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NUCLEAR DATA SENSITIVITY COEFFICIENTS FOR

A (^{233}U - ^{232}Th) FUELED LMFBR

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ABSTRACT

Sensitivity coefficients for the nuclear data of the principal constituents of a representative ^{233}U - ^{232}Th fueled LMFBR have been generated. Generalized perturbation coefficients for several reactor parameters were computed with the VARI code and ENDF/B Version 4 data for a homogeneous one-dimensional spherical model. The following ten reactor parameters were studied: eigenvalue; breeding ratio; inner core conversion ratio; outer core conversion ratio; central reaction rate ratios of f^{02} , c^{23} , and c^{02} relative to f^{23} ; and the central material reactivity worths of ^{233}U , ^{232}Th , and ^{23}Na . Total (energy-integrated) and energy-dependent sensitivity coefficients were obtained for each of these parameters to each of the following nuclear data: σ_f for ^{233}U , ^{234}U , ^{232}Th , and ^{233}Pa ; σ_c for ^{233}U , ^{234}U , ^{232}Th , ^{233}Pa , ^{23}Na , SS316, and fission products; $\bar{\nu}$ for ^{233}U and ^{232}Th ; and σ_{inel} for ^{232}Th . These data are combined with estimated data uncertainties and with observed large differences in recent data evaluations to project the impact on integral parameters calculated for a ^{233}U - ^{232}Th fueled LMFBR.

INTRODUCTION

Recent emphasis on the proliferation resistance of nuclear fuels has renewed interest in the ^{233}U - ^{232}Th fuel cycle. Currently, the use of ^{233}U and thorium as fuel for both thermal and fast reactors is under intensive design analysis. Early integral measurements made on these systems are being re-analyzed and there is also considerable activity in the measurement and evaluation of basic microscopic nuclear data for these materials. Interest in these activities has been heightened by the recent evaluations of Smith et. al.,¹ which propose sizable changes (relative to the current ENDF/B evaluations) for several of the cross sections of ^{233}U and thorium. To assist in the interpretation of these current studies, sensitivity coefficients for the nuclear data of the principal constituents of a representative ^{233}U - ^{232}Th oxide LMFBR have been generated. These coefficients are useful in spotlighting the nuclear data of most importance in reactor design and in the evaluation of the effects of changes and/or uncertainties in nuclear data on the prediction of reactor parameters.

NUCLEAR DATA UNCERTAINTIES

Even though many cross section measurements are now performed to within 2% accuracy, the disagreement among independent measurements is in many cases much greater. Sometimes these discrepancies can be traced to inconsistent normalizations, however for many of the materials of interest there still exist large ranges where the only available measurements differ by more than 20%. A brief summary of the estimated cross section uncertainties for a ^{233}U - ^{232}Th oxide fueled LMFBR is given in Table 1. It is evident from these estimates that unacceptably large cross section uncertainties still exist for these isotopes. The fission cross section of ^{233}U has a 3-5% uncertainty over the entire energy range of interest for LMFBR design, while the uncertainty in the ^{232}Th capture cross section ranges from at least 10% to 20%. The uncertainties in the cross sections of the principal structure materials range from 5% to 20%. The application of appropriate nuclear data sensitivity coefficients to these uncertainties can provide estimates of the uncertainties in calculated reactor performance parameters.

Table 1. Estimated Cross Section Uncertainties

		Energy (keV)					
	Ref.	10^{-1}	10^0	10^1	10^2	10^3	10^4
^{233}U (n,f)	2						
(n,γ)							
$\bar{\nu}$	3						
^{232}Th (n,f)	1						
(n,γ)							
(n,n')							
$\bar{\nu}$							
^{16}O (n,n)	4						
^{23}Na (n,n)	4						
(n,γ)							
Fe,Ni,Cr (n,n)	5						
(n,n')							
(n,γ)	4						

MODEL DESCRIPTION AND CALCULATIONAL METHODS

The reactor composition used for generating the sensitivity coefficients corresponds to the beginning-of-equilibrium cycle for a typical mixed (^{233}U - ^{232}Th) oxide fueled LMFBR. This model corresponds to the "Pu-free" designs being considered in the current Proliferation Resistant LMFBR Core Design Studies (PRLCDS). Multigroup cross sections were produced by MC²-2 for each of the homogeneous core compositions and for the blanket composition using ENDF/B Version 4 nuclear data. The twelve broad group energy structure is consistent with previous studies.⁶⁻⁸ To reduce the number of isotopes used in the sensitivity calculations, isotopes were combined to form materials. The structural materials (Fe, Ni, Cr, Mo, and Mn) were combined to form stainless steel; the fission products (^{135}Xe , ^{149}Sm , and the three lumped fission products of ^{233}U) were combined to form a single lumped fission product pair. Furthermore, cross sections corresponding to the inner core composition were used throughout the model, except for ^{233}U and ^{232}Th , which used the appropriate cross sections in each of the regions.

A one-dimensional search was made for the critical core radius of the spherical model, maintaining the ratio of core zone volumes and the thicknesses of the blanket and reflector regions. This four region spherical model was then represented in the sensitivity calculations using a uniform mesh spacing of 25, 7, 14, and 4 mesh, respectively in the inner core, outer core, radial blanket, and reflector regions.

The VARI-1D code⁹ was used to compute generalized sensitivity coefficients. The results quoted herein utilized generalized perturbation theory (which does not include an artificial adjustment of $\bar{\nu}$). The sensitivity coefficients are of the form $(dX/X)/(d\sigma/\sigma)$, where dX/X is the fractional change in a given reactor parameter, and $d\sigma/\sigma$ is the fractional change in a given cross section (which produces dX). For some of the principal cross sections of ^{233}U and ^{232}Th ($\sigma_{n,f}^{23}$, $\sigma_{n,\gamma}^{23}$, ν^{23} , $\sigma_{n,f}^{02}$, $\sigma_{n,\gamma}^{02}$, $\sigma_{n,n'}^{02}$, ν^{02}), the sensitivity coefficients have been computed as a function of energy, that is, the nuclear data was changed over each of the 12 broad group energy ranges individually. The total or energy integrated change in a reactor parameter was also obtained by changing the nuclear data over the entire energy range.

Sensitivity coefficients were computed for the following ten reactor parameters:

- Eigenvalue, k
- Breeding Ratio
- Inner Core Conversion Ratio
- Outer Core Conversion Ratio

Central Reaction Rate Ratios

$$^{232}\text{Th} (n,\gamma)/^{233}\text{U}(n,f)$$

$$^{232}\text{Th} (n,f)/^{233}\text{U}(n,f)$$

$$^{233}\text{U} (n,\gamma)/^{233}\text{U}(n,f)$$

Central Material Reactivity Worths

$$^{233}\text{U}$$

$$^{232}\text{Th}$$

$$^{23}\text{Na}$$

The reaction rate ratios are all reported relative to the ^{233}U fission rate and correspond to the central (first) mesh point. The definitions of the breeding and core conversion ratios include production in ^{232}Th and ^{234}U and destruction of ^{233}U , ^{235}U , and ^{233}Pa . Protactinium-233 was included as fissile material in the definition of the breeding ratio because it β^- decays with a 27.0 day half-life to ^{233}U . The central material worths correspond to the addition of the material into the central (first) mesh only.

SENSITIVITY COEFFICIENTS

The total, or energy integrated, sensitivity coefficients are listed in Table 2. These coefficients represent the percent change in a particular integral parameter resulting from a uniform 1% increase in cross section over the entire energy range (thermal - 10 MeV). These data give a good indication of the relative sensitivity of the principal cross sections. These coefficients can be interpolated, or extrapolated to estimate the effects of small changes in the magnitude (such as renormalization) of a cross section. As would be anticipated, the sensitivities for this ^{233}U -Th fueled system are similar to the sensitivities for a ^{239}Pu -U fueled system.¹⁰ The results in Table 2 clearly show the primary importance of the ^{233}U and ^{232}Th nuclear data. A 1% increase in σ_f^{23} increases k_{eff} by 0.58% $\Delta k/k$, decreases the breeding ratio by 0.88%, and reduces the central reactivity worths of ^{232}Th and sodium by 1.1% and 2.2%, respectively. A 1% increase in σ_c^{23} decreases k_{eff} by .035% $\Delta k/k$, increases the breeding ratio by .081%, and reduces the central reactivity worth of sodium by 0.4%. A 1% increase in $\bar{\nu}$ for ^{233}U increases k_{eff} by ~1%. The results in Table 2 also indicate that the sensitivities of these integral parameters to σ_c for ^{233}Pa and fission products are quite small. It may be noted that current uncertainties (see Table 1) for even the principal cross sections of ^{233}U and ^{232}Th are much larger than 1%, and therefore, are likely to produce significant uncertainties in calculated integral parameters, such as eigenvalue, breeding ratio, and material reactivity worths. Energy-dependent (i.e., as a function of the 12 broad group energy ranges) sensitivity coefficients were computed for each of the ten integral parameters listed in Table 2 for the following ^{233}U and

Table 2. Total (Energy Integrated) Sensitivity Coefficients^a
for a ²³³U-Th Fueled LMFBR

Nuclear Data	$\delta k/k$	Breeding Ratio	Inner Core Conversion Ratio	Outer Core Conversion Ratio	Central Reaction Rate Ratios			Central Material Reactivity Worths		
					f^{02}/f^{23}	c^{02}/f^{23}	c^{23}/f^{23}	^{233}U	^{232}Th	Na
Fission:										
^{233}U	0.5832	-0.8836	-0.9412	-0.9467	-0.6372	-1.0344	-1.0558	0.1019	-1.0657	-2.2450
^{234}U	0.0008	-0.0001	-0.0000	0.0000	0.0003	-0.0000	-0.0000	-0.0004	-0.0011	-0.0290
^{232}Th	0.0149	0.0015	0.0005	0.0005	0.9907	-0.0005	0.0006	-0.0170	-0.0687	-0.3964
^{233}Pa	0.0002	-0.0004	-0.0004	-0.0002	-0.0001	0.0000	0.0000	-0.0000	-0.0002	-0.0066
Capture:										
^{233}U	-0.0358	-0.0814	-0.0876	-0.0882	0.0361	-0.0047	0.9927	-0.0574	-0.0130	-0.4432
^{234}U	-0.0008	0.0017	0.0025	-0.0001	0.0009	-0.0001	-0.0002	-0.0001	-0.0009	-0.0250
^{232}Th	-0.3477	0.8088	0.9536	0.9594	0.3465	0.9501	-0.0664	0.1045	0.9771	-2.3523
^{233}Pa	-0.0021	-0.0048	-0.0055	-0.0031	0.0022	-0.0002	-0.0005	-0.0001	-0.0032	-0.0915
^{23}Na	-0.0017	-0.0009	-0.0001	-0.0001	0.0018	-0.0002	-0.0003	0.0012	-0.0012	-0.6548
SS316	-0.0299	-0.0154	-0.0027	-0.0024	0.0300	-0.0033	-0.0062	0.0147	-0.0139	-0.8330
Fission Product	-0.0046	0.0009	-0.0003	-0.0003	0.0048	-0.0004	-0.0011	0.0008	-0.0059	-0.2119
Nu:										
^{233}U	0.9677	-0.0023	-0.0000	-0.0013	-0.0001	0.0000	0.0000	0.7692	-0.9656	-0.2513
^{232}Th	0.0265	0.0025	0.0000	0.0001	-0.0001	0.0000	0.0000	-0.0105	-0.1037	-0.6901
Inelastic Scattering:										
^{232}Th	-0.0082	0.0121	0.0334	0.0324	-0.3630	0.0371	0.0421	0.0193	0.1012	0.5689

^aThis is the percent change in integral parameter per percent change (increase) in cross section uniformly over the entire energy range.

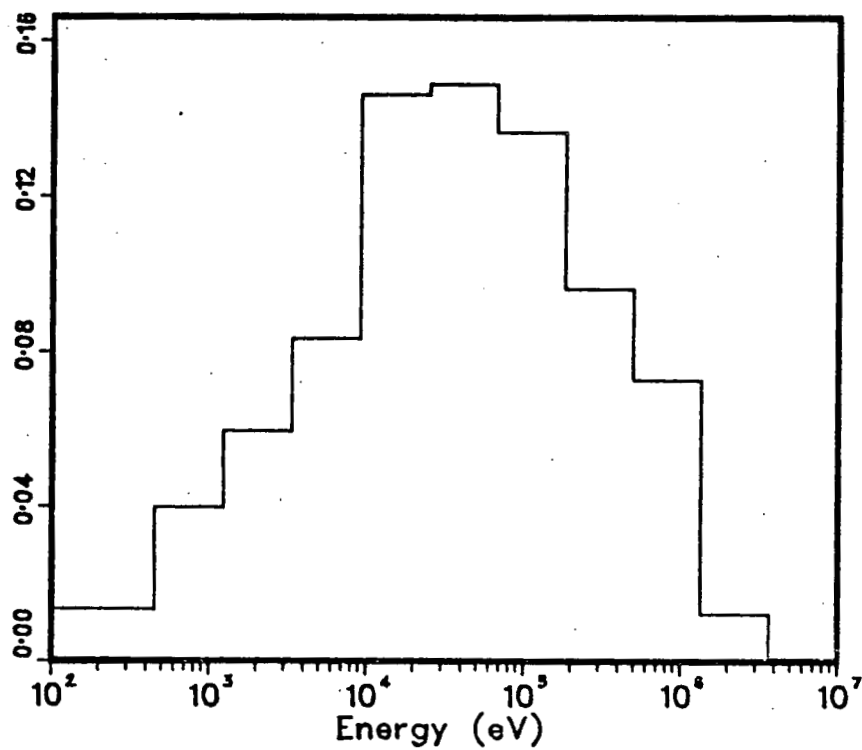


Fig. 1. Percent Change in Breeding Ratio
Per Percent Increase in σ_c^{02} .

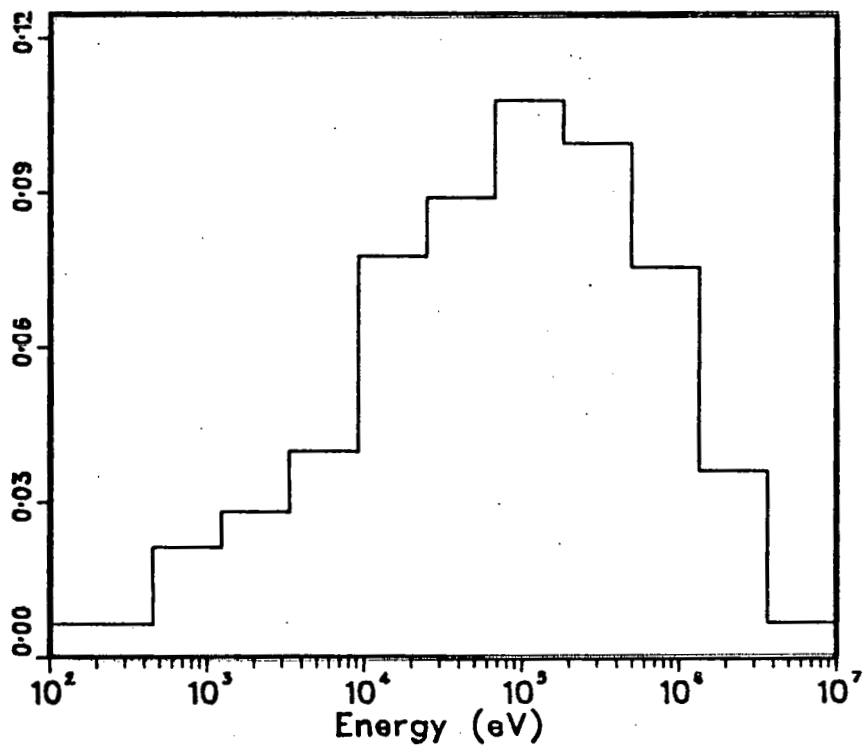


Fig. 2. Percent Change in Eigenvalue
Per Percent Increase in σ_f^{23} .

^{232}Th cross sections: σ_f^{23} , σ_f^{02} , σ_c^{23} , σ_c^{02} , ν^{23} , ν^{02} , and $\sigma_{n,n}^{02}$. Some of these results are illustrated in Figs. 1 and 2. The percent change in eigenvalue per percent increase in σ_f^{49} as a function of energy is shown in Fig. 1. This sensitivity is comparable in both shape and magnitude to the corresponding sensitivity of eigenvalue to σ_f^{49} in mixed (^{239}Pu , U)-oxide fueled LMFBRs.¹⁰ The shape or energy-dependence of this sensitivity reflects the flux weighting of σ_f^{23} with a peak in the 100-500 keV range. The percent change in breeding ratio per percent increase in σ_c^{02} as a function of energy is shown in Fig. 2. As before, the shape of this sensitivity reflects the flux weighting of the cross section (in this case, σ_c^{02}). It is important to note the peak in this curve is much broader and is shifted to lower energies (around 10 - 200 keV) compared to Fig. 1. This shift in sensitivity to lower energies is the result of the very sharp increase in σ_c^{02} at lower energies. In this ^{233}U -Th fast reactor model, 63% of the neutron captures in thorium occur below 67 keV.

COMPARISON OF CALCULATED INTEGRAL PARAMETERS USING RECENT ^{233}U AND THORIUM EVALUATIONS

Projections have been made using the sensitivity results from this study with proposed changes in the ENDF/B evaluations. It should be noted that preliminary ENDF/B Version 5 data were not yet available. Comparisons have been made with an initially proposed (i.e., pre-preliminary) ENDF/B Version 5 evaluation (noted herein as ENDF/B-5P) in order that these calculated projections might be useful in the evaluation process. The subsequent preliminary evaluations for both ^{233}U and Th are significantly different than the ENDF/B-5P evaluations used herein. An additional comparison is made using a recent Th evaluation¹ (noted herein as ANL-2/78).

Because of the primary importance of ^{233}U fission and Th capture cross sections, the large differences between their recent evaluations and the ENDF/B Version 4 evaluations can be expected to produce significant changes in calculated reactor parameters. The percent difference as a function of energy in ^{232}Th capture cross section of ENDF/B-5P relative to ENDF/B-4 is shown in Fig. 3. The thorium capture cross section of ENDF/B-5P is 5-10% smaller (than ENDF/B-4) from 0.1 to 60 keV and ~20% smaller from 60-400 keV. This reduction in σ_c^{02} would produce a 4.0% increase in eigenvalue (relative to the ENDF/B-4 data). Two-thirds of this effect is produced by the differences in σ_c^{02} above 67 keV. In fact, ~2.3% δk results from the ~22% difference in σ_c^{02} between 67 and 500 keV. The percent difference as a function of energy in ^{233}U fission cross section of ENDF/B-5P relative to ENDF/B-4 is shown in Fig. 4. These differences are small (< 0.5-1.0%) and both positive and negative below 500 keV. Above 500 keV the ^{233}U fission cross section of ENDF/B-5P is larger by ~3-8%. The overall effect of these differences in σ_f^{23} upon eigenvalue are small (~0.2% δk larger with ENDF/B-5P).

The calculated breeding ratio will also be strongly effected by the differences in σ_c^{02} and σ_f^{23} shown in Figs. 3 and 4. The reduced thorium

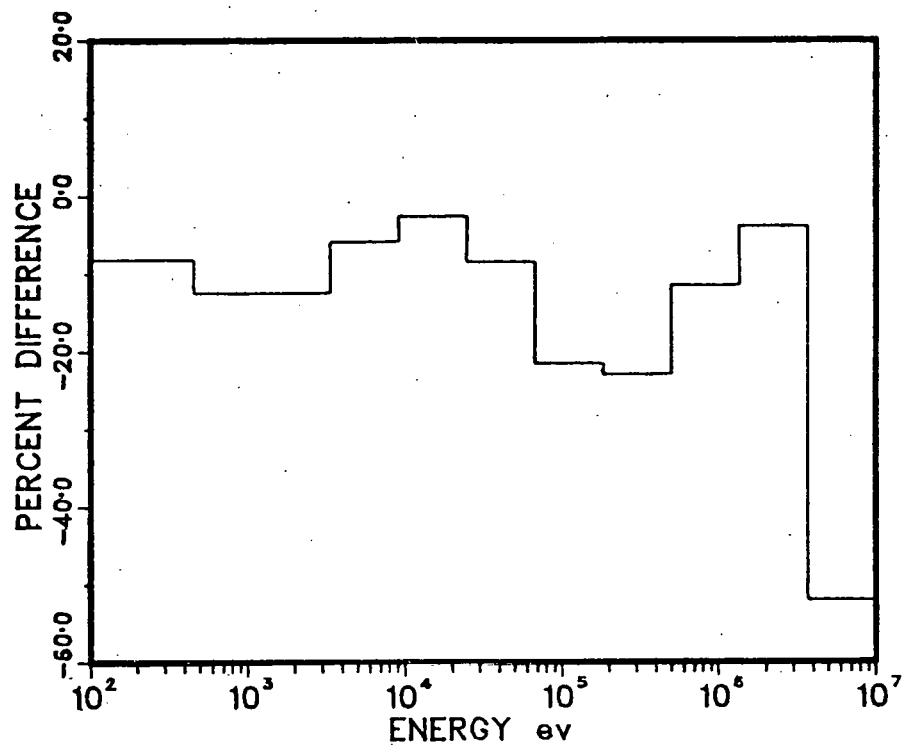


Fig. 3. ^{232}Th (N,Gamma) Percent Difference
ENDF/B-5P vs. ENDF/B-4.

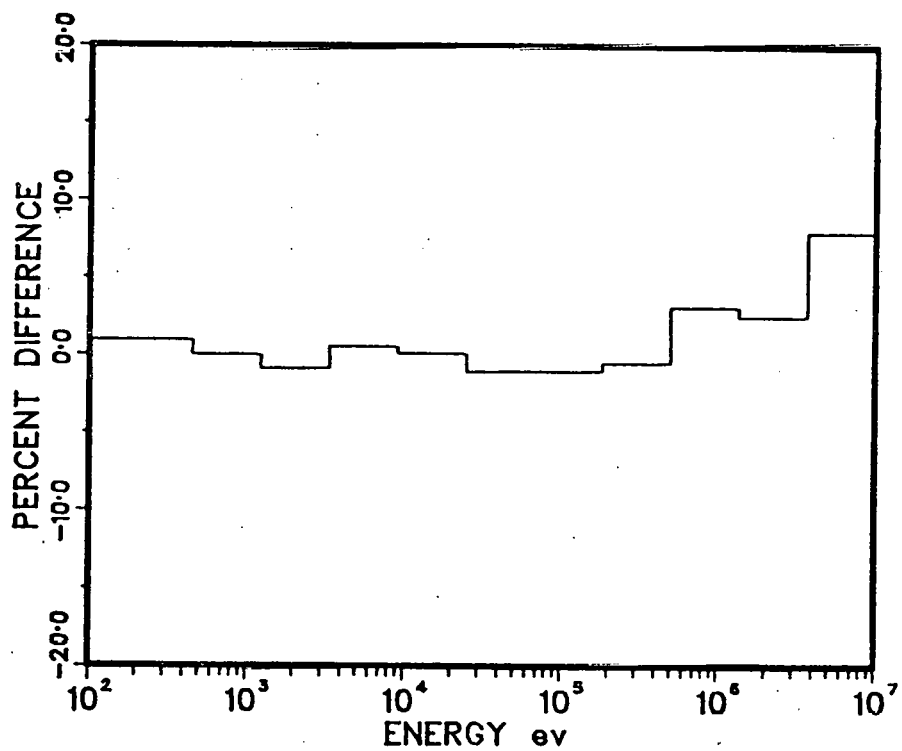


Fig. 4. ^{233}U (N,Fission) Percent Difference
ENDF/B-5P vs. ENDF/B-4.

capture cross section of ENDF/B-5P will decrease the breeding ratio by $\sim 11.8\%$. Sixty percent of this change (i.e., $\sim 7.1\% \delta BR$) occurs from 67-500 keV and 24% occurs below 67 keV. The small differences in σ_f^{23} change the breeding ratio by $\sim 0.3\%$ (lower in ENDF/B-5P).

Calculations were made for this same one-dimensional ^{233}U -Th oxide reactor model using the ENDF/B-5P evaluations of ^{233}U and thorium, and the ANL-2/78 evaluation of thorium. The nuclear data for all the remaining materials was ENDF/B-4. These results, as summarized in Table 3, indicate large changes in several important integral parameters as projected above with the sensitivity coefficients. The eigenvalue is $\sim 4.8\%$ larger (relative to ENDF/B-4) with ENDF/B-5P and $\sim 4.1\%$ larger with ANL-2/78. The breeding ratio is reduced 10.5% with ENDF/B-5P and 9.1% with ANL-2/78. As projected, these large changes in both eigenvalue and breeding ratio result principally from the differences in the thorium capture cross section. Of the 11.2% reduction (ENDF/B-5P relative to ENDF/B-4) in c^{02}/f^{23} , only 0.1% results from the increase in f^{23} and 11.1% results from the decrease in c^{02} . Table 3 also indicates these data have only slight impact on the power splits and significant effects (5-10%) on central reactivity worths. Clearly the large changes discussed for these principal cross sections strain the validity of linearly extrapolating with these sensitivity coefficients. Furthermore, such a large change in eigenvalue would require a corresponding significant change (such as enrichment) which could compensate for some of these changes (such as in breeding ratio). In fact, an enrichment adjustment back to critical reduce the change in breeding ratio by almost 50% with a corresponding large change in fissile inventory.

SUMMARY

Sensitivity coefficients for the nuclear data of the principal constituents of a representative ^{233}U - ^{232}Th fueled LMFBR have been generated. These data were found to be very similar to the analogous data in the ^{239}Pu - and ^{235}U -fueled systems. It is noted, however, that nuclear data uncertainties are much larger for ^{233}U and ^{232}Th than ^{235}U and ^{239}Pu . Furthermore, recent evaluations show significant differences for some of the most sensitive nuclear data for these systems. The energy-dependent sensitivity coefficients obtained in this study should be helpful in assessing the impact of data changes on the integral parameters of a ^{233}U - ^{232}Th system.

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Table 3. Integral Parameter Comparisons with ENDF/B-4

Integral Parameter	ENDF/B-4	ENDF/B-5P	$\frac{\text{ENDF/B-5P}}{\text{ENDF/B-4}}$	ANL-2/78	$\frac{\text{ANL-2/78}}{\text{ENDF/B-4}}$
Eigenvalue, k	1.00000	1.04831	1.04831	1.04104	1.04104
Power Splits, $\frac{P(\text{IC})}{P(\text{OC})}$	1.40517	1.40437	0.99943	1.40311	0.99853
Conversion Ratio					
Inner Core	0.80442	0.71284	0.88616	0.72739	0.90424
Outer Core	0.64074	0.58801	0.88650	0.57813	0.90229
Breeding Ratio	1.17912	1.05568	0.89531	1.07210	0.90923
Central Reaction Rate Ratios					
f^{02}/f^{23}	0.0039725	0.0041456	1.04356	0.0041744	1.05082
C^{02}/f^{23}	0.11581	0.10280	0.88766	0.10488	0.90567
C^{23}/f^{23}	0.091793	0.093683	1.02060	0.093577	1.01944
Central Material Reactivity Worths ($\delta k/k / 10^{24}$ atoms)					
^{233}U	7.5606(-4)	6.9261(-4)	0.91608	6.9992(-4)	0.92573
^{232}Th	-5.9642(-5)	-5.2837(-5)	0.88590	-5.4098(-5)	0.90705
Na	5.7631(-7)	5.3874(-7)	0.93481	6.2425(-7)	1.08318

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