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**ACCURATE NUCLEAR FUEL
BURNUP ANALYSES**

**THIRTEENTH
QUARTERLY PROGRESS REPORT
DECEMBER 1964 - FEBRUARY 1965**

B. F. Rider
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J. P. Peterson, Jr.
R. S. Seymour
J. L. Jaech
F. R. Smith

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GENERAL ELECTRIC

ATOMIC POWER EQUIPMENT DEPARTMENT
SAN JOSE, CALIFORNIA

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FOREWORD

Accurate measurements of fuel burnup are required to aid in reactor design for high burnup fuels and to aid in evaluating nuclear fuel costs. The usefulness of current radiochemical methods is limited because: (a) limited availability of long-lived radioactive isotopes among the fission products; (b) the accuracy with which these fission products can be measured because of uncertainties in their physical constants; and (c) the volatile nature of the few available isotopes. Mass spectrometric techniques are being investigated to obtain a more accurate burnup analysis by measuring the quantity of the nonradioactive refractory fission products produced from a variety of fuels. By using the accurate isotope dilution technique on stable fission products, errors that limit the final accuracy of radiochemical measurements are eliminated, such as errors in counting efficiencies, decay schemes, and decay constants, as well as those found in out-of-pile and in-pile decay corrections.

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SUMMARY

The development of accurate methods for the determination of nuclear fuel burnup began on the present program in December 1961. The first twelve quarterly reports appeared as GEAP-4053-1, GEAP-4053-2, GEAP-4082, GEAP-4137, GEAP-4201, GEAP-4278, GEAP-4361, GEAP-4430, GEAP-4503, GEAP-4621, GEAP-4716, and GEAP-4776. Mass spectrometric analysis of stable fission product nuclides is being studied as a means to improve accuracy. One of the most promising and stable fission products is neodymium and, in particular, Nd-148.

During this quarter, the calculation of burnup from U, Pu, and Nd mass spectrometric measurements has been programmed for a digital computer. The program utilizes an iterative method to correct for the burnout and decay of the various species of interest to achieve a more accurate value than has been hitherto possible without very time-consuming hand calculations.

An interlaboratory comparison of standard lanthanide solutions with Phillips Petroleum Company has been completed. No bias between sites was found in the primary solutions used to calibrate neodymium spike solutions for isotopic dilution mass spectrometry.

The rhenium filament material on hand was found to be high in natural barium content which interfered with barium and cerium mass analyses. By using the boric acid addition technique on tantalum filaments, the cerium analyses on irradiated U-235, U-233, and Pu-239 foils from capsules GEV-1 and -2 are proceeding smoothly.

Measurements of relative fission yields from GEV-1 and -2 are nearing completion. Absolute thermal fission yield measurements for stable fission products in the heavy mass peak of the fission yield curve will begin shortly on five MTR-irradiated capsules recently received.

PROGRAM PROGRESS

During this quarter, the calculation of burnup in irradiated uranium fuel from U, Pu, and Nd mass spectrometric measurements has been programmed for a digital computer. In addition, work on the absolute thermal fission yield measurements for stable fission products (including Nd-148) on the heavy mass peak of the fission yield curve is progressing on schedule.

CALCULATION OF NUCLEAR FUEL BURNUP

The calculation of burnup in irradiated nuclear fuel (containing no Th-232 or U-233) from the mass spectrometric determination of uranium, plutonium, and stable fission products can be tedious if performed manually. With machine computation, it is possible to obtain more accurate burnup values by applying corrections normally neglected in the interest of simplicity. In addition, values for the capture-to-fission ratio, α , for U-235 and Pu-239 are obtained.

The required calculations have been programmed in a free style FORTRAN code called BURNUP⁽¹⁾ which is available on request. In this code, burnup in MWd/ton is calculated from U, Pu, and Nd mass spectrometric analyses. The calculation of burnup from heavy element isotopic composition could be based on the measured changes in U-236:U-238 and U-235:U-238 ratio changes caused by irradiation. However, these two ratios are sensitive to U-238 contamination. A more sensitive measure of burnup is the change in the U-236:U-235 ratio which is independent of U-238 but is dependent on a knowledge of the capture-to-fission ratio in U-235, α_5 . To make use of the latter relationship, α_5 is first calculated from the data. On the basis of this calculation, samples are arranged in three sets: S-1, S-2, and S-3. Set S-1 includes the samples which contain a small amount of U-238 contamination. For these samples, the average α_5 of the uncontaminated samples is used together with the U-236:U-235 ratio

for the U-235 burnup calculations. Set S-2 includes the sample for which an acceptable α_5 cannot be calculated because of statistical scatter. For these samples, the input α_5 is used. Set S-3 includes all normal samples from which an average α_5 is calculated for use in subsequent steps. Each set is further divided into either subset 1 for samples containing large amounts of pre-irradiation plutonium or subset 2 for samples which do not. For subset 1, the capture-to-fission ratio for Pu-239, α_9 , is calculated from the data. For subset 2, the input α_9 is used.

The uranium and plutonium isotopic composition of the sample is calculated from the measured isotopic ratios corrected for occasional traces of U-238 by the average α_5 , and for impurities contained in the isotopic diluent, such as U-234, in the U-233 added. An initial atom percent fission is computed for U-235, Pu-239, Pu-241, and U-238 from the change in the heavy element isotopic composition according to equations described elsewhere. (2)

A correction is then made for the U-236 burnout based on an integrated exposure (nv_0t) obtained from the U-235 depletion. The U-238 burnout correction, determined from the change in the plutonium content (including Pu-239 and Pu-241 fissions and Pu-241 decay correction) is made. Finally, an iteration of the initial set of calculations, with the data corrected as described, yields final values for the atom percent fission of each fissionable species. In addition, the concentrations of uranium and plutonium (calculated from the sample volume, and spike volume and concentration) are adjusted to a pre-irradiation total heavy element basis for use with the subsequent neodymium data.

Stable fission product Nd-148, -146, and -145 atom concentrations in the irradiated fuel (each of which is directly proportional to burnup) are computed from measured ratios of each isotope to Nd-150, used as an isotopic diluent. Corrections are made for:

1. Burnout of each isotope.
2. Production of Nd-142 from fission product Pr-141 by neutron absorption.

3. Natural neodymium contamination as indicated by the residual Nd-142 which does not occur in fission.
4. Small amounts of fission product Nd-150 in the Nd-150 spike position.
5. Isotopic impurities in the Nd-150 isotopic diluent.

From the effective fission yields, determined from the various sources of fission as previously computed from the heavy element data, and the adjusted heavy element concentration, the total atom percent fission is calculated for each sample. The capture-to-fission ratio for Pu-239 is obtained from the heavy element data and a comparison of the results for atom percent fission obtained by both methods. Finally, the total atom percent fission is converted to burnup in MWd/t.

The program takes 15 to 20 seconds set-up time plus 1 to 3 seconds machine time per sample in a Philco 2000 digital computer. Burnup analyses calculated this way are more accurate and less expensive than hand calculations.

The instructions for the calculation of burnup as programmed appear in Appendices I and II. They will be useful to those who want to carry through a few hand calculations as well as to those who may want to follow the reasoning behind the computation. The equations apply equally as well to uranium fuels which contain initial plutonium as to those fuels which do not. Use is made of changes in the heavy element isotopic ratios to supplement stable fission product analyses. Since corrections are included for known nuclear reactions, the burnup calculations should be applicable to fuels up to very high exposures.

PROGRESS ON ABSOLUTE FISSION YIELD MEASUREMENTS

To minimize laboratory bias in the absolute fission yield determinations to be made on stable fission product nuclides by isotopic dilution mass spectrometry, neodymium and lanthanum standard solutions were exchanged with Phillips Petroleum Company. As can be seen in Table 1, the agreement between sites by EDTA titration is excellent and there is no bias between sites in their primary solutions which are used to calibrate neodymium spike solutions

used in the isotopic dilution analysis.

TABLE 1. Interlaboratory Comparisons of Lanthanide Standard Solutions

<u>Lanthanide Solution</u>	<u>Laboratory where prepared</u>	<u>Results, molarity</u>	
		<u>GE-Vallecitos</u>	<u>Phillips-CPP</u>
Ia	GE-VAL	0.01103 ₆	0.01103
Nd	GE-VAL	0.00869 ₄	0.00870 ₀
Nd	Phillips-CPP	0.00726 ₃	0.00725 ₈

For the fission yield measurements of neodymium, rhenium metal filaments have been very satisfactory. The rhenium metal (supplied by Chase Brass and Copper Company, Inc.) contains some impurities. The major impurity is 100 ppm of natural molybdenum. The natural barium present seriously interferes with the analysis of fission product barium and cerium isotopes. However, for these isotopes, tantalum filaments which are not so contaminated are being used successfully. As a further insurance against barium interference in the cerium analysis, borax is added and the CeO^+ ions are analyzed. During the last month of the quarter, five capsules were received from Phillips Petroleum Company for analysis of absolute thermal fission yields of stable fission products. Emphasis will be placed on the heavy mass yield peak of the fission yield curve for several fissionable isotopes. There is one capsule each of Pu-239, Pu-241, and U-233. The other two capsules contain U-235. Each capsule was irradiated in the MTR to a substantial burnup to permit the absolute number of fissions to be calculated from the heavy element mass loss. The chemistry shielded facility has been prepared to receive these capsules for analysis in the near future.

FUTURE WORK

Analysis of irradiated foils of U-235, U-233, and Pu-239 from capsules GEV-1 and -2 for stable fission products are nearing completion. Cerium and barium analyses which had been adversely affected by natural barium interference in the rhenium filaments described are proceeding smoothly on tantalum filaments. Because of its implication with respect to whether recycle plutonium

could be handled manually in refabrication, the Pu-236 and Pu-238 content of plutonium formed in uranium oxide irradiated in a boiling-water reactor will be determined as a function of MWd/t. In addition, separation and determination of the stable fission product, neodymium, in irradiated UO_2 as it has been developed and used in this program will be written in standard form and submitted to the uranium burnup task force of the American Society for Testing and Materials, Committee E-10 Sub V, for consideration for adoption as an industrially standardized method.

REFERENCES

1. B. F. Rider, C. P. Ruiz, J. P. Peterson, Jr., J. L. Jaech, and R. S. Seymour, "BURNUP: A Code for Calculation of Nuclear Fuel Burnup from U, Pu, and Nd Mass Spectrometric Measurements," GEAP-4811 (to be published).
2. B. F. Rider and C. P. Ruiz, "Determination of Atom Percent Fission in Uranium Fuel," in Progress in Nuclear Energy Series IX, Analytical Chemistry, 3, Part 2, C. E. Crouthamel ed., Pergamon Press (1962).

APPENDIX I

SELECTED SYMBOLS FOR BURNUP CALCULATIONS
IN ORDER OF APPEARANCE IN APPENDIX II

<u>Symbol</u>	<u>Meaning</u>
$M_{3/8}, M_{5/8}$	Isotopic ratios of U-233 and U-235 to U-238 in the <u>mixture</u> of U-Pu mixed spike and sample.
$M_{6/5}, M_{4/5}$	Isotopic ratios of U-236 and U-234 to U-235 in the <u>mixture</u> of U-Pu mixed spike and sample.
$R_{2/9}, R_{0/9}, R_{1/9}$	Isotopic ratios of Pu-242, -240, and -241 to Pu-239 in the "As <u>Received</u> " (unspiked) sample.
$M_{2/9}$	Isotopic ratios of Pu-242 to Pu-239 in the <u>mixture</u> of U-Pu mixed spike and sample.
V_{SA}, V_{SP}	<u>Volume</u> of <u>sample</u> and <u>volume</u> of <u>spike</u> added to the mixture of U-Pu mixed spike and sample.
$M_{42/50}, M_{48/50},$ $M_{46/50}, M_{45/50}$	Isotopic ratios of Nd-142, -148, -146, and -145 to Nd-150 in the <u>mixture</u> of Nd-150 spike and sample.
V_{SA}^*, V_{SP}^*	<u>Volume</u> of <u>sample</u> and <u>volume</u> of <u>spike</u> added to the mixture of Nd-150 spike and sample.
$S_{4/3}, S_{8/3}, S_{9/2}$	Isotopic ratio of U-234 and U-238 to U-233, and of Pu-239 to Pu-242, in the U-Pu mixed <u>spike</u> solution.
S_3	Atoms per milliliter of U-233 in the U-Pu mixed <u>spike</u> .

$C_{2/9}, C_{3/8}$

Isotopic ratio of Pu-242 to Pu-239 and U-233 to U-238 in the mixed calibration standard prepared from NBS standards No. 949 and No. 950.

 C_9/C_8

Ratio of Pu-239 to U-238 in the mixed calibration standard.

 $R_{3/8}$

Ratio of U-233 to U-238 in the "As Received" (unspiked) samples. $R_{3/8} = 0$ for non-Th-232, non-U-233 fuels.

 $P_{2/9}, P_{3/8}$

Ratio of Pu-242 to Pu-239 and the ratio of U-233 to U-238 in the primary calibration mixture of calibration standard and U-Pu mixed spike.

 $S_{50/42}, S_{50/48}, S_{50/46}, S_{50/45}$

Isotopic ratio of Nd-150 to Nd-142, -148, -146, and -145 in the Nd-150 spike.

 A_{50}

Atoms of Nd-150 per milliliter in the Nd-150 spike.

 N_4^o, N_5^o, N_8^o

Fraction of original heavy element atoms (mass > 228) which were U-234, U-235 and U-238, respectively.

 $R_{6/5}^o$

The ratio of U-236 to U-235 in the fuel before irradiation.

 $R_{5/8}^o, R_{2/8}^o, R_{9/8}^o, R_{0/8}^o, R_{1/8}^o$

The ratio of U-235, Pu-242, Pu-239, Pu-240, and Pu-241 to U-238 in the fuel before irradiation.

 t

The decay time (in seconds) from the end of irradiation until the measurement.

 t^*

The irradiation time in seconds.

$\alpha_5, \alpha_9, \alpha_1$

Effective neutron capture-to-fission ratio for U-235, Pu-239, and Pu-241, respectively.

G

$G = 0.064$. If c is the ratio of the U-238 fission rate to the fission rate from all other sources expressed as equivalent U-235 fission rate so that,

$$c = \frac{\nu_5(\epsilon-1)}{\nu_8-1-\alpha_8} \approx 1.6(\epsilon-1) \text{ where } \nu_5 = 2.44 \pm 0.02$$

neutrons per fission of U-235, $\nu_8 = 2.67 \pm 0.30$ neutrons per fission of U-238, $\alpha_8 = 0.13 \pm 0.02$ effective ratio of U-238 (n, γ) capture-to-fission cross sections averaged over a fission spectrum, and ϵ = fast fission factor. Since $(\epsilon-1) \approx 0.04 N_8^0$, $c \approx 1.6(0.04)N_8^0$. Let $G = 1.6(0.04) = 0.064$ so that $c \approx G N_8^0$.

 $\sigma_5, \sigma_6, \sigma_1$

Neutron absorption cross section of U-235, U-236, and Pu-241, respectively (expressed in square centimeters).

 $\sigma_{45}, \sigma_{48}, \sigma_{46}, \sigma_{42}, \sigma_{41}$

Neutron absorption cross section of Nd-145, -148, -146, -142, and Pr-141, respectively (expressed in square centimeters).

 $\nu_9/\nu_5, \nu_1/\nu_5$

Ratio of the number of neutrons per fission of Pu-239 and Pu-241 to U-235, equal to 1.17 and 1.25, respectively.

 λ_1

Decay constant of Pu-241 expressed in seconds.

K

A value that has been chosen to determine when α_9 can be calculated from the data with reasonable accuracy, usually = 0.1 or 0.2.

 $C_{50/42}, C_{50/48}, C_{50/46}, C_{50/45}, C_{48/42}$

Ratios of Nd-150 to Nd-142, -148, -146, and -145, and the ratio of Nd-148 to Nd-142 in natural neodymium contamination.

V	Maximum <u>value</u> permitted for the standard deviation of the mean for the average α_5 .
V ₁	Minimum <u>value</u> permitted for average α_5 .
V ₂	Maximum <u>value</u> permitted for average α_5 .
V ₃	Conversion coefficient from total atom fission fraction to MWd/ton.
V ₄	Minimum permitted individual <u>value</u> of α_9 .
V ₅	Maximum permitted individual <u>value</u> of α_9 .
V ₆	Ratio of concentration of heavy element sample dilution to the concentration of the neodymium sample dilution.
V ₇	Minimum permitted individual <u>value</u> of α_5 .
V ₈	Maximum permitted individual <u>value</u> of α_5 .
V ₉	Minimum acceptable <u>value</u> for $\bar{\alpha}_{93}^*$.
V ₁₀	Maximum acceptable <u>value</u> for $\bar{\alpha}_{93}^*$.
V ₁₁	Maximum acceptable <u>value</u> for $S\alpha_{93}^*$.
V ₁₂	Minimum acceptable <u>value</u> for K_2 .
V ₁₃	Maximum acceptable <u>value</u> for K_2 .
V ₁₄	Maximum acceptable number of standard deviations α_5 may deviate from the $\bar{\alpha}_5$.

V_{15}	Maximum acceptable <u>value</u> for K_3 .
V_{16}	Minimum acceptable <u>value</u> for K_3 .
V_{17}	Maximum acceptable <u>value</u> for $M_{48/50}$.
V_{18}	Minimum acceptable <u>value</u> for $M_{48/50}$.
V_{19}	Maximum allowable <u>value</u> for J .
K_2	Calculated quantity, ideally 0, to test agreement between Nd-148 and Nd-145 plus -146.
K_3	Calculated quantity, ideally 0, to test agreement in atom percent fission derived from neodymium and heavy element isotopic data.
$Y_{05}, Y_{85}, Y_{65}, Y_{55}, Y_{15}$	Fission <u>yield</u> of Nd-150, Nd-148, Nd-146, Nd-145, and Pr-141, respectively, in thermal fission of U-235.
$Y_{09}, Y_{89}, Y_{69}, Y_{59}, Y_{19}$	Fission <u>yield</u> of Nd-150, -148, -146, -145, and Pr-141, respectively, in thermal fission of Pu-239.
$Y_{01}, Y_{81}, Y_{61}, Y_{51}, Y_{11}$	Fission <u>yield</u> of Nd-150, -148, -146, -145, and Pr-141, respectively, in thermal fission of Pu-241.
$Y_{08}, Y_{88}, Y_{68}, Y_{58}, Y_{18}$	Fission <u>yield</u> of Nd-150, -148, -146, -145, and Pr-141, respectively, in fast fission of U-238.
α_{51}	Effective neutron capture-to-fission ratio for U-235 calculated from Equation (1) in Appendix II.
$\bar{\alpha}_5$	Average of all acceptable α_{51} values.

$S\alpha_{51}$	Standard deviation of a single observation of α_{51} .
H	Ratio of final U-235 enrichment to initial value.
N_6^*	Correction factor for U-236 burnout.
$M_{6/5}^*$	U-236 burnout corrected value of $M_{6/5}$.
F_{51}, F_{52}, F_{53}	Fraction of heavy element atoms which fissioned as U-235 as calculated from three different equations.
F_9, F_1, F_8	Fraction of heavy element atoms which fissioned as Pu-239, Pu-241, and U-238, respectively.
F	Total fraction of heavy element atoms which fissioned.
M_8, M_4, M_5, M_6	Isotopic abundance of U-238, -234, -235, and -236 (in percent) in the irradiated sample.
A, B, C, D	Intermediate constants in the calibration of the U-233 plus Pu-242 mixed spike (A and B) or in the determination of $R_{9/8}$ of the sample (C and D).
$R_{9/8}, R_{0/8}, R_{1/8}, R_{2/8}$	Ratio of Pu-239, -240, -241, and -242 to U-238 in the irradiated sample.
W	Exposure in $nv_0 t$ divided by σ_5 .
X	Arbitrary statistic to determine whether α_9 can be calculated from the data.
$R_{1/8}^{***}$	Ratio of Pu-241 to U-238 corrected for decay during and after irradiation.

A_8 Atoms of U-238 per milliliter of sample. P Pu-239 captures per milliliter of sample. α_{91}

Capture-to-fission ratio for Pu-239 (first calculation).

* , ** , ***

One, two, or three asterisks indicate that one, two, or three corrections were applied to the value.

 Q

Correction factor for U-238 burnout.

 $Q_{3/8}, Q_{5/8}$ U-238 burnout corrected values for $M_{3/8}$ and $M_{5/8}$. $\Delta_1 \dots \Delta_{14}$

Calculated constants for neodymium equations.

 $M_{T58} \dots F_{T8}$ Summarized terminal values for $M_{5/8}$ through F_8 from heavy element calculations required for use in neodymium calculations. $E_{50}, E_{48}, E_{46}, E_{45}, E_{41}$ Effective fission yields of Nd-150, -148, -146, -145, and Pr-141 in the irradiated sample. $E_{0/8}, E_{0/6}, E_{0/5}$ Ratio of the effective fission yields of Nd-150 to Nd-148, -146, and -145, respectively. A_{48}, A_{46}, A_{45} Atoms of Nd-148, -146, and -145, respectively, per milliliter of sample. T_8, T_{56}, T_{568}

Fissions per milliliter of sample from the Nd-148, Nd-(145+146), and the average of these two values, respectively.

 Z

Heavy element atoms per milliliter of sample on a pre-irradiation basis.

W_T^*	Neutron exposure (nv ₀ t).
σ_f	Average effective fission cross section for all combined heavy element atoms in the fuel.
K_1	$K_1 = 1/E_{0/8}^* (M_{48/50})$.
A_{42}	Nd-142 <u>a</u> toms per milliliter of sample formed by [Pr-141(n, γ)Pr-142] and subsequent decay to Nd-142. This is the Nd-142 which is not natural contamination.
A_{42}^*	Nd-142 <u>a</u> toms per milliliter of sample as measured.
A_{42}^{**}	Nd-142 <u>a</u> toms per milliliter of sample from natural Nd contamination equal to $A_{42}^* - A_{42}$.
$M_{50/42}^*$	Corrected ratio of Nd-150 to natural Nd-142.
$A_{48}^*, A_{46}^*, A_{45}^*$	Nd-148, -146, and -145 <u>a</u> toms per milliliter of sample corrected for influence of Nd-142 formed from Pr-141.
A_{461}, A_{462}	Nd-146 <u>a</u> toms per milliliter of sample formed from [Nd-145(n, γ)Nd-146] when $\sigma_{46} \neq 0$ and when $\sigma_{46} = 0$, respectively (values 1 and 2).
A_{463}, A_{464}	Nd-146 <u>a</u> toms per milliliter of sample formed from fission where $\sigma_{46} \neq 0$ and when $\sigma_{46} = 0$, respectively (values 3 and 4).
A_{465}	Burnout corrected Nd-146 <u>a</u> toms per milliliter of sample (value 5 and final).
A_{481}, A_{482}	Nd-148 <u>a</u> toms per milliliter of sample formed from fission when $\sigma_{48} \neq 0$ and when $\sigma_{48} = 0$, respectively (value 1 and 2).

A_{483}	Burnout corrected Nd-148 <u>atoms</u> per milliliter of sample (value 3 and final value).
$T_8^*, T_{56}^*, T_{568}^*, Z^*$	Burnout corrected values of T_8 , T_{56} , T_{568} , and Z .
F_{88}, F_{56}, F_{568}	Total initial heavy element atom <u>fraction</u> fissioned as calculated from Nd-148, from Nd-145 + Nd-146, and from Nd-145 + Nd-146 + Nd-148. The double subscript on the Nd-148 value is to distinguish this value from F_8 used for the U-238 contribution to the total fission fraction.
MWd/t	<u>Megawatt days</u> per <u>ton</u> from Nd analysis.
J	Ratio of natural Nd-148 contamination to stable fission product Nd-148.
F_{92}	Atom <u>fraction</u> fission from fission of Pu-239 calculated from total fission fraction as determined from Nd minus F_8 , F_5 , and F_1 (value 2 and final value of F_9).
α_{92}	Capture-to-fission ratio for Pu-239 (value 2).
α_{93}	Experimentally measured value of α_9 (value 3 and final calculation of α_9).
$\bar{\alpha}_{93}^*$	Average of all acceptable α_{93} values.
$S_{\alpha_{93}}^*$	<u>Standard deviation</u> for a single observation of α_{93} .
SUM	<u>Sum</u> of all heavy element ratios to U-238.
4, 5, 6, 8, 9, 0, 1, 2, F, T ATOM PCT	Atom percent of U-234, -235, -236, -238, Pu-239, -240, -241, -242, fission, and total heavy element <u>atom percent</u> .

APPENDIX II

INSTRUCTIONS FOR CALCULATION OF NUCLEAR FUEL BURNUP
FROM U, Pu, AND Nd MASS SPECTROMETRIC MEASUREMENTS

- A. Blend an aliquot of dissolved spent fuel solution with mixed U-233 + Pu-242 spike according to "Determination of Uranium and Plutonium Concentrations and Isotopic Abundances," General Electric Company Report, APED-4527, (May 1, 1964); and record values for $M_{3/8}$, $M_{5/8}$, $M_{6/5}$, $M_{4/5}$, $R_{2/9}$, $R_{0/9}$, $R_{1/9}$, $M_{2/9}$, V_{SA} , and V_{SP} .
- B. Blend an aliquot of the same spent fuel solution with Nd-150 spike according to the procedure outlined in "Accurate Nuclear Fuel Burnup Analyses XII," USAEC Report, GEAP-4776, (December 1, 1964); and record $M_{42/50}$, $M_{48/50}$, $M_{46/50}$, $M_{45/50}$, V_{SA}^* , and V_{SP}^* .
- C. Also, record a series of constants, some of which may vary from one batch of samples to the next. Spike dependent constants are $S_{4/3}$, $S_{8/3}$, $S_{9/2}$, S_3 , $C_{2/9}$, $C_{3/8}$, C_9/C_8 , $R_{3/8}$, $P_{2/9}$, $P_{3/8}$, $S_{50/42}$, $S_{50/48}$, $S_{50/46}$, $S_{50/45}$, and A_{50} . Fuel dependent constants are N_4^o , N_5^o , N_8^o , $R_{6/5}^o$, $R_{5/8}^o$, $R_{2/8}^o$, $R_{9/8}^o$, $R_{0/8}^o$, $R_{1/8}^o$, t and t^* . Reactor dependent constants are α_5 , α_9 , α_1 , G , σ_5 , σ_6 , σ_1 , σ_{45} , σ_{48} , σ_{46} , σ_{42} , and σ_{41} . Other constants are v_9/v_5 , v_1/v_5 , λ_1 , K , $C_{50/42}$, $C_{50/48}$, $C_{50/46}$, $C_{50/45}$, $C_{48/42}$, V , V_1 , V_2 , V_3 , V_4 , V_5 , V_6 , through V_{19} . Fission yield constants include Y_{05} , Y_{85} , Y_{65} , Y_{55} , Y_{15} , Y_{09} , Y_{89} , Y_{69} , Y_{59} , Y_{19} , Y_{01} , Y_{81} , Y_{61} , Y_{51} , Y_{11} , Y_{08} , Y_{88} , Y_{68} , Y_{58} , and Y_{18} . A base set of constants are programmed in the code and only changes from the base set need be supplied.
- D. Some preliminary calculations separate the samples into three sets.
1. Error in α_5 from the U-234 (n, γ) U-235 reaction can be avoided by adding U-234 to U-235 in both pre- and post-irradiation samples. Hence, for each sample calculate

$$M_{4/8}^{**} = (M_{4/5})(M_{5/8}) - (S_{4/3})(M_{3/8})$$

$$M_{5/8}^{***} = M_{4/8}^{**} + M_{5/8}$$

$$R_{5/8}^{o*} = R_{5/8}^o (1 + N_4^o/N_5^o)$$

$$\alpha_{51} = \left[\frac{(M_{6/5})(M_{5/8}) - (R_{6/5}^o)(R_{5/8}^o)}{R_{5/8}^{o*} - M_{5/8}^{***} - (M_{6/5})(M_{5/8}) + (R_{6/5}^o)(R_{5/8}^o)} \right]$$

If $V_7 > \alpha_{51} > V_8$, reject that sample noting this fact.

2. For the remaining samples, $\bar{\alpha}_{51} = \frac{\sum \alpha_{51}}{n}$, and

$$s_{\alpha_{51}} = \sqrt{\frac{\sum \alpha_{51}^2 - (\sum \alpha_{51})^2/n}{n-1}}$$

3. For each acceptable sample, calculate $(\alpha_{51} - \bar{\alpha}_{51})$. Form a set (S-1) of those samples for which this quantity exceeds $V_{14} \cdot (s_{\alpha_{51}})$.
4. For the remaining samples, recalculate $\bar{\alpha}_{51}$ and $s_{\alpha_{51}}$, calling the new values $\bar{\alpha}_{51}^*$ and $s_{\alpha_{51}}^*$. These new values are based on m samples.
5. Test to see if $V_1 < \bar{\alpha}_{51}^* < V_2$ and $s_{\alpha_{51}}^* / \sqrt{m} < V$. If both conditions hold, the m samples used in calculating these quantities form set S-3. If not, all samples are in set S-2, and S-1 and S-3 are both empty.

E. From this point, calculations differ for each set. Start with set S-3, and calculate the following for each S-3 sample.

1. $H = M_{5/8} / R_{5/8}^o$

2. $N_6^* = \frac{(\sigma_5 - \sigma_6)}{\sigma_5} \left[\frac{1-H}{H^{\sigma_6/\sigma_5-H}} \right]$

3. Multiply each $M_{6/5}$ value by N_6^* to get a corrected $M_{6/5}^*$.

$$4. \text{ Re-compute } \alpha_{51}^{**} = \left[\frac{(M_{6/5}^*)(M_{5/8}) - (R_{6/5}^O)(R_{5/8}^U)}{R_{5/8}^{O*} - M_{5/8}^{***} - (M_{6/5}^*)(M_{5/8}) + (R_{6/5}^O)(R_{5/8}^O)} \right]$$

$$5. \text{ Find the average of these values: } \bar{\alpha}_{51}^{**} = \frac{\sum \alpha_{51}^{**}}{m}$$

6. Error in F_{53} from the U-234 (n, γ) U-235 reaction can be avoided by adding U-234 to U-235 in both pre- and post-irradiation samples.

Calculate

$$M_{6/5}^{**} = M_{6/5}^* \left(\frac{M_{5/8}}{M_{4/8}^{**} + M_{5/8}} \right)$$

$$R_{6/5}^{O*} = R_{6/5}^O \left(\frac{1}{1 + N_4^O/N_5^O} \right)$$

$$7. F_{53} = N_5^O \left[\frac{M_{6/5}^{**} - R_{6/5}^{O*}}{M_{6/5}^{**} + \bar{\alpha}_{51}^{**} (1 + M_{6/5}^{**})} \right]$$

$$8. M_8 = 100 / [M_{4/8}^{**} + M_{5/8} (1 + M_{6/5}^*) + 1]$$

$$9. M_4 = (M_8)(M_{4/8}^{**})$$

$$10. M_5 = (M_8)(M_{5/8})$$

$$11. M_6 = (M_8)(M_{5/8})(M_{6/5}^*)$$

$$12. R_9 = 100 / (1 + R_{0/9} + R_{1/9} + R_{2/9})$$

$$13. R_0 = (R_9)(R_{0/9})$$

$$14. R_1 = (R_9)(R_{1/9})$$

$$15. R_2 = (R_9)(R_{2/9})$$

$$16. A = \frac{P_{2/9} - C_{2/9}}{1 - (P_{2/9})(S_{9/2})}$$

$$17. \quad C = \frac{1 - (M_{2/9})(S_{9/2})}{M_{2/9} - R_{2/9}}$$

$$18. \quad B = \frac{P_{3/8} - C_{3/8}}{1 - (P_{3/8})(S_{8/3})}$$

$$19. \quad D = \frac{1 - (M_{3/8})(S_{8/3})}{M_{3/8} - R_{3/8}}$$

where $R_{3/8} = 0$

$$20. \quad R_{9/8} = (C_9/C_8) \left(\frac{AC}{BD} \right)$$

$$21. \quad R_{0/8} = (R_{0/9})(R_{9/8})$$

$$22. \quad R_{1/8} = (R_{1/9})(R_{9/8})$$

$$23. \quad R_{2/8} = (R_{2/9})(R_{9/8})$$

$$24. \quad W = \ln \left[\frac{1}{1 - \left(\frac{R_{5/8}^o - M_{5/8}}{R_{5/8}^o} \right)} \right]$$

$$25. \quad X = R_{9/8}^o \left(\frac{1 - e^{-2W}}{W} \right)$$

$$X = 2R_{9/8}^o \quad \text{when } W \leq 0$$

$$26. \quad R_{1/8}^{***} = R_{1/8} e^{\lambda t} + \left(\frac{1 + \alpha_1}{\alpha_1} \right) \left(\frac{\lambda_1 t^* \sigma_5}{\sigma_1 W} \right) (R_{2/8} - R_{2/8}^o)$$

$$27. \quad A_8 = \frac{V_{SP}}{V_{SA}} (S_3)(D)$$

$$28. F_{51} = N_8^0 [R_{5/8}^0 - M_{5/8} - (M_{6/5}^*) (M_{5/8}) + (R_{6/5}^0) (R_{5/8}^0)]$$

$$29. P = \left[(R_{0/8} - R_{0/8}^0) + (R_{1/8}^{***} - R_{1/8}^0) + (R_{2/8} - R_{2/8}^0) \left(\frac{1 + \alpha_1}{\alpha_1} \right) \right]$$

For the remaining steps, divide the S-3 set into further sub-sets, depending on the value of X in (24). If $X \geq K$, call it S-3-1; if $X < K$, call it S-3-2.

$$30a. \alpha_{91} = \frac{\text{S-3-1}}{(R_{9/8}^0 - R_{9/8} - P)}$$

$$30b. F_{91} = N_8^0 P / \alpha_{91}$$

$$31a. F_9 = N_8^0 P / \alpha_{91}$$

$$31b. F_1 = \frac{N_8^0}{\alpha_1} (R_{2/8} - R_{2/8}^0)$$

$$32a. F_1 = \frac{N_8^0}{\alpha_1} (R_{2/8} - R_{2/8}^0)$$

$$32b. F_{81} = G N_8^0 \left[F_{53} + \left(\frac{v_9}{v_5} \right) F_{91} + \left(\frac{v_1}{v_5} \right) F_1 \right]$$

$$33a. F_8 = G N_8^0 \left[F_{53} + \left(\frac{v_9}{v_5} \right) F_9 + \left(\frac{v_1}{v_5} \right) F_1 \right]$$

$$33b. F^* = F_{53} + F_{91} + F_1 + F_{81}$$

$$34a. F = F_{53} + F_9 + F_1 + F_8$$

$$34b. MWd/t^{**} = v_3 F^*$$

$$35a. MWd/t^{**} = v_3 F$$

F. Compute values for S-1 as follows. This set will exist only if there is a set S-3. Otherwise, all data will form set S-2.

$$1. F_{52} = N_5^0 \left[\frac{M_{6/5} - R_{6/5}^0}{M_{6/5} + \bar{\alpha}_{51}^{**} (1 + M_{6/5})} \right] \quad (\text{use } \bar{\alpha}_{51}^{**} \text{ from Sec. E-5})$$

$$2. M_{5/8}^* = R_{5/8}^0 - \frac{F_{52}}{N_8^0} (1 + \bar{\alpha}_{51}^{**})$$

$$3. H = M_{5/8}^* / R_{5/8}^0$$

$$4. N_6^* = \frac{(\sigma_5 - \sigma_6)}{\sigma_5} \left(\frac{1-H}{H \sigma_6 / \sigma_5 - H} \right)$$

5. Multiply each $M_{6/5}$ value by N_6^* to get a corrected $M_{6/5}^*$ value.

$$\text{Set } M_{6/5}^{**} = M_{6/5}^* \left(\frac{M_{5/8}}{M_{4/8}^{**} + M_{5/8}} \right) \text{ and } R_{6/5}^{o*} = R_{6/5}^o \left(\frac{1}{1 + N_4^o/N_5^o} \right)$$

$$6. F_{52}^* = N_5^o \left[\frac{M_{6/5}^{**} - R_{6/5}^{o*}}{M_{6/5}^{**} + \bar{\alpha}_{51}^{**} (1 + M_{6/5}^{**})} \right]$$

$$7. M_{5/8}^{**} = R_{5/8}^o - \frac{F_{52}^*}{N_8^o} (1 + \bar{\alpha}_{51}^{**})$$

$$8. M_{8/8}^* = M_{5/8}^{**}/M_{5/8}$$

$$9. M_{3/8}^* = (M_{8/8}^*) (M_{3/8})$$

$$10. M_{4/8}^* = (M_{4/5}) (M_{5/8}^{**}) - (S_{4/3}) (M_{3/8}^*)$$

$$11. M_8^* = 100/[M_{4/8}^* + M_{5/8}^{**} (1 + M_{6/5}^*) + 1]$$

$$12. M_4^* = (M_8^*) (M_{4/8}^*)$$

$$13. M_5^* = (M_8^*) (M_{5/8}^{**})$$

$$14. M_6^* = (M_5^*) (M_{6/5}^*)$$

$$15. R_9 = 100/(1 + R_{0/9} + R_{1/9} + R_{2/9})$$

$$16. R_0 = (R_9) (R_{0/9})$$

$$17. R_1 = (R_9) (R_{1/9})$$

$$18. R_2 = (R_9) (R_{2/9})$$

$$19. A^* = \frac{P_{2/9} - C_{2/9}}{1 - (P_{2/9}) (S_{9/2})}$$

$$20. \quad C^* = \frac{1 - (M_{2/9})(S_{9/2})}{M_{2/9} - R_{2/9}}$$

$$21. \quad B^* = \frac{P_{3/8} - C_{3/8}}{1 - (P_{3/8})(S_{8/3})}$$

$$22. \quad D^* = \frac{1 - (M_{3/8}^*)(S_{8/3})}{M_{3/8}^* - R_{3/8}}$$

$$23. \quad R_{9/8}^* = (C_9/C_8)(A^*C^*/B^*D^*)$$

$$24. \quad R_{0/8}^* = (R_{0/9})(R_{9/8}^*)$$

$$25. \quad R_{1/8}^* = (R_{1/9})(R_{9/8}^*)$$

$$26. \quad R_{2/8}^* = (R_{2/9})(R_{9/8}^*)$$

$$27. \quad W^* = \ln \left[\frac{1}{1 - \frac{(R_{5/8}^O - M_{5/8}^{**})}{R_{5/8}^O}} \right]$$

$$28. \quad X^* = R_{9/8}^O \left(\frac{1 - e^{-2W}}{W} \right)$$

$$X^* = 2R_{9/8}^O \text{ when } W \leq 0$$

$$29. \quad R_{1/8}^{**} = R_{1/8}^* e^{\lambda_1 t} + \left(\frac{1 + \alpha_1}{\alpha_1} \right) \left(\frac{\lambda_1 t^* \sigma_5}{\sigma_1 W^*} \right) (R_{2/8}^* - R_{2/8}^O)$$

$$30. \quad A_8^* = (V_{SP}/V_{SA})(S_3)(D^*)$$

$$31. \quad F_{51}^* = N_8^O [R_{5/8}^O - M_{5/8}^{**} - (M_{6/5}^*)(M_{5/8}^{**}) + (R_{6/5}^O)(R_{5/8}^O)]$$

$$32. \quad P^* = \left[(R_{0/8}^* - R_{0/8}^O) + (R_{1/8}^{**} - R_{1/8}^O) + (R_{2/8}^* - R_{2/8}^O) \left(\frac{1 + \alpha_1}{\alpha_1} \right) \right]$$

For the remaining steps, divide the S-1 set into two further subsets, depending on the value of X^* in (27). If $X^* \geq K$, call it S-1-1; if $X^* < K$, call it S-1-2.

S-1-1

$$33a. \alpha_{91}^* = \frac{P^*}{(R_{9/8}^o - R_{9/8}^* - P^*)}$$

$$34a. F_9^* = N_8^o P^* / \alpha_{91}^*$$

$$35a. F_1^* = \frac{N_8^o}{\alpha_1} (R_{2/8} - R_{2/8}^o)$$

$$36a. F_8^* = G N_8^o \left[F_{52}^* + \left(\frac{v_9}{v_5} \right) F_9^* + \left(\frac{v_1}{v_5} \right) F_1^* \right]$$

$$37a. F^{**} = F_{52}^* + F_9^* + F_1^* + F_8^*$$

$$38a. MWd/t^{**} = V_3 F^{**}$$

S-1-2

$$33b. F_{91}^* = N_8^o P^* / \alpha_9$$

$$34b. F_1^* = \frac{N_8^o}{\alpha_1} (R_{2/8} - R_{2/8}^o)$$

$$35b. F_{81}^* = G N_8^o \left[F_{52}^* + \left(\frac{v_9}{v_5} \right) F_{91}^* + \left(\frac{v_1}{v_5} \right) F_1^* \right]$$

$$36b. F^{***} = F_{52}^* + F_{91}^* + F_1^* + F_{81}^*$$

$$37b. MWd/t^{**} = V_3 F^{**}$$

G. Next, compute values for S-2 as follows. This set exists only if S-1 and S-3 do not.

$$1. F_{52} = N_5^o \left[\frac{M_{6/5} - R_{6/5}^o}{M_{6/5} + \alpha_5 (1 + M_{6/5})} \right]$$

$$2. M_{5/8}^* = R_{5/8}^o - \frac{F_{52}}{N_8^o} (1 + \alpha_5)$$

$$3. H = M_{5/8}^* / R_{5/8}^o$$

$$4. N_6^* = \frac{(\sigma_5 - \sigma_6)}{\sigma_5} \left(\frac{1 - H}{H \sigma_6 / \sigma_5 - H} \right)$$

5. Multiply each $M_{6/5}$ value by N_6^* to get a corrected $M_{6/5}^*$ value.

$$\text{Set } M_{6/5}^{**} = M_{6/5}^* \left(\frac{M_{5/8}}{M_{4/8}^{**} + M_{5/8}} \right) \text{ and } R_{6/5}^{o*} = R_{6/5}^o \left(\frac{1}{1 + N_4^o / N_5^o} \right)$$

$$6. \quad F_{52}^* = N_5^o \left[\frac{M_{6/5}^{**} - R_{6/5}^{o*}}{M_{6/5}^{**} + \alpha_5 (1 + M_{6/5}^{**})} \right]$$

$$7. \quad M_{5/8}^{**} = R_{5/8}^o - \frac{F_{52}^*}{N_8^o} (1 + \alpha_5)$$

Steps (8) through (32) are the same as in set (S-1). Make the same test on X to form subsets S-2-1 and S-2-2. Proceed as with S-1-1 and S-1-2.

H. Compute the correction factor for U-238 burnout, Q.

1. For S-1 or S-2 calculate as follows:

$$Q^* = \left[1 + R_{9/8}^* + P^* \left(\frac{1 + \alpha_9}{\alpha_9} \right) + \left(F_{81}^* / N_8^o \right) - R_{9/8}^o \right]^{-1} \leq 1$$

2. For S-3 calculate as follows:

$$Q = \left[1 + R_{9/8} + P \left(\frac{1 + \alpha_9}{\alpha_9} \right) + \left(F_{81} / N_8^o \right) - R_{9/8}^o \right]^{-1} \leq 1$$

3. Multiply the input columns $M_{3/8}$ and $M_{5/8}$ by Q^* or Q whichever is applicable, and call these values $Q_{3/8}^*$ and $Q_{5/8}^*$ or $Q_{3/8}$ and $Q_{5/8}$, respectively. Re-do the analysis using these values for $M_{3/8}$ and $M_{5/8}$.

4. Finally, arrange all the $M_{6/5}^*$ in descending order. List the corresponding, corrected values for the following quantities: R_9 , R_0 , R_1 , R_2 , $R_{9/8}$, $M_{6/8}$, $M_{5/8}$. Graphically plot each value versus $M_{6/5}^*$ and visually inspect the proximity of each point to a smooth curve. Recheck or reanalyze the input data for any outlying points.

I. If neodymium mass spectrometric measurements are available, calculate for each case as follows:

$$1. \quad \Delta_1 = \left(\frac{1}{S_{50/42}} - \frac{1}{C_{50/42}} \right)$$

$$2. \Delta_2 = \left(\frac{1}{C_{50/48}} - \frac{1}{S_{50/48}} \right)$$

$$3. \Delta_3 = \left(\frac{1}{C_{50/46}} - \frac{1}{S_{50/46}} \right)$$

$$4. \Delta_4 = \left(\frac{1}{C_{50/45}} - \frac{1}{S_{50/45}} \right)$$

$$5. \Delta_5 = \left(\frac{1}{C_{50/42} S_{50/48}} - \frac{1}{S_{50/42} C_{50/48}} \right)$$

$$6. \Delta_6 = \left(\frac{1}{C_{50/42} S_{50/46}} - \frac{1}{S_{50/42} C_{50/46}} \right)$$

$$7. \Delta_7 = \left(\frac{1}{C_{50/42} S_{50/45}} - \frac{1}{S_{50/42} C_{50/45}} \right)$$

$$8. \Delta_8 = \left(\frac{-1}{C_{50/42}} \right)$$

9. For each sample. if $V_{17} < M_{48/50} < V_{18}$ print "Sa Size Error".

For each sample, define F_T as a value from the output of the heavy element analysis. This will be either F (2nd iteration, Section E-34a for S-3-1), or F^* (2nd iteration, Section E-33b for S-3-2), or F^{**} (2nd iteration, Section F-37a for S-1-1 or S-2-1), or F^{***} (2nd iteration, Section F-36b for S-1-2 or S-2-2).

IMPORTANT: These are to be taken from the 2nd iteration after adjustment by Q or Q^* .

Also, define:

$$\left. \begin{aligned} F_{T5} &= F_{53} \text{ or } F_{52}^* \\ F_{T9} &= F_9, F_{91}, F_9^*, \text{ or } F_{91}^* \\ F_{T1} &= F_1 \text{ or } F_1^* \\ F_{T8} &= F_8, F_{81}, F_8^*, \text{ or } F_{81}^* \end{aligned} \right\}$$

All from the 2nd iteration,
as was F_T .

$$10. E_{50} = 1/F_T (F_{T5}Y_{05} + F_{T9}Y_{09} + F_{T1}Y_{01} + F_{T8}Y_{08})$$

$$11. E_{48} = 1/F_T (F_{T5}Y_{85} + F_{T9}Y_{89} + F_{T1}Y_{81} + F_{T8}Y_{88})$$

$$12. E_{46} = 1/F_T (F_{T5}Y_{65} + F_{T9}Y_{69} + F_{T1}Y_{61} + F_{T8}Y_{68})$$

$$13. E_{45} = 1/F_T (F_{T5}Y_{55} + F_{T9}Y_{59} + F_{T1}Y_{51} + F_{T8}Y_{58})$$

$$14. E_{41} = 1/F_T (F_{T5}Y_{15} + F_{T9}Y_{19} + F_{T1}Y_{11} + F_{T8}Y_{18})$$

$$15. E_{0/8}^* = E_{50}/E_{48}$$

$$16. E_{0/6}^* = E_{50}/E_{46}$$

$$17. E_{0/5}^* = E_{50}/E_{45}$$

$$18. \Delta_9 = E_{0/8}^*/C_{50/42}$$

$$19. \Delta_{10} = E_{0/6}^*/C_{50/42}$$

$$20. \Delta_{11} = E_{0/5}^*/C_{50/42}$$

$$21. \Delta_{12} = 1 - E_{0/8}^*/C_{50/48}$$

$$22. \Delta_{13} = 1 - E_{0/6}^*/C_{50/46}$$

$$23. \Delta_{14} = 1 - E_{0/5}^*/C_{50/45}$$

$$24. A_{48} = V_6 \left(\frac{V_{SP}^*}{V_{SA}^*} \right) (A_{50}) \left(\frac{\Delta_1^M_{48/50} + \Delta_2^M_{42/50} + \Delta_5}{\Delta_9^M_{48/50} + \Delta_{12}^M_{42/50} + \Delta_8} \right)$$

$$25. \quad A_{46} = V_6 \left(\frac{V_{SP}^*}{V_{SA}^*} \right) (A_{50}) \left(\frac{\Delta_1^M M_{46/50} + \Delta_3^M M_{42/50} + \Delta_6}{\Delta_{10}^M M_{46/50} + \Delta_{13}^M M_{42/50} + \Delta_8} \right)$$

$$26. \quad A_{45} = V_6 \left(\frac{V_{SP}^*}{V_{SA}^*} \right) (A_{50}) \left(\frac{\Delta_1^M M_{45/50} + \Delta_4^M M_{42/50} + \Delta_7}{\Delta_{11}^M M_{45/50} + \Delta_{14}^M M_{42/50} + \Delta_8} \right)$$

$$27. \quad T_8 = A_{48} / E_{48}$$

$$28. \quad T_{56} = \frac{A_{46} + A_{45}}{E_{46} + E_{45}}$$

$$29. \quad T_{568} = \frac{A_{48} + A_{46} + A_{45}}{E_{48} + E_{46} + E_{45}}$$

30. Obtain several output values from heavy element analysis. **IMPORTANT:**
Use values from 1st iteration, before adjustment for Q or Q*.

Define:

$$M_{T58} = M_{5/8} \text{ for previous subset S-3}$$

$$M_{T58} = M_{5/8}^* \text{ for previous subset S-1 or S-2}$$

$$M_{T48} = M_{4/8}^* \text{ for previous subset S-3}$$

$$M_{T48} = M_{4/8} \text{ for previous subset S-1 or S-2}$$

$$R_{T98} = R_{9/8} \text{ for previous subset S-3}$$

$$R_{T98} = R_{9/8}^* \text{ for previous subset S-1 or S-2}$$

$$R_{T08} = R_{0/8} \text{ for previous subset S-3}$$

$$R_{T08} = R_{0/8}^* \text{ for previous subset S-1 or S-2}$$

$$R_{T18} = R_{1/8}^{***} \text{ for previous subset S-3}$$

$$R_{T18} = R_{1/8}^{**} \text{ for previous subset S-1 or S-2}$$

$$R_{T28} = R_{2/8} \text{ for S-1, S-2, and S-3}$$

$$A_{T8} = A_8 \text{ for previous subset S-3}$$

$$A_{T8} = A_8^* \text{ for previous subset S-1 or S-2}$$

$$W_T = W \text{ for previous subset S-3}$$

$$W_T = W^* \text{ for previous subset S-1 or S-2}$$

31. Calculate:

$$Z = A_{T8} (1 + M_{T58} + M_{T48} + M_{6/5}^* M_{T58} + R_{T98} + R_{T08} + R_{T18} e^{-\lambda_1 t} + R_{T28} + T_{568}/A_{T8})$$

$$32. W_T^* = nv_o t = \frac{W_T}{\sigma_5}$$

$$33. \sigma_f = \frac{\ln\left(\frac{Z}{Z - T_{568}}\right)}{W_T^*}$$

$$34. A_{42} = E_{41} \sigma_f \sigma_{41} Z \left[\frac{e^{-\sigma_f W_T^*}}{(\sigma_{41} - \sigma_f)(\sigma_{42} - \sigma_f)} + \frac{e^{-\sigma_{41} W_T^*}}{(\sigma_f - \sigma_{41})(\sigma_{42} - \sigma_{41})} + \frac{e^{-\sigma_{42} W_T^*}}{(\sigma_f - \sigma_{42})(\sigma_{41} - \sigma_{42})} \right]$$

$$35. K_1 = 1 - 1/E_{0/8}^* (M_{48/50})$$

$$36. \quad A_{42}^* = V_6 \frac{V_{SP}^*}{V_{SA}^*} (A_{50}) \left[\frac{1 - \frac{1}{S_{50/42} M_{42/50}} - \frac{1 - 1/S_{50/48} (M_{42/50})}{K_1}}{\frac{1}{M_{42/50}} - C_{50/42} + \frac{C_{50/42} - C_{48/42} M_{48/50}}{K_1}} \right]$$

$$37. \quad A_{42}^{**} = A_{42}^* - A_{42} \quad (\text{if } A_{42}^{**} \leq 0, \text{ set it } = 0)$$

$$38. \quad M_{42/50}^* = (M_{42/50}) (A_{42}^{**}/A_{42}^*)$$

$$39. \quad A_{48}^* = V_6 \left(\frac{V_{SP}^*}{V_{SA}^*} \right) (A_{50}) \left(\frac{\Delta_1 M_{48/50} + \Delta_2 M_{42/50}^* + \Delta_5}{\Delta_9 M_{48/50} + \Delta_{12} M_{42/50}^* + \Delta_8} \right)$$

$$40. \quad A_{46}^* = V_6 \left(\frac{V_{SP}^*}{V_{SA}^*} \right) (A_{50}) \left(\frac{\Delta_1 M_{46/50} + \Delta_3 M_{42/50}^* + \Delta_6}{\Delta_{10} M_{46/50} + \Delta_{13} M_{42/50}^* + \Delta_8} \right)$$

$$41. \quad A_{45}^* = V_6 \left(\frac{V_{SP}^*}{V_{SA}^*} \right) (A_{50}) \left(\frac{\Delta_1 M_{45/50} + \Delta_4 M_{42/50}^* + \Delta_7}{\Delta_{11} M_{45/50} + \Delta_{14} M_{42/50}^* + \Delta_8} \right)$$

$$42. \quad A_{461} = E_{45} \sigma_f \sigma_{45} Z \left[\frac{e^{-\sigma_f W_T^*}}{(\sigma_{45} - \sigma_f)(\sigma_{46} - \sigma_f)} + \frac{e^{-\sigma_{45} W_T^*}}{(\sigma_f - \sigma_{45})(\sigma_{46} - \sigma_{45})} + \frac{e^{-\sigma_{46} W_T^*}}{(\sigma_f - \sigma_{46})(\sigma_{45} - \sigma_{46})} \right]$$

$$43. \quad A_{462} = E_{45} \sigma_f \sigma_{45} Z \left[\frac{-e^{-\sigma_f W_T^*}}{(\sigma_{45} - \sigma_f) \sigma_f} - \frac{e^{-\sigma_{45} W_T^*}}{(\sigma_f - \sigma_{45}) \sigma_{45}} + \frac{1}{\sigma_f \sigma_{45}} \right]$$

$$44. \quad A_{463} = E_{46} Z \left(\frac{\sigma_f}{\sigma_{46} - \sigma_f} \right) \left(e^{-\sigma_f W_T^*} - e^{-\sigma_{46} W_T^*} \right)$$

$$45. \quad A_{464} = E_{46} Z \left(1 - e^{-\sigma_f W_T^*} \right)$$

$$46. \quad A_{465} = A_{46}^* \left(\frac{A_{464} + A_{462}}{A_{461} + A_{463}} \right)$$

$$47. \quad A_{481} = E_{48} Z \left(\frac{\sigma_f}{\sigma_{48} - \sigma_f} \right) \left(e^{-\sigma_f W_T^*} - e^{-\sigma_{48} W_T^*} \right)$$

$$48. \quad A_{482} = E_{48} Z \left(1 - e^{-\sigma_f W_T^*} \right)$$

$$49. \quad A_{483} = A_{48}^* (A_{482}/A_{481}) \quad \text{and } J = \frac{A_{42}^{**} (C_{48/42})}{A_{483}}$$

$$50. \quad T_8^* = A_{483}/E_{48} \quad \text{If } J > V_{19} \text{ print "Hi J" and set } T_8^* = 0$$

$$51. \quad T_{56}^* = \frac{A_{465} + A_{45}^*}{E_{46} + E_{45}} \quad \text{If } J > V_{19} \text{ print "Hi J" and set } T_{56}^* = 0$$

$$52. \quad K_2 = \left(\frac{T_8^*}{T_{56}^*} - 1 \right)$$

$$\text{If } V_{12} > K_2 > V_{13}; \quad T_{568}^* = T_8^* \text{ and print "Nd inconsistent".}$$

$$\text{If } V_{12} < K_2 < V_{13}; \quad T_{568}^* = \frac{T_8^* + T_{56}^*}{2}.$$

$$53. \quad Z^* = A_{T8} (1 + M_{T58} + M_{T48} + M_{6/5}^* M_{T58} + R_{T98} + R_{T08} + R_{T18} e^{-\lambda_1 t} \\ + R_{T28} + T_{568}^*/A_{T8})$$

$$54. \quad F_{88} = T_8^*/Z^*$$

$$55. \quad F_{56} = T_{56}^*/Z^*$$

$$56. \quad F_{568} = T_{568}^*/Z^*$$

$$57. \quad K_3 = \left(\frac{F_{568}}{F_T} - 1 \right)$$

$$\text{If } V_{15} < K_3 < V_{16}; \text{ set } F_{568} = 0 \text{ and print "Nd/HE inconsistent"}$$

$$58. \quad \text{MWd/t} = V_3 F_{568}$$

$$59. \quad F_{92} = F_{568} - F_{T5} - F_{T8} - F_{T1}$$

For previously defined subsets S-1-1, S-2-1, and S-3-1

60. α_{92} = either α_{91} from Section E-30a, or α_{91}^* from Section F-33a

$$61. \alpha_{93} = \left(\frac{F_{T9}}{F_{92}} \right) \alpha_{92}$$

For previously defined subsets S-1-2, S-2-2, and S-3-2

$$62. \alpha_{93} = (F_{T9}/F_{92}) \alpha_9$$

63. For all samples excluding those for which $V_4 > \alpha_{93} > V_5$

$$\bar{\alpha}_{93} = \frac{\sum \alpha_{93}}{n}, \text{ and}$$

$$S\alpha_{93} = \sqrt{\frac{\sum \alpha_{93}^2 - (\sum \alpha_{93})^2/n}{n-1}}$$

64. For each acceptable sample calculate $\alpha_{93} - \bar{\alpha}_{93}$. Exclude from $\bar{\alpha}_{93}$ all samples for which this quantity exceeds $V_{14}(S\alpha_{93})$, recalculate $\bar{\alpha}_{93}$ and $S\alpha_{93}$ calling new values $\bar{\alpha}_{93}^*$ and $S^*\alpha_{93}$. These values are based on m samples.

65. Test to see if $V_9 < \bar{\alpha}_{93}^* < V_{10}$ and $S^*\alpha_{93}/\sqrt{m} < V_{11}$. If both conditions hold, the value for $\bar{\alpha}_{93}^*$ is acceptable. If either condition does not hold set $\bar{\alpha}_{93}^* = \alpha_9$.

66. For all subsets, recompute F_{T9} , F_{T8} , and F_T (Section I-9) using α_{93} from Section I-61 or $\bar{\alpha}_{93}^*$ from Section I-65 in place of α_9 , α_{91} , or α_{91}^* . Call these final values F_{T9}^* , F_{T8}^* , F_T^* .

$$67. MWd/t^* = V_3 F_T^*$$

68. Arrange the samples in numerical order, and print out the following information.

$M_4, M_5, M_6, M_8, R_9, R_0, R_1, R_2, F_T, F_{T5}, F_{T9}, F_{T1}, F_{T8}, MWd/t^*,$
 $\alpha_{51}, \alpha_{93}, F_{88}, F_{56}, F_{568}, MWd/t, R_{9/8}, A_8, Z^*,$ and $J.$

$$69. \text{ SUM} = 1 + M_{5/8} + M_{6/5} M_{5/8} + M_{4/8}^{**} + R_{9/8} + R_{0/8} + R_{1/8} e^{\lambda_1 t} + R_{2/8} \\ + (F_T^*) \left(\frac{1}{N_{8Q}^O} \right)$$

$$4 \text{ ATOM PCT} = (M_{4/8}^{**}) (100) / \text{SUM}$$

$$5 \text{ ATOM PCT} = (M_{5/8}) (100) / \text{SUM}$$

$$6 \text{ ATOM PCT} = (M_{6/5}) (M_{5/8}) (100) / \text{SUM}$$

$$8 \text{ ATOM PCT} = 100 / \text{SUM}$$

$$9 \text{ ATOM PCT} = (R_{9/8}) (100) / \text{SUM}$$

$$0 \text{ ATOM PCT} = (R_{0/8}) (100) / \text{SUM}$$

$$1 \text{ ATOM PCT} = (R_{1/8}) (e^{\lambda_1 t}) (100) / \text{SUM}$$

$$2 \text{ ATOM PCT} = (R_{2/8}) (100) / \text{SUM}$$

$$F \text{ ATOM PCT} = (F_T^*) \left(\frac{100}{N_{8Q}^O} \right) / \text{SUM}$$

$$T \text{ ATOM PCT} = (4 + 5 + 6 + 8 + 9 + 0 + 1 + 2 + F) (\text{ATOM PCT})$$

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