irradiation data at constant fuel power and variable flux level into graded irradiation data at variable fuel power and constant flux level. It estimates the extent to which graded fuel has been irradiated. It prepares a table of maximum-to-minimum ratios of fuel specific power for constant flux cases, rejecting those cases having ratios above some limiting value. It provides a new input to the QUICK economics code by both modifying and extending the data produced by the ALTHAEA code. PROTEUS also calculates analytical curve fits for each isotope as burnup or flux-time.

Appendix A presents a review of least squares technique and of simple exponential fitting.

Appendix B contains a detailed description of a modified version of the Westcott formalism to express reaction rates in terms of effective cross section ratios. This model is involved in calculations both by ALTHAEA and by PROTEUS. In the Westcott formula, the intensity of neutron flux and its energy spectrum are expressed by ϕ_0 and the index r , respectively. These terms have been modified by the ALTHAEA code to better simulate spectral hardening and self-shielding of the major plutonium resonances.

Appendix C contains a Fortran II program of the PROTEUS code.

Appendix D gives a sample printout of a PROTEUS computation.

DISCUSSION

FUELING METHODS

ALTHAEA, when operated as a point burnup code, can conveniently simulate two fueling methods - batch and graded.

Batch Fueling

ALTHAEA can simulate batch fueling on the basis of two assumptions. One is that the fuel is shuffled during the irradiation so that each element of the fuel "sees" the same neutron flux at the same time, even though the flux level and spectrum vary with time. The other assumption is that the neutrons produced in excess of those needed to maintain the chain reaction are absorbed by a control system that does not change the neutron spectrum. This technique of not changing the spectrum is used if graded and batch fuel cycle data are to be prepared from the same ALTHAEA run. The technique of spectral hardening by the control system can be used for an ALTHAEA run that is not to be converted into graded fuel cycle data.

In batch irradiation the reactivity limited lifetime is reached when the excess reactivity calculated by ALTHAEA just compensates for the estimated neutron leakage. An idealized example of the computed batch instantaneous reactivity (X_{mult}) is shown in Figure 1. The minimum value of k_{∞} is shown as the horizontal line labeled "minimum k_{∞} ." When the value of X_{mult} falls below the minimum k_{∞} line, the reactor is considered to be subcritical and the irradiation is terminated. The excess reactivity (indicated by the crosshatched area above the minimum k_{∞} curve but below the instantaneous k_{∞}) is assumed to be adsorbed in a control system that does not change the neutron spectrum.

Graded Fueling

In the graded system, the reactor fueling is arranged so that the excess neutrons (loosely indicated by the crosshatched area above the minimum k_{∞} line) are absorbed in fuel elements deficient in neutron reproduction (the crosshatched area below the minimum k_{∞} line). Since the

FIGURE 1
ALTHAEA Reactivity as a Function of Irradiation Time

X_{mult} curve away almost as a straight line, the average $k_{\infty} A_{\text{mult}}$ of all fuel in the reactor will remain above the minimum k_{∞} line for essentially twice as long in the graded cycle (A_{mult}) as in the batch cycle.

An idealized instance of the graded mode is typified in automatic fueling whereby fresh fuel is continually fed to the reactor while the most depleted fuel is steadily withdrawn. The fuel in the reactor therefore consists of fuel elements having all the intermediate compositions of the burned fuel. Although the interaction of these fuel elements upon each other is difficult to estimate, the two extreme cases that bracket the more likely conditions can be readily analyzed. These are designated as "non-interacted" and "fully interacted" graded cycles.

In a noninteracted graded cycle it is assumed that adjacent fuel elements, although grossly different in isotopic compositions, do not affect the neutron spectrums of one another, even though excess neutrons are made available from fresh fuel to more depleted fuel. A noninteracted graded fuel at a constant flux level but in a spectrum that can vary with the change in concentrations of the various fuel isotopes during the burnup.

In a fully interacted graded cycle, it is assumed that excess neutrons flow to the depleted fuel region and that the neutron energy spectrum is the same for all fuel in the reactor. (This spectrum is the average spectrum of the entire fuel element composition.) A fully interacted graded cycle is equivalent to irradiating fuel at a constant flux level and in a constant spectrum throughout the burnup.

In practice, most thermal reactors on the graded cycle perform intermediately to the extremes described here. The noninteracted graded case described here is unfair to the plutonium fuel cycles because the initial neutron spectrum required is harder than that likely to exist. The spectral index for a fully graded cycle is usually the lowest of all of the systems considered because it has the lowest enrichment requirement.

The reactivity limited lifetime of a fuel element in the graded cycle is reached when the total number of neutrons produced since startup is equal to the number of neutrons absorbed in the fuel plus the number lost

by leakage or otherwise not accounted for during the burnup. ALTHAEA computes the ideal situation by simply averaging the instantaneous reactivity values, disregarding any skewed flux-time relationship. Since no neutron absorptions in a control system are included in this averaging, the minimum value of k_{∞} for criticality can be increased to provide for control sufficient for operation.

ALTHAEA Simulations of Fueling

The primary operating criterion of a power reactor, aside from safety, is that a constant heat rating must be preserved. To achieve this in the ALTHAEA simulation of batch irradiation, the flux is varied inversely as the effective fission cross section* of the fuel. Thus, the specific power of the fuel element, which is the product of the flux and the fission cross section, is constant throughout the burnup. This is shown in Figure 2 for the batch case by the X_{mult} and X_{flux} curves for both U-235 enriched uranium and plutonium-in-natural uranium fueling of a water reactor. Of these two fuels, U-235 enriched uranium requires less flux change to maintain the same power. The reason for this is that plutonium formed from the burning out of U-235 has a cross section larger than that of U-235.

During a graded calculation, the reactor flux level is fixed, while the effective fission cross section varies, so that the specific power of a given fuel element is not constant, and the fuel may not produce the desired power level throughout its lifetime, as shown in Figure 3 by the curves A_{mult} and A_{power} .

It is possible to specify a flux that will make the average specific power equal to the desired value, provided the average fission cross section during the burnup is known, thus simulating the fully interacted graded mode. An iterative ALTHAEA calculation is required to compute a fully interacted graded irradiation case with an assigned specific power. In this process, an average spectral index and an average flux level are computed from the previous run and are compared with the values used to compute the

*Throughout this report, it will be assumed that the effective fission cross section of the fuel is appropriately weighted by the energy of fission for each isotope.

FIGURE 2
ALTHAEA Flux and Reactivity as Functions of Irradiation Time at
Constant Power (Batch Fueling at a Constant Power of 20 MW/ton)

FIGURE 3
ALTHAEA Power and Reactivity as a Function of Irradiation Time at
Constant Flux (Graded Fueling at an Average Power of 20 MW/ton)

previous runs. After two or three successive calculations, the estimated spectral index and flux level will be sufficiently close to the resulting averages that no further iteration is warranted. This can save several successive ALTHAEA burnup calculations, which are time consuming and, for many survey purposes, add no significant accuracy to the mass balances.

An alternate method of calculating graded irradiations is to use the ALTHAEA code to calculate batch (namely, constant power) irradiation of the fuel until the graded reactivity limited lifetime (A_{mult}) is surpassed. The power level of the fuel from these ALTHAEA data is constant and equals the average value. This is not true for an actual graded irradiation (Figure 3), wherein the instantaneous power level of the fuel is usually greater than the average value initially, and decreases to its lowest value just before fuel discharge.

PROTEUS CALCULATIONS

While the data direct from ALTHAEA indicate that the total time of the graded run is correct, the rate at which events occur within the interval requires some adjustment. Having a proper time scale for burn-out of the initial fuel is particularly important to the economics of the fuel cycle wherein the proper mass balances at the end of each accounting period are significant. ⁽²⁾

Code Functions

The PROTEUS code adjusts the time scale by first determining ⁽²⁾ the flux level that would have given the same average specific power with a constant flux for some specific terminal k_{∞} value. It then constructs a graded irradiation time scale based on the principle that the product of time and the graded flux is constant. It will be shown (p. 16) that the formula for the graded flux is the flux-time integration weighted by the effective cross section of the fuel. The PROTEUS code also indicates the maximum-to-minimum heat generation experienced by a fuel element in this graded cycle mode, but this does not include a cosine flux distribution correction.

With minor programming changes PROTEUS could also be altered to simulate, from the same ALTHAEA data, reactors operating at several different specific fuel powers. This would be quite a straightforward change, since the code curve-fits the data versus time, and the time scale can be altered to reflect the changes in specific power. If isotopic decay were important, altering PROTEUS would be a poor practice because satisfactory corrections cannot easily be made for isotopic effects. For example, if PROTEUS were to convert an ALTHAEA run at a specific power of 15 MW/ton to a run at 5 MW/ton the results would be in error because of no provision for sufficient Pu-241 decay. Similarly, a thorium irradiation at 15 MW/ton, converted to 30 MW/ton, would be in error because this would increase the conversion of Pa-233 to U-234 and decrease the yield of U-233. PROTEUS cannot easily reflect these effects, although in some cases approximations would be satisfactory.

PROTEUS sometimes introduces small errors because it fixes a flux level to establish an average fuel power, but uses ALTHAEA calculations of flux spectral index variations with time. The resulting variations in the specific fuel power may be slightly in error because the relative number of epithermal fissions will change with the spectral index, even though the flux level is "constant."

Code Operations

One primary contribution of the PROTEUS code is that both a batch and a graded irradiation case can be obtained from one ALTHAEA burnup calculation and that these two will have the same average specific power. Otherwise, three or more ALTHAEA calculations would be required: (1) a batch irradiation, (2) an approximate graded irradiation, and (3) at least one iteration of the graded irradiation calculation. Another feature of PROTEUS is that cases with different burnup termination criteria can be conveniently constructed from a single ALTHAEA calculation. These cases can be used (1) to determine the effect of a finite number of fuel discharges upon the graded exposure, (2) to determine uncertainties in neutron leakage, and (3) to determine, to a lesser extent, the uncertainties in parasitic absorption allowances.

The graded irradiation calculation made by the PROTEUS code is for the noninteracted case wherein the distribution of neutron energies represented by the spectral index r is determined by the local population of fuel isotopes in the fuel. This case differs from the fully interacted graded model which can at present be obtained by iterating ALTHAEA. Noninteracted graded irradiation calculations are computed in PROTEUS from a batch irradiation calculation performed by ALTHAEA.

The basis of the conversion of batch irradiation data to noninteracted graded data is that the burnup at the graded in-reactor time τ (that is, at constant flux) must be the same as that at the batch irradiation time t (that is, at constant specific power), provided that

$$\tau \phi^*(T) = t \phi^*(t), \quad (1)$$

where T is the total in-reactor time and ϕ^* is the graded irradiation flux, which depends on the in-reactor time. The conversion, as defined by this equation, affects neither the initial nor the terminal conditions (which are a function of τ), but only the conditions at times intermediate to these. Thus $\tau = 0$ when $t = 0$, and $\tau = T$ when $t = T$; but, in general, $\tau \neq t$ when $0 < t < T$. Equation (1) is based on the assumption that the degree of burnup achieved in a constant power irradiation is uniquely determined by the product of the irradiation time and the effective flux during that time.

In essence, the PROTEUS code receives sets of isotopic compositions, sets of cross sections, and an exposure, all of which may be considered as functions of time; PROTEUS then represents them analytically as functions of the dummy variable $\xi = t \phi^*(t)$. From these functions, the properties of the graded irradiated fuel at each economic accounting period can be determined. The formula for the n^{th} accounting period is, from Equation (1),

$$\xi_n = (n - 1) \delta \tau \phi^*(T), \quad (2)$$

where $\delta \tau$ is the interval between accounting periods. An accounting period of six months is required by current AEC regulations. At these intervals the burnup charges and use charges on the fuel are declared and paid.

An advantage of this technique is that it is independent of the criterion (the minimum k_{∞} value) used to terminate the burnup in ALTHAEA. This is true for batch cases as well, and PROTEUS is often used to construct batch irradiation cases for QUICK.⁽²⁾ PROTEUS can actually produce final end points (that is, reactivity limited exposures) for any assigned values of k_{∞} . Thus, simulation of reactors with different leakages requires only the ALTHAEA run. For batch calculations only the properties of the fuel near the terminal time are represented analytically. PROTEUS can also compute graded data for terminal criteria other than those for which the batch case was computed.

An outline of the computational sequence performed by PROTEUS is shown in Table I. The relationship between PROTEUS and the other computer codes used in fuel cycle analysis work is shown in Figure 4.

TABLE I

THE PROTEUS SEQUENCE OF COMPUTATIONS

1. Reads in the ALTHAEA data for a constant power irradiation and determines the in-reactor time, if any, at which the maximum-to-minimum heat transfer limit is exceeded.
2. Inspects the isotopic concentration arrays to determine the portion that will be represented by a polynomial and the portion that will be represented by an exponential curve fit.
3. Computes by the technique of least squares a polynomial expression for the in-reactor time as a function of the appropriate k_{∞} (that is, X_{mult} for batch irradiation, or A_{mult} for graded irradiation) and determines the time corresponding to the specified terminal value. The terminal in-reactor time is either this time or the heat transfer limiting time, whichever is less.
4. Computes an analytical representation of the isotopic compositions and the exposure: (a) in batch cases a function of the in-reactor time in the vicinity of the terminal time, and (b) in graded cases as a function of the parameter $\xi = t\phi^*$ for the entire time.
5. Obtains the fuel properties at each accounting period either from ALTHAEA data in batch cases or from the functions in graded cases. The initial properties of the fuel are supplied by ALTHAEA for both cases, and the final properties are derived from the analytical functions.

FIGURE 4
The Sequence of Fuel Cycle Analysis Computations

Operation of the PROTEUS code is illustrated by a comparison of the changes in U-235 concentration versus time for irradiation at constant specific power and with noninteracted graded fuel. Figure 5 shows these changes for a simulated BWR with an initial uranium enrichment of 3.05 percent. The figure also shows calculations for two different terminal values of k_{∞} -- 1.040 and 1.0175.

The concentration for constant specific power operation is not affected by the terminal k_{∞} , but the concentrations for constant flux operation are different. Because the flux level during a constant specific power irradiation increases as the fuel becomes depleted, the graded flux for longer in-reactor times (that is, lower terminal k_{∞}) will also become greater. Thus, the fuel will tend to burn out faster in these cases. This explains the relationship of the two noninteracted graded cases in Figure 5.

Determination of the Graded Flux

To determine the graded flux it is necessary to know the flux level that will give an average specific power equal to the batch specific power. It can be shown that this flux is simply the cross-section weighted time average of the batch flux. Let

- T = in-reactor time, days
- E = reactor exposure, MWd/ton
- ρ = initial density of the fuel, g/cc
- ϕ = neutron flux, neutrons/cm²-sec (i. e., Westcott Flux, see Appendix B)
- K = constant
- = (gram/ton) (MW-sec/MeV)
- ψ = effective macroscopic fission cross section of the fuel weighted by energy of fission, MeV/cm, or

$$\psi = \sum_{i=1}^n y_i \sigma_i^f e_i \quad (3)$$

where

- n = number of fissile isotopes in the fuel
- y = number density of a given isotope

FIGURE 5
Isotopic Concentration of U-235 in a Boiling Water Reactor (BWR)
Simulation

σ^f = effective fission cross section

e = energy of fission;

therefore

$$E = \int_0^T \frac{K}{\rho} \phi(t) \psi(t) dt . \quad (4)$$

An example of the relationship between the graded flux, ϕ^* , calculated by PROTEUS and the actual and averages fluxes calculated by ALTHAEA is shown in Figure 6. These data are for an extreme example that of a plutonium enriched spike in a boiling water reactor simulation. The initial composition of the plutonium spike was 93 percent Pu-239 and 7 percent Pu-240. The initial fission cross section of the spike fuel was high; but, because the Pu-239 burned out at a much faster rate than the Pu-241 being formed, the initial cross section decreased significantly as the burnup progressed. The flux level, therefore, was greatly increased to compensate for the diminished fission cross section. In the example, the flux level increased by a factor of 1.6 during the first half of the lifetime and by a factor of 100 over the entire reactivity limited lifetime of 1.81 years.

The noninteracted graded irradiation calculation is illustrated by Figure 7 wherein the total power generated by the plutonium spike is shown as a function of in-reactor time. This function is, by definition, linear for batch irradiation. In graded irradiation, most of the power is generated while the fuel is fresh. For example, 50 percent of the power produced in the graded case was generated in the first 35 percent of the residence time.

From Equation (4) ϕ^* is defined by

$$E = \frac{K}{\rho} \phi^* \int_0^T \psi(t) dt$$

or

$$\phi^* = \frac{\int_0^T \phi(t) \psi(t) dt}{\int_0^T \psi(t) dt} \quad (5)$$

FIGURE 6
Actual and Average Flux Levels for Batch Irradiation of a Plutonium Spike in a BWR Simulation

FIGURE 7
Power Generation for Batch and Noninteracted Graded Irradiation of a
Plutonium Enriched Spike in a BWR Simulation

This expression can be simplified for computational purposes by recalling that $\phi(t)$ was computed by ALTHAEA such that

$$\phi(t) \psi(t) = q_o, \text{ a constant.}$$

Substituting this expression into Equation (1) gives

$$\phi^* = \frac{\int_0^T q_o dt}{\int_0^T \frac{q_o}{\phi(t)} dt} = \frac{q_o T}{q_o \int_0^T \frac{dt}{\phi(t)}}$$

so that

$$\phi^*(T) = \frac{T}{\int_0^T \frac{dt}{\phi(t)}} \quad (6)$$

The integral in this equation cannot be calculated exactly, because the flux, or $\phi(t)$, available to PROTEUS is in the form of an array. Thus, a numerical integration is required

$$\int_0^{T_n} \frac{dt}{\phi(t)} \simeq \frac{1}{2} \sum_{i=1}^n (t_i - t_{i-1}) \times \left(\frac{1}{\phi_i} + \frac{1}{\phi_{i-1}} \right) \quad (7)$$

If the same total amount of heat is to be generated within the same period of time in an irradiation with the constant flux ϕ^* , then the READ subroutine of PROTEUS makes a computation in which the denominator of Equation (6) is represented by Equation (7).

From Equation (1), the graded in-reactor time τ_m that corresponds to the batch time of $T/2$ is

$$\tau_m \phi^*(T) = \frac{T}{2} \phi^*(T/2)$$

$$\frac{\tau_m}{T} = 1/2 \frac{\phi^*(T/2)}{\phi^*(T)}$$

or, from Figure 6

$$\begin{aligned}\frac{\tau_m}{T} &= 0.50 \times \frac{2.85 \times 10^{12}}{4.08 \times 10^{12}} \\ &= 0.35 \text{ or } 35\%.\end{aligned}$$

This calculation is actually the opposite of the PROTEUS calculation, in which a graded time is specified and multiplied by the graded flux to obtain a value for the adjusted variable ξ . A value for each dependent variable is then found as a function of ξ .

PROTEUS Results

A fuel cost calculation example was completed with and without PROTEUS to illustrate the adjustments that PROTEUS can make upon ALTHAEA data. An ALTHAEA computation of a slightly enriched uranium simulation of a water moderated and cooled reactor was used. In this case, the ALTHAEA code was instructed to burn the fuel until the time average k_∞ of the fuel became 1.00 as shown by the Direct ALTHAEA Graded Burnup curve of Figure 8. Under such circumstances, the k of a batch loaded reactor would be far below 1. (These general distinctions between batch and graded fueling have been illustrated in Figures 1, 2, and 3.) For batch cycle fuel costs, the ALTHAEA data can be used directly by instructing the code to provide end point data when the instantaneous k_∞ of the fuel passes through an assigned minimum value of k_∞ ($k_\infty = 1.030$ for example). Fuel costs for this example are shown in Table II. For an initial indication of graded fuel cycle costs, ALTHAEA can also be instructed to provide end point data, with the simple time averaged k of the fuel passing through an assigned minimum value of k_∞ ($k_\infty = 1.040$, which is greater than the k_∞ for the batch case above to provide control allowance). Figure 8 shows also the irradiation time and k_∞ curves for various final k_∞ . Fuel costs based upon this approximation are also shown on Table II. With this one ALTHAEA computation, both batch and graded fuel cycle costs can be estimated as shown in Table II, although the graded cycle costs will be off because the method involves a conceptual error in that the specific power of the fuel is constant. This is shown by the horizontal line in Figure 9. As previously discussed, this constant power is achieved by the automatic variation of neutron flux in the ALTHAEA code.

FIGURE 8
Reactivity of a Fuel as a Function of Final k_{∞} for ALTHAEA and PROTEUS Graded Burnups

TABLE II
 MINIMUM FUEL COSTS BASED
 ON A SINGLE COMPUTER BURNUP CALCULATION
 USING ALTHAEA

Initial Fuel Enrichment, wt%	Initial Reactivity	Batch Cycle (Final $k_{\infty} = 1.030$)		Graded Cycle Final Average $k_{\infty} = 1.040$	
		Fuel Exposure, MWd/MT	Fuel Cost, mills/kWh _e	Fuel Exposure, MWd/MT	Fuel Cost, mills/kWh _e
1.98	1.104	11,441	2.458	20,144	1.719
2.37	1.149	16,549	2.134	30,482	1.528
2.77	1.185	21,212	2.039	39,398	1.505
3.16	1.213	25,438	2.031	47,408	1.539
3.56	1.236	29,372	2.062	54,744	1.599
3.95	1.255	33,106	2.115	61,581	1.675
4.34	1.271	36,655	2.178	68,023	1.759

FIGURE 9
Specific Power of Fuel for Different k_{∞} Values

For large power reactors, the flux for graded cycle is essentially constant with time, and PROTEUS makes this correction with a resulting change in specific fuel power, as shown by the sloping curves in Figure 9. This degree of variation in specific fuel power can be indicated from the variation in flux levels from the original ALTHAEA data.

The most important correction made by PROTEUS is to adjust the U-235 concentration versus time, as computed by ALTHAEA. It is significant to note that while ALTHAEA shows U-235 to burn out nonlinearly, the PROTEUS correction shows it to burn out more rapidly. This particular correction is important to fuel costing wherein the initial fuel is financed as an asset at an interest rate different from the general interest rate. For example, the current USAEC use charge is 4.75 percent on slightly enriched uranium, but the general interest rate for a private utility is from 10 to 12.5 percent. In Figure 10, the earlier burnout of U-235, as shown by PROTEUS, results in an earlier transfer of funds from a 4.75 percent interest rate to a 10 to 12.5 interest rate. This is reflected in the data shown in Table III.

The graded cycle shown in Figure 8 is highly idealized in that it assumes nearly continuous charge-discharge of fuel as opposed to discrete fuel movements often involving sizable fractions of the reactor core load. PROTEUS can simulate this latter situation by assigning a higher minimum value to k_{∞} . A stopping point of 1.10, rather than 1.04, is shown in Figure 8, and the resulting effect on fuel specific power is shown in Figure 9. For each of these k_{∞} values, PROTEUS supplies a complete listing of isotope concentrations with time so that fuel costs can be computed appropriately. The assignment of higher k_{∞} values to simulate discrete rather than continuous fuel discharge is developed in the next section.

Neutron Losses to the Control System

Neutron losses can be divided into four groups: (1) fission product absorption, (2) cladding and structural material absorption, (3) neutron leakage, and (4) control system absorption. All four categories are properly accounted for by the ALTHAEA burnup code when used in

FIGURE 10
Comparative Burnout of U-235 for ALTHAEA and PROTEUS Graded Burnups

TABLE III

MINIMIZED GRADED FUEL CYCLE COSTS

Working Capital Interest Rate, <u>%/yr</u>	Fuel Use Charge Rate, <u>%/yr</u>	<u>From ALTHAEA</u>			<u>Corrected by PROTEUS</u>		
		<u>Minimum Fuel Cost, mills/kWh</u>	<u>Fuel Enrichment at Minimum</u>	<u>Fuel Exposure at Minimum</u>	<u>Minimum Fuel Cost, mills/kWh_e</u>	<u>Fuel Enrichment at Minimum</u>	<u>Fuel Exposure at Minimum</u>
12.5	4.75	1.776	2.946	24,980	1.782	3.072	26,050
12.5	10.0	2.002	2.865	23,490	2.017	2.978	24,400
12.5	12.5	2.107	2.838	22,980	2.127	2.944	23,800

one dimension. However, when used as zero dimension only fission product absorption and structural absorption are accounted for. The PROTEUS code serves the function of correcting for control and leakage. A perfect graded system (continuous charging and discharging of fuel) would theoretically sustain no loss of neutrons into the control system. But in actual practice some loss of neutrons must be incurred.

With graded fuel management, some fuel elements have reactivity contributions of less than unity, and others more than unity, but the net is a reactivity slightly greater than unity. The more depleted fuel, with a reactivity less than unity, absorbs excess neutrons from the highly reactive elements, acting much like control rods.

Figure 11 shows a typical curve for reactivity versus time for a fuel element in a reactor simulation with graded fuel management. The graded reactor in the figure is fueled with elements whose reactivity history will be identical. The reactor is ready for discharge when the excess reactivity equals zero. At this point, if perfect neutron exchange exists, Regions 1 and 2 balance the reactivity deficiencies of Regions 3 and 4, and the reactor has no control losses; but at this point it must be refueled. When Region 4 is discharged, Regions 1, 2, and 3 are left, causing an excess reactivity which can be attributed to Region 1 because the reactivities of Regions 2 and 3 balance one another. The excess for a linear reactivity curve would be

$$\begin{aligned} k_{\text{excess}_1} &= k_{\text{max}} \left(\frac{\frac{R-1}{2}}{\frac{R-1}{2} + 1} \right) \\ &= k_{\text{max}} \left(\frac{R-1}{R+1} \right), \end{aligned} \quad (7)$$

where

R = number of regions.

When the new fuel is added, its contribution to excess reactivity is shown as k_{max} . This excess reactivity is evenly distributed through the entire reactor; thus, $k_{\text{excess}_0} = k_{\text{max}}/R$.

FIGURE 11
Linear Reactivity Curve

The average excess for linear reactivity between refuelings is one-half the maximum; thus, for the entire reactor

$$k_{\text{control}} = \frac{k_{\text{max}}}{R + 1} \left(\frac{1 + \frac{R - 1}{R + 1}}{R} \right)$$

$$= \frac{k_{\text{max}}}{R + 1} \quad (8)$$

In the PROTEUS code, a more general form of this equation simply integrates the average reactivity worth for each region instead of assuming linearity as shown in Figure 11.

Table IV shows the average losses to the control system calculated by PROTEUS in milli-k for various initial enrichments irradiated to reactivity limited lifetimes on a graded cycle. The number of regions in a reactor, or the frequency of refueling, is based on a practical time interval between refuelings--here chosen to be 11 months. The loss of neutrons to a control system is relatively constant over the range of exposures from 20,000 to 46,000 MWd/ton.

TABLE IV
CONTROL SYSTEM REQUIREMENTS
FOR A SIMULATED PRESSURIZED WATER REACTOR (PWR)
WITH 11 MONTHS BETWEEN DISCHARGES

<u>Fuel Exposure, MWd/ton</u>	<u>Number of Regions</u>	<u>K_{max}, milli-k</u>	<u>Average Control Requirements, milli-k</u>
13,102	2	149	64
20,587	4	185	65
38,067	5	213	66
33,675	6	236	67
41,159	7	255	65
46,767	7	271	65
52,282	8	285	63

Below 20,000 and above 46,000 the loss rate is less. The reduction in loss to the control system for long exposures is due to a self-shielding effect. For although the addition of more enriching material will eventually produce more exposure, the fuel is self-shielded at time zero and produces a smaller initial excess reactivity per gram of fissile fuel. The cases experiencing lower exposures also show a reduction in control losses. If U-235 is used as a fuel, it is evident that the immediate breeding of plutonium makes the curve nonlinear, so that a greater exposure is achieved than would have been predicted from the initial reactivity.

For a single fuel exposure the effect of increasing the number of discharges per fuel element lifetime is to decrease the loss to the control system, as shown in Table V.

TABLE V
AVERAGE CONTROL SYSTEM REQUIREMENT
AS A FUNCTION OF THE NUMBER OF REGIONS
FOR A SIMULATED PWR FUEL
WITH AN EXPOSURE OF 20,000 MWd/ton

<u>Time Between Discharges</u>	<u>Number of Regions</u>	<u>Average Control Requirement, milli-k</u>
11 months	4	65.0
6 months	7	38.2
1 month	42	6.8
1 day	1260	0.2

This system of accounting for control requirements allows the zero-dimensional mode of the ALTHAEA code to make a better simulation of practical graded fuel management.

ANALYTICAL REPRESENTATION OF ALTHAEA DATA

The accurate representation of ALTHAEA data by simple analytical functions is the most difficult part of the PROTEUS calculation. In order to obtain a reasonable compromise between accuracy and speed, three principles were followed.

1. Every set of data, regardless of the variable that it represents, should be handled in the same general manner.
2. The accuracy of the curve fitted to a set of data points should be the best for those points whose ordinates have the highest values.
3. Only a minimal amount of input data should be required to supplement the ALTHAEA data.

A set of data points to be curve-fitted is divided in two separate parts. In the portion that contains the higher values, a third order polynomial is used; in the portion containing the lower values, an exponential function is used. In the most common cases, the maximum and minimum values of the function occur on the boundaries of the region, and the division is made arbitrarily by specifying that neither the ratio of the maximum to the minimum value of the dependent variable in the portion to be fitted by a polynomial nor the slope of the curve in this region should exceed 10. If these criteria are satisfied over the entire interval, the exponential portion of the fit will be omitted. Some more arbitrary and less accurate fits are made for the cases when a maximum or minimum, or both, are contained within the region. When only the data in a limited portion of the interval are fitted, the polynomial is used exclusively. The techniques of least squares and of the exponential approximation are described in Appendix A.

REFERENCES

1. E. T. Merrill. ALTHAEA, Part I. A One-Dimensional Two-Group Diffusion Code with an Effective Four-Group Burnup, BNWL-462 (To be published).
2. E. A. Eschbach, D. E. Deonigi, and S. Goldsmith. QUICK - A Simplified Fuel Cost Code, HW-71812. January 2, 1962.
3. Cornelius Lanczos. Applied Analysis, Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1956.
4. R. D. Crout. A Short Method for Evaluating Determinants and Solving Systems of Linear Equations with Real or Complex Coefficients, AIEE Transactions, Vol. 60, pp. 1235-40, 1941.
5. E. A. Eschbach and R. L. Watts. Unpublished Data, Battelle-Northwest Laboratory, Richland, Washington.
6. C. H. Westcott. The Specification of Neutron Flux and Effective Cross Sections in Reactor Calculations, CRRP-662. August 15, 1956.
7. P. F. Gast. "Physics of Plutonium in Thermal Reactors," Plutonium as a Power Reactor Fuel, HW-75007. December, 1962.
8. F. G. Dawson and L. H. Steves. Comparison of Westcott Spectrum with the Gas and Water Kernel Models. Determination of the Neutron Temperature and Epi-Thermal Index, HW-75278. October, 1962.
9. C. H. Westcott. Effective Cross Section Values for Well-Moderated Thermal Reactor Spectra (3rd Edition, Corrected) CRRP-960. November 1, 1960.
10. R. L. Murray. Nuclear Reactor Physics, Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1957.
11. R. C. Liikala. Westcott Parameters Derived from the RBU Basic Library for a Δ -4 Cutoff, HW-77389. April 25, 1963.

APPENDIX A

BASIS OF THE ANALYTICAL EXPRESSIONS USED IN THE PROTEUS CODE

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Each set of empirical data produced by the ALTHAEA code is represented in PROTEUS by a combination of an exponential and a polynomial function. The coefficients of the exponential are calculated so that they will exactly match three selected data points; the coefficients of the polynomial are calculated by the principle of least squares.⁽³⁾ Actually, the polynomial is used to represent the difference between the empirical data points and a linear approximation--a technique which improves the accuracy of the fit and reduces the computing time.

The following two sections describe the basis for the expressions contained in the program.

Exponential Expression

The exponential expression has the form

$$y(x) = b[1 - e^{-p(x-x_0)}] + y_0 \quad . \quad (A1)$$

The arbitrary coefficients b and p can be determined by specifying that the curve will pass through the data points (x_1, y_1) and (x_2, y_2) in addition to (x_0, y_0) . A formula for each of these coefficients is quite simple if the independent variables are equally spaced (that is, $x_2 - x_1 = x_1 - x_0$) for then

$$\begin{aligned} \frac{y_2 - y_0}{y_1 - y_0} &= \frac{1 - e^{-p(x_2 - x_0)}}{1 - e^{-p(x_1 - x_0)}} \\ &= 1 + e^{-1/2 p(x_2 - x_0)} \quad . \quad (A2) \end{aligned}$$

Therefore

$$p = \frac{2}{x_2 - x_0} \ln \left(\frac{y_1 - y_0}{y_2 - y_1} \right) \quad . \quad (A3)$$

Substituting Equation (A3) into Equation (A1), with $x = x_1$ and $y = y_1$, gives

$$b = \frac{(y_1 - y_0)^2}{y_2 - 2y_1 + y_0} \quad . \quad (A4)$$

Unfortunately, x_1 is seldom exactly halfway between s_0 and x_2 , and the coefficients p and b must be obtained by an iterative calculation based on the two data points that bracket the center of the interval. As a first approximation, Equations (A3) and (A4) are used with a value of y_1 determined by a linear interpolation between the bracketing values. Subsequent approximations are made by adjusting y_1 such that the error in the representation of one of the chosen data points is reduced to zero. Equation (A3) is always used to calculate p , but it is more convenient to use the following alternative expression to calculate b :

$$b = \frac{y_2 - y_0}{1 - e^{-p(x_2 - x_0)}} \quad . \quad (A5)$$

Adequate convergence is usually obtained within five iterations. This calculation is contained in the EXPC subroutine of the PROTEUS code.

Least Squares Polynomial

An m^{th} order polynomial expression has the form

$$y(x) = a_0 + a_1x + a_2x^2 + \cdots + a_mx^m \quad , \quad (A6)$$

where the coefficients of the polynomial $a_0, \dots, a_m$ can be determined by the principle of least squares, as described in the following paragraphs.

The differences between the ordinates given by Equation (A6) and the y coordinates of the actual data points are called residuals--namely, for $x = x_i$, the residual δ_i is:

$$\delta_i = y_i - \sum_{j=0}^m a_j x_i^j \quad . \quad (A7)$$

The best principle of least squares states that the curve (of a given order) that best represents the data is that curve for which the sum of the squares of the residuals is a minimum. In other words, the coefficients $a_0, a_1, \dots, a_m$ of the m^{th} order polynomial that provides the best representation to n given

data points are determined when $\sum_{i=1}^m \delta_i^2$ has its smallest possible value.

It is necessary to have at least $1 + m$ empirical data points and it may be assumed that each of the points has equal importance or weighting.

Let

$$\begin{aligned} f(a_0, a_1, \dots, a_m) &\equiv \sum_{i=1}^n \delta_i^2 \\ &= \sum_{i=1}^n y_i^2 - \sum_{j=0}^m a_j x_i^j^2 ; \end{aligned} \quad (\text{A8})$$

then, the least squares principle will be expressed by the set of equations obtained by differentiating Equation (A8) with respect to each of the a 's and by equating each result to zero. For example, the p^{th} equation of this set is:

$$\frac{\partial f}{\partial a_p} = -2 \sum_{i=1}^n x_i^p \delta_i = 0 .$$

With Equation (A7), this can be written as

$$\sum_{i=1}^n x_i^p \sum_{j=0}^m a_j x_i^j - y_i^2 = 0 ,$$

or

$$a_0 \sum_{i=1}^n x_i^p + a_1 \sum_{i=1}^n x_i^{p+1} + \dots + a_m \sum_{i=1}^n x_i^{p+m} = \sum_{i=1}^n x_i^p y_i . \quad (\text{A9})$$

There will be m of these equations--namely, $p = 1, 2, \dots, m$.

For convenience, define the set of variables $a_0, a_1, \dots, a_m$ as the $m + 1$ component vector $\underline{A}$. Let the coefficients of the a 's in the set of simultaneous equations be designated as the $(m + 1)$ by $(m + 1)$ matrix $\underline{D}$. Finally, let the terms on the right-hand side of the equations be represented by the $m + 1$ component vector $\underline{C}$. With this notation, the set of simultaneous equations can be compactly written as the matrix equation

$$\underline{D} \underline{A} = \underline{C},$$

which has the solution

$$\underline{A} = \underline{D}^{-1} \underline{C}. \quad (\text{A10})$$

The coefficients of an m^{th} order polynomial that will represent n empirical data points determined by the principle of least squares are given, therefore, by the product of the inverse of the matrix

$$D = \begin{pmatrix} n & \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 & \dots & \sum_{i=1}^n x_i^m \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 & \dots & \dots & \dots \\ \sum_{i=1}^n x_i^2 & \dots & \dots & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{i=1}^n x_i^m & \dots & \dots & \dots & \sum_{i=1}^n x_i^{2m} \end{pmatrix}$$

and the column vector

$$C = \begin{pmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \\ \vdots \\ \sum_{i=1}^n x_i^m y_i \end{pmatrix}$$

There are many standard routines⁽⁴⁾ by which this product can be computed, but the better ones recognize that $\underline{D}$ is symmetrical.

It should be noted that it is not usually desirable to obtain $\underline{D}^{-1}$ explicitly* unless the computation is to be repeated with a different $\underline{C}$. Also, because of round-off errors in the computation, an iterative calculation is often required to obtain the polynomial coefficients with sufficient precision.^(4, 5)

* A general rule for the construction of the inverse of a matrix is that each entry in the inverted matrix equals the cofactor of the corresponding entry in the transposed original matrix divided by the determinant of the original matrix. (The transpose of a matrix is formed by interchanging rows and columns.)

APPENDIX B

THE WESTCOTT REACTION RATE FORMULA

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THE WESTCOTT REACTION RATE FORMULA

The cross-section and flux notation used in the ALTHAEA and PROTEUS codes is based on that of Westcott.⁽⁶⁾ However, because the Westcott system was devised for well-moderated neutron interactions with extremely dilute fuel, the ALTHAEA version of this system has been extensively modified to apply also to a harder spectrum. The modifications include primarily:

- 1) Corrections to the reaction cross sections in order to account for the resonance shielding.⁽⁷⁾
- 2) Prescriptions relating the effective neutron temperature to the temperature of the moderator.⁽⁸⁾
- 3) Provisions for introducing a fast fission factor and other geometric effects.

A discussion of these items follows a discussion of the basic Westcott formulation.

Basis of Westcott's Formulation

The Westcott system is based on the usual formula for the reaction rate

$$R = \int_0^{\infty} N \sigma(v) n(v) v \, dv \quad , \quad (B1)$$

where

R = reaction rate, events/cm³-sec

N = number density of a given isotope, number/cm³

v = speed of the neutron with respect to the given isotope,
cm/sec

σ = cross section for the reaction, cm²

n = neutron density, number/cm³.

It is understood the value of σ in Equation (B1) corresponds to some particular reaction (that is, fission, capture, etc.).

Westcott's reaction rate formula is essentially an integrated form of Equation (B1):⁽⁹⁾

$$R = N \hat{\sigma} n_o v_o, \quad (B2)$$

where

$$\begin{aligned} \hat{\sigma} &= \text{the effective cross section for the reaction, cm}^2 \\ n_o &= \text{the total neutron density, number/cm}^3 \\ v_o &= \text{a representative neutron speed, cm/sec.} \end{aligned}$$

Because N , n_o , and v_o can be specified in a given situation, the problem of calculating the reaction rate changes from that of integrating Equation (B1) to that of calculating an effective cross section for the reaction.

An expression for the effective cross section can be obtained by equating the right-hand sides of Equations (B1) and (B2):

$$N \hat{\sigma} n_o v_o = N \int_0^{\infty} \sigma(v) n(v) v dv.$$

Solving this for $\hat{\sigma}$ and noting that by definition

$$n_o = \int_0^{\infty} n(v) dv$$

gives

$$\hat{\sigma} = \frac{\int_0^{\infty} \sigma(v) n(v) v dv}{v_o \int_0^{\infty} n(v) dv}. \quad (B3)$$

It is evident that when every neutron has just the right speed, or v_o , Equations (B1) and (B2) become identical, and the effective cross section will equal $\sigma(v_o) \equiv \sigma_o$ (that is, the cross section at the speed v_o). The same result will be obtained in the more realistic situation wherein the reaction cross section is inversely proportional to the neutron speed--a $1/v$ cross section.*

* A material having such a cross section is said to be a "1/v absorber."

A cross section that varies as $1/v$ can be expressed in the form

$$\sigma(v) = \frac{\sigma_o v_o}{v} \quad . \quad (B4)$$

Substituting this relation into Equation (B3) gives

$$\hat{\sigma} = \sigma_o \frac{\int_0^{\infty} n(v) dv}{\int_0^{\infty} n(v) dv} \quad ,$$

so that $\hat{\sigma} = \sigma_o$ for a $1/v$ absorber.

Two things concerning the above result should be emphasized. The effective cross section for a $1/v$ absorber is completely independent of the neutron speed distribution, and there is no restriction on the choice of the representative neutron speed v_o . Thus, $\hat{\sigma}$ will equal the cross section evaluated at whatever neutron speed is specified in the defining equation [that is, Equation (B2)], regardless of the distribution of neutron speeds.

In most cases a $1/v$ approximation is not adequate--mainly because of resonance peaks, as shown in Figure B1. However, much of the simplicity of the approach outlined for $1/v$ absorbers can be retained by introducing a "non- $1/v$ " correction factor, so that the effective cross section is given by the product $g\sigma_o$.⁽¹⁰⁾ The g factor is obtained from experimentally determined cross-section values as will be shown. Note that the neutron speed distribution must be specified in order to evaluate g .

Maxwellian Distribution of Neutron Speeds

The speeds of neutrons completely in equilibrium with the atoms of a moderator are accurately represented by Maxwell's gas equation.⁽¹⁰⁾

$$n(v)dv = n_o A v^2 e^{-B^2 v^2} dv \quad , \quad (B5)$$

FIGURE B1
Fission Cross Section for Pu-239 as a Function of the Speed of the Incident Neutron

where

$n(v)dv$ = number of neutrons having a speed between v and $v + dv$, number/cm³

n_0 = total neutron density, number/cm³

v = neutron speed, cm/sec

and

$$A = 4\pi \left(\frac{m}{2\pi kT} \right)^{3/2}$$

$$B = \left(\frac{m}{2kT} \right)^{1/2},$$

where

m = neutron mass

= 1.6747×10^{-24} grams

k = Boltzmann's constant

= 1.38044×10^{-16} erg/°K or 8.6164×10^{-5} eV/°K

T = effective neutron temperature, °K.

The effect of the parameter T is shown by Figure B2 wherein Equation (B5) is graphed for three different values of the temperature. It is evident from the figure that the most probable neutron velocity (hereafter denoted as v_p) is a function of the temperature, and can be obtained by equating the first derivative with respect to velocity of Equation (B5) to zero. This gives

$$v_p = \sqrt{\frac{2kT}{\pi m}} \quad (B6)$$

E_p , the energy that corresponds to this velocity, is $1/2 mv_p^2$ so that from Equation (B6) one obtains $E_p = kT$.

The temperature of well thermalized neutrons--those in thermal equilibrium with the moderator--is essentially that of the moderator.

A convenient reference point, therefore, is room temperature, 293 °K.

Let this temperature and the corresponding most probable velocity be denoted as T_0 and v_0 , respectively. From Equation (B6) the most probable velocity for room temperature neutrons is found to be 2200 meters per second, while the corresponding energy is 0.0253 eV. Note that the most

FIGURE B2
Maxwellian Distribution of Neutron Speeds at Three Different Temperatures

probable velocity for a Maxwellian distribution at temperature T is related to the most probable velocity for a room temperature distribution by the expression

$$v_p(T) = v_o \sqrt{\frac{T}{T_o}} .$$

The average velocity associated with the Maxwellian distribution can be found by substituting Equation (B5) into the defining relation

$$\bar{v} \equiv \frac{\int_0^{\infty} v n(v) dv}{\int_0^{\infty} n(v) dv} \quad (B7)$$

to obtain

$$\bar{v} \equiv A \int_0^{\infty} v^3 e^{-B^2 v^2} dv ,$$

with the result* that

$$\bar{v} = \sqrt{\frac{8kT}{\pi m}} . \quad (B8)$$

* The integral is most conveniently evaluated by changing the variable to $X = B^2 v^2$, for then

$$\begin{aligned} \bar{v} &= \frac{A}{2B^4} \int_0^{\infty} x e^{-x} dx = \frac{A}{2B^4} (x + 1) e^{-x} \Big|_0^{\infty} \\ &= \frac{A}{2B^4} \end{aligned}$$

Combining Equation (B8) with Equation (B6) for $T = T_0$ (that is, $v_p(T_0) = v_0$) gives the following relationship between the average velocity at a temperature T and the most probable velocity at room temperature:

$$\frac{\bar{v}}{v_0} = \sqrt{\frac{4T}{\pi T_0}} \quad (B9)$$

It is convenient at this point to introduce the average cross section $\bar{\sigma}$ and to relate it to the effective cross section $\hat{\sigma}$. The defining relation for the average cross section is

$$\bar{\sigma} = \frac{\int_0^{\infty} \sigma(v)n(v)v \, dv}{\int_0^{\infty} n(v)v \, dv} .$$

Comparing this formula with Equation (B3), which defines $\hat{\sigma}$, and with Equation (B7) shows that for an effective cross section at room temperature

$$\hat{\sigma} = \bar{\sigma} \frac{\bar{v}}{v_0} \quad (B10)$$

The "non-1/v" factor g can be defined as the ratio

$$g = \frac{\hat{\sigma}}{\sigma_0} .$$

Substituting the value of the effective cross section from Equation (B10) gives

$$g = \left(\frac{\bar{\sigma}}{\sigma_0} \right) \left(\frac{\bar{v}}{v_0} \right) .$$

With Equation (B9), this can be written

$$g(T) = \frac{\bar{\sigma}}{\sigma_0} \sqrt{\frac{4T}{\pi T_0}} \quad (B11)$$

Equation (B11) is actually used to compile the g factors as a function of temperature for various fuel isotopes.⁽¹⁰⁾

The Westcott Flux Spectrum

In the following discussion it will be convenient to characterize the neutron speed distribution $n(v)$ as a flux ϕ , where

$$\phi = n(v)v ,$$

and to consider the neutron energy $E = 1/2 mv^2$ as the independent variable.* The functional dependence of the neutron flux upon the energy is called a flux spectrum.

The thermal reactor flux spectrum assumed by Westcott is a combination of Maxwellian distribution for the low or thermal neutron energies, a $1/E$ distribution for the high or epithermal energies, and a joining or cutoff function.⁽³⁾ The joining function is a particularly sensitive formulation because some important near-thermal resonances lie near the cutoff point (see Figure B1). Much of the disagreement among various investigators in this field is in their choice of a joining function.

The equation for the flux spectrum suggested by Westcott has the form⁽⁸⁾

$$\phi(E) = \frac{E}{(kT)^2} e^{-E/kT} + \frac{\beta\Delta}{E} , \quad (B12)$$

where

ϕ = neutron flux, number/cm²-sec

E = neutron energy, eV

T = neutron temperature, °K

k = Boltzmann constant

β = epithermal-to-thermal flux ratio

Δ = joining function between the Maxwellian and the $1/E$ tail.

For thermal energies, Equation (B12) will be essentially a Maxwellian distribution. For epithermal energies, Equation (B12) will be essentially a $1/E$ variation, in accordance with theoretical calculations for slowing down

* This is energy with respect to the target nucleus and is not an absolute value.

in a nonabsorbing medium.⁽⁷⁾ (Note that the $1/E$ approximation is most accurate for slowing down in hydrogen and holds fairly well in all media for energies sufficiently below those of fission neutrons.)

The joining function originally suggested by Westcott was designed to be zero for energies less than some "cutoff energy," μkT , and 1 for energies greater than this.* Westcott later modified the step function approach in order to present data based on four different formulations of Δ . These are shown in Figure B3. The $\Delta 4$ formulation is generally used, however.⁽¹¹⁾

Using the neutron spectrum represented by Equation (B12) gives the following formula for the effective cross section.⁽³⁾

$$\hat{\sigma} = \sigma_0(g + rs) \quad , \quad (B13)$$

where

$$\begin{aligned} \sigma_0 &= \text{"2200 m/sec cross section," cm}^2 \\ g &= \text{non-1/v factor for thermal energies} \\ s &= \text{non-1/v factor for epithermal energies} \\ r &= \text{spectral index.} \end{aligned}$$

Both g and s are functions of the neutron temperature, except when the absorber obeys the $1/v$ law. In this case, $g = 1$, and $s = 0$. The spectral index r is a parameter that characterizes the fraction of epithermal neutrons in the spectrum and is related to β , the epithermal-to-thermal flux ratio, by the expression

$$r = \frac{\beta}{1 + b\beta} \quad , \quad (B14)$$

where

$$b = \frac{4}{\sqrt{\pi\mu}} \quad . \quad (B15)$$

Finally, the computational formula used to obtain the s factor⁽³⁾ is

$$s = \frac{\Sigma}{\sigma_0} \sqrt{\frac{4T}{\pi T_0}} - bg \quad , \quad (B16)$$

*Note that the ratio of the cutoff energy to the most probable energy in the Maxwellian is simply μ , which in the $\Delta 4$ formulation is 3.681.

FIGURE B3
Westcott Cutoff, or Joining, Functions

where Σ is the infinite dilution resonance integral in cm^2 , and g is obtained from Equation (B11).

Improved Techniques Used by ALTHAEA

Even though the Westcott system is limited to well moderated reactors, its very simplicity makes it useful in a survey code such as ALTHAEA, and a number of modifications to the system have extended its applicability. These modifications, and the techniques used by the ALTHAEA code can be described as follows:

1. Cross sections are determined from a four-group structure made up of
 - a) a high energy fast group (6 MeV to 0.2 MeV) capable of including n-2n reactions of all isotopes being considered,
 - b) a slowing-down group to 0.683 eV,
 - c) a resonance absorption group to thermal energies, and
 - d) a thermal group. (The fast, slowing-down, and resonance absorption groups are combined to form the Westcott "s".)
2. The Westcott "r", or spectral index, is calculated as a function of cell geometry, blackness of the cell (a function of the material cross sections), and some calibratable coefficient.
3. The neutron temperature is calculated as a function of the moderator temperature, cell blackness, and a calibratable constant.
4. The spectrum, cross sections and neutron temperature are all calculated by an iterative process.
5. The resonances are handled by using lumped resonance parameters (a function of fuel temperature) to account for Doppler broadening and self-shielding. These parameters are available in the two intermediate energy groups for both absorption and fission cross sections. The cross-shielding effect is included during the self-shielding calculation. This calculation

- includes the lumped resonance parameters of all other isotopes whose resonances overlap that of the isotope being considered.
6. Burnup equations are solved by means of the Runge-Kutta technique, which is essentially an inverted Simpson's rule. The Runge-Kutta burnup system, based on the rate of change of spectrum and/or isotopic concentration, determines the time-step length and how often the cross sections are calculated.
 7. The external P_3 cell calculation used requires only 2 or 3 seconds. This calculation supplies the ALTHAEA code with the thermal flux depression (a function of fuel blackness), the fast effect contribution, and a lumped nonfuel absorption cross section.
 8. The cross section library is derived automatically from the RBU cross section library.

APPENDIX C

PRINTOUT OF THE PROTEUS CODE
AND ITS KEY SUBROUTINES

```

* LABEL
C 905 PROTEUS MAIN PROGRAM
C
C CONTROL CARD FORMAT 5I2,13,12,2F5.0,1X,A4,1X,A4,F8.4,F8.0,4F8.4
C
C COLUMNS
C
C M1=0, WILL DO GRADED THEN RETURN AND DO BATCH CASES 01-02
C =1, FOR BATCH ONLY
C =2, FOR GRADED ONLY
C
C LS=0, PROGRAM WILL START WITH FIRST MELEAGER CASE 03-04
C =1, PROGRAM WILL START WITH THE
C CASE NUMBER IN COLUMNS 27-30
C LSTP=0, PROGRAM WILL END WITH LAST MELEAGER CASE 05-06
C =1, PROGRAM WILL END WITH CASE PRECEDING THE
C CASE NUMBER IN COLUMNS 32-35
C N9=0, FOR EXIT AT END OF JOB 07-08
C =N, NUMBER OF CHAIN LINK TO BE CALLED AT END OF JOB
C
C NBUG=0, FOR MINIMUM PRINTOUT 09-10
C =1, FOR COMPLETE PRINTOUT
C
C ITAPE=0, NORMAL OPERATION-INPUT TAPE IS B-8 11-13
C =N, INPUT TAPE IS B-N
C
C IRECYC=0, NORMAL OPERATION-NEEDS TWO GRADED ENDPOINTS 14-15
C =1, FOR ONE GRADED END POINT
C
C DAYS=0, THEORETICAL GRADED - NORMAL OPERATION 16-20
C =D, DAYS BETWEEN SHUT-DOWN TO REFUEL
C (IF D IS GREATER THAN ZERO, EN2 SHOULD BE SET EQUAL
C (TO 1+ ALLOWANCE FOR LEAKAGE AND NON-INTERACTION
C (IN THE FUEL)
C
C FACTOR=0, NORMAL OPERATION 21-25
C =F, MULTIPLIER FOR NON-INTERACTION
C
C SHUS= CASE NUMBER FOR START IF M2=1 27-30
C STP= CASE NUMBER FOR EXIT 32-35
C
C PERIOD=0, NORMAL OPERATION(SIX MONTH ECONOMIC PERIOD) 36-43
C =P, TIME IN DAYS BETWEEN ECONOMIC CALCULATIONS
C
C RATE=0, NORMAL OPERATION 44-51
C =R, GREATEST MAX TO MIN HEAT TRANSFER RATIO ALLOWED
C
C EN1= FINAL K FOR BATCH CASES 52-59

```

C-1

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```

C      EN2=      FINAL K FOR GRADED CASES                                60-67
C
C
C
COMMON ICOM,COM
COMMON X,Y,N4N,M10,THIS,IS,EN,M2,KOP,M1,MQ,JJ,ID9,AAA,RATE,STP
COMMON RI,RA,MSZ,CUT,SDENS,I8,IREFCYC,DAY,EEN2,EXPT,FACTOR
C
DIMENSION ICOM(20),COM(80)
DIMENSION MQ(45),EN(3),Y(45,150),X(150),AAA(22),BP(45),DATA(150,5)
1,XY(20),XX(21,22),A(10),XXI(15,15),CHECK(15,16),CP(45),IS(45),
2TX(3),Z(45,150),BB(45,10),W(150),EY(150),B(21),JJ(45),T(150),
3NB7(2),MM(45),ERROR(5),N4N(2,3),EXPT(150)
C
C
MSZ=44
A(1)=6H      NO
A(2)=2HNE
A(3)=6H      OMI
A(4)=4HTTED
A(5)=6HQUESTI
A(6)=6HONABLE
A(7)=6HPART O
A(8)=6HMITTED
C
THIS=5H THE
XXX=4HXXXX
XXXX=6H XXXXX
M=4
M9=1
C
C
WRITE OUTPUT TAPE 3,1003
C
READ INPUT TAPE 2,1000,M1,LS,LSTP,N9,NBUG,I8,IREFCYC,DAYS,FACTOR,
XSHUS,STP,PERIOD,RATE,EN,CUT
C
WRITE OUTPUT TAPE3,1000,M1,LS,LSTP,N9,NBUG,I8,IREFCYC,DAYS,FACTOR,
XSHUS,STP,PERIOD,RATE,EN,CUT
C
PERIOD=PERIOD*86400.*1.E-7
C
4 IF (RATE-1.0) 5,5,6
5 RATE=10000.0
C
6 IF (N9) 7,7,10
7 PRINT 1002
PAUSE

```

C-2

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```

C
10 IF (M1) 11,11,12
11 M1=2
   MRR=1
   GO TO 15
12 IF (M1-3) 15,11,13
13 M1=1

C
15 IF (LSTP) 20,20,17
17 STP=4H9999

C
20 IF (EN(1)) 21,21,22
21 EN(1)=1.030
22 IF (EN(2)) 23,23,24
23 EN(2)=1.040
24 EN(3)=EN(2)
   IF (I8) 26,25,26
25 I8 = 8

C
26 IF (FACTOR) 28,27,28
27 FACTOR=1.0
28 IF (PERIOD) 30,29,30
29 PERIOD=1.5759
30 WRITE OUTPUT TAPE 3,1000,M1,LS,LSTP,N9,NBUG,I8,IREFCYC,DAYS,FACTOR,
   XSHUS,STP,PERIOD,RATE,EN,CUT

C
   EEN2=EN(2)
   DAY=DAYS
   WRITE OUTPUT TAPE 3,1025

C
31 CALL RDYTP(7)
35 GO TO (40,36,36),M9
36 CALL RDYTP(5)
37 GO TO (40,40,38),M9
38 READ INPUT TAPE 5,2070,MHUS
   CALL COMPAR (MHUS,XXXX,6,J)
   GO TO (38,60,38),J

C
40 CALL RDYTP(I8)
42 IF (LS) 43,43,45

C
43 READ INPUT TAPE 18,2076,MHUS
44 CALL COMPAR (MHUS,THIS,6,J)
   GO TO (43,46,43),J

C
45 READ INPUT TAPE 18,4005,SSS
   CALL COMPAR (SSS,SHUS,4,J)
   GO TO (45,46,45),J

```



```

C
46 BACKSPACE 18
49 GO TO (70,50,60),M9
50 WRITE OUTPUT TAPE 5,2070,XXXX
   GO TO 70
C
60 READ INPUT TAPE 5,1035,CMULT,DMULT,EMULT,Y(13,1),Y(14,1),M10,ID9
   CALL COMPAR (M10,XXX ,4,J)
   GO TO (62,980,62),J
C
62 NT=1
63 N1=1
64 NN=2
65 X(2)=10.0**5
66 NZ=1
67 N5=1
   READ INPUT TAPE 5,4000,THIS,AAA
69 GO TO 306
C
70 CALL READ
   KOP=KOP
   IF (M10-9999) 71,980,71
C
71 N5=N4N(2,3)
72 IF (N5-2) 80,80,86
C
80 LCM=2
81 GO TO 952
C
86 CMULT=Y(13,1)
87 DMULT=Y(13,N5)
88 EMULT=Y(14,N5)
   DO 89 J=1,3
89 TX(J)=0.0
C
90 GO TO (100,91),M9
91 L=N4N(1,1)
92 J=N4N(1,2)
93 WRITE OUTPUT TAPE 5,1035,CMULT,DMULT,EMULT,Y(13,L),Y(14,J),M10,ID9
   WRITE OUTPUT TAPE 5,4000,THIS,AAA
C
C
100 NT=1
   GO TO (101,325),M1
C
101 NL=NT+12
   N1=N4N(1,NT)
   N4=N4N(2,NT)

```

```

102 I4=(N4-N1+1)/20+1
    NN=(N4-N1+1)/I4
    M=4
C
    GO TO (105,106,110),NT
105 IX=NN
    GO TO 110
106 IA=NN
C
110 IF (N4-N1-4) 111,116,116
111 M=N4-N1
C
112 KK=M+1
113 DO 114 J=KK,4
114 B(J)=0.0
C
116 MG=(N4-N1+1)/I4+1
118 AN=MG
C
120 IF (N1-1) 125,125,130
125 NZ=N1+I4
126 GO TO 135
130 NZ=N1
C
135 DO 140 J=N1,N4
137 XK=Y(NL,N1)-Y(NL,J)
139 DO 140 L=1,M
140 DATA(J,L)=XK** (L-1)
C
145 AH=(X(N4)-X(NZ))/(Y(NL,NZ)-Y(NL,N4))
150 DO 155 J=N1,N4,I4
153 W(J)=AH*(Y(NL,NZ)-Y(NL,J))+X(NZ)
155 W(J)=W(J)-X(J)
C
    XNZ=X(NZ)
    GO TO 165
C
160 AH=(Y(29,N4)-Y(29,NZ))/(Y(14,NZ)-Y(14,N4))
    DO 161 J=N1,N4,I4
    W(J)=AH*(Y(14,NZ)-Y(14,J))+Y(29,NZ)
161 W(J)=W(J)-Y(29,J)
    XNZ=Y(29,NZ)
    GO TO 205
C
165 DO 200 I=1,M
170 DO 200 J=1,M
175 XX(I,J)=0.0
180 DO 185 L=N1,N4,I4

```

```

185 XX(I,J)=XX(I,J)+DATA(L,I)*DATA(L,J)
190 IF(I-J) 195,200,195
195 XX(J,I)=XX(I,J)
200 CONTINUE
C
205 DO 220 J=1,M
210 XY(J)=0.0
215 DO 220 I=N1,N4,I4
220 XY(J)=XY(J)+DATA(I,J)*W(I)
C
225 DO 230 J=1,M
230 XX(J,M+1)=XY(J)
235 CALL CROUT5 (XX,B,M,20,6)
C
C
      IF (NBUG) 245,252,245
245 GO TO (246,247,248),NT
C
246 WRITE OUTPUT TAPE 3,1071,M10,ID9
      GO TO 250
247 WRITE OUTPUT TAPE 3,1072,M10,ID9
      GO TO 250
248 WRITE OUTPUT TAPE 3,1073,M10,ID9
C
250 WRITE OUTPUT TAPE 3,1080,          AH,XNZ, (B(J),J=1,M)
251 WRITE OUTPUT TAPE 3,1065
C
252 SUMX=0.0
255 DO 285 I=N1,N4
      GO TO (256,256,257),NT
C
256 XTIT=X(I)
      GO TO 260
257 XTIT=Y(29,I)
C
260 EY(I)=B(I)
265 DO 270 J=2,M
270 EY(I)=EY(I)+DATA(I,J)*B(J)
271 EY(I)=AH*(Y(NL,NZ)-Y(NL,I))+ XNZ -EY(I)
275 ERR=XTIT-EY(I)
276 PERR=ERR/XTIT
280 SUMX=SUMX+ABSF(PERR)
C
283 IF (NBUG) 284,285,284
284 WRITE OUTPUT TAPE 3,1090,1,Y(NL,I),XTIT,          EY(I),ERR,PERR
285 CONTINUE
C
291 ERROR(NT)=SUMX/AN

```

```

292 IF (ERROR(NT)-0.01) 302,293,293
293 LCM=4
C
302 GO TO (310,303,306),M9
303 WRITE OUTPUT TAPE 5,1020,AH,X(NZ),(B(J),J=1,4)
304 GO TO 310
C
306 READ INPUT TAPE 5,1020,AH,X(NZ),(B(J),J=1,4)
307 NL=NT+12
C
310 TX(NT)=0.0
313 XK=Y(NL,M1)-EN(NT)
315 DO 316 L=1,M
316 TX(NT) = TX(NT) +B(L)*XK**(L-1)
318 XK=Y(NL,NZ)-EN(NT)
319 TX(NT) = AH*XK-TX(NT) + XNZ
320 CONTINUE
C
325 NT=NT+1
GO TO (101,327,160,340),NT
C
327 GO TO (340,101),M1
C
C
340 IF (DMULT-EN(1)) 342,342,341
341 TX(1) = X(N5)
342 IF (EMULT-EN(2)) 344,344,343
343 TX(2) = X(N5)
TX(3)=Y(29,N5)
344 CONTINUE
C
C
NC=1
IF (NBUG) 345,348,345
345 WRITE OUTPUT TAPE 3,2050
346 WRITE OUTPUT TAPE 3,2060,EN(M1),TX(1),TX(2),TX(3)
C
348 IF (CMULT-EN(M1))350,350,354
350 LCM=6
GO TO 948
C
354 IF (TX(M1)) 356,356,358
356 TX(NT)=1.0
357 LCM=4
358 CONTINUE
C
C
C

```

```

360 GO TO (390,409,361),M9
361 DO 364 K=1,MSZ
    READ INPUT TAPE 5,1020,BP(K),CP(K),(BB(K,J),J=1,4),LBATCH
    READ INPUT TAPE 5,1020,(BB(K,J),J=5,10),IS(K)
364 CONTINUE
365 GO TO 551
C
390 GO TO (391,400),M1
C
391 LP=TX(1) /X(2)+1.0
    MELK=(PERIOD+0.01)/X(2)
    AM=MELK
C
    DO 392 J=1,LP,MELK
        AJ=J-1
        AJ=AJ/AM
        IF (ABSF(X(J)-AJ*PERIOD)-0.10) 392,409,409
392 CONTINUE
C
    DO 396 K=1,MSZ
        IS(K)=1
        MQ(K)=LP+4
        IF (MQ(K)-N5) 394,394,393
393 MQ(K)=N5
394 JJ(K)=LP-3
        IF (JJ(K)) 395,395,396
395 JJ(K)=1
396 CONTINUE
C
        LBATCH=2
        N5=MQ(1)
        GO TO 410
C
400 DO 401 J=1,N5
401 X(J)=X(J)*Y(29,J)
C
409 LBATCH=1
C
C
410 DO 500 K=1,MSZ
415 M=4
420 IF(Y(K,2)-10.0**(-24)) 425,425,330
425 DO 430 J=1,10
430 BB(K,J)=0.0
435 BP(K)=0.0
436 CP(K)=0.0
440 GO TO 500
C

```

```

330 J=IS(K)
    GO TO (331,332),J
331 GO TO (445,446),LBATCH
445 N1=1
    GO TO 447
446 N1=JJ(K)
C
447 N4=MQ(K)
    N2=(N5-1+N4)/2-2
    DX=(X(N5-1)-X(N4))/2.0+X(N4)
    IF (N4-N5) 333,336,336
C
332 N1=MQ(K)
    N4=N5
    N2=(N1+1)/2-2
    DX=(X(N1)-X(1))/2.0+X(1)
C
333 IF (DX-X(N2)) 336,334,334
334 N2=N2+1
    GO TO 333
C
C
336 IF (N4-N1-4) 337,339,339
337 M=N4-N1
    KK=M+1
    DO 338 J=KK,4
338 BB(K,J)=0.0
C
339 GO TO (362,366),LBATCH
366 BP(K)=0.0
    CP(K)=0.0
    I4=1
    GO TO 367
C
362 I4=(N4-N1)/25+1
    BP(K)=(Y(K,N4)-Y(K,N1))/(X(N4)-X(N1))
    CP(K)=Y(K,N1)
C
C
367 DO 368 J=N1,N4
    DO 368 L=1,M
368 DATA(J,L)=X(J)**(L-1)
C
370 DO 389 I=1,M
375 DO 389 J=1,M
380 XX(I,J)=0.0
385 DO 386 L=N1,N4,I4
386 XX(I,J)=XX(I,J)+DATA(L,I)*DATA(L,J)

```

```

      IF (I-J) 388,389,388
388 XX(J,I)=XX(I,J)
389 CONTINUE
C
C
455 DO 460 J=N1,N4,I4
460 W(J)=Y(K,J)-BP(K)*(X(J)-X(N1))-CP(K)
C
465 DO 481 J=1,M
470 XY(J)=0.0
475 DO 476 I=N1,N4,I4
476 XY(J)=XY(J)+DATA(I,J)*W(I)
481 CONTINUE
C
485 DO 486 J=1,M
486 XX(J,M+1)=XY(J)
C
487 CALL CROUT5 (XX,B,M,20,6)
488 DO 489 J=1,M
489 BB(K,J)=B(J)
   BB(K,10)=X(N1)
C
      CALL EXPC (X,Y,MQ,IS,BB,N5)
C
      IF (K-KOP) 500,499,500
499 IY=(N5-N1+1)/I4
C
500 CONTINUE
C
C
501 M=4
C
      DO 550 K=1,MSZ
      IF (BP(K)+CP(K)+BB(K,1)) 506,550,506
506 SUMX=0.0
507 IF (NBUG) 509,508,509
508 IF (K-KOP) 550,510,551
509 WRITE OUTPUT TAPE 3,2040,K,M10,MQ(K),IS(K)
      WRITE OUTPUT TAPE 3,1085,BP(K),CP(K),(BB(K,J),J=1,10)
      WRITE OUTPUT TAPE 3,1065
C
510 GO TO (511,512),LBATCH
511 N1=1
      N4=N5
      GO TO 513
512 N1=JJ(K)
      N4=MQ(K)
C

```

```

C
513 DO 537 I=N1,N4
      J=IS(K)
      IF (I-1) 521,521,522
521 EY(I)=Y(K,I)
      GO TO 528
522 IF (I-MQ(K)) 514,516,515
514 GO TO (519,516),J
515 GO TO (516,519),J
C
516 EY(I)= BB(K,6)*(1.0-EXP(-BB(K,5)*(X(I)-BB(K,8))))+BB(K,7)
517 GO TO 528
C
519 EY(I)=BB(K,1)
520 DO 525 J=2,M
525 EY(I)=EY(I)+DATA(I,J)*BB(K,J)
      EY(I)=EY(I)+BP(K)*(X(I)-BB(K,10))+CP(K)
528 ERR=EY(I)-Y(K,I)
529 PERR=ERR/Y(K,N5+1)
530 SUMX=SUMX+ABS(ERR)
535 IF (NBUG) 536,537,536
536 WRITE OUTPUT TAPE 3,1090,I,X(I),Y(K,I),      EY(I),ERR,PERR
537 CONTINUE
C
540 AN4=N4-N1+1
541 IF (K-KOP) 546,542,546
542 ERROR(3)=SUMX/(AN4*Y(K,N5+1))
543 IF (ERROR(3)-.020) 546,544,544
544 LCM=4
C
546 IF (NBUG) 547,550,547
547 SUMX=SUMX/AN4
548 WRITE OUTPUT TAPE 3,2075,SUMX
550 CONTINUE
C
551 IF (IP-3) 553,552,553
552 CALL PDUMP
553 GO TO (560,554,560),M9
C
554 DO 557 K=1,MSZ
556 WRITE OUTPUT TAPE 5,1020,BP(K),CP(K),(BB(K,J),J=1,4),LBATCH
557 WRITE OUTPUT TAPE 5,1020,(BB(K,J),J=5,10),IS(K)
C
C
C
560 GO TO (600,590),M1
C
590 S2=1.0/RA

```



```

      S1=RI
      GO TO 720
C
C
C
600 PER=PERIOD
620 LP=TX(1) /PER +1.0
C
630 T(1)=0.0
      IF (LP=2) 641,635,635
635 DO 640 L=2,LP
640 T(L)=T(L-1)+PER
C
641 LT=LP+1
642 T(LT)=TX(1)
C
      DO 643 L=1,LT
643 X(L)=T(L)*1.0E+07
C
      GO TO (653,645),LBATCH
645 DO 646 K=1,MSZ
      DO 646 L=1,LP
      KK=L+(MELK-1)*(L-1)
      Z(K,L)=Y(K,KK)
646 CONTINUE
      MG=LT
      GO TO 654
C
653 MG=1
C
654 DO 675 K=1,MSZ
      I=IS(K)
      DO 675 L=MG,LT
      IF (T(L)-BB(K,9)) 655,655,656
655 GO TO (659,657),I
656 GO TO (657,659),I
C
657 Z(K,L)= BB(K,6)*(1.0-EXP(-BB(K,5)*(T(L)-BB(K,8))))+BB(K,7)
      GO TO 671
C
659 Z(K,L)=0.0
      DO 665 I=1,M
665 Z(K,L)=Z(K,L)+BB(K,I)*T(L)**(I-1)
      Z(K,L)=BP(K)*(T(L)-BB(K,10))+CP(K)+Z(K,L)
C
671 IF (Z(K,L)) 672,675,675
672 Z(K,L) = 0.0
675 CONTINUE

```

```

C
685 MK=1
686 NT=1
    AAA(22)=1HB
    WRITE OUTPUT TAPE 7,4000,THIS,AAA,M10,ID9
690 DO 695 L=1,LP
    WRITE OUTPUT TAPE 7,4001,Z(13,L),Z(14,L),Z(12,L),X(L),Z(11,L),
    1 SDENS,MK,M10,ID9
    WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=1,10),Z(15,L),Z(16,L),Z(17,L)
    WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=18,28),Z(30,L),Z(31,L)
    WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=32,44)
    WRITE OUTPUT TAPE 7,4004
695 CONTINUE
700 MK=2
    L=LT
    WRITE OUTPUT TAPE 7,4001,EN(1),Z(14,L),Z(12,L),X(L),Z(11,L),SDENS,
    1 MK,M10,ID9
    WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=1,10),Z(15,L),Z(16,L),Z(17,L)
    WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=18,28),Z(30,L),Z(31,L)
    WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=32,44)
    WRITE OUTPUT TAPE 7,4004
C
C
C
715 GO TO (946,720,720),M1
C
C
720 NT=2
    CFT=TX(3)*1.0E-07
722 PER=PERIOD*TX(3)
C
750 LP=TX(2) /PERIOD+1.0
755 T(1)=0.0
760 LT=LP+1
765 T(LT)=TX(2)*TX(3)
    IF (LP-2) 774,770,770
770 DO 775 L=2,LP
775 T(L)=T(L-1)+PER
774 DO 776 L=1,LT
776 X(L)=T(L)/CFT
    IF(DAY)777,780,777
777 CALL KFINAL(BB,EN,EEN2,KINF,BP,CP,TX,X(LP+1),DAY,FACTOR)
    GO TO(778,780),KINF
778 DO 779 I=1,150
779 X(I)=EXPT(I)
    GO TO 71
780 CONTINUE
C

```

```

C      DO 882 K=1,MSZ
        I=IS(K)
      860 DO 882 L= 1,LT
        IF (T(L)-BB(K,9)) 861,861,862
      861 GO TO (865,863),I
      862 GO TO (863,865),I
C      863 Z(K,L)= BB(K,6)*(1.0-EXP(-BB(K,5)*(T(L)-BB(K,8))))+BB(K,7)
      864 GO TO 877
C      865 Z(K,L)=0.0
      870 DO 875 I=1,M
      875 Z(K,L)=Z(K,L)+BB(K,I)*T(L)**(I-1)
        Z(K,L)=BP(K)*(T(L)-BB(K,10))+CP(K)+Z(K,L)
C      877 IF (Z(K,L)) 881,882,882
      881 Z(K,L) = 0.0
      882 CONTINUE
C
C
C
C      904 MK=1
        AAA(22)=1HG
        WRITE OUTPUT TAPE 7,4000,THIS,AAA,M10,ID9
      905 DO 910 L=1,LP
        WRITE OUTPUT TAPE 7,4001,Z(13,L),Z(14,L),Z(12,L),X(L),Z(11,L),
          1 SDENS,MK,M10,ID9
        WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=1,10),Z(15,L),Z(16,L),Z(17,L)
        WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=18,28),Z(30,L),Z(31,L)
        WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=32,44)
        WRITE OUTPUT TAPE 7,4004
      910 CONTINUE
      915 MK=3
        L=LP+1
        G=TX(3)*1.0E-12
        WRITE OUTPUT TAPE 7,4003,Z(13,L),EN(2),Z(12,L),G,X(L),Z(11,L),
          1SDENS,MK,M10,ID8
        WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=1,10),Z(15,L),Z(16,L),Z(17,L)
        WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=18,28),Z(30,L),Z(31,L)
        WRITE OUTPUT TAPE 7,4002,(Z(K,L),K=32,44)
        WRITE OUTPUT TAPE 7,4004
      945 CONTINUE
C      948 GO TO (952,951,949),M9
      949 READ INPUT TAPE 5,1042,(ERROR(L),L=1,3),IX,IA,N5,IY,LCM
      950 GO TO 952
      951 WRITE OUTPUT TAPE 5,1042,(ERROR(L),L=1,3),IX,IA,N5,IY,LCM

```

```

C
952 SS=S2/S1
    WRITE OUTPUT TAPE 3,1026,M10,ID9,A(LCM+1),A(LCM+2),CMULT,DMULT,
    1 EMULT,N5,IX,IA,IY,(ERROR(J),J=1,3),SS,G
C
    G=0.0
953 IX=0
954 IA=0
955 N4=0
956 DO 957 J=1,5
957 ERROR(J)=0.0
958 S1=0
959 S2=0
960 M=4
961 IY=0
962 LCM=0
963 CMULT=0.0
964 DMULT=0.0
965 EMULT=0.0
C
    GO TO (70,70,60),M9
C
C
980 IF (MRR) 985,985,981
981 MRR=0
    M1=1
    GO TO (982,982,983),M9
C
982 CALL RDYTP(I8)
    GO TO (42,984,38),M9
C
983 REWIND 5
    GO TO 38
C
984 WRITE OUTPUT TAPE 5,1035,(ERROR(J),J=1,5),XXX,ID9
    END FILE 5
    REWIND 5
    M9=3
    GO TO 38
C
C
985 WRITE OUTPUT TAPE 7,2077,XXXX
    END FILE 7
    REWIND 7
    GO TO (986,986,994),M9
986 CALL RDYTP(I8)
C
990 GO TO (994,991,994),M9

```

```

991 WRITE OUTPUT TAPE 5,1035,(ERROR(J),J=1,5),XXX,ID9
992 END FILE 5
993 REWIND 5
C
994 IF (N9-1) 995,997,997
995 WRITE OUTPUT TAPE 3,1006
PRINT 1007
PAUSE77777
CALL EXIT
C
997 SENSE LIGHT 0
SENSE LIGHT 1
WRITE OUTPUT TAPE 3,1008,N9
CALL CHAIN (N9,4)
C
C
1000 FORMAT(5I2,I3,I2,2F5.0,1X,A4,1X,A4,F8.4,F8.0,4F8.4)
1001 FORMAT (6X,A4)
1002 FORMAT (20X,24HHANG TAPES - PRESS START///)
1003 FORMAT (1H1///10X,7HPROTEUS////)
1005 FORMAT (1H1)
1006 FORMAT(12HONORMAL EXIT)
1007 FORMAT(20X,29HREMOVE AND SAVE LABELED TAPES/////)
1008 FORMAT(26HONORMAL EXIT, CALLING LINK,I3)
1015 FORMAT (1H0//)
1020 FORMAT (1P6E13.6,I2)
1025 FORMAT (1H1///42X,35H SUMMARY OF PROTEUS CALCULATIONS///
1120H CASE INPUT K INFINITY VALUES DATA
2POINTS POLY FIT PER CENT ERRORS HEAT TRANS /
3119H NUMBER COMMENT INITIAL FINAL FINAL AVE TOT XM
4 AM Y XMULT AMULT Y FIS MAX/MIN G FLUX //)
1026 FORMAT (1X,A4,A1,
1 3X,2A6,2X,3F8.3,6X,4I4,2X,2P2F8.3,F9.3,0PF11.3,1PE13.4//)
1035 FORMAT (5F10.7,25X,A4,A1)
1045 FORMAT (1H1///40X,41H END POINT NUMBER FINAL K INFINITY//
1 41X,I8,20X,F8.4//
1 41X,I8,20X,F8.4//
1 41X,I8,20X,F8.4//
1 41X,I8,20X,F8.4//
1 41X,I8,20X,F8.4//
1 41X,I8,20X,F8.4//)
1042 FORMAT (3E11.4,5I5,12X,6H XXXXX)
1065 FORMAT (111H0 N X Y
1 CALCULATED Y ERROR PERCENT ERROR//)
1071 FORMAT (1H1// 33X,43HIN REACTOR TIME AS A FUNCTION OF XMULT -
1 A4,A1//)
1072 FORMAT (1H1// 33X,43HIN REACTOR TIME AS A FUNCTION OF AMULT -
1 A4,A1//)

```

```

1073 FORMAT (1H1// 33X,43H      GRADED FLUX AS A FUNCTION OF AMULT  -
1      A4,A1///)
1080 FORMAT (30X,
1      6H AH = 1PE12.4,18X,
1      6H BH = 1PE12.4//30X,
1      6H B0 = 1PE12.4, 18X,
1      6H B1 = 1PE12.4//30X,
1      6H B2 = 1PE12.4, 18X,
1      6H B3 = 1PE12.4///)
1085 FORMAT (44X,30H      POLYNOMIAL COEFFICIENTS///30X,
1      5HBP = 1PE11.4,10X,5HCP = E11.4,10X,5HB0 = E11.4//30X,
1      5HB1 = 1PE11.4,10X,5HB2 = E11.4,10X,5HB3 = E11.4//30X,
1      5HB5 = 1PE11.4,10X,5HB6 = E11.4,10X,5HB7 = E11.4//30X,
1      5HB8 = 1PE11.4,10X,5HB9 = E11.4, 10X,5HB10= E11.4//)
1090 FORMAT (110,1P4E20.4,2PF15.3)
2010 FORMAT (1H0)
2040 FORMAT (1H1/25H      CALCULATION FOR K = 12,6X,A4,I15,I5///)
2050 FORMAT (1H1/30X,48H  BATCH TIME      GRADED TIME      GRADED FLU
1X //)
2060 FORMAT (1H 12X,1P4E15.5)
2070 FORMAT (A6)
2075 FORMAT (1H0/20X,17H AVERAGE ERROR = 1PE16.4)
2076 FORMAT (A6)
2077 FORMAT (A6,125X,1H )
4000 FORMAT (A5,20A6,2A1,A4,A1)
4001 FORMAT (2F9.7,44X,1PE11.4,11X,2E11.4,0PF6.3,9X,I2,4X,A4,A1)
4002 FORMAT (1P13E10.3)
4003 FORMAT (2F9.7,44X,1P4E11.4,0PF6.3,9X,I2,4X,A4,A1)
4004 FORMAT (119X,1H )
4005 FORMAT (127X,A4)
      END
*      LABEL
C 906      SUBROUTINE READ OF PROTEUS
      SUBROUTINE READ
C
      COMMON ICOM,COM
      COMMON X,Y,NN, ID8,THIS,I4,EN,M2,KOP,M1,MK,JJ,ID9,AAA,RATE,STP
      COMMON RI,RA,MSZ,CUT,SDENS,I8,IRECYC,DAY,EEN2,EXPT,FACTOR
C
      DIMENSION ICOM(20),COM(80)
      DIMENSION Y(45,150),X(150),NN(2,3),EN(3),I4(45),MK(45),JJ(45),
1EP(2,2),AAA(22),S(150),EXPT(150)
C
      MX=1
      M2=M2
      M = I8
      XXX=5H XXXX
C

```

```

      CUT1=10.0+CUT
      CUT2=10.0-CUT
C
10 READ INPUT TAPE M,4000,THUS,AAA,ID8,ID9
   CALL COMPAR (STP,ID8,4,J)
   GO TO (11,13,11),J
11 CALL COMPAR (THUS,XXX, 5,J)
12 GO TO (15,13,15),J
13 ID8=9999
   REWIND 18
   GO TO 500
C
15 CALL COMPAR (THUS,THIS,5,J)
20 GO TO (10,40,10),J
C
40 DO 75 J=1,150
45 READ INPUT TAPE M,4001,Y(13,J),Y(14,J),RI,RA,Y(12,J),Z,Y(11,J),
   1 SDENS,LT
   X(J)=Z*1.0E-07
   EXPT(J)=X(J)
50 READ INPUT TAPE M,4002,(Y(K,J),K=1,10),(Y(K,J),K=15,17)
   READ INPUT TAPE M,4002,(Y(K,J),K=18,28),(Y(K,J),K=30,31)
   READ INPUT TAPE M,4002,(Y(K,J),K=32,44)
60 READ INPUT TAPE M,4004,JUNK
C
   IF (1.0/(RA*RI)-RATE) 70,70,76
C
70 IF (LT-1) 76,75,71
71 IF (LT-3) 45,72,76
72 IF (IRECYC) 2,2,76
   2 GO TO (73,76),MX
73 MX=2
   GO TO 45
75 CONTINUE
C
76 IF (J-2) 77,77,80
77 NM(2,3)=J
78 GO TO 500
C
80 IF (X(J)-X(J-1)) 81,81,85
81 J=J-1
84 GO TO 80
85 N5=J-1
   IF (DAY) 86,87,86
86 Q=X(N5)*1.E7/86400.
   NR=Q/DAY+1.0
   RNR=NR
   DAYS=Q/RNR

```

READ

READ

READ

READ

READ

READ

```

      CONK=(Y(13,1)-EEN2      )*((1.0+(RNR-1.0)/(RNR+1.0))/(2.0*RNR))
      EN(2)=EEN2+CONK*FACTOR
      EN(3)=EN(2)
C
      87 Y(13,J+1)=0.0
      88 Y(14,J+1)=0.0
      Y(29,1)=Y(12,1)*1.0E+12
C
      DO 90 J=2,N5
      S(J)=0.5*(X(J)-X(J-1))*(1.0/Y(12,J)+1.0/Y(12,J-1))+S(J-1)
      Y(29,J)=X(J)/S(J)*1.0E+12
      90 CONTINUE
C
C
      LL=2
C
      93 DO 95 L=1,LL
      EP(1,L)=EN(L)+.035
      95 EP(2,L)=EN(L)-.035
C
C
      105 DO 114 L=1,LL
      106 IF (EP(2,L)-Y(L+12,N5)) 107,114,114
      107 IF (EP(1,L)-Y(L+12,N5)-.01) 108,108,111
      108 DO 109 J=1,2
      109 EP(J,L)=Y(L+12,N5)
      110 GO TO 114
C
      111 EP(1,L)=EP(1,L)+Y(L+12,N5)-EP(2,L)
      112 EP(2,L)=Y(L+12,N5)
      114 CONTINUE
C
C
      115 DO 165 L=1,LL
      116 J=0
      117 J=J+1
      119 IF (Y(L+12,J)-EP(1,L)) 120,120,117
      120 NN(1,L)=J-3
      121 IF (J-3) 122,122,125
      122 EP(1,L)=EP(1,L)-.01
      123 IF (EP(1,L)-EN(1)) 125,125,116
C
      125 IF (Y(L+12,J)-EP(2,L)) 140,140,130
      130 J=J+1
      135 IF (J-N5) 125,140,140
      140 NN(2,L)=J+2
C
      145 IF (NN(1,L)-1) 146,147,147

```

READ

READ
READ
READ


```

146 NN(1,L)=1
147 IF (NN(2,L)-N5) 150,150,148
148 NN(2,L)=N5
C
150 J1=NN(1,L)
151 J2=NN(2,L)
152 DO 155 J=J1,J2
153 IF (Y(L+12,J)-Y(L+12,J+1)) 154,154,155
154 NN(1,L)=J+1
155 CONTINUE
C
156 IF (NN(2,L)-NN(1,L)-4) 157,160,160
157 NN(2,L)=NN(1,L)+5
160 IF (NN(2,L)-N5) 165,165,161
C
161 NN(2,L)=N5
165 CONTINUE
C
170 NN(1,3)=1
    LL=1+M1/2
175 NN(2,3)=NN(2,LL)
    N5=NN(2,3)
C
C
    IF (N5-8) 176,180,180
176 DO 177 K=1,MSZ
    MK(K)=N5
    I4(K)=1
    Y(K,N5+1)=Y(K,N5)
177 CONTINUE
    J=0
    GO TO 400
C
180 DO 300 K=1,MSZ
181 IF (Y(K,2)-1.0E-24) 182,182,184
C
182 MK(K)=1
    I4(K)=1
183 GO TO 300
C
184 IF (K-12) 200,187,200
C
C
187 I4(12)=1
    Y(12,N5+1)=Y(12,N5)
    DO 188 J=1,N5
    IF (Y(12,1)*10.0-Y(12,J)) 189,188,188
188 CONTINUE

```

READ
READ
READ

```

C      MK(12)=N5
      GO TO 300
189  C      MK(12)=J
      GO TO 300
C
C
C
200  NHUMP=1
      IF (Y(K,1)-Y(K,N5-1)) 202,202,201
201  ML=1
      I4(K)=1
      LX=1
      LH=1
      YAK=Y(K,1)-Y(K,2)
      GO TO 204
C
202  ML=2
      I4(K)=2
      LX=N5
      LH=N5
      YAK=Y(K,N5)-Y(K,N5-1)
C
204  DO 225 J=2,N5
      GO TO (205,210),ML
C
205  L=J
      GO TO (206,215),NHUMP
206  YAP=Y(K,L-1)-Y(K,L)
      YAD=Y(K,L)-Y(K,L+1)
      IF (YAD/ABSF(YAD)-YAP/ABSF(YAP)) 220,207,208
207  IF (ABSF(YAP)*10.0-ABSF(YAK)) 230,220,220
208  NHUMP=2
      LH=L
      GO TO 214
C
210  L=N5-J+1
      GO TO (211,215),NHUMP
211  YAP=Y(K,L+1)-Y(K,L)
      YAD=Y(K,L)-Y(K,L-1)
      IF (YAP/ABSF(YAP)-YAD/ABSF(YAD)) 213,212,220
212  IF (ABSF(YAK)*10.0-YAP) 230,220,220
213  NHUMP=2
      LH=L
C
214  IF (Y(K,L)-CUT2*Y(K,LX)) 225,230,230
C
215  IF (Y(K,L)-Y(K,LX)) 230,230,225

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```

C
220 IF (Y(K,LX)-CUT1*Y(K,L)) 225,230,230
225 CONTINUE
C
230 GO TO (235,240),ML
235 IF (N5-L-2) 236,250,250
236 L=N5
    GO TO 250
C
240 IF (L-3) 241,250,250
241 L=1
C
250 MK(K)=L
    Y(K,N5+1)=Y(K,LH)
C
300 CONTINUE
C
C
    J=0
400 DO 407 K=1,MSZ
405 IF (Y(K,1)-1.0*10.0**(-J-4)) 407,407,406
406 IF (Y(K,1)-1.0*10.0**(J-3)) 410,407,407
407 CONTINUE
    J=J+1
    GO TO 400
410 KOP=K
    Y(KOP,N5+1)=Y(KOP,1)
C
C
500 RETURN
C
4000 FORMAT (A5,20A6,2A1,A4,A1)
4001 FORMAT (2F9.7,29X,2F5.5,5X,E11.4,11X,2E11.4,F6.3,9X,I2)
4002 FORMAT (13E10.3)
4004 FORMAT (A6)
    END
* LABEL
C 430 SUBROUTINE EXPC
    SUBROUTINE EXPC (X,Y,MQ,IS,BB,N5)
C
    DIMENSION X(150),Y(45,150),IS(45),MQ(45),BB(45,10)
    MSZ=44
C
    DO 300 K=1,MSZ
        L=MQ(K)
        ML=IS(K)
C
210 GO TO (215,220),ML

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```

215 N0=L
    N2=N5
    GO TO 225
220 N2=L
    N0=1
C
225 XX=(X(N2)+X(N0))/2.0
    N1=(N0+N2)/2-2
    DO 230 J=N1,N2
    GO TO (226,227),ML
226 L=N5-J
    GO TO 228
227 L=J
C
228 IF (XX-X(L)) 235,235,230
230 CONTINUE
C
    N1=(N0+N2)/2
    GO TO 240
235 N1=J-1
C
240 DELX=(X(N2)-X(N0))/2.0
    AVEX=(X(N2)+X(N0))/2.0
    YM=Y(K,N1)+(Y(K,N1+1)-Y(K,N1))*(AVEX-X(N1))/(X(N1+1)-X(N1))
    P=LOGF((Y(K,N2)-YM)/(YM-Y(K,N0)))/DELX
    B=(Y(K,N2)-Y(K,N0))/(1.0-EXPF(P*(X(N2)-X(N0))))
C
    DO 250 I=1,40
    Z1=B*(1.0-EXPF(P*(X(N1)-X(N0))))+Y(K,N0)
    ERROR=(Y(K,N1)-Z1)/Y(K,N1)
    IF (ABSF(ERROR)-0.00001) 260,260,245
C
245 YM=Y(K,N1)+YM-Z1
    P=LOGF((Y(K,N2)-YM)/(YM-Y(K,N0)))/DELX
    B=(Y(K,N2)-Y(K,N0))/(1.0-EXPF(P*(X(N2)-X(N0))))
250 CONTINUE
C
260 BB(K,5)=-P
    BB(K,6)=B
    BB(K,7)=Y(K,N0)
    BB(K,8)=X(N0)
    L=MQ(K)
    BB(K,9)=X(L)
300 CONTINUE
    RETURN
    END
* LABEL
CCRT5 SUBROUTINE CROUT5 MODIFIED FOR PROTEUS

```

```

C      SUBROUTINE CROUT5 (A,C,N,NC,NF)
C      SOLVES A SYSTEM OF N LINEAR ALGEBRAIC EQUATIONS IN N UNKNOWN BY
C      THE CROUT METHOD (MAX N=15) - ACCURACY IS IMPROVED TO A MAXIMUM OF
C      SIX SIGNIFICANT FIGURES
C
C      A IS N,N+1 MATRIX OF INPUT COEFFICIENTS
C      C IS N,1 COLUMN MATRIX OF UNKNOWN AS OUTPUT
C      NC IS MAX NUMBER OF ITERATIONS TO BE PERMITTED (6 - 10 IS ADVISED)
C      NF IS NUMBER OF SIGNIFICANT FIGURES OF ACCURACY REQUIRED IN
C      BALANCE OF TWO SIDES OF EACH EQUATION (NOT TO EXCEED 6)
C
C      REF- AIEE TRANS 1941 VOL 60 P1235-1240
C      DIMENSION A(21,22),B(21,22),D(21),AA(21),C(21)
C      KOUNT = 0
C      NIL=1
C      ZOUNDS=0.0
C      SIG=10.0**NF
1  DO 2 I=1,N
C      D(I)=0.0
C      AA(I)=A(I,N+1)
2  B(I,1)=A(I,1)
4  DO 3 I=1,N
3  B(1,I+1)=A(1,I+1)/A(1,1)
C      KOUNT=KOUNT+1
C      DO 6 L=2,N
C      DO 6 I=L,N
C      S=0.0
C      T=0.0
C      DO 6 J=2,L
C      S=S+B(I,J-1)*B(J-1,L)
C      B(I,L)=A(I,L)-S
C      T=T+B(L,J-1)*B(J-1,I+1)
6  B(L,I+1)=(A(L,I+1)-T)/B(L,L)
7  C(N)=B(N,N+1)
C      DO19 I=2,N
C      K=N-I+1
C      S=0.0
C      DO 8 L=2,I
C      KL=K+L-1
8  S=S+C(KL)*B(K,KL)
19 C(K)=B(K,N+1)-S
C      DO 20 I=1,N
20 C(I)=C(I)+D(I)
C      DO 10 I=1,N
C      D(I)=0.0
C      DO 9 J=1,N
9  D(I)=D(I)-A(I,J)*C(J)
C      A(I,N+1)=D(I)+AA(I)

```

```

10 D(I)=C(I)
DO 14 I=1,N
  ZZ=0.
  DO 5 J=1,N
    5 ZZ=ZZ+C(J)*A(I,J)
    ZZ=ABSF(AA(I)-ZZ)
    Z=ABSF(AA(I))
    IF (Z) 18,13,18
18 IF (1.0-Z) 12,13,17
17 Z=10.0*Z
    ZZ=10.0*ZZ
    GO TO 18
11 IF (1.0-Z) 12,13,13
12 Z=0.1*Z
    ZZ=0.1*ZZ
    GO TO 11
13 ZZ=ZZ*SIG
    IF (1.0-ZZ) 15,15,14
15 IF (KOUNT - NC) 4,4,16
16 NIL=2
    ZOUNDS=MAX1F(ZOUNDS,ZZ)
14 CONTINUE
    GO TO (21,22), NIL
22 AA1 = ZOUNDS/FLOATF(NF)
    IFE = 1
21 DO 23 I=1,N
23 A(I,N+1)=AA(I)
    RETURN
    END
* LABEL
C1KFI KFINAL-A PROGRAM TO SIMULATE ACTUAL GRADED OPERATION
SUBROUTINE KFINAL(C,EN,EEN2,KINF,B,A,T,TIME,DAY,FACTOR)
DIMENSION C(45,10),EN(3),B(45),A(45),T(3)
NR=TIME/(86400.*DAY)+1.0
IF(NR-1)95,95,96
95 RNR=1.
GO TO 97
96 RNR=NR
97 X=TIME/(86400.*RNR)
SUMK=0.
DO 101 I=1,NR
  CONK=0.
  DI=I-1
  XX=T(3)*DI*TIME*1.0E-07/RNR
  DO 100 J=1,4
100 CONK=CONK+C (13,J)*XX** (J-1)
  CONK=CONK+A(13)+B(13)*(XX-C(13,10))
101 SUMK=SUMK+(CONK-EEN2)/(2.0*RNR)

```

CONNEW=EEN2+SUMK*FACTOR		
TEST=ABSF.((CONNEW-EN(2))/CONNEW)		
IF(TEST-2.0E-3)111,111,110		
110 CONTINUE		
EN(2)=CONNEW		
EN(3)=EN(2)		
KINF=1		
IF(NBUG-2)120,120,111		
120 NBUG=NBUG+1		
RETURN		
111 KINF=2		
RETURN		
END		
* FAP		110-2001
COUNT 100		110-2002
ENTRY COMPAR		110-2003
* COMPAR SUBROUTINE--TWO POSSIBLE CALLING SEQUENCES		110-2004
* CALL COMPAR(A,B,N,M)		110-2005
* A IS THE BEGINNING ADDRESS OF THE 1ST. COMPARISON ITEM		110-2006
* B IS THE BEGINNING ADDRESS OF THE 2ND. COMPARISON ITEM		110-2007
* N IS THE NUMBER OF CHARACTERS TO BE COMPARED		110-2008
* M =1 IF A IS GREATER THAN B		110-2009
* M =2 IF A EQUALS B		110-2010
* M =3 IF A IS LESS THAN B		110-2011
*		110-2012
* CALL COMPAR(A,I,B,J,N,M)		110-2013
* A,B,N,M THE SAME AS ABOVE		110-2014
* I IS THE POSITION OF THE FIRST CHARACTER IN A		110-2015
* J IS THE POSITION OF THE FIRST CHARACTER IN B		110-2016
COMPAR SXA SET1+1,4		110-2017
SXA RET,1		110-2018
STI HOLD		110-2019
LDI 5,4	LOOK AT THE FIFTH	110-2020
IIL 7400	INSTRUCTION FOLLOWING THE	110-2021
OFT HOLD+1	TSX,4 AND SEE IF THE LIST	110-2022
TRA LIST4	IS 4 OR 6 ARGUMENTS.	110-2023
CLA* 2,4	ROUTINE FOR 6 ARGUMENTS	110-2024
TSX ARITH,1	SET POSITION OF FIRST	110-2025
STA SHFA	CHARACTER IN 1ST. ARGUMENT	110-2026
STA SHFA1		110-2027
CLA* 4,4	DO THE SAME FOR	110-2028
TSX ARITH,1	THE SECOND ARGUMENT	110-2029
STA SHFB		110-2030
STA SHFB1		110-2031
CLA 3,4	STORE ADDRESS OF	110-2032
STA TEST+1	SECOND ARGUMENT	110-2033
AXT 5,1		110-2034
SXA NOCHAR,1		110-2035

	AXT	7,1	SET EXIT TO CALLING	110-2036
	SXA	RET+2,1	PROGRAM TO TRA 7,4	110-2037
	AXT	3,1		110-2038
	SXA	ARGB,1		110-2039
	AXT	6,1		110-2040
	SXA	SET1+2,1		110-2041
	TRA	LISA		110-2042
LIST4	AXT	3,1	ROUTINE FOR 4 ARG. LIST	110-2043
	SXA	NOCHAR,1		110-2044
	AXT	5,1	SET RETURN TO CALLING	110-2045
	SXA	RET+2,1	PROGRAM AT TRA 5,4	110-2046
	AXT	2,1		110-2047
	SXA	ARGB,1		110-2048
	AXT	0,1	SET SHIFTS TO ZERO AS	110-2049
	SXA	SHFB,1	CHARACTERS ARE LEFT	110-2050
	SXA	SHFA,1	ADJUSTED	110-2051
	SXA	SHFB1,1		110-2052
	SXA	SHFA1,1		110-2053
	CLA	2,4	STORE ADDRESS OF	110-2054
	STA	TEST+1	SECOND ARGUMENT	110-2055
	AXT	4,1		110-2056
	SXA	SET1+2,1		110-2057
LISA	CAL*	1,4		110-2058
	SLW	MQA		110-2059
	CLA	1,4		110-2060
	STA	SHFA-1		110-2061
ARGB	CAL*	** ,4		110-2062
	SLW	MQB		110-2063
NOCHAR	CLA*	** ,4	PICK UP NO OF CHARACTERS	110-2064
	PDX	0,4	TO BE COMPARED	110-2065
	AXT	1,1		110-2066
TEST	CAL	MQB	PICK UP UNUSED PORTION	110-2067
	LDQ	** ,1	AND NEXT CHARACTERS OF ARG. B	110-2068
SHFB	LGL	**	LEFT ADJUST WORD	110-2069
	SLW	STORE		110-2070
	XCL			110-2071
SHFB1	ARS	**		110-2072
	SLW	MQB		110-2073
	CAL	MQA	PICK UP UNUSED PORTION	110-2074
	LDQ	** ,1	AND NEXT CHARACTERS OF	110-2075
SHFA	LGL	**	ARG. A, LEFT ADJUST, AND	110-2076
	PAI			110-2077
	XCL			110-2078
SHFA1	ARS	**		110-2079
	SLW	MQA		110-2080
	PIA			110-2081
	TXL	AGAIN+1,4,6	TRA TO MASK IF LAST PIECE TO COMP	110-2082
	TXI	*+1,4,-6		110-2083

	LAS	STORE	COMPARE WORDS	110-2084
	TRA	SET1	FIRST IS GREATER	110-2085
	TRA	AGAIN	THEY ARE THE SAME	110-2086
SET3	CLA	THREE	FIRST IS SMALLER	110-2087
	TRA	SET1+1		110-2088
SET2	CLA	TWO		110-2089
	TRA	SET1+1		110-2090
SET1	CLA	ONE		110-2091
	AXT	**,4		110-2092
	STO*	**,4		110-2093
	TOV	++1		110-2094
RET	AXT	**,1		110-2095
	LDI	HOLD		110-2096
	TRA	**,4		110-2097
ARITH	SUB	ONE	ROUTINE TO SET THE	110-2098
	ARS	18	NUMBER OF BITS TO	110-2099
	XCA		SHIFT LEFT TO LEFT	110-2100
	MPY	SIX	ADJUST CHARACTERS IN	110-2101
	XCA		WORD	110-2102
	TRA	1,1		110-2103
AGAIN	TXI	TEST,1,1		110-2104
	ANA	STORE,4	MASK UNUSED CHAR. OF ARG. A	110-2105
	SLW	MQA	AND SAVE THE RESULT	110-2106
	CAL	STORE	MASK OFF UNUSED CHARACTERS	110-2107
	ANA	STORE,4	OF ARG. B AND SAVE	110-2108
	SLW	MQB	THE RESULT	110-2109
	CAL	MQA	COMPARE THE REMAINING	110-2110
	LAS	MQB	PORTIONS OF THE TWO ARGS.	110-2111
	TRA	SET1	A IS GREATER THAN B	110-2112
	TRA	SET2	THEY ARE EQUAL	110-2113
	TRA	SET3	A IS LESS THAN B	110-2114
ONE	PZE	0,0,1		110-2115
TWO	PZE	0,0,2		110-2116
THREE	PZE	0,0,3		110-2117
	OCT	777777777777		110-2118
	OCT	777777777700		110-2119
	OCT	777777770000		110-2120
	OCT	777777000000		110-2121
	OCT	777700000000		110-2122
	OCT	770000000000		110-2123
STORE	PZE			110-2124
SIX	DEC	6		110-2125
HOLD	PZE			110-2126
	OCT	777777700000		110-2127
MQA	PZE			110-2128
MQB	PZE			110-2129

APPENDIX D

SUMMARY OF PROTEUS CALCULATIONS

SUMMARY OF PROTEUS CALCULATIONS

CASE NUMBER	COMMENT	INPUT K INITIAL	INFINITY VALUES			DATA POINTS				POLY FIT XMULT	PER CENT AMULT	ERRORS Y FIS	HEAT TRANS	
			FINAL	FINAL	AVE	TOT	XM	AM	Y				MAX/MIN	G FLUX
2350	NONE	1.375	0.837	1.014		17	0	8	17	0.	0.038	0.077	2.887	4.1397E-11
2351	NONE	1.432	0.805	1.006		23	0	8	23	0.	0.014	0.045	4.016	3.3875E-11
2352	NONE	1.461	0.784	1.004		28	0	9	28	0.	0.010	0.045	5.090	2.8584E-11
2353	QUESTIONABLE	1.048	0.941	1.008		5	0	4	5	0.	8.764	0.000	1.112	6.5132E-11
2354	NONE	1.484	0.755	1.008		36	0	10	36	0.	0.006	0.057	6.976	2.1876E-11
2355	NONE	1.298	0.862	1.012		13	0	7	13	0.	0.063	0.110	2.111	4.8648E-11
2356	NONE	1.478	0.765	1.005		33	0	9	33	0.	0.005	0.051	6.251	2.4162E-11
2400	NONE	1.400	0.832	1.013		17	0	8	17	0.	0.045	0.052	3.030	4.3080E-11
2401	NONE	1.460	0.800	1.004		23	0	8	23	0.	0.016	0.046	4.222	3.5296E-11
2402	NONE	1.491	0.779	1.002		28	0	9	28	0.	0.011	0.042	5.362	2.9805E-11
2404	NONE	1.518	0.749	1.005		36	0	9	36	0.	0.004	0.051	7.386	2.2846E-11
2405	NONE	1.174	0.892	1.006		9	0	7	9	0.	0.176	0.133	1.457	6.0206E-11
2406	NONE	1.438	0.815	1.011		20	0	8	20	0.	0.026	0.057	3.659	3.8580E-11
2407	NONE	1.511	0.760	1.008		33	0	9	33	0.	0.006	0.045	6.692	2.4829E-11
2408	NONE	1.477	0.792	1.007		25	0	8	25	0.	0.011	0.038	4.737	3.2548E-11
2450	NONE	1.420	0.828	1.012		17	0	7	17	0.	0.031	0.056	3.145	4.4409E-11
2451	NONE	1.483	0.796	1.002		23	0	8	23	0.	0.018	0.043	4.385	3.6417E-11
2452	NONE	1.516	0.780	1.011		27	0	8	27	0.	0.008	0.035	5.529	3.0770E-11
2454	NONE	1.545	0.745	1.005		36	0	9	36	0.	0.005	0.055	7.754	2.3464E-11
2455	NONE	1.179	0.887	1.004		9	0	7	9	0.	0.201	0.148	1.485	6.2264E-11

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