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ANALYSIS OF PROTEUS LWHCR PHASE II EXPERIMENTS PERFORMED USING THE AARE MODULAR SYSTEM AND JEF BASED LIBRARIES

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ABSTRACT

The capability of the AARE modular code system and JEF-1 based nuclear data libraries to analyse LWHCR lattices is investigated by calculating the wet and dry cells of the PROTEUS-LWHCR Phase II experiment. The results are compared to those obtained using several cell codes. Main features of AARE, such as the self-shielding of resonance cross sections in the whole energy range, the generation of adequate fission source spectra, the accurate calculation of migration areas, and the efficiency of the elastic removal correction are investigated. In particular, it is shown that AARE can predict the k_∞ void coefficient well with a 1% deviation from experiment, whereas the other codes give larger deviations.

INTRODUCTION

Existing spectrum codes and related nuclear data libraries were mainly developed for design calculations of Light Water or Fast Breeder reactors. Therefore many simplifications were considered. For example, the resonance and fast energy ranges (in the case of LWR-codes), and the lowest resonance and thermal ranges (in the case of FBR-codes) are treated in a way, which is not always adequate for Light Water High Conversion Reactor (LWHCR) calculations. This can lead to conflicting calculational results especially in the determination of eigenvalues, reaction rates, and void coefficients. Therefore the development of suitable methods and the generation of adequate nuclear data libraries is a key issue in assessing the feasibility of a LWHCR core.

In this framework the new general purpose code system AARE (Advanced Analysis for Reactor Engineering)[1] was created and JEF (Joint Evaluated File) based nuclear data libraries were generated.[2] In this paper the capability of the AARE modular system and JEF based nuclear data libraries to analyse LWHCR lattices is investigated by calculating the PROTEUS-LWHCR Phase II experiment.[3] The results are compared to those previously published where several cell codes, including WIMS-D, MICROX-2, KARBUS, and SPEKTRA were used.

AARE, a PSI (Paul Scherrer Institute) update of the DANDE (applied nuclear DAta, core Neutronics DEpletion) system from Los Alamos, is a flexible code package which allows applications to a broad class of reactor types. It includes as well burn-up and sensitivity codes. Within AARE the coupling and reformatting programme TRAMIX, a PSI update of TRANSX-CTR, and the one-dimensional discrete-ordinates transport code ONEDANT are available. TRAMIX is able to shield resonance data in the whole energy range using the intermediate resonance absorption shielding method of resolved resonances (IR method) by calculating isotope dependent

Goldstein-Cohen λ factors and energy dependent Dancoff corrections, to compute accurately fission spectra from fission matrices, to correct elastic scattering matrices for differences between actual flux and library weighting flux, and to produce a variety of library formats which can be used in most transport and diffusion codes.

Particular features of AARE, such as the self-shielding of resonance cross-sections in the whole energy range important for structural materials and actinides (including the low energy resonances of heavy actinides such as the capture resonance of ^{242}Pu at 2.7eV), the shielding of oxygen resonances in the MeV range, the generation of adequate fission source spectra, the accurate calculation of migration areas with transport cross sections obtained using the inflow formula, the choice of different group structures, and the efficiency of the elastic removal correction are investigated. Also analysed is the IR method by making a comparison with an accurate pointwise slowing down calculation in the resolved resonance range using the cell code MICROX-2.

For the sake of consistency all cross-sections are taken from the JEF file. The cross section generation scheme NJOY (version 6/83) has been employed to produce MATXS formatted nuclear data libraries in 70, 193, and 308 groups for use in the AARE system. Additionally, the editing module MICROR was utilized for creating the MICROX-2 libraries (FD, GG, GAR data files), and the canadian module WIMSR was tested and updated to generate with the management code WILMA a JEF based library for the code WIMS-D (WIMS-JEF library). The preprocessed WIMS81 data library was used for comparison.

Eigenvalues, migration areas, reaction rate ratios of important actinides, and void coefficients are computed and compared with the series of experiments (Phase II) currently performed at the PROTEUS-LWHCR facility. PROTEUS includes a central test zone of mixed oxide fuel PuO_2/UO_2 characterized by a volumetric moderator/fuel ratio of 0.48. Cores 7-8 indicate, respectively, the fully watered and dry core. Both cores consist of a three region cell with fuel pin, steel cladding, and moderator. Experimental errors on the standard types of reaction rate ratios were found to be between $\pm 1.5\%$ and $\pm 2.0\%$. For the fission of ^{241}Pu and the capture of ^{242}Pu the errors are $\pm 3.0\%$[3].

RESULTS

Table I summarizes some calculated-to-experimental (C/E) values for reaction rates and k_∞, and computed absolute values for migration areas (M^2) obtained using the AARE system. The IR method was utilized, and cross sections were shielded in the whole energy range. A cell flux weighted fission spectrum for the whole cell (converged spectrum) was determined iteratively. The elastic removal correction was utilized in the case of 70 neutron group calculations. Throughout the whole paper F9 denotes the fission rate of ^{239}Pu per atom, C8 the capture (i.e. (n,γ)) rate of ^{238}U per atom, F8 the fission rate of ^{238}U per atom, F5 the fission rate of ^{235}U per atom, F1 the fission rate of ^{241}Pu per atom, and C2 the capture rate of ^{242}Pu per atom.

Table I shows that all investigated energy structures and JEF data libraries give generally a good prediction of experiments. Furthermore, the migration area calculations agree well for both cores within 1% for all energy structures. The use of 70 neutron groups together with previously mentionned AARE options gives small deviations from the results carried out with finer energy structures. However, the prediction of the capture rate of ^{242}Pu in Core 7 improves with increasing number of energy groups, and is accurate within 1.3% when using the 308 neutron group MATXS library. This is because TRAMIX is able to shield the main resonance of ^{242}Pu

Core	Core 7			Core 8		
Number of groups in the library	70	193	308	70	193	308
k_∞	0.995	0.998	0.999	0.995	0.999	0.998
M^2 [cm^2]	43.6	43.9	44.0	203.7	202.7	202.6
C8/F9	1.004	1.005	1.000	0.997	0.987	1.003
F8/F9	1.008	1.031	1.020	0.975	0.974	0.988
F5/F9	1.016	1.028	1.037	1.003	1.009	1.003
F1/F9	1.036	1.050	1.028	0.998	1.009	1.010
C2/F9	0.953	0.964	0.987	1.246	1.260	1.256

Table I: Calculation/experiment (C/E) values for reaction rate ratios and k_∞, and computed migration areas (M^2) for Core 7 and Core 8 obtained using AARE and different self-shielded JEF MATXS libraries

(at 2.7 eV) and the 308 neutron group structure allows a very detailed energy representation around 2.7 eV.

Tables II and III give a comparison between the results from AARE, MICROX-2, WIMS-D/JEF and those previously published from other codes such as WIMS-D, KARBUS, and SPEKTRA)[3,4,5] for Core 7 and Core 8.

Generally it is found that the systematic use of JEF based nuclear data libraries improves the consistency of the results in both cores. This is particularly true in the case of Core 8 where the neutron spectrum is harder (see Fig. 1). In calculations of voided cores the values of fast cross sections are important, and JEF-1 data are supposed to account for more recent measurements compared to ENDF/B-IV or to older evaluations. A significant improvement is achieved in the prediction of reaction rates relevant to the neutron balance, such as the capture and the fission of ^{238}U relative to the fission of ^{239}Pu. This is because various resonance parameters have been reevaluated in JEF. The maximum deviation from experiment (about 25%) occurs in the capture of ^{242}Pu in the voided lattice. Since all methods reproduce this discrepancy, it appears that JEF-1 fast data of ^{242}Pu are not adequate for LWHCR calculations.

Main reactivity discrepancies between the WIMS-JEF and the WIMS81 library are found to come primarily from ^{238}U, ^{239}Pu and ^{240}Pu absorption and fission cross sections.[6] As far as single reactions are concerned the fission of ^{241}Pu is predicted less accurately by the WIMS81 library, since unshielded cross sections are used. The fact that the WIMS-JEF k_∞ is less accurate is due to several individual effects. WIMS-D overestimates systematically the capture rate of ^{242}Pu in Core 7 by up to 60%, since this code utilizes infinite dilution low energy cross sections, and the main contribution to C2 in Core 7 comes from the 2.7 eV resonance. For both cores large discrepancies (up to 10%) between calculated migration areas M^2 (important for deducing k_∞ in the experiments) originate, when using the two different WIMS libraries. Following major reasons for these deviations were found. First, the self-scattering term in non-moderators is transport corrected only in the case of the WIMS-JEF library. Second, oxygen

Code	KARBUS	SPEKTRA	WIMS-D	WIMS-D	AARE	MICROX-2
Library	KEDAK-4	DATUBS-4	WIMS81	WIMS-JEF	MATXS	FD GG GAR
Number of groups	69	35	69	69	70	193
k_∞	0.986	1.004	1.012	0.982	0.995	0.992
M^2 [cm^2]	46.5	45.2	48.1	44.4	43.6	44.3
C8/F9	1.036	1.001	0.982	1.021	1.004	1.009
F8/F9	1.024	1.025	1.030	1.017	1.008	1.002
F5/F9	1.012	1.064	0.995	1.009	1.016	1.035
F1/F9	1.008	1.067	1.054	1.012	1.036	1.009
C2/F9	1.552	1.057	1.732	1.617	0.953	1.090

Table II: Calculation/experiment (C/E) values for reaction rate ratios and k_∞, and computed migration areas (M^2) for Core 7 obtained using different methods and nuclear data libraries

Code	KARBUS	SPEKTRA	WIMS-D	WIMS-D	AARE	MICROX-2
Library	KEDAK-4	DATUBS-4	WIMS81	WIMS-JEF	MATXS	FD GG GAR
Number of groups	69	35	69	69	70	193
k_∞	0.984	0.988	1.037	0.997	0.995	0.983
M^2 [cm^2]	-	193.7	219.7	200.4	203.7	-
C8/F9	1.082	1.040	1.007	0.993	0.997	1.022
F8/F9	1.047	1.002	1.026	0.984	0.975	0.990
F5/F9	1.006	1.020	1.013	0.998	1.003	0.998
F1/F9	0.967	1.000	1.152	0.997	0.998	0.997
C2/F9	1.138	1.120	0.962	1.211	1.246	1.226

Table III: Calculation/experiment (C/E) values for reaction rate ratios and k_∞, and computed migration areas (M^2) for Core 8 obtained using different methods and nuclear data libraries

and ^{238}U scattering cross sections in the fast energy range are found to be smaller in the case of the WIMS81 library. This is important since the migration area is mostly contributed to in the highest energy range.[6]

The small differences between MICROX-2 and AARE reaction rates from 193 group calculations (see Tables I-III) are primarily due to the pointwise solution of slowing down equations, to the linear interpolation in the fast energy range, and to the two zone homogeneization in MICROX-2. The slight MICROX-2 overestimate of the capture of ^{238}U in Core 8 could partly be due to the linear interpolation in the fast energy range.

An overestimate of the fission of ^{235}U (relative to the fission of ^{239}Pu) in Core 7 (about 3.5%) occurs in the case of each fine group AARE calculation (see Table I). This is consistent with MICROX-2 where an accurate pointwise shielding of resonance cross sections is performed (see Table II). Therefore we may suppose a slight overprediction of ^{235}U fission in the thermal and resolved resonance ranges up to 82 eV, quantitatively confirming previous studies.

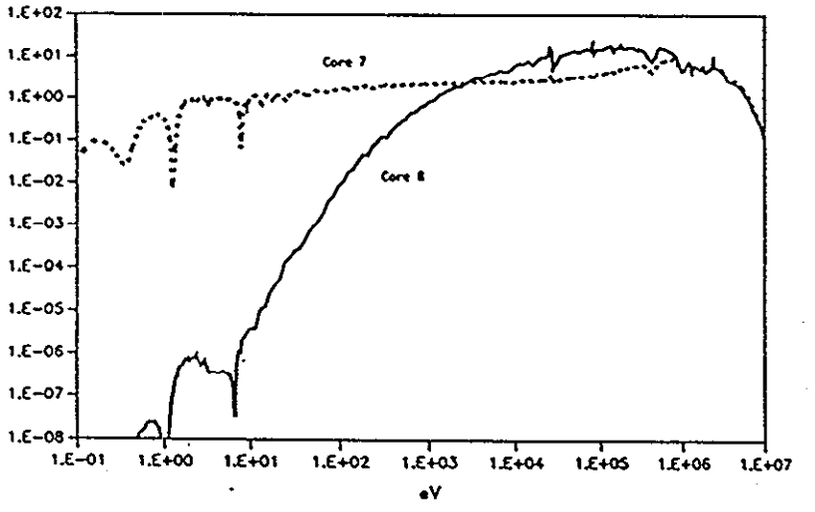

Fig. 1: Averaged neutron spectra of both cores expressed per unit of lethargy computed using AARE

In the following analysis the main features of AARE, such as an adequate self-shielding of resonance cross sections in the whole energy range of importance for structural materials and actinides (including the low energy resonances of heavy actinides), the shielding of oxygen resonances in the MeV range, the generation of adequate fission source spectra, and the efficiency of the removal correction are investigated.[7] Furthermore k_∞ void coefficients are given.

Comparison between IR and NR methods

It comes out that the intermediate resonance absorption shielding method of resolved resonances (IR method) used in AARE does a surprising good job of representing the resonance effects in watered LWHCR tight lattices. This is because in contrast to the usual methods the

Goldstein-Cohen λ factors are calculated and are therefore problem dependent. Particularly, it is found that the narrow resonance approximation (NR method) leads to a bad prediction of C2 in Core 7 even if many fine groups are used (C/E of 1.100 with 308 groups). The use of appropriate λ parameters (IR method) improves systematically eigenvalues and relevant reaction rate ratios of Core 7.

This is especially true when coarser group structures are considered, where the resonance cross section shape is averaged over a larger energy width and the λ-parameter method becomes more effective (i.e. k_∞ C/E of 0.995 versus 0.982, C8/F9 C/E of 1.004 versus 1.044 in the case of 70 group AARE calculations). Obviously, results for the voided Core 8 are almost independent on the specific treatment of resonance cross sections (all λ's of interest are almost 1 in the fast energy range).

Self-shielding of cross sections of structural materials

The effect of self-shielding of structural material cross sections is not important for watered LWHCR lattices such as Core 7. However, the use of unshielded structural material cross sections could lead to some shortcomings in the analysis of voided LWHCR lattices. Since the cell spectrum is rather hard (see Fig. 1), more fast neutrons would be absorbed in the resonances of structural materials (in the keV range). Therefore the fast neutron flux and current, and consequently k_∞ and migration area, would be underestimated.

The use of infinite dilution structural material cross sections leads to a relative decrease in k_∞ of 0.1% in Core 7 (C/E of 0.994 versus 0.995) and of 0.6% in Core 8 (C/E of 0.989 versus 0.995) and in a 1.5% decrease of migration area in Core 8 (200.7 versus 203.7 cm^2), when performing 70 group AARE calculations. All other measured reaction rate ratios remain practically unchanged.

Self-shielding of oxygen resonances

If oxygen resonances (in the MeV range) are not self-shielded, the migration area increases by 2%, whereas k_∞ for the dry lattice increases by as much as 1.1% in the case of 70 group AARE calculations. This is because the fast flux and current of fully voided lattices would be overestimated.

The effect of self-shielding of high energy oxygen resonances is found to be minor in the case of Core 7 (the migration area increases by 1%, whereas k_∞ and all reaction rates remain practically unchanged) because the cell spectrum is soft (see Fig. 1). This effect becomes negligible, when using a detailed energy representation in the MeV range.

Use of different fission source spectra

Three fission spectra have been used for comparison, namely the converged spectra of both cores, and the WIMS spectrum pertaining to the WIMS81 library (i.e. the same as that of ^{235}U in an infinite moderator). It is seen that the converged fission spectra of Core 7 and Core 8 are almost identical in the important energy range (see Fig. 2). This is because the resulting neutron spectra of both cores, which obviously differ considerably in the thermal, epithermal, and resonance energy ranges, are quite similar at high energies (see Fig. 1). Furthermore the WIMS spectrum gives a reasonable estimate of the correct fission spectrum. This spectrum is

found to be slightly harder (compare with Fig. 2).

If the WIMS spectrum is used instead of the converged cell spectrum, k_∞ increases weakly by 0.3% in Core 7 and by 0.5% in Core 8, due to a slight increase of the fission of ^{238}U (i.e. by 1.1% in Core 8) and therefore of the migration area (i.e. by 0.5% in Core 8). Thus the WIMS spectrum is adequate for LWHCR lattice calculations.

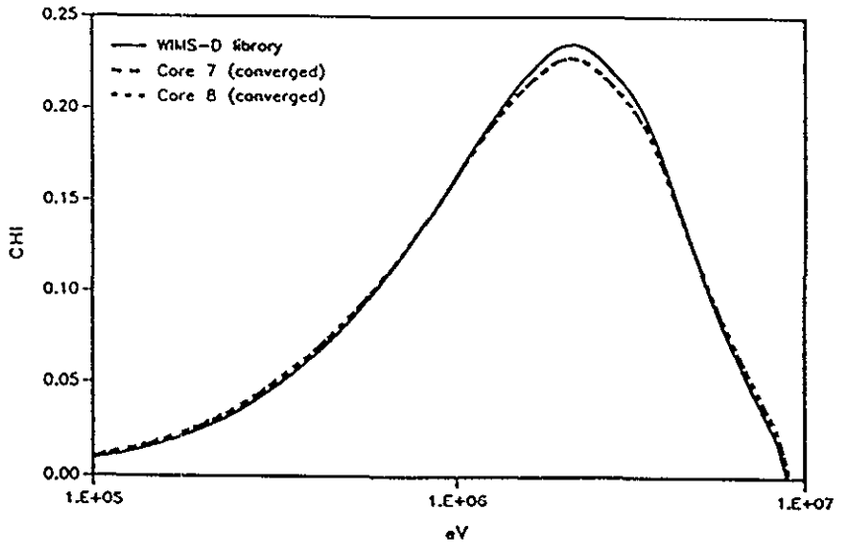

Fig. 2: Different fission spectra utilized in this analysis

Effect of elastic removal correction

In AARE the elastic removal correction can be applied to account for differences between the real flux and the model library flux. As already pointed out in Table I the values obtained with the elastic correction tend to reproduce those from more detailed fine group calculations.

The results from 70 group AARE calculations of Core 8 without elastic adjustment are less accurate (i.e. k_∞ C/E of 1.006 versus 0.995, C8/F9 C/E of 0.974 versus 0.997, M^2 of 200.7 versus 203.7 cm^2). However, the effect of the elastic correction is minor in Core 7, because the shape of the library flux is similar to that of the cell flux.

The k_∞ void coefficients

An accurate prediction of the k_∞ void coefficient for an LWHCR is particularly difficult due to its being the sum of large changes in individual reaction rates caused by the strong change of the cell spectrum. Therefore, sophisticated numerical methods and accurate data are needed.

In Table IV the k_∞ void coefficients α_v due to the full voidage of the PROTEUS test lattice are given. Experimental results are compared to those obtained with AARE, WIMS-D, MICROX-2, KARBUS, and SPEKTRA. It is shown that the use of finer group structures improves systematically all results. The prediction of the void coefficient is excellent within

Code	Library	Number of groups	k_∞ Void coefficient α_v
Experiment	-	-	+4.2±0.9
WIMS-D	WIMS81 JEF	69 69	+6.7 +5.7
KARBUS	KEDAK-4	69	+4.0
SPEKTRA	DATUBS-4	35	+2.6
MICROX2	JEF	193	+2.6
AARE	JEF	$70^{\text{no el.c.}}$ $70^{\text{with el.c}}$ 193 308	+5.3 +4.2 +4.3 +4.1

Table IV: Void coefficient α_v between 0 and 100% void (expressed in 10^{-4}/% void) for PROTEUS-LWHCR Phase II test lattice

less than 1% in the case of AARE with 193 and 308 neutron groups. The same accuracy can be reached with the 70 neutron group structure when applying the elastic removal correction in AARE. If uncorrected elastic removal and self-scattering cross sections are used, the void coefficient is similar to that from WIMS-D and MICROX-2. The underestimate of MICROX-2 comes primarily from the approximate self-shielding of unresolved resonances of actinides and of resolved resonances of structural materials in the keV and MeV range. The same trend would be shown by AARE, when the cross sections of structural materials would be taken at infinite dilution. The good prediction of KARBUS is in contrast with the single reaction rates (compare with Table II and Table III).

CONCLUSIONS

The present analysis dealt with the neutronics of clean LWHCR lattices. The results from the calculations were compared with experiment. From the study presented following conclusions can be reached.

The WIMS group structure is adequate for quick cell spectrum calculations of watered as well as voided LWHCR fresh cores.

AARE appears able to predict the void coefficient of clean LWHCRs well. This is so even if the 70 neutron group structure is used, due to the effectiveness of the elastic scattering correction. For the PROTEUS-LWHCR test lattices, the difference between calculated and experimental k_∞ void coefficients (0 to 100%) is 1.1 x 10^{-4}/% void if no elastic correction is used, and 0.1 x 10^{-4}/% void if the correction is included. The experimental error (1σ) of $\pm$0.9 x 10^{-4}/% void should, of course, be borne in mind.

The global fission spectrum used in the WIMS81 data library is found to be suitable for LWHCR calculations.

An accurate estimate of reaction rates of heavy actinides with low energy resonances (such as the capture of ^{242}Pu) can only be achieved by using self-shielded cross sections in the whole energy range (including the low energy range) and a fine group structure around these resonances.

The JEF evaluation is found to be generally adequate for LWHCR calculations. However, ^{235}U fission appears to be slightly overpredicted in the lower resonance energy range, and fast ^{242}Pu capture cross sections (above 1 keV) seem to be too high.

Using AARE in connection with JEF data, a better consistency is achieved compared to previously published results.

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