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Progress Report

Applied Nuclear Data

Research and Development

January 1—March 31, 1978

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APPLIED NUCLEAR DATA RESEARCH AND DEVELOPMENT
QUARTERLY PROGRESS REPORT
January 1 - March 31, 1978

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ABSTRACT

This progress report describes the activities of the
Los Alamos Nuclear Data Group for the period January 1 through
March 31, 1978. The topical content is summarized in the
contents.

I. THEORY AND EVALUATION OF NUCLEAR CROSS SECTIONS

A. R-Matrix Analysis of the Four-Nucleon System (G. M. Hale and D. C. Dodder)

In addition to containing several reactions of interest in applications,
the four-nucleon system offers numerous tests of the charge-independence proper-
ties of nuclear forces. In our most ambitious analysis to date, we are attempt-
ing to account for data from ten independent reactions in two different compound
systems with a single set of charge-independent R-matrix parameters. The pro-
gress of this work during the last quarter is outlined below, by compound
system.

^{4}Li. Fitting the data for p + ^{3}He elastic scattering determines the iso-
spin-1 parameters of the four-nucleon R-matrix. Small improvements in our al-
ready good fit[1] to these data were obtained by allowing absorption in more
partial waves to reproduce the magnitude of the reaction cross section observed
in recent measurements.[2] A more systematic treatment of parameters in the dis-
tant levels appears to be consistent with simple properties of the effective
p + ^{3}He interaction.

^{4}He. The energy range of the six independent particle reactions considered
in this system has been extended to energies close to 30 MeV excitation in ^{4}He

in order to better determine levels in the 20-30 MeV region. This extension has involved the addition of many new measurements, particularly for the d + d reactions. The fit to these higher energy data, while at present only qualitative, is expected to improve as better values for parameters of the upper isospin-0 levels are found.

A major development in the analysis has been the discovery that, when reasonable gamma-ray widths are added in the levels whose particle widths have been determined by analyzing data from the particle reactions described above, a satisfactory description of the photo-absorption reactions on ^{4}He[^{4}He(γ,p)T, ^{4}He(γ,n)^{3}He, and ^{4}He(γ,d)D] is obtained. This development removes the apparent contradiction between the isospin-1 level ordering that best explains p + ^{3}He scattering data[3] and that which had been thought to account best for ^{4}He(γ,p) and ^{4}He(γ,n) measurements.[4]

B.   R-Matrix Analysis of π-N Scattering   (D. C. Dodder)

An earlier analysis of the π-N scattering that went up to 100 MeV pion laboratory energy has been extended to 300 MeV pions. This analysis simultaneously fits p(π^+,π^+)p, p(π^-,π^-)p, and p(π^-,π^0)n experiments with a set of charge-independent reduced widths and Coulomb-corrected eigenenergies. Other Coulomb differences between the two charge states are explicitly calculated by the R-matrix program. A preliminary fit to the data has been obtained neglecting the inelastic channels. Pion production and gamma-emission channels are now being put in before the analysis is extended to higher energies.

The differential cross sections from these scattering experiments are used at the Los Alamos Meson Physics Facility (LAMPF) for calibrating a number of experiments, and the R-matrix program EDA is useful for providing predictions at angles and energies where experimental measurements are not available.

C.   Calculation of the ^{88}Y(n,γ) Cross Section Using Gamma-Ray Strength Functions   (E. D. Arthur)

The use of the systematic behavior of gamma-ray strength functions has been suggested[5] as a means by which neutron capture cross sections can be calculated for nuclei where little or no experimental data exist. The gamma-ray strength function is defined by

$$\frac{<\Gamma_\gamma>}{<D>} = \int_0^{S_n} f_{E1}(\varepsilon_\gamma) \; \varepsilon_\gamma^3 \rho(S_n - \varepsilon_\gamma) d\varepsilon_\gamma \quad , \tag{1}$$

where S_n is the neutron binding energy, ρ is the level density of the compound system, and the electric dipole gamma-ray strength function $f_{E1}(\varepsilon_\gamma)$ is assumed to have a giant dipole resonance (GDR) form given by

$$f_{E1}(\varepsilon_\gamma) = \frac{k \, \varepsilon_\gamma \, \Gamma_{GDR}}{(\varepsilon_\gamma \Gamma_{GDR})^2 + (\varepsilon_\gamma^2 - E_{GDR}^2)^2} \quad . \tag{2}$$

The $f_{E1}(\varepsilon_\gamma)$ function is expected to vary smoothly from nucleus to nucleus, whereas the ratio of the average gamma-ray width to the average level spacing $2\pi<\Gamma_\gamma>/<D>$, the quantity that is generally used to normalize neutron capture calculations, can vary drastically between nearby nuclei. We have explored the magnitude and variation of gamma-ray strength functions by fitting neutron capture cross sections for nuclei from [85]Rb to [99]Tc. We considered only E1 contributions and took the giant dipole resonance width and position [Γ_{GDR} and E_{GDR} in Eq. (2)] from photonuclear data. The E1 gamma-ray strength functions extracted for several compound systems are shown in Fig. 1. From the analysis of [85,87]Rb and [90,91,92]Zr(n,γ) data, the strength function $f_{E1}(\varepsilon_\gamma)$ was determined, within the accuracy of the fit, to be identical for isotopes of the same element. Since recent experimental results[6-8] are available for the [88]Sr, [89]Y, and [90,91,92]Zr(n,γ) reactions, we believe the extracted strength functions to be particularly reliable for these cases.

We have applied the gamma-ray strength function obtained for the ^{90}Y compound system through the [89]Y(n,γ)[90]Y reaction to the case of neutron capture on [88]Y. Even with a reasonable knowledge of the gamma-ray strength function, care must be taken in the determination of the level density expression appearing in Eq. (1), since for the case of the [89]Y compound system, the integration extends past 11 MeV, a particularly high value. We thus constrained the [89]Y compound nucleus level density to fit nuclear level information at low excitation energies and observed resonance spacings determined from systematics at the neutron binding energy.

The results of the present preliminary calculation of the [88]Y(n,γ) cross section are shown in Fig. 2 and are compared to the results of our earlier
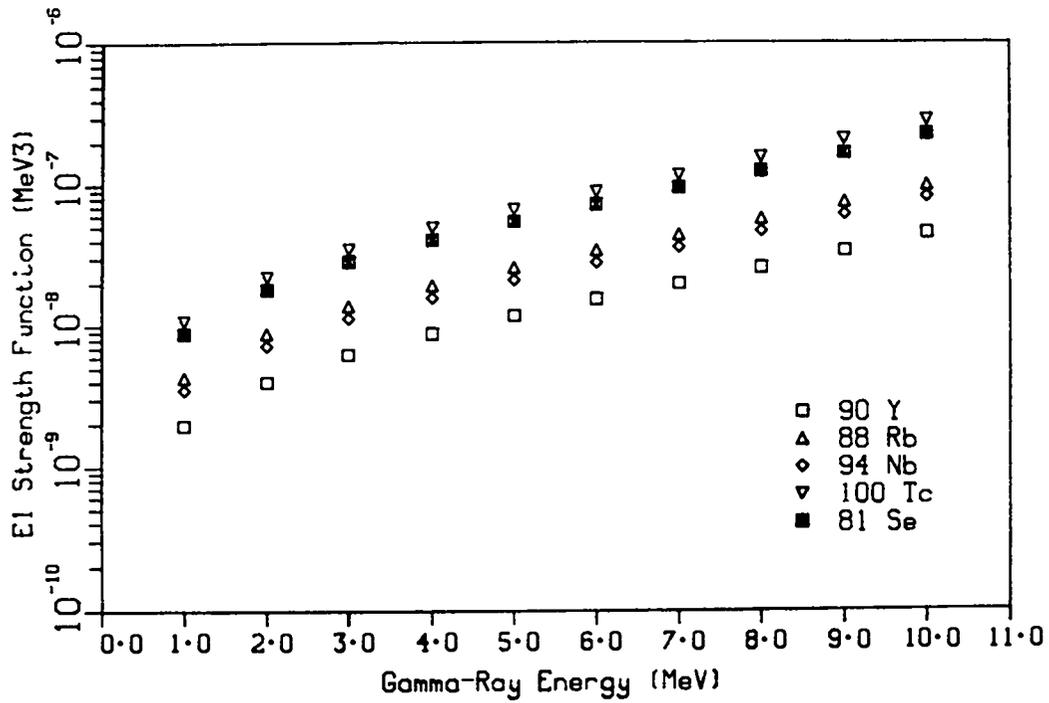
Fig. 1.

Compound nucleus E1 gamma-ray strength functions extracted from neutron capture data.
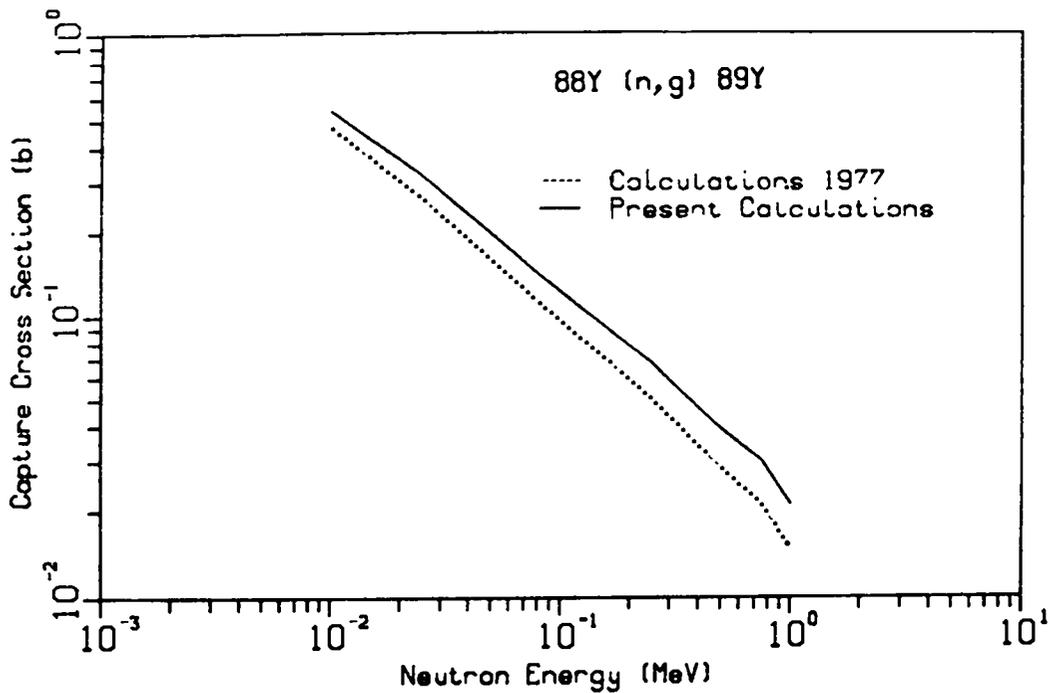
Fig. 2.

A comparison of the present ^{88}Y(n,γ) cross section calculation using the ^{90}Y E1 gamma-ray strength function with our earlier calculated results.

calculation.[9] For the previous calculation, phenomenological expressions were used to fit the behavior of $<D>$ and $<\Gamma_\gamma>$ in the mass region from A = 80-100, with an estimated uncertainty in their determination of 50 to 25%, respectively.

D. (α,n) Cross Sections of Minor Isotopes of Magnesium (D. G. Foster, Jr., E. D. Arthur, and A. H. Wells)

Passive methods for nondestructive assaying of plutonium have become an important element of nuclear-safeguards research. In support of this effort, we have calculated the (α,n) cross sections of ^{25}Mg and ^{26}Mg up to the maximum energy of naturally occurring alpha particles (approximately 5.5 MeV). We have also calculated the secondary neutron energy spectrum. The calculations were performed using the GNASH code, with optical-model parameters for neutrons, protons, and alpha particles taken from recent work by Flynn et al.[10] We found it necessary to decrease Flynn's radius of the real alpha potential somewhat, however, in order to improve agreement with the low-energy ^{26}Mg(n,α)^{29}Si cross section measured by Bair and Willard.[11] We took the parameters for the discrete levels from a computer listing of ENSDF.[12]

The alpha particle is heavy enough relative to magnesium nuclei that the center-of-mass motion smears the neutron spectrum significantly. Since GNASH does not calculate angular distributions, we have assumed isotropy in the center-of-mass system and calculated the resulting laboratory spectrum in a separate operation. Figure 3 illustrates the results for 5.6-MeV alpha particles. We have also calculated the slowing-down spectrum of alpha particles from plutonium in a mixture of PuO_2 and MgO, but we have not yet combined the two operations to obtain the neutron spectrum that results.

E. Correlated Error Data for n + ^{9}Be Evaluated Cross Sections (P. G. Young and D. W. Muir)

Covariance data files have been derived for the Los Alamos Scientific Laboratory-Lawrence Livermore Laboratory (LASL-LLL) evaluation[13] of n + ^{9}Be cross sections. Error data are included for the total, elastic, discrete inelastic [used to represent the ^{9}Be(n,2n) reaction], total (n,2n), (n,γ), (n,p), (n,d), (n,t), and (n,α) reactions. In most cases the error data are based either on the scatter of experimental data or on quoted uncertainties. Correlations in energy are included in the uncertainties for each reaction type and are generally divided into "long" and "short" range components. Correlations across reaction type are provided for MT = 51-83, the pseudolevels used to represent the ^{9}Be(n,2n)
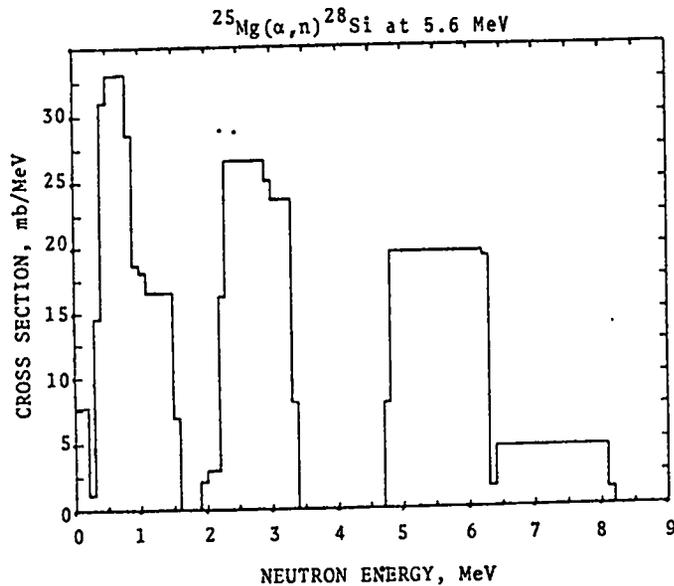
$^{25}Mg(\alpha,n)^{28}Si$ at 5.6 MeV

Fig. 3.
Calculated spectrum of neutrons from the
$^{25}Mg(\alpha,n)^{28}Si$ reaction for 5.6 MeV alpha
particles assuming isotropy in the center-
of-mass system.

reaction.[13] In addition, the elastic and total (n,2n) covariances include im-
plicit correlations with the reactions from which they are derived.

The complete ^9Be data file will be provided to the Brookhaven National
Laboratory (BNL) and Radiation Shielding Information Center (RSIC) data centers
upon completion of data testing activities at the Los Alamos Scientific Labor-
atory.

F.   COMNUC Code Development   (D. G. Madland)

The following changes have been incorporated into the statistical reaction
model code COMNUC (HEAVY).[14]

1.   The prescription for calculating the number of contributing partial waves
at a given energy has been modified to yield a larger value of ℓ_{max}.

2.   The continuum fission calculation has been changed in order to better rep-
resent the physical situation at the fission barrier.[15] The changes af-
fect first, second, and third chance fission calculations.

3.   Discrete fission channels (up to a maximum of 10) have been introduced
into the second and third chance fission calculations.[15]

4. The routine GILCAM, from the code GNASH,[16] has been incorporated into the nuclear level-density calculation. GILCAM adjusts the parameters of the Gilbert and Cameron formulation[17] of the (continuous) level density so that discrete and continuous level densities are smoothly joined. An additional option now exists by which the boundary condition of one level at zero excitation energy may be invoked.

5. Cross sections for all open channels can now be punched in ENDF format for up to 50 bombarding energies per calculation.

A sensitivity of calculated cross sections to the choice of the branching ratio energy grid, in certain cases, and to the incident neutron transmission coefficient energy grid in certain other cases, has led to the conclusion that the end point conditions used in the spline interpolation scheme of COMNUC are not optimal. Two alternative spline packages are being studied for possible use in the code. In the meantime, the problem can be circumvented by clustering three to five grid points near each end of the grid.

G. ^{242}Pu Evaluation (D. G. Madland and P. G. Young)

An evaluation of the neutron-induced reactions on ^{242}Pu has been undertaken for an energy range of 1 keV to 20 MeV. The evaluation will be primarily calculational as little data exist (scant data on the total and capture cross sections and a fair amount of fission cross-section data are available). Combined shape and compound-elastic spherical optical-model calculations, direct coupled-channel inelastic calculations, and Hauser-Feshbach statistical reaction model calculations have been performed on an energy grid of 125 points. Total, shape and compound elastic, (n,n'), (n,xn), (n,xnf), and (n,γ) cross sections have been calculated. The results are under study.

H. ^{233}U Evaluation (L. Stewart, D. G. Madland, and P. G. Young)

Several of the planned updates discussed in the previous quarterly report[18] have been completed. A paper on the evaluation has been submitted and accepted for the San Diego June 1978 American Nuclear Society Meeting.

I. Phase I Reviews (L. Stewart)

Partial reviews of the Version V preliminary evaluations for ^{238}U, ^{240}Pu, and ^{241}Pu have been made and the results reported to the National Nuclear Data

Center and to the principal evaluators. Severe problems in the gamma-ray files were outlined for Pb, and the (n,2n) spectra for Au were not possible from physical considerations. The cut-off energies for spectral information for a number of materials were found to be incorrect and Brookhaven National Laboratory will incorporate these corrections into the Version V files.

II.   NUCLEAR CROSS-SECTION PROCESSING

A.   Cross Sections for the Assessment of ^{233}U-^{232}Th Fuel Cycles   (R. E. MacFarlane)

Because of the recent interest in proliferation resistant replacements for the plutonium-using breeder reactor fuel cycle, a national program is under way to assess various reactor types using ^{233}U and ^{232}Th. New evaluations of the cross sections for these two isotopes are being developed, but they will not be available in time to influence the studies now under way. However, because of the importance of these studies, it has been decided to make pre-preliminary versions of these evaluations available. We have processed these pre-preliminary ENDF/B-V evaluations into two different multigroup libraries using the NJOY code. The first set is in the 50 group format of LIB-IV,[19] and the second is in the 42 group FTR-300S format.[20] The results have been sent to General Electric; Westinghouse Advanced Reactor Division; Westinghouse Hanford Engineering Development Laboratory; Combustion Engineering, Inc; Atomics International; and the National Nuclear Data Center at Brookhaven National Laboratory.

B.   Multigroup Cross Sections for the Actinides   (D. W. Muir, R. E. MacFarlane, and R. J. Barrett)

Multigroup neutron and photon-production cross sections for the long-lived curium and californium isotopes were processed with NJOY into the standard TD-Division format (30 neutron groups, 12 photon groups, separate edit vectors, and P_0 - P_4 neutron scattering tables). Isotopes included are ^{245}Cm, ^{246}Cm, ^{247}Cm, ^{248}Cm, ^{249}Cf, ^{250}Cf, ^{251}Cf, and ^{252}Cf. Basic evaluated data were taken from ENDF/B, preliminary Version V (tapes T944 and T945). Revision of some of these evaluated data seems likely before the issuance of ENDF/B-V in final form, expected to occur by late 1978, so users are advised to exercise some caution in using these multigroup sets. Together with ^{242}Pu, ^{241}Am, ^{243}Am, and ^{244}Cm, which were processed previously from ENDF/B-IV, this work makes available to LASL users a fairly complete (although preliminary) set of multigroup neutron cross sections for neutronics studies on the higher actinides.

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C. Analysis of PCS Doppler Calculations (R. B. Kidman)

The Processing Code Subcommittee (PCS) of the Code Evaluation Working Group has additionally specified that the Doppler effect be computed between temperatures of 300 and 2100 K on the ZPR-6-7 infinite medium composition.

The LASL results have been analyzed in detail with exact perturbation theory. Some results are shown in Table I. Temperature changes of the ^{238}U cross sections cause most of the Doppler effect, and most of this occurs in the resolved resonance absorption region. Iron contributes about 10% of the Doppler effect, which comes mostly from one group that includes the large iron resonance at 1150 eV. Plutonium-239 exhibits a small positive Doppler effect because rather large changes in both the fission and capture cross sections have nearly equal and opposite effects on the eigenvalue.

Groupwise effects and sensitivities are available for all materials and reactions. The purpose has been to gain a better understanding of the Doppler effect and to prepare for useful discussions of probable causes of differences as the results come in from other laboratories.

TABLE I

BREAKDOWN OF DOPPLER EFFECT

Decomposition	$\delta k \ (10^{-3})$	% of ΔK
Total eigenvalue change (ΔK) in going from 300 to 2100 K	-31.15	100.0
^{238}U	-28.50	91.5
Fe	- 3.08	9.9
^{239}Pu	1.44	-4.6
All other materials	- 1.01	3.2
^{238}U resolved resonance absorption	-22.29	71.6
^{238}U unresolved resonance absorption	- 6.12	19.6
Fe absorption in group 19 (749→1230 eV)	- 2.57	8.3
^{239}Pu nu-fission	6.67	-21.4
^{239}Pu absorption	- 5.23	16.8

D. P_0 to P_7 Scattering Tables for ^{1}H and ^{12}C (D. W. Muir and R. J. Barrett)

We have completed the processing of cross-section sets for ^{1}H and ^{12}C using NJOY and basic evaluated data either from ENDF/B-IV or ENDF/B-IV with LASL modifications (in the case of ^{12}C). The ^{12}C changes were made by P. G. Young in order to improve the angle and energy distributions of inelastic neutrons.[21] Parameters of the NJOY calculations are listed in Table II. The neutron and photon energy-group boundaries for the special multigroup structure are listed in Table III.

The TRANSX code[22] was modified to produce the neutron output tables in the ANISN format described in Table II. This new output capability should prove very useful in supplying NJOY cross sections to users of all codes in the ANISN "family" (ANISN, MORSE, TDA, DOT, etc.). The neutron tables have been written to photostore. The number of neutron groups is 37 and the table length 41, with the kerma factor occupying the first position for each group. The gamma-ray production data are available in card form.

TABLE II

NJOY RUN PARAMETERS FOR ^{1}H AND ^{12}C

Legendre order	7
Neutron group structure	Special (see Table III)
Photon group structure	Special (see Table III)
Table length	No. energy groups + 4
Weighting function	Flat, with 300° thermal spike added
Temperature	0 K
Dilution	Infinite
Output format	ANISN[a]

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[a]BCD; FIDO; $(2\ell+1)$-factor included; neutrons and photons in separate tables.

TABLE III

NEUTRON AND PHOTON ENERGY BOUNDARIES (ev)

Group Boundaries	Neutron Energy	Photon Energy
1	1.96 + 7[a]	1.40 + 7
2	1.69 + 7	1.00 + 7
3	1.49 + 7	8.00 + 6
4	1.42 + 7	7.00 + 6
5	1.38 + 7	6.00 + 6
6	1.28 + 7	5.00 + 6
7	1.22 + 7	4.00 + 6
8	1.11 + 7	3.00 + 6
9	1.00 + 7	2.50 + 6
10	9.05 + 6	2.00 + 6
11	8.19 + 6	1.50 + 6
12	7.41 + 6	1.00 + 6
13	6.38 + 6	7.00 + 5
14	4.97 + 6	4.50 + 5
15	4.72 + 6	3.00 + 5
16	4.07 + 6	1.50 + 5
17	3.01 + 6	1.00 + 5
18	2.39 + 6	7.00 + 4
19	2.31 + 6	4.50 + 4
20	1.83 + 6	3.00 + 4
21	1.11 + 6	2.00 + 4
22	5.50 + 5	1.00 + 4
23	1.58 + 5	
24	1.11 + 5	
25	5.25 + 4	
26	2.48 + 4	
27	2.19 + 4	
28	1.03 + 4	
29	3.35 + 3	
30	1.23 + 3	
31	5.83 + 2	
32	1.01 + 2	
33	2.90 + 1	
34	1.07 + 1	
35	3.06 + 0	
36	1.13 + 0	
37	4.14 − 1	
38	1.00 − 5	

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[a]Read as 1.96×10^{7}.

E.   Processing Code Development   (R. E. MacFarlane)

A paper[23] describing the capabilities of the NJOY processing code was pre-
sented at the RSIC Multigroup Cross Section Seminar held at Oak Ridge National
Laboratory (ORNL) on March 14-16, 1978. A second paper[24] describing the shield-
ing factor method for producing effective cross sections, as implemented in the
MINX/SPHINX and CCCC code interface system, was presented at the same meeting.
A third paper[25] describing improved methods for applying the shielding factor
method in reactor calculations was presented at the American Nuclear Society
Topical Meeting on Advances in Reactor Physics, Gatlinburg, TN (April 1978).

III. FISSION PRODUCTS AND ACTINIDES: YIELDS, YIELD THEORY, DECAY DATA, DEPLE-
     TION, AND BUILD-UP

A.   Fission Yield Theory   [R. E. Pepping (University of Wisconsin), D. G.
      Madland, C. W. Maynard (University of Wisconsin), T. R. England, and P. G.
      Young]

Several coding errors have been found, and fission product yields have been
recomputed for the case of ε_2 as the only parameter describing fission fragment
shapes. Yields have also been computed allowing both ε_2 and ε_4 to vary. For
the latter case, in order to minimize computation cost, only the GMAX (minimum
potential energy) and SUM cases (described previously[26]) were run. In the case
of SUM yields, an approximation is used in which the product of the fragment
level densities is assumed to be Gaussian. Results are summarized in Table IV.
Fragment yield distributions tend to be fairly flat with a very shallow valley.

Using values of the pairing and shell correction energies computed directly
from the Seeger formula,[27] computed yields tend to show a systematic even-odd
mass effect that is not yet understood. The effect disappears if experimental
values[28] are used for these energies instead. In practice, the fragment ground
state is assumed to be described by the available experimental information, and
the Seeger formula is used to extrapolate to shapes other than that of the
ground state.

Work is currently under way to improve the agreement between measured values
of the spacings of neutron levels and those predicted by the Gilbert and
Cameron[29] formula being used. This will result in a redetermination of the
shell and pairing correction terms in such a way that the total single-particle
correction (shell + pairing) is unchanged.

TABLE IV

SUMMARY OF RECENT YIELD CALCULATIONS

	$\langle \nu_p \rangle$	$\langle E_\gamma \rangle$	$\langle Q \rangle$	$\langle KE \rangle$	PL	PL/118
I. ϵ_2 only varying						
A. $\delta = 2.0$ fm						
GMAX	2.132	7.044	201.	181	112	3.4
YMAX	2.044	7.721	201	181	112	3.5
SUM	1.646	7.046	202	184	112	3.1
B. $\delta = 2.44$ fm						
GMAX	1.823	7.026	199	179	109	1.5
YMAX	2.085	7.101	200	179	114	2.
SUM	1.954	6.419	200	181	114	1.5
C. $\delta = 3.0$ fm						
GMAX	3.1	6.5	198	174	99	33
YMAX	3.6	5.5	199		105	49
SUM	3.0	5.6	199	175	105	12
II. ϵ_2, ϵ_4 varying						
A. $\delta = 2.0$ fm						
GMAX	5.3	6.1	200	161	112	36
SUM	4.9	6.9	200	162	112	43
B. $\delta = 2.4$ fm						
GMAX	5.6	6.8	199	157	112	11.5
SUM	5.1	8.1	199	160	118	1
C. $\delta = 3.0$ fm						
GMAX	6.145	5.3	199	155	109	15
SUM	5.86	5.8	199	156	109	20.

Legend:

$\langle \nu_p \rangle$ = Upper bound on prompt neutrons. Zero kinetic energy assumed.

$\langle E_\gamma \rangle$ = Total energy available for prompt gammas.

$\langle KE \rangle$ = Total kinetic energy of fragments (infinite separation).

PL = Location of light mass peak.

PL/118 = Ratio of mass yield at PL to that at 118.

B.   ENDF/B-V Yields   [T. R. England, D. G. Madland, W. B. Wilson, R. E. Schenter (Hanford Engineering Development Laboratory), B. F. Rider (General Electric Company), and J. Liaw (University of Oklahoma)]

Version V-D of the evaluated yields in the revised ENDF/B format was found to contain an error in all 20 sets. These were redone and sent to BNL for distribution with the actinide files.

Various integral tests using conservation principles on the yields are being reported in a paper prepared for the American Nuclear Society Gatlinburg Topical Meeting on Advances in Reactor Physics (April 10, 1978). For all 20 yield sets, the paper includes computation of prompt and delayed neutrons at equilibrium, the average prompt and delayed energy release, plots of yields, charge dispersion, even-odd effects, etc., and comparisons with experiment.

A summary of the ENDF/B yield data has been distributed to the CSEWG Fission Product and Actinide Data Subcommittee.

C.   Delayed Neutron Emission Probabilities for ENDF/B-V   (T. R. England and N. L. Whittemore)

For use in the ENDF/B-V fission-product files and yield evaluations, the delayed emission probabilities have now been completed for 102 precursors; further changes will not be made for the yield evaluation, and changes are not expected for the fission product files.

Table V lists the values in percent (the Pn value is column 5). DPN is the uncertainty; where DPN is zero, the Pn value was estimated based on energetics. The estimated values are expected to be correct only within a factor of ~2, although previous experience indicates an average uncertainty of $\lesssim$50%. Forty-nine of the Pn values are measured, and fifty-three are estimated. However, the estimated values are either small or apply to nuclides having small cumulative yields. The estimated values account for only $\lesssim$10% of the total delayed neutron yields and are, fortunately, not important in intended applications.

The half-lives listed in Table V (column 7) will not necessarily be identical to the values in ENDF/B-V. A similar listing of Pn values has appeared in previous progress reports. Some values in Table V have been changed slightly as noted in the footnotes to the table. Computations using these Pn values and ENDF/B-V yields will be reported at the American Nuclear Society San Diego meeting in June.

These data have been distributed to the CSEWG Fission Product and Actinide Data Subcommittee.

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TABLE V

102 DELAYED NEUTRON BRANCHING RATIOS (Pn) AND HALF-LIVES RECOMMENDED
FOR INCORPORATION IN ENDF/B-V EVALUATION [a]
2-10-78

GP	Nuclide	QB	BN	PN(%)	DPN[a]	HL	DHL[a]	Ref HL	Ref PN
4	ZN 300790	8.66	7.65	1.1	0.0	2.74	0.04	4	3
4	GA 310790	6.06	5.70	0.15	0.0	2.86	0.04	4	3
4	GA 310800	9.44	8.50	0.92	0.0	1.66	0.02	1	3
4	GA 310810	7.44	5.13	5.0	0.0	1.23	0.01	1	3
5	GA 310820	12.35	8.12	16.00	0.0	0.60	0.01	1	3
5	GA 310830	11.41	3.20	56.0	0.0	0.31	0.01	1	3
4	GE 320830	8.49	8.11	0.17	0.0	1.9	0.4	1	3
4	GE 320840	7.54	4.15	10.	0.0	1.2	0.3	1	3
6	GA 320850	9.84	5.04	20.	0.0	0.234	0.0	2	3
6	GE 320860	8.91	3.92	22.	0.0	0.259	0.0	2	3
3	AS 330840	9.99	9.06	0.13	0.06	5.6	0.3	1	1
4	AS 330850	9.05	4.10	23.	3.	2.03	0.01	1	1
5	AS 330860	11.35	6.22	10.5	2.2	0.9	0.2	1	1
5	AS 330870	10.41	4.11	44.	0.14	0.73	0.06	1	1
3	SE 340870	7.27	6.40	0.21	0.03	5.60	0.16	1	1
4	SE 340880	6.33	4.85	0.15	0.09	1.52	0.06	1	1
5	SE 340890	8.63	6.15	5.0	1.5	0.41	0.04	1	1
5	SE 340900	7.47	3.92	11.	0.0	0.555	0.0	2	3
5	SE 340910	10.31	5.72	21.	8.	0.27	0.08	1	1
1	BR 350870	6.54	5.46	2.37	0.18	55.6	0.1	1	1,5
2	BR 350880	8.91	7.15	6.8	0.4	16.0	0.2	1	1,5
3	BR 350890	8.68	5.22	13.	3.	4.38	0.03	1	1,5
4	BR 350900	9.91	6.21	21.	2.	1.92	0.06	1	1,5
5	BR 350910	9.18	4.57	11.	2.	0.542	0.008	1	1,5
5	BR 350920	12.01	6.21	22.	6.	0.362	0.012	1	1
6	BR 350930	10.43	3.46	41.	0.0	0.201	0.0	2	3
4	KR 360920	5.48	5.06	0.033	0.003	1.85	0.01	1	1
4	KR 360930	8.15	6.30	2.0	0.2	1.29	0.01	1	1,5
6	KR 360940	6.56	4.33	2.2	1.4	0.208	0.009	1	1
5	KR 360950	9.45	6.22	9.5	0.0	0.50	0.0	2	3
3	RB 370920	7.60	7.35	0.012	0.001	4.50	0.02	1	1
3	RB 370930	6.07	5.14	1.42	0.14	5.85	0.04	1	1,5
4	RB 370940	9.18	7.17	10.4	0.8	2.76	0.02	1	1,5
5	RB 370950	7.87	4.64	8.7	0.6	0.384	0.005	1	1,5
6	RB 370960	10.76	6.62	14.	1.0	0.201	0.002	1	1,5
6	RB 370970	9.03	3.92	30.	4.	0.170	0.002	1	1,5
6	RB 370980	12.11	6.39	15.0	2.4	0.119	0.007	1	1
6	RB 370990	10.07	3.09	41.	0.0	0.076	0.005	1	3

TABLE V (continued)

GP	Nuclide	QB	BN	PN(%)	DPN[a]	HL	DHL[a]	Ref HL	Ref PN
5	SR 380970	7.10	6.81	0.10	0.0	0.43	0.03	1	3
5	SR 380980	5.37	4.67	0.53	0.0	0.80	0.10	1	3
5	SR 380990	8.45	6.16	3.4	2.4	0.6	0.2	1	1
4	SR 381000	6.40	4.11	5.0	0.0	1.046	0.0	2	3
4	Y 390971	5.77	5.22	1.6	0.3	1.13	0.04	1	1
4	Y 390970	5.77	5.22	0.33	0.0	3.7	0.1	4	3
5	Y 390981	8.26	7.55	4.	2.	0.65	0.05	4	4
4	Y 390980	8.26	7.55	0.54	0.0	2.	0.15	4	3
4	Y 390990	6.51	4.44	1.2	0.8	1.4	0.2	1	1
5	Y 391000	9.59	7.18	5.5	0.0	0.756	0.0	2	2
3	ZR 401040	4.88	4.57	0.11	0.0	3.783	0.0	2	3
5	ZR 401050	7.96	6.80	1.4	0.0	0.559	0.0	2	3
2	NB 411030	5.39	5.05	0.13	0.0	15.669	0.0	2	3
5	NB 411040	8.51	7.69	0.71	0.0	1.00	0.0	2	3
4	NB 411050	6.57	4.86	2.9	0.0	1.80	0.0	2	3
5	NB 411060	9.66	7.25	5.5	0.0	0.535	0.0	2	3
4	MO 421090	7.39	6.69	0.53	0.0	1.033	0.0	2	3
4	MO 421100	5.62	4.50	1.3	0.0	1.892	0.0	2	3
1	TC 431090	6.28	4.98	1.7	0.0	50.00	0.0	2	3
5	TC 431100	9.19	7.41	3.1	0.0	0.83	0.0	2	3
4	AG 471220	9.17	7.98	1.4	0.0	1.5	0.5	4	3
5	AG 471230	7.28	5.08	4.6	0.0	0.39	0.03	1	3
5	CD 481280	5.54	5.24	0.11	0.0	0.83	0.03	4	3
3	IN 491271	6.44	5.55	0.83	0.0	3.76	0.03	1	3
3	IN 491270	6.44	5.55	0.83	0.0	2.0	0.0	2	3
3	IN 491280	9.07	7.79	1.7	0.0	0.84	0.06	1	3
5	IN 491291	7.31	5.32	3.8	0.0	0.99	0.02	1	3
4	IN 491290	7.31	5.32	3.8	0.0	2.5	0.2	1	3
5	IN 491300	9.69	7.42	4.9	0.0	0.58	0.01	1	3
6	IN 491310	8.39	5.02	10.	0.0	0.28	0.01	1	3
6	IN 491320	12.31	6.97	24.	0.0	0.13	0.04	1	3
4	SN 501330	7.24	7.11	0.02	0.0	1.47	0.03	1	3
4	SN 501340	6.07	3.43	17.	7.	1.04	0.02	1	1
6	SN 501350	8.08	5.03	8.6	0.0	0.291	0.0	2	3
2	SB 511341	8.69	7.35	0.086	0.012	10.4	0.1	1	1
4	SB 511350	7.52	3.86	14.	2.	1.71	0.02	1	1,5
5	SB 511360	9.54	5.20	23.	8.	0.82	0.02	1	1
6	SB 511370	8.40	3.61	20.	0.0	0.284	0.0	2	3
2	TE 521360	4.40	4.02	0.9	0.4	17.5	0.2	1	1
4	TE 521370	6.48	5.63	2.2	0.5	2.8	0.7	1	1

TABLE V (continued)

GP	Nuclide	QB	BN	PN(%)	DPN[a]	HL	DHL[a]	Ref HL	Ref PN
4	TE 521380	5.34	3.84	5.6	1.6	1.4	0.4	1	1
5	TE 521390	7.61	5.02	6.3	0.0	0.424	0.0	2	3
2	I 531370	5.77	4.45	7.2	0.7	24.5	0.1	1	1,5
3	I 531380	7.48	5.86	2.6	0.3	6.53	0.08	1	1
4	I 531390	6.77	3.89	10.2	0.9	2.38	0.07	1	1
5	I 531400	8.93	5.35	22.	6.	0.60	0.01	1	1
5	I 531410	7.42	3.52	39.	13.	0.47	0.03	1	1
4	I 531420	9.74	5.44	16.	0.0	0.196	0.0	3	3
4	I 531430	7.76	3.28	18.	0.0	0.328	0.0	3	3
4	XE 541410	5.85	5.79	0.043	0.003	1.73	0.01	1	1,5
4	XE 541420	4.34	3.93	0.41	0.03	1.24	0.03	1	1
5	XE 541430	6.65	5.59	1.2	0.0	0.30	0.03	1	3
5	XE 541440	4.67	3.84	0.73	0.0	1.00	0.0	2	3
2	CS 551410	5.06	4.65	0.053	0.004	24.9	0.2	1	1
4	CS 551420	7.06	6.20	0.19	0.10	1.71	0.01	1	1,5
4	CS 551430	5.73	4.09	1.6	0.2	1.78	0.01	1	1,5
4	CS 551440	8.05	6.16	2.8	0.7	1.002	0.005	1	1,5
5	CS 551450	6.07	3.83	14.	2.	0.585	0.008	1	1,5
5	CS 551460	8.54	6.45	13.4	0.7	0.335	0.007	1	1
5	CS 551470	6.97	4.01	25.	3.	0.21	0.03	1	1
5	BA 561490	6.20	6.05	0.03	0.0	0.917	0.0	2	3
4	BA 561500	4.87	4.41	0.24	0.0	1.798	0.0	2	3
4	LA 571490	5.36	4.48	0.81	0.0	2.864	0.0	2	3
5	LA 571500	7.68	6.73	0.94	0.0	0.648	0.0	2	3

LEGEND

GP — Approximate decay group (6 groups).
QB — Maximum beta-decay energy of precursor (MeV).
BN — Neutron binding energy in daughter (MeV).
PN — Neutron emission probability (%) of daughter.
DPN — Uncertainty in PN.
HL — Precursor in half-life (s).
DHL — Uncertainty in half-life (s).

[a]DHL for half-lives taken from ENDF/B-IV; DPN for estimated PN values are inserted as zero for ready identification.

REFERENCES

1. Experimental values based on a revision of the preliminary review by G. Rudstan, "Status of Delayed Neutron Data," Proc. of the IAEA 2nd Advisory Panel on Fission Product Nuclear Data (Sept. 1977) (to be published). The data were revised by a delayed neutron subgroup organized by this panel.

2. Half-lives from ENDF/B-IV as tabulated in T. R. England and R. E. Schenter, "ENDF/B-IV Fission-Product Files: Summary of Major Nuclide Data," Los Alamos Scientific Laboratory report LA-6116-MS (1975).

3. PN values based on a least-squares fit of experimental values to the form PN = A*(QN-BN)**B, T. R. England. BN and QN are based on G. T. Garvey, W. J. Gerace, R. L. Jaffe, and I. Talmi, "Set of Nuclear-Mass Relations and A Resultant Mass Table," Rev. Mod. Phys. 41, No. 4, Part 11 (Oct. 1969).

4. Values supplied by P. L. Reeder, personal communication, Reeder to England, 3/28/78.

5. C. W. Reich recommendation (letter to England, 1/31/78). Wither the PN value or its uncertainty, or both, differ from the preliminary values of Ref. 1. An unweighted average rather than an inverse variance weighting was used, and, in some cases having more than one measurement from the same laboratory, the values were first averaged and treated as a single quantity in the final weighting. A total of 48 precursors were reexamined for possible changes by this procedure.

D.   ANS 5.1 Decay-Heat Standard   (T. R. England, W. B. Wilson, R. J. LaBauve, and N. L. Whittemore)

Completion of this initial standard has been upgraded to Priority 1 by the American Nuclear Society. The committee met on March 3 to consider new experimental data for ^{239}Pu and an extension of the standard to 10^9 s as an immediate goal, and the long-term needs as to additions to the standard.

In preparation for this meeting, a number of comparisons between calculations using ENDF/B-IV data[30] and recent, unpublished total decay heat experiments at LASL and ORNL were made. Gamma-spectra comparisions were also made but not reported at the ANS 5.1 Meeting.

Figure 4 shows the ratio of the ^{233}U, ^{235}U, and ^{239}Pu LASL calormetric measurements to calculation. The ^{233}U and ^{235}U data agree with calculation well within uncertainties ($\tilde{<}$3 and ~5% , respectively, for ^{235}U and ^{233}U, for both calculation and experiment). Uranium-233 is not currently incorporated into the standard. All results are based on a 20 000 s thermal irradiation.

Plutonium-239 measurements are ~10% higher than calculation. This anomally has not been explained, although a considerable effort has been expended to find errors in the data base and experiment. This effort is continuing.

Figure 5 compares the ORNL measurments (extrapolated to a 20 000 s irradiation) with calculation. The LASL ^{239}Pu values of Fig. 4 are repeated for convenient comparison. ORNL Measurements are in much better agreement with calculation than the LASL experiment; ORNL values agree with uncertainties. The increase of measured values over calculation at ~500 s (also evident in Fig. 4) appears, without question, to be due to an error in ENDF/B-IV data. Again, we have not located this error, but the primary problem is the discrepancy with the LASL experiment.

Figure 6 shows the ratio of the LASL and ORNL experimental values based on extrapolating the ORNL values to a 20 000 s irradiation, and Figs. 7 and 8 show comparisons for an infinite and burst irradiation for ^{239}Pu.

The ANS 5.1 Standards Committee resolved several issues which will permit a comprehensive standard to be released that will include ^{235}U, ^{238}U, and ^{239}Pu. The most important are:

1.   The ^{239}Pu data will be combined in a generalized least-squares program at HEDL for the time range of 1-10^5s.

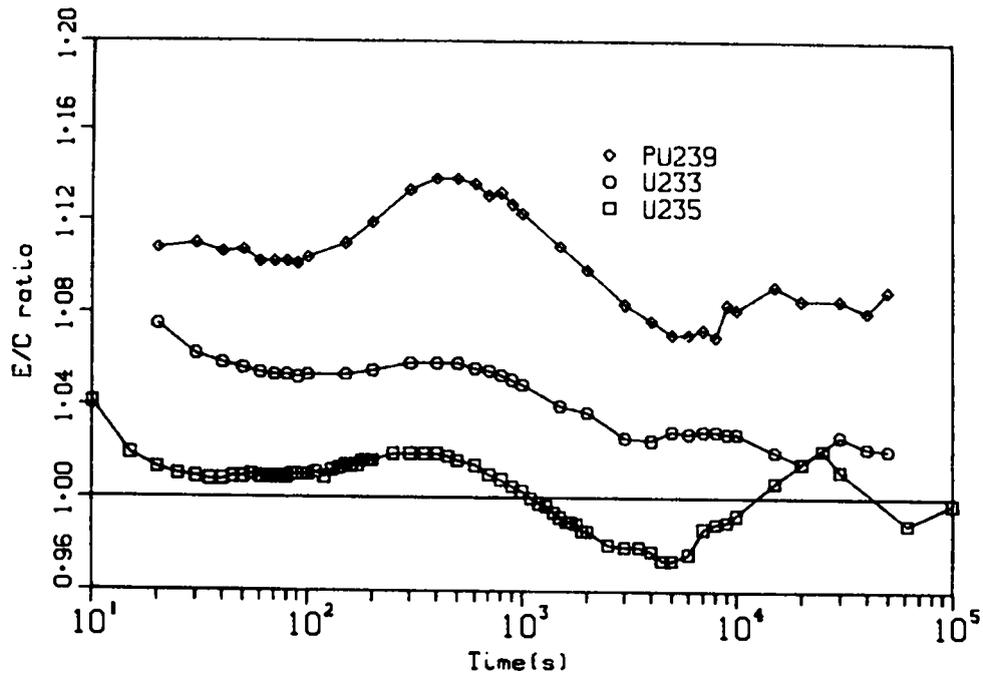2.   The standard will be extended at LASL to 10^9 s using calculated values.

Fig. 4.

Ratio of LASL decay heat measurements to calcula-
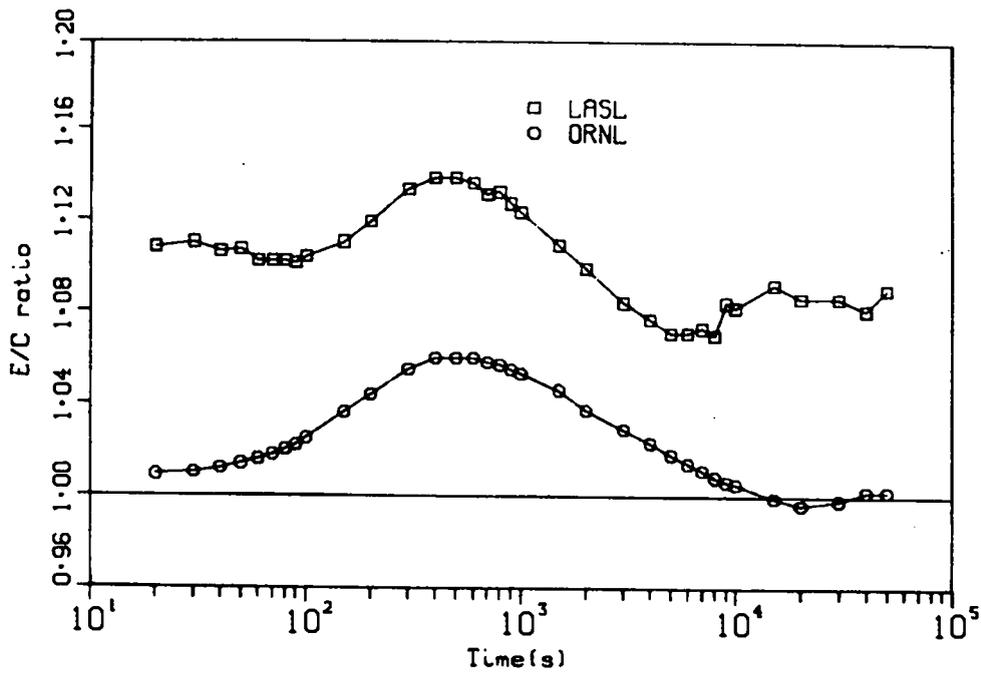tions (CINDER-10, ENDF/B-IV) 20 000 s irradiation
(Yarnell experiment).

Fig. 5.

[239]Pu decay heat ratio of experiment to calculation
20 000 s irradiation calculation uses ENDF/B-IV (Ref.
30) 2/24/78.

Fig. 6.
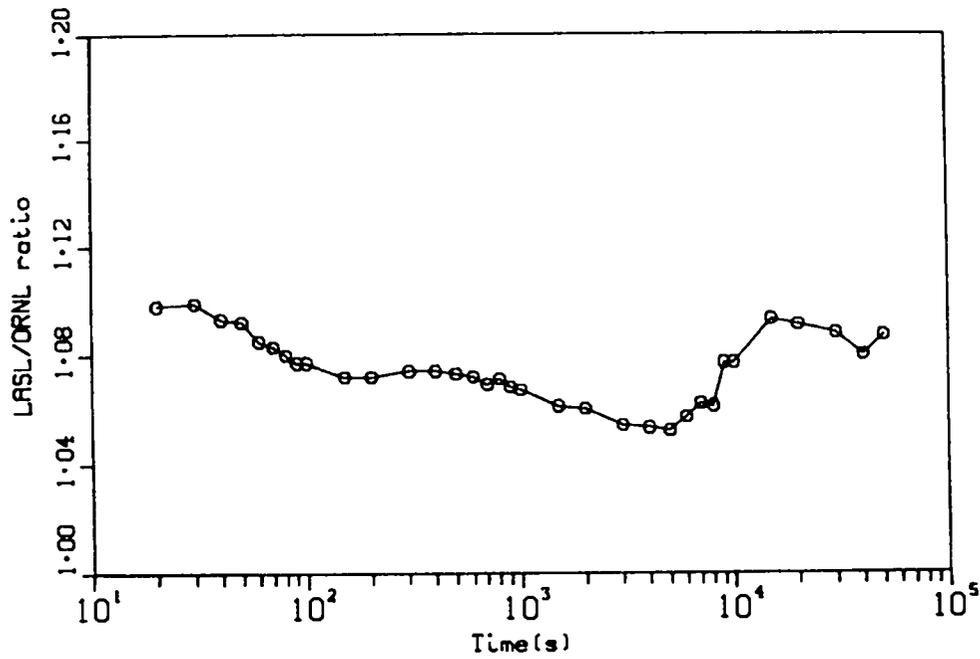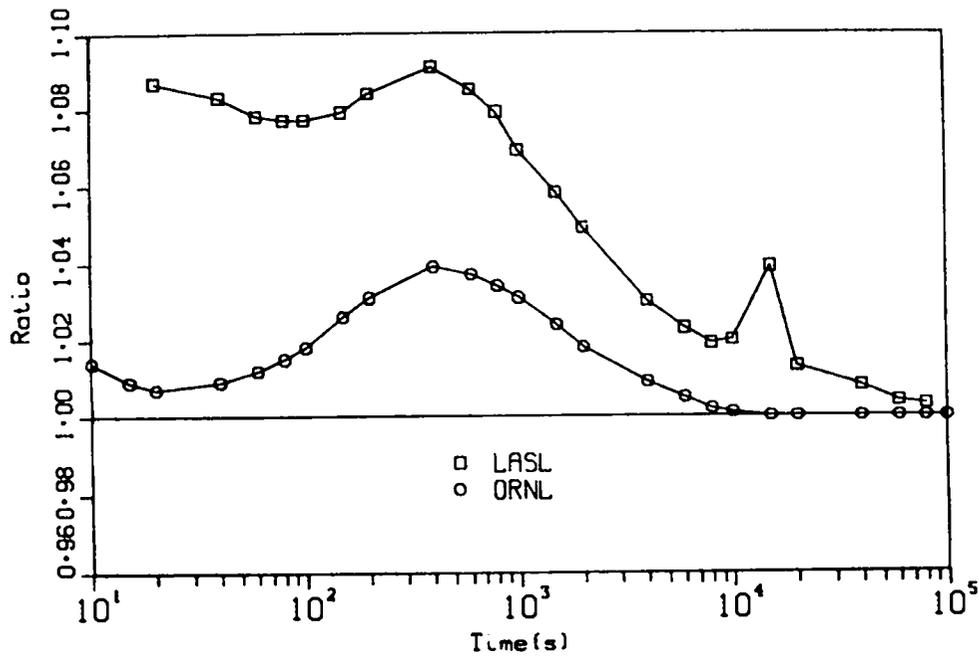^{239}Pu decay heat ratio LASL to ORNL 20 000 s
irradiation 2/24/78.

Fig. 7.
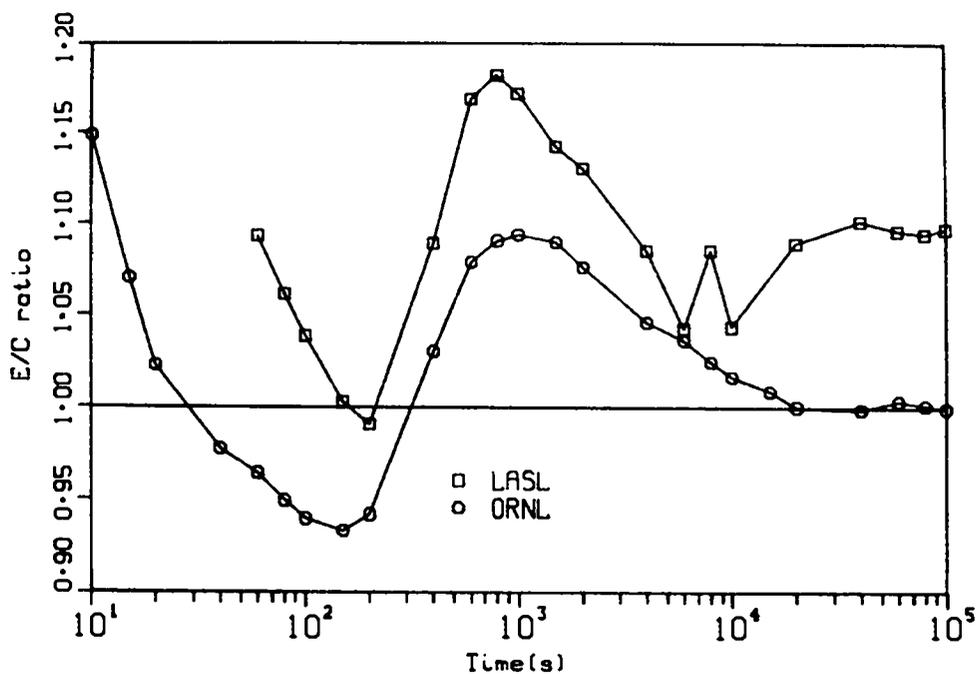^{239}Pu comparison for infinite irradiation.

Fig. 8.
Pulse comparison ratio of experiment to calculation
(MeV/f-s) 2/24/78.

3. A table of upper limit corrections for the effect of neutron absorption in
    fission products will be generated at LASL and a section prepared for the
    standard detailing the use of the table and user options.

4. The ^{239}Pu combined values will be provided to LASL and there combined with
    calculations extending the time range. The result will be fitted in a non-
    linear least-squares program for final incorporation into the standard.

5. Uncertainties at long cooling times (without absorption) will be reexamined
    at HEDL.

The intent is to complete a preliminary standard during May for consideration by
ANS 5 and ANSI.

E. Library for Processed ENDF/B Aggregate Fission-Product Spectra (R. J.
    LaBauve. T. R. England, and D. C. George)

    The PEFPYD library of processed ENDF/B aggregate fission-product spectra
and yield data is being generated again using the more accurate normalization
described in the last progress report.[31] This work is about 95% complete.

    The new library data for beta-decay energy from a thermal pulse of neutrons
on ^{235}U was collapsed into an 11-group structure shown in Table VII and fit with

linear combinations of exponential functions as described in Ref. 32. The fitted analytic functions were then used to compute the beta-decay energy spectra resulting from a 20 000 hr irradiation of ^{235}U with a 10^4 flux of thermal neutrons for each of the 11 groups. (See Ref. 32 for details of method used in this calculation.) The results were then compared with those from a CINDER-10 calculation of this same case, and this comparison is shown in Table VII. Note the remarkable agreement now achieved with the new normalization.

F. UK Fission Product Data File (T. R. England)

A. Tobias has supplied a combined ENDF/B and UK file of activation and fission-product decay data. The file is primarily of interest in that it contains >300 products having spectral data (compared to 181 in ENDF/B-IV). It is also of interest in checking for gross errors in the ENDF/B-V file.

G. Gas Content (T. R. England and N. L. Whittemore)

Plots of noble gases and halogen content for various fissionable nuclides and irradiation conditions have been completed and supplied to the Nuclear Regulatory Commission. The plots include content (densities) of radioactive and stable products and also the beta and gamma energy-release rates. A total of 60 plots were supplied.

H. Examination of the Gunst, Connor, and Conway Experiments as a Potential Benchmark for Fission-Product Absorption in Thermal Reactors (W. B. Wilson and T. R. England)

For the Electric Power Research Institute (EPRI), the Bettis Atomic Power Laboratory (BAPL) fission-product absorption experiments of Gunst, Connor, and Conway[33,34] have been considered as potential benchmarks because they represent the largest accumulation of experimental data describing parasitic neutron absorption by fission products generated in a highly-irradiated thermal reactor fuel, ^{233}U. The nature and limitations of the results of these experiments and values produced in EPRI-CINDER[35] comparison calculations have been previously summarized.[36]

Comparison calculations of values of the reported barns-per-fission (b/f) quantities $\hat{\sigma}_{eff}$, $\hat{\sigma}_{2200}$, and $\hat{I}$ have heretofore been performed for ^{233}U sample #46 with a simplified representation of the ~3 year history of irradiation, cooling, and measurement periods. This simplified history consists of 72 time steps, each

TABLE VI

BROAD GROUP ENERGY BOUNDARIES AND PERCENT DECAY ENERGY IN EACH GROUP FOR U-235 THERMAL PULSE

Group No.	Lower Energy Bound (MeV)	Upper Energy Bound (MeV)	Percent Decay Energy-Gammas	Percent Decay Energy-Betas
1	0.1	0.4	7.4	4.6
2	0.4	0.9	32.2	12.9
3	0.9	1.35	19.1	14.1
4	1.35	1.8	16.5	14.6
5	1.8	2.2	5.9	12.3
6	2.2	2.6	6.9	10.9
7	2.6	3.0	3.6	9.1
8	3.0	4.0	5.0	13.7
9	4.0	5.0	2.7	5.0
10	5.0	6.0	0.6	2.1
11	6.0	7.0	0.1	0.7

TABLE VII

20 000 hr THERMAL IRRADIATION OF ^{235}U
(Percent Difference Between CINDER-10 and Approximate Method for Beta-Energy Release)

Cooling Time (s)	Group 1 0.1-0.4 MeV	Group 3 0.9-1.35 MeV	Group 5 1.8-2.2 MeV	Group 8 3.0-4.0 MeV	Group 10 5.0-6.0 MeV	Total all Groups
1.0×10^{-4}	0.6	1.4	1.0	1.7	2.8	1.4
1.0×10^{-1}	0.6	1.3	0.9	1.5	2.5	1.3
1.0×10^{0}	0.6	1.3	0.8	1.5	2.4	1.2
1.0×10^{1}	0.8	1.5	0.7	1.3	3.5	1.2
1.0×10^{2}	1.1	1.7	0.9	2.5	11.5	1.6
1.0×10^{3}	1.2	2.0	0.8	3.6	4.1	1.7
1.0×10^{4}	0.9	1.7	-0.1	0.8	1.2	1.3
1.0×10^{5}	0.7	1.1	-0.2	-0.3	0.5	1.5
1.0×10^{5}	1.6	-0.9	-0.3	-0.3	0.6	1.1
1.0×10^{7}	1.2	-2.3	0.4	0.0	3.1	0.2
1.0×10^{8}	-4.2	-5.6	-3.7	1.1	-0.7	-4.1
1.0×10^{9}	-0.2	-0.4	-0.8	3.5	0.4	-0.1

describing characteristic time segments with time-averaged group flux values produced from the detailed, monitored flux history reported in Ref. 34.

In order to determine the validity of such a simplified treatment of the flux history, companion calculations for ^{233}U sample #44 have been performed with a complete 1692 time-step history and with a simplified history similar to that used in previous calculations. Results of these companion calculations, compared to BAPL values in Table VIII, demonstrate the validity of the use of simplified flux histories in these calculations.

I. Identification of Major Fission-Product Absorbers (W. B. Wilson and T. R. England)

A modified version of the EPRI-CINDER code has been developed to group corresponding linearized nuclide concentrations and to order major neutron absorbers relative to importance as absorbers. The temporal contributions of major neutron absorbers to the total parasitic absorption throughout a typical LWR fuel life-time have been evaluated and will be reported at the May 22 Seminar on Nuclear Data Problems for Thermal Reactor Applications at Brookhaven National Laboratory, sponsored by EPRI.

J. Other Studies for the Electric Power Research Institute (T. R. England, W. B. Wilson, R. J. LaBauve, and N. L. Whittemore)

1. For use in an EPRI funded experiment at Intelcom Rad Tech, 150-group beta and gamma spectra were provided for ^{235}U and ^{239}Pu thermal fission. The irradiation times were 35 day and 1000 s for ^{235}U and 20 000 and 1000 s for ^{239}Pu. Multigroup spectra were supplied at 0, 1, 10, 10^2, 10^3, 10^4, and 10^3 s of cooling.

2. Using the CINDER-10 code, the most important contributors to decay heat were tabulated for a "typical" LWR reactor. The power level was constant at 80 w/cm^3 for 30 000 hr. Four group LWR cross sections were used to account for (n,γ) coupling. All nuclides contributing $\gtrsim 2\%$ to the total heating between 0.1 and 10^9 s following shutdown were tabulated, including beta and gamma components, total component heating, noble gas, and halogen content, etc.

K. Q-2 Studies (T. R. England and N. L. Whittemore)

Several calculations were made for LASL Group Q-2 for a highly specialized reactor design using the CINDER-10 code.

TABLE VIII

MEASURED AND CALCULATED VALUES OF $\hat{\sigma}_{eff}$, $\hat{\sigma}_{2200}$, and $\hat{I}$, SAMPLE 44

Elapsed Hours	Irad Cycle	$\hat{\sigma}_{eff}$ (b/f) BAPL Meas	Calc	EPRI-CINDER Calc 72-TS	1692-TS	$\hat{\sigma}_{2200}$ (b/f) BAPL Meas	Calc	EPRI-CINDER Calc 72-TS	1692-TS	$\hat{I}$ (b/f) BAPL Meas	Calc	EPRI-CINDER Calc 72-TS	1692-TS
1640.12	2	159.3	139.7	131.04	130.32	146.0	126.2	116.13	115.43	194.7	198.1	217.66	217.37
2720.17	3	126.5	113.8	108.43	107.26	120.6	100.0	93.54	92.40	85.2	200.2	214.75	214.36
3453.99	4	210.3	218.0	193.98	196.51	193.3	202.5	178.07	180.56	248.3	226.4	231.16	231.72
3668.99	4	102.1	101.2	95.33	95.90	80.4	87.5	80.77	81.33	317.1	200.0	211.48	211.64
5667.99	7	82.3	80.3	77.07	77.35	66.0	67.0	63.11	63.38	237.7	194.5	202.36	202.42
6449.04	8	107.1	111.8	104.88	104.11	88.9	97.8	90.46	89.71	264.9	204.1	208.35	208.15
6836.04	8	78.3	77.2	74.46	74.28	61.6	63.7	60.51	60.33	241.6	195.2	201.62	201.54
8176.66	10	72.9	70.0	68.64	67.56	56.8	56.9	55.10	54.05	234.2	191.2	196.61	196.18
9517.83	12	80.2	83.3	78.59	78.38	63.9	70.2	65.23	65.03	240.3	192.8	195.56	195.55
9862.83	12	65.9	67.2	64.97	64.99	49.7	54.4	51.88	51.89	237.3	187.6	191.79	191.81
11220.66	14	61.1	62.9	60.99	60.93	45.7	50.5	48.26	48.21	226.6	183.6	187.02	187.01
13047.66	17	65.7	68.3	64.60	65.15	50.3	56.1	52.22	52.75	228.3	181.9	182.89	183.12
13441.66	17	55.3	57.9	55.90	56.17	40.0	46.0	43.72	43.99	226.4	177.9	179.79	179.90
16240.66	21	60.5	63.3	60.16	60.04	46.5	51.9	48.64	48.51	213.1	174.2	174.57	174.57
16585.66	21	53.0	54.3	52.39	52.45	38.8	43.2	41.07	41.13	216.3	170.1	171.46	171.48
18058.66	22	50.3	52.3	50.54	50.57	34.9	41.4	39.43	39.47	235.6	167.7	168.59	168.61
19067.66	23	49.0	50.0	48.92	48.40	36.3	39.3	38.02	37.51	195.0	165.2	165.95	165.73
19762.66	24	55.6	58.5	55.77	55.73	41.8	47.7	44.85	44.81	212.2	166.8	166.55	166.58
20223.66	24	48.7	49.9	48.13	48.20	35.1	39.3	37.42	37.49	209.5	162.9	163.35	163.38
22770.16	25	54.2	56.4	53.24	53.43	41.5	45.8	42.56	42.74	196.5	164.1	163.22	163.32
23179.16	25	47.0	48.6	46.67	46.82	34.6	38.2	36.18	36.32	190.6	160.4	160.39	160.45
25814.16	25	46.3	48.0	46.56	46.70	33.0	37.7	36.17	36.31	204.5	159.6	158.82	158.87

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