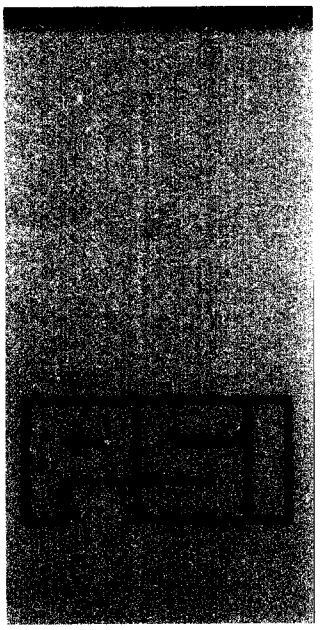
PSI-Bericht Nr. 32
JEF REPORT 11
Juni 1989



Paul Scherrer Institut
JEF REPORT 11

Labor für Reaktorphysik und Systemtechnik

Validation of LWR Calculation Methods and JEF-1 Based Data Libraries by TRX and BAPL Critical Experiments

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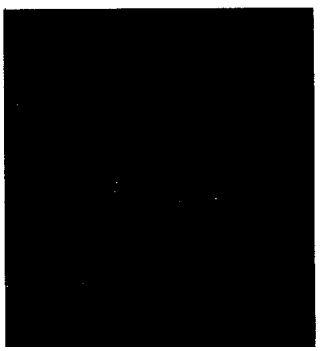
A Report on work done in the frame of JEF activity under the leadership of OECD NEA DATA BANK (BANQUE DE DONNEES DE L'AEN OCDE)



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Validation of LWR calculation methods and JEF-1 based data libraries by TRX and BAPL critical experiments

by

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Abstract

In this report the capability of various code systems widely used at PSI (such as WIMS-D, BOXER, and the AARE modules TRAMIX and MICROX-2 in connection with the one-dimensional transport code ONEDANT) and JEF-1 based nuclear data libraries to compute LWR lattices is analysed by comparing results from thermal reactor benchmarks TRX and BAPL with experiment and with previously published values.

It is shown that with the JEF-1 evaluation eigenvalues are generally well predicted within 8 mk (1 mk = 0.001) or less by all code systems, and that all methods give reasonable results for the measured reaction rate ratios within or not too far from the experimental uncertainty. This is consistent with previous similar studies.

Zusammenfassung

In diesem Bericht wird die Eignung verschiedener im PSI verbreitet benützter Code-Systeme (wie WIMS-D, BOXER, und der AARE Moduln TRAMIX und MICROX-2 in Verbindung mit dem eindimensionalen Transportprogramm ONEDANT) und von auf JEF-1 beruhenden Wirkungsquerschnittsbibliotheken zur Berechnung von LWR-Gittern untersucht. Zu diesem Zweck werden die Resultate für die thermischen Benchmark-Experimente TRX und BAPL mit den Messungen und früher publizierten Werten verglichen.

Es wird gezeigt, dass die Eigenwerte mit der JEF-1 Evaluation von allen Code-Systemen gut innerhalb von 8 mk (1 mk = 0.001) oder weniger berechnet werden, und dass alle Methoden vernünftige Resultate für die gemessenen Reaktionsratenverhältnisse innerhalb oder nicht weit von der Messunsicherheit ergeben. Dies ist konsistent mit früheren ähnlichen Studien.

Contents

1 INTRODUCTION

Light water reactors (LWR) are still an important component of modern reactor fuel management strategies. A lot of effort was devoted in the past to the development and to the validation of adequate spectrum codes for design calculation of LWRs, and various accurate neutronic calculations have been performed using specific methods and nuclear data libraries [1], [2], [3], [4].

However, the frequent utilization of the existing code systems for calculations of LWR configurations requires a continuous and rigorous verification and validation of the quality of the results, especially when new nuclear data are used.

Therefore we decided to select well known critical LWR experiments and recalculate them with the different code systems available at the Paul Scherrer Institute (PSI), and with the newest nuclear data files. The code (systems) are BOXER, WIMS-D, and the AARE (cell) codes TRAMIX and MICROX-2 in connection with the one-dimensional transport code ONEDANT.

BOXER [2] is a code developed at PSI for the calculation of two-dimensional light water reactor configurations, consisting of core neutronics and depletion modules.

WIMS-D [5] is a comprehensive code for reactor lattice cell calculations including depletion in a wide variety of reactor types. It is especially designed for the analysis of moderated systems.

AARE (Advanced Analysis for Reactor Engineering) [6] is a PSI update of the DANDE (applied nuclear DAta, core Neutronics and DEpletion) [7] system from Los Alamos. It is a flexible, new code package which allows applications to a broad class of reactors. Additionally to DANDE it includes general purpose burn-up and sensitivity modules. Particularly the coupling and reformatting (cell) programme TRAMIX [8], a PSI update of TRANSX-CTR [9], and the integral transport theory spectrum code MICROX-2 [10] from General Atomics are available in AARE. TRAMIX is a general purpose code, and MICROX-2, which was especially developed for high temperature reactor applications, is generally suitable for calculations of not too heterogeneous systems.

The main objective of this study is to achieve a code comparison obtained using the same source of nuclear data, on the basis of a simple geometric model.

Previous work was performed using ENDF/B data [1], [2]. In this study all calculations were carried out systematically with the JEF-1 evaluation [11].

JEF-1 is a computer-readable repository of (mainly) new neutron and photon data in the energy range up to 20 MeV. Together with the recently evaluated fusion file EFF-1 [12] it is the newest standard european data source for thermal reactor, fast reactor, shielding as well as fusion-blanket analysis.

The experiments analysed in this report were selected by the "Cross Section Evaluation Working Group" (CSEWG) [13]. These are water moderated lattices of slightly enriched (1.3%) uranium rods with a diameter of 0.9830 cm in a triangular lattice (TRX-1 through TRX-4) and water moderated critical lattices of 1.311 weight percent enriched uranium oxide rods with a diameter of 0.9728 cm in a triangular pattern (BAPL-1 through BAPL-3) respectively. Because these experiments were well measured, they are especially suitable for testing LWR methods and nuclear data libraries. Particularly, the accuracy of ^{235}U fission spectrum and fission resonance integral, of ^{238}U fission cross sections, inelastic scattering, shielded resonance and thermal capture cross sections can be checked. The scattering and thermal absorption cross sections of water are very important also.

In Section 2 the processing scheme for the JEF-1 based libraries is discussed. In Section 3 a detailed description of the main features of the spectrum codes employed at PSI is given. This facilitates the understanding of the results and of the technical discussion presented in Section 5. Section 4 is devoted to the description of the computational model (including geometric approach and codes used)

employed in the reference calculations presented in Section 5. Moreover, in Section 5 the influence of more sophisticated models on the results from the reference calculations is investigated.

Finally, Section 6 gives some conclusions from this study.

2 NUCLEAR DATA

All calculations are based on specific JEF-1 data libraries for the (cell) codes TRAMIX, BOXER, WIMS-D and MICROX-2. In this section a description of these libraries is given. More detail is given in [14].

2.1 Pointwise and groupwise libraries

2.1.1 Processing scheme

Pointwise and groupwise files to be processed further for making working libraries for TRAMIX, WIMS-D, and MICROX-2 were generated using the Los Alamos NJOY system (Version 6/83 with updates up to mid 1987 [15]).

First, pointwise PENDF cross sections (see Ref. [16]) were processed into an ENDF/B like format using the NJOY modules RECONR, BROADR, UNRESR, HEATR and THERMR. The RECONR module reconstructs pointwise (energy-dependent) cross sections using ENDF/B resonance parameters and interpolation schemes (identified by an integer parameter). Resonance cross sections are calculated with an extended version of the methods of RESEND [17]). BROADR Doppler-broadens and thins pointwise cross sections using the method of SIGMA modified for better behaviour at high temperatures and low energies [18]. UNRESR computes effective self-shielded pointwise cross sections in the unresolved-resonance region using the methods of ETOX [19]. HEATR generates pointwise heat production cross sections (kerma factors) and radiation-damage-energy production cross sections. THERMR produces incoherent inelastic energy-to -energy matrices for free or bound scatterers, coherent elastic cross sections for crystalline materials, and incoherent elastic cross sections. The PENDF files were produced using the JEF-1, the revised JEF-1.1, and the fusion oriented EFF-1 European evaluations [11], [20], [12]. These PENDF files include pointwise cross sections for almost all available isotopes (about 300) and temperatures up to 3000 K. The thermal region was treated according to the free gas model. For particular isotopes such as H in H_2O coherent and incoherent thermal $S(\alpha, \beta)$ matrices were included based on the recent JEF-1 evaluation [21].

Second, various GENDF multigroup cross section files were constructed using the GROUPR module. For comparison purposes, among the four group structures described in Ref. [14] only the 70 group WIMS-BOXER (used in BOXER, basically in WIMS-D, and in TRAMIX) and the 193 group GA-MICROX structures [14] (used in MICROX-2 and in TRAMIX) were considered in the present study.

GROUPR generates self-shielded groupwise vector cross sections, group-to-group neutron scattering matrices, and photon production matrices using pointwise ENDF and PENDF data. The cross sections are written onto groupwise cross section files GENDF in ENDF/B like format [22]. Vectors for all reaction types, matrices for reactions producing neutrons, including fission together with mixed data pertaining to fission yields of prompt and delayed neutrons were calculated for different degrees of anisotropy at different temperatures and background cross sections.

The narrow-resonance Bondarenko flux model was employed for light isotopes. Shielded multigroup cross sections of heavier resonance nuclides were estimated using the method of the flux slowing

down calculator assuming a single resonance absorber in a non-absorbing moderator. This appears to be consistent with the resonance formalism employed in WIMS-D. A brief description of the GENDF libraries is given in subsections 2.1.2-2.1.3, whereas Sections 2.2-2.5 report on the working libraries.

2.1.2 70 group WIMS-BOXER structure GENDF JEF-1 library

The energy structure of the WIMS-BOXER library consists of the standard 69 group WIMS structure and one additional group from 10 MeV to 14.918 MeV. This library contains JEF-1 neutron P_0 and P_1 self-shielded temperature dependent data pertaining to most important isotopes for LWR and light water high converter reactor calculations. 42 thermal energy groups below 4 eV with upscatter are considered. The dry WIMS-D input spectrum [14] was utilized for collapsing PENDF data into multigroup cross sections. For accurate leakage calculations oxygen and carbon cross-sections (including all fast resolved resonances between 1 MeV and 10 MeV) were self-shielded using the method of the flux calculator applied in the whole energy range. Generally, the self-shielding of resonance cross sections of certain light elements is found to be important for correct calculations in hard spectra systems, if these elements are high density materials (such as oxygen in UO_2 lattices) and if a coarse group structure in the MeV range is used. In these cases, the energy representation of resonances is not accurate enough, so that self-shielding is needed.

2.1.3 193 group GA-MICROX structure GENDF JEF-1 library

This library contains JEF-1 P_0 through P_3 self-shielded data at 296 K and is mainly intended for high temperature reactors, LWR and light water high converter reactor calculations. 103 thermal energy groups below 4.6 eV with upscatter are considered. The boundaries of the first 92 fast energy groups are taken from the GAM-II energy structure, whereas in the thermal range below 2.38 eV the boundaries coincide with the energy points of the MICROX code. Dry and wet WIMS-D input spectra [14] were utilized for collapsing PENDF data into multigroup cross sections. The wet spectrum was used for hydrogen, deuterium and oxygen.

2.2 TRAMIX JEF-1/EFF-1 libraries

The GENDF files of different neutron energy structures have been converted into MATXS format suitable for further processing with TRAMIX, using the NJOY module NMATXS (MAT70 and MAT193 libraries). The MATXS file is a cross section library in a flexible format designed to generalize the existing standard CCCC files ISOTXS, BRKOXS, GRUPXS [23]. In this processing the available $S(\alpha,\beta)$ library matrices were utilized for water, heavy water, carbon, beryllium, and for oxygen in UO_2.

2.3 MICROX-2 JEF-1 libraries

GENDF and PENDF data files can be edited into the FDTAPE, GGTAPE and GARTAPE input files for MICROX-2 using the PSI-NJOY coupling module MICROR [24]. The FDTAPE data file contains fine group dilution- and temperature- dependent cross sections in the fast energy range. The GGTAPE data file consists of two sections which include infinite dilute P_0 and P_1 cross sections in the fast and thermal energy ranges respectively. MICROX-2 uses only the thermal section of the GGTAPE, which contains pointwise cross sections with upscatter calculated using the free gas model or the available coherent and incoherent scattering $S(\alpha,\beta)$ matrices. The GARTAPE data file contains pointwise

Doppler-broadened resonance cross sections in the resolved resonance range. Fine energy points (up to the keV range) may be defined according to the criterion of equidistant lethargy or velocity spacing to be used in MICROX-2 for an accurate self-shielding of the resolved resonance range (as a solution of slowing down equations in two zones).

Starting from the GENDF data in 193 groups and from the pointwise PENDF library from NJOY (see previous section), FDTAPE, GGTAPE, and GARTAPE data libraries were generated. The FDTAPE data set includes 92 neutron group self-shielded cross sections up to P_3. Individual fission spectra for main actinides are included. The thermal part of the GGTAPE consists of 101 energies and includes scattering matrices for main moderators, i.e. hydrogen, deuterium, carbon and oxygen (KERN=1 in the MICROX-2 terminology). The addition of GGTAPE scattering matrices for actinides did not modify the results and the conclusions presented in this report. The GARTAPE contains pointwise, Doppler-broadened resonance cross sections in the resolved resonance range. It has been generated on the basis of equidistant velocity spacing (resulting in a larger density of points at higher energies compared to the equidistant lethargy spacing). Doing in this way, the GARTAPE allows additionally a suitable analysis of intermediate spectra [25]. The generation of an alternative GARTAPE with constant lethargy spacing did not affect substantially the results presented in this study. Data for each library isotope are tabulated at 14457 energy points between 0.414 eV and 8.0072 keV.

2.4 WIMS-D JEF-1 data library

Starting from the 70 group WIMS-BOXER GENDF files, a 69 neutron group library for the code WIMS-D (WIMSJEF library) was generated (the first (highest) energy group of the WIMS-BOXER library was cut out). Hereby the NJOY module WIMSR was applied to transform the GENDF cross-sections into a form suitable for being used as input to the Canadian WIMS library management programme, WILMA [26], [27]. In the processing with WIMSR and WILMA the relevant data were calculated by considering all explicitely represented reaction types on the GENDF files. A global fission spectrum, based primarily on data for ^{235}U fission, was taken over from the standard WIMS81 library (WIMS spectrum, [14]). The version of the WIMSR module currently used was a specially updated one [14]. The modified version of the WIMSR module allowed a transport correction for the self-scattering cross section, the selection of a given dilution for evaluating scattering data and a generalized "inflow" computation of the transport cross section using an alternative problem-specific current read from the CCCC standard interface file RMFLUX [23]. WIMSR was also modified in such a way that the slowing down power on the GENDF file is evaluated at infinite dilution. An important modification to WIMSR was related to the resonance tabulations, whereby the original background cross-section grid was shifted in each energy group by the product of the potential scattering cross section and the Goldstein-Cohen λ-factor for the resonance absorber. This considers the fact that the total background cross-section in WIMS-D consists of the contributions from all isotopes including the tabulated resonance absorber. The WIMS-D library consists of transport corrected P_0 data for most nuclides. The "inflow" transport correction is computed for all nuclides using a representative standard weighting current [14]. For the principal moderator isotopes (hydrogen, deuterium, oxygen and carbon) P_0 and P_1 cross-sections are available.

2.5 BOXLIB JEF-1 library

The BOXLIB cross section library used in BOXER was generated from JEF-1 basic nuclear data using the ETOBOX code, the library processing code of ELCOS (Eir-Lwr-COde-System) [28]. The methods

involved in this processing are slightly different from those used in NJOY, particularly in the treatment of resonances [29], [30].

The BOXLIB JEF-1 based library contains neutron cross sections collapsed to 70 groups. It consists of most important isotopes including fission products for LWR calculations. The group structure is the same as in the 70 group NJOY produced libraries (cf. Section 2.1.2). However, the upper boundary of the thermal range is 1.3 eV instead of 4 eV, so that the number of thermal (upscatter) groups is only 37. P_0 and P_1 scattering matrices (P_2 transport corrected) are given for all isotopes. In addition to the group cross sections BOXLIB contains point data in the resonance range. The weighting spectrum is a fission spectrum in the fast range (above 183 keV), a 1/E spectrum between 1.3 eV and 183 keV, and a modified Maxwellian spectrum in the thermal range. BOXLIB contains a fixed fission spectrum for each fissile nuclide collapsed with the above weighting spectrum for the incident neutrons.

In the resolved resonance range point cross sections are reconstructed from the resonance parameters given in JEF-1. The four models used for the resonance parameters in the ENDF/B format are included in ETOBOX. Then the cross sections are Doppler broadened by numerical integration of the thermal excitation kernel [29]. Self-shielded unresolved resonance cross sections are computed from the distributions of the resonance parameters given in JEF-1 according to the statistical model and Doppler broadened by means of the Ψ and χ functions [30]. The narrow resonance approximation is used to evaluate the self-shielding.

In the fast range (E > 907 eV) the resonance cross sections (both resolved and unresolved resonances) are collapsed to groups for three temperatures (20, 1100, and 2800 °C) and 4 values of the dilution cross section (10, 100, 1000 barns, and ∞). In the resonance range between 1.3 eV and 907 eV (important low energy resonances of plutonium isotopes are included) pointwise lists of cross sections are produced for three to seven temperatures (depending on the nuclide). For the unresolved resonances these lists are produced for the above four dilutions and three temperatures. In contrast to the GAR file used in MICROX-2, where the points are equidistant, the number of points per lethargy unit depends on the variation of the cross sections with lethargy, so that the cross section values between the points can be accurately reconstructed by interpolation. The minimum lethargy spacing of the points is 10^{-4}. As an example, the lists for ^{238}U number 3813 points between 1.3 and 907 eV. Near the resonance peaks BOXLIB has a considerably higher density of points than the GAR file.

In the thermal range (10^{-5} eV < E < 1.3 eV) infinite dilute cross sections are collapsed into groups for a number of temperatures dependent on the specific isotope. The thermal scattering matrices for most nuclides are calculated by the free gas model. For the moderator nuclides and especially for hydrogen in water the $S(\alpha,\beta)$ matrices given in JEF-1 are used.

3 SPECTRUM CELL CODES

All calculations were performed using BOXER, WIMS-D, and the AARE (cell) codes TRAMIX and MICROX-2 in connection with the one-dimensional transport programme ONEDANT. In the following section a detailed description of these code (systems) is given.

3.1 BOXER

BOXER is a part of ELCOS [28]. It includes modules for cell, two-dimensional, and burn-up calculations. BOXER is an extensive code system developed at PSI for calculations of light water reactor configurations. For the purpose of the following investigations, the cell code in BOXER is described here in more detail.

In the resonance range between 1.3 and 907 eV the flux is computed in 4000 to 5000 lethargy points using a collision probability method [31]. For this calculation the geometry of the cell is simplified to two zones (resonance or fuel zone and moderator smeared with gap and clad). The lists of energy points for different nuclides are combined as follows: All the points of the resonance nuclide with the highest density are considered. Points from the lists for the other resonance nuclides are inserted where they are necessary to represent the total macroscopic cross sections accurately. The collision probabilities are calculated with the approximation of spatially flat and isotropic source per zone. The slowing down source is determined with the assumption that the scattering is isotropic in the center of mass system. The energy independent Dancoff factor calculated for the cylindrical cell is corrected by a fit to the exact values determined by a Monte Carlo method for square lattices [3] and an elaborate numerical integration for hexagonal cells [32]. The pointwise flux in the resonance zone is then used as the weighting function for collapsing the resonance cross sections into groups. By this method the overlap between the resonances of a particular nuclide as well as of different nuclides is explicitly taken into account.

The resonance cross sections in the fast energy range above 907 eV (both resolved and unresolved resonances) are interpolated as a function of temperature and dilution cross section using a Bondarenko like formalism similar to that in TRAMIX. The effect of the self-shielding of the resonance cross sections on the dilution cross sections for the other resonance nuclides is taken into account by an approximate interpolation scheme. The interpolation versus dilution cross section and temperature is performed by formulas which were fitted to tables of calculated self-shielded cross sections for 21 dilutions and 6 temperatures. The formulas reproduce the calculated values with an accuracy better than 1% for dilution cross sections greater than 5 barns.

The fluxes in 70 groups and in each zone are calculated by means of an integral transport method [33]. The fission source is assumed to be flat over all zones containing fissile nuclides. The scattering source in each zone can be flat or represented by a polynomial of the radius. The fission spectrum for the cell is a linear combination of the fission spectra of the individual fissile nuclides weighted by the product of density, $\nu\sigma_f$, and the BOXLIB weighting spectrum. In the epithermal range (above 1.3 eV) P_1 corrected isotropic scattering is used. In the thermal range P_1 anisotropy (P_2 corrected) can be taken into account. In the whole energy range the "inflow" transport correction is used. The cells are calculated with white boundary conditions or with the outgoing partial current from a previously calculated cell as a fixed source at the periphery.

For the leakage calculation the macroscopic cross sections in 70 groups are homogenized over the cell using flux-volume weighting, and modified by a rehomogenization procedure [34]. The leakage is determined by a zero-dimensional B_1 transport calculation [35]. The buckling can be given in the input or the critical buckling can be searched for.

3.2 WIMS-D

WIMS-D is a comprehensive standard code for reactor lattice cell calculations including burn-up calculations in a wide variety of reactor types [5]. WIMS-D is a complex code primarily intended for the calculation of moderated systems. The geometry can be either fuel rods or plates, in regular arrays or clusters. WIMS-D contains tabulations of temperature dependent resonance integrals accurately evaluated for homogeneous mixtures of moderator and absorber at many energy points. Equivalence theorems are utilized to obtain few-group effective cross sections in heterogeneous problems. The Goldstein-Cohen treatment based on the intermediate resonance absorption shielding method of resolved resonances (IR method) using fixed IR-parameters is employed. Self-shielding of resonance

cross sections is performed in the energy range between 9 keV and 4 eV. Outside of this energy range all cross sections are taken at infinite dilution, which is suitable for well thermalized system analysis. More precisely the resonance treatment is based on equivalence theorems which are similar for infinite lattices of rods or bundles of plates. These theorems relate in each case the heterogeneous problem to an equivalent homogeneous problem by means of a suitable rational approximation for the fuel self-collision probability. They take account of a first order correction for the interaction between resonances of several isotopes. In WIMS-D the resonance groups have been chosen so as to provide uniform distribution of resonances in lethargy and in cases of a single resonance in a group it is placed near the lethargy centre of the group. Therefore it is assumed that the disadvantage factors outside resonances are energy independent and may be set equal to unity.

The main feature of WIMS-D consists in calculating a detailed flux spectrum in all 69 library groups in each of the principal regions of the lattice: fuel, can, coolant and in clusters also bulk moderator, these regions being coupled through collision probabilities, then condensing the groups to obtain few-group constants, solving the few-group transport equation in fine spatial mesh, modifying the solution to take leakage into account, and then again expanding the resulting fluxes at all mesh points to the original 69 groups, assuming that the subdivision of flux within a transport group at a given mesh point is such as that calculated before for the corresponding region, to obtain region and point reaction rates for chosen nuclides. The transport equation can be solved either in an integral form (collision probabilities) or in a differential form (discrete-ordinates method). Hereby a global library fission spectrum is utilized. First order anisotropy of scattering is taken into account. Leakage can be calculated either by the B_1-method or the diffusion theory method. In the latter case the effect of cell heterogeneity can be accounted for either by simple flux and volume weighting of transport cross sections or, in cylindrical geometry only, by Benoist's theory of directed diffusion coefficients with or without correlation terms.

3.3 AARE

AARE, a PSI update of the DANDE [7] (applied nuclear DAta, core Neutronics DEpletion) system from Los Alamos, is a new flexible code package which allows applications to a broad class of reactor types. It includes the one-dimensional discrete-ordinates transport code ONEDANT and the two-dimensional discrete-ordinates transport code TWODANT, as well as burn-up and sensitivity codes. AARE has been extensively tested and benchmarked with respect to the analysis of fusion, fast reactors, light water high converter reactors, as well as high temperature reactors.

ONEDANT is a modular computer program designed to solve the one-dimensional, time-independent, multigroup discrete-ordinates form of the Boltzmann transport equations. The modular construction of the code package separates the input processing, the transport equation solving, and the post-processing, or edit, functions into distinct, independently executable code modules, connected to one another solely by means of binary interface files.

TWODANT is the analogous to ONEDANT in two dimensions.

In AARE, ONEDANT and TWODANT are used in connection with the interface coupling programmes TRAMIX and MICROX-2, and with the B_N module SOLVERB for leakage calculations. These codes, which are linked together with special data files in CCCC format [23], are described in the next two subsections.

3.3.1 TRAMIX and SOLVERB

TRAMIX is a flexible computer (cell) code that reads nuclear data from a library in MATXS format (in any group structure) and produces groupwise cross-sections which can be read into most transport codes (particularly into ONEDANT and TWODANT). Any order of scattering approximation (smaller than or equal to the maximum available on the MATXS library) can be chosen. Nuclear data can be produced for neutron, photon, or coupled transport. Options include adjoint tables, mixtures, self-shielding based alternatively on the Bondarenko formalism or on the IR method by considering Dancoff corrections for different geometric models, group collapse, homogenization, thermal upscatter, prompt or steady-state fission, transport corrections, elastic removal corrections, and flexible response-function edits. In contrast to the other codes presented in this section, TRAMIX has a very general and efficient fission spectrum capability. Using an iterative procedure, it is able to generate problem dependent zone fission spectra. Moreover the self-shielding procedure is applied to the whole energy range, which includes thermal resolved resonances of heavy actinides, unresolved resonances of main actinides and high energy resolved resonances of structural materials. The λ factors needed in the IR method are calculated for each isotope as a function of the neutron energy in terms of an approximative reconstruction of cold resonances on the basis of Bright-Wigner formulas [8].

SOLVERB [6] was developed for leakage cell calculations based on the B_N method. Alternatively the diffusion approach can be considered, particularly when the P_1 scattering matrices are not available on the cross section library. This code includes an automatic procedure for determining buckling factors (B^2) and eigenvalues (k_{eff} and k_∞), homogenizes the cell using cell fluxes and currents, and utilizes the Behrens-Lohnert method to account for the streaming effects when calculating the migration area.

3.3.2 MICROX-2

MICROX-2 is an integral transport theory spectrum code which solves the neutron slowing down and thermalization equations on a detailed energy grid for a two region lattice cell. MICROX-2 was developed for the efficient and rigorous preparation of broad group neutron cross sections for poorly moderated systems such as fast breeder reactors in addition to the well moderated thermal reactors such as high temperature reactors as well as LWRs. Additionally to the cross sections, cell eigenvalues (k_{eff} and k_∞) and reaction rates in any group structure are delivered. The fluxes in the two regions are coupled by transport corrected collision probabilities for the generation of the region-wise transfer probabilities in the fast- and resonance-energy ranges. The computation of these collision probabilities is based upon the spatially flat neutron emission approximation and the transport (modified P_0) approximation of anisotropic scattering effects, simulated through the use of the transport mean free path instead of the total mean free path. The collision probability calculation also utilizes an energy dependent Dancoff correction factor algorithm, and is performed on an ultra-fine energy grid using GAR data including temperature dependent Doppler-broadened resonance cross-sections at 15000 energy mesh points (selected with the criteria of constant lethargy or velocity spacing) between 8 keV and 0.414 eV for each nuclide. Thus, the model of resonance treatment is similar to that of BOXER, except of the different distribution of energy points. A second level of heterogeneity can be treated, i.e. the inner region may include two different types of grains (particles). MICROX-2 accounts explicitely for overlap and interference effects between different resonance levels in both the resonance and thermal energy range, and allows for the simultaneous treatment of leakage and resonance self-shielding in doubly heterogeneous lattice cells. With the help of GAR data the lowest energetic part of the unresolved range can be shielded. Additionally, a linear Bondarenko-interpolation between sets of temperature- and dilution-dependent FDTAPE fine group data prepared by the NJOY

module MICROR (approximative self-shielding of fast range, including the fast part of the unresolved range) can be requested above a flexible value (less than 8 keV) which determines the upper energy boundary for the pointwise resonance calculation. The interpolation scheme used is less sophisticated than in BOXER. Up to P_3 in the fast energy range, and P_1 order of scattering in the thermal range are considered. Neutron leakage effects are treated by performing fine group and hyperfine point B_1 slowing down (fast and resonance-energy ranges), or P_0 plus DB^2 thermalization (thermal range) calculations in each region. Energy-dependent bucklings (positive, zero, or negative) are supplied as input. A buckling search as a solution of the collapsed (with the fine flux) two group (a fast and a thermal group with thermal cut off at 2.38 eV) B_1 equations can be turned on. The treatment of leakage is essentially similar as in WIMS-D. For the preparation of adequate groupwise cross sections the activation of the buckling search may be important in the case of systems characterized by a strongly space dependent spectrum (see Section 6). Zone fission spectra may be constructed as linear combinations of fission spectra for various fissionable actinides available on the FDTAPE. The detailed neutron flux and current spectra are used for collapsing the basic neutron cross sections into cell-averaged and region-averaged broad-group cross sections and scattering transfer arrays (up to P_1). The present algorithm allows the maximum number of fast broad groups to be equal to the number of groups available on the FDTAPE (i.e. 92 in the case of our library), and the maximum number of thermal broad groups to be equal to one third of the number of points available on the thermal part of the GGTAPE, this because of the trapezoidal rule used in the broad group cross section preparation (i.e. 33 in the case of our libraries). Broad group P_2 and P_3 scattering transfer arrays may be determined with P_2 and P_3 weighting spectra obtained from an extended transport approximation. The broad group cross sections produced by MICROX-2 may be used either in diffusion- or transport-theory codes, and especially in the AARE system (ONEDANT and TWODANT) via an XSLIB output format, one of the simplest Los Alamos card image formats [36].

4 COMPUTATIONAL MODEL

In order to make a quick but valid code comparison the same physical model as defined in a previous study at PSI [1] was considered, in which the reactor assembly was reduced to the basic cell of its interior lattice (first option in the ENDF-202 Benchmark specification book [13]). The resulting cell consists of four zones, i.e. fuel, vacuum gap, clad, and moderator (vacuum gap and clad are smeared in the case of WIMS-D and BOXER calculations).

A cell calculation (with white outer boundary conditions to simulate an infinite lattice) for the central lattice of each of the TRX and BAPL experiments was performed, followed by a homogenized-cell leakage calculation. In the leakage calculation either a measured energy independent buckling is given in the case of one-region lattices (TRX-1, TRX-2, BAPL-1, BAPL-2, BAPL-3), or the critical buckling is searched for in the case of two-region lattices (TRX-3, TRX-4), assuming that the (unknown) multiplication factor k_{eff} is a priori equal to 1 [1].

Although this model simulates only approximatively the whole reactor (complex three dimensional geometry including reflector, spacer sheets and top lattice plates is approximated with a 0-dimensional model), it is able to give a very accurate prediction of various parameters including eigenvalues and reaction rate ratios. This is because the reactor center is almost not disturbed by the outer zones, and the interior lattice is large compared to the whole reactor (see next section).

Through the whole paper ϱ^{28} denotes the ratio of epithermal-to-thermal ^{238}U captures, δ^{25} the ratio

of epithermal-to-thermal ^{235}U fissions, with a thermal cut off of 0.625 eV, δ^{28} the ratio of ^{238}U fissions to ^{235}U fissions, C^* the ratio of ^{238}U captures to ^{235}U fissions, and k_∞ the infinite multiplication factor, each of these parameters taken at the reactor center. k_{eff} refers to the global multiplication factor of the whole reactor, and M^2 to the migration area of the cell, the ratio between cell averaged one group diffusion coefficient and absorption cross section, a quantity related to the total number of neutrons leaking out of the cell.

For the sake of completeness and for a better understanding and judgement of the results presented in the next section the experimental results for k_{eff}, ϱ^{28}, δ^{25}, δ^{28} and C^* (E), and their relative errors in percent (ΔE) are given in Table 1 for each of the experiments [13]. The relative errors in k_{eff} were derived from those in the bucklings (except TRX-3 and TRX-4) [1]. Particularly it has been already pointed out that these errors are always small compared to the calculation error [1].

Experiment	TRX-1		TRX-2		TRX-3		TRX-4	
Values	E	ΔE	E	ΔE	E	ΔE	E	ΔE
k_{eff}	1.000	±0.26	1.000	±0.091	/	/	/	/
ϱ^{28}	1.320	±1.6	0.837	±1.0	3.03	±1.7	0.481	±2.3
δ^{25}	0.0987	±1.0	0.0614	±1.3	0.231	±1.3	0.0358	±1.4
δ^{28}	0.0946	±4.3	0.0693	±5.1	0.167	±4.8	0.0482	±4.1
C^*	0.797	±1.0	0.647	±0.9	1.255	±0.9	0.531	±0.8

Experiment	BAPL-1		BAPL-2		BAPL-3	
Values	E	ΔE	E	ΔE	E	ΔE
k_{eff}	1.000	±0.06	1.000	±0.06	1.000	±0.04
ϱ^{28}	1.39	±0.7	1.12	±0.9	0.906	±1.1
δ^{25}	0.084	±2.4	0.068	±1.5	0.052	±1.9
δ^{28}	0.078	±5.1	0.070	±5.7	0.057	±5.3

Table 1: Reaction rate ratios (E), and measurement relative errors in % (ΔE) for TRX and BAPL experiments

BOXER, TRAMIX and MICROX-2 were systematically employed for the preparation of self-shielded broad group cross sections from the basic libraries described in previous section, to be used further in the AARE system (as far as spectrum and leakage calculations are concerned), whereas WIMS-D was utilized for both the multigroup cross section preparation (self-shielding of resonances), the spectrum, and the leakage calculation. Doing in this way a code system comparison seems to be worthwhile. WIMS-D may as well be used as a standalone code for the preparation of adequate multigroup cell and region averaged cross sections to be used in the AARE system. However, the results from the entire WIMS-D calculations presented in this study were found to match very well those obtained with AARE (ONEDANT and SOLVERB) and WIMS-D cross sections, if the transport model (i.e. number of meshes, order of anisotropy, and so on) is the same.

A detailed description of the computational model follows. First, an explanation of the methodology of the preparation of self-shielded multigroup cross sections is given for each code system. Second, the way is shown how the spectrum and leakage calculations are performed in AARE.

In BOXER the cell was modelled by three zones, i.e. fuel, clad smeared with gap, and moderator. The hexagonal shape of the cell was taken into account for the calculation of the Dancoff factor. In addition, the calculated Dancoff factor was multiplied by an input factor less than, but close to unity to take into account the reduced number of neighbours for the peripheral fuel rods. The resonance cross sections were self-shielded by a flux calculation in approximately 4250 points between 907 eV and 1.3 eV and by a Bondarenko type interpolation above 907 eV. P_1 macroscopic 70 neutron group self-shielded cross sections for each zone as well as microscopic capture and fission cross sections (for the computation of the reaction rate ratios) and the BOXER fission spectrum for the cell were output to be further used in AARE. Hereby a management module was written at PSI for converting BOXER cross sections into XSLIB format.

For two region MICROX-2 calculations, gap, aluminum cladding and moderator had to be smeared into one homogenized zone, and calculations were carried out using zone-averaged atomic densities (two zone model). For each experiment, the required input Dancoff factor and the reference (almost constant) moderator cross section (taken in the resonance range of the fuel) were determined by performing a WIMS-D resonance calculation in three zones (fuel, homogenized vacuum gap and clad, and moderator) for an infinite hexagonal lattice, using the WIMSJEF library. The (alternative) use of a tabulation (maximum 19 points) of appropriate Dancoff factor and moderator cross section input pairs from WIMS-D (aimed to a more accurate interpolation of the energy dependent Dancoff factor) did not significantly change the results presented in this report. We checked the Dancoff factors obtained using this method against Carlvik tables [32]. To this end the Dancoff factor was recalculated accurately using a cubic interpolation in two variables (i.e. the moderator to fuel ratio and the moderator cross section) for a hexagonal lattice, and the reference moderator cross section was estimated with TRAMIX and MAT70. These two values could be reproduced well within less than 1% by performing a WIMS-D resonance calculation with the two zone model. However, the Dancoff factor used in this study (i.e that obtained using WIMS-D and the three zone approach) was found to be about maximum 5% higher for the same moderator cross section, which agrees with previous studies [3]. The use of the two-zone Dancoff factor would result in about maximum 0.2% decrease of MICROX-2 eigenvalues in the case of one-region lattice calculations (i.e. for TRX-1, TRX-2, and BAPL experiments).

The library fission spectrum pertaining to ^{235}U in an infinite moderator was employed, which is suitable for LWR calculations. The upper energy boundary for the pointwise resonance calculation on the basis of the GAR file was set at 4 keV. This is reasonable, since all important resolved resonances of ^{238}U being lower than 4 keV are accounted for in the pointwise slowing down calculation. Doing in this way the unresolved range of ^{235}U (between 80 eV and 4 keV) is not shielded. However, this results in a negligible error, due to the fact that the neutron spectrum of the TRX and BAPL reactors is soft and that the ^{235}U cross sections are almost infinite dilute. Above 4 keV cross sections of uranium isotopes were shielded using a Bondarenko like linear interpolation. This guarantees the shielding of the unresolved range of ^{238}U and the upper part of that of ^{235}U, but is found not to be important for these experiments. The input buckling was set to zero.

Self-shielded cell and region (fuel and moderator, the last consisting of smeared aluminum clad and water) averaged materialwise microscopic cross sections in a very detailed 113 neutron group structure (consisting of 92 fast groups, the maximum number allowed, and 21 collapsed broad thermal groups with constant lethargy spacing) were delivered in XSLIB format for use in the AARE system. Within this processing a small approximation was introduced in the spatial collapsing of moderator cross sections, since the same spectrum had to be considered for collapsing both the clad and the water thermal cross sections. However, the use of a larger number of thermal broad groups (i.e. 33, the

maximum number allowed), which diminishes the effect of the weighting spectrum, did not influence the results discussed in the next section.

As far as TRAMIX is concerned, this code reads in MATXS formatted cross sections (from MAT70 or MAT193 in our specific case), computes group dependent Dancoff factors for hexagonal lattices using the Sauer-Bonalumi formula (which is in most cases an accurate approximation [8]), shields data in the whole energy range (including cladding and moderator, this feature is found not to be important for LWR calculations) using the IR method by computing the λ factors, and produces directly group-ordered GOXS formatted macroscopic zone cross sections (in the terminology of the CCCC files [23]). Either the weighting function on the MATXS library or a more suitable spectrum in the CCCC format RMFLUX are used for collapsing the fission matrices on the MATXS file to generate a problem oriented space dependent fission spectrum. In addition, if the correct flux is known from a previous transport calculation, the original library removal cross section may be corrected (elastic removal correction [8,9]) to account for differences between this flux and the library flux. This correction is helpful especially when the basic library has a coarse group structure, or, of course, when the correct flux differs considerably from the library flux. As shown in a previous study, the use of the elastic removal correction is able to improve the accuracy of the calculated void coefficient in the case of intermediate spectra [25].

For spectrum calculations, XSLIB formatted cross sections from BOXER and MICROX-2 are converted into the more compact GOXS format using ONEDANT (the Solver module in Block V is turned off [36]). Transport cross sections and zone fission spectra belonging to XSLIB are added into the GOXS library by means of an internal management module written at PSI.

In any case (the cross sections may come from BOXER, MICROX-2, or TRAMIX) a cell calculation for the central lattice of each of the TRX and BAPL experiments is performed using ONEDANT, the GOXS data file, and white outer boundary conditions to simulate an infinite lattice.

SOLVERB is applied to solve the B_1 integral leakage equations using the flux solution from ONEDANT (in the RMFLUX format), the geometry- and material-related specifications (GEODST, NDXSRF, and ZNATDN CCCC files) and the GOXS cross section library. Either the spectrum with input buckling (in the case of TRX-1, TRX-2, BAPL-1, BAPL-2 and BAPL-3) or the fundamental mode spectrum (in the case of TRX-3 and TRX-4) are determined iteratively (the "inflow" transport correction is computed until convergence in the transport cross section is achieved), and one-group collapsed cross sections, eigenvalues, total and group dependent migration areas are delivered. Flux files are renormalised with respect to the B_1 spectrum.

Last, ONEDANT is utilized (in connection with some internal management modules written at PSI in the case of GOXS cross sections coming from BOXER) to determine all required reaction rate ratios. In this calculation, two CCCC files are used, i.e. the regular total flux by interval (RTFLUX) from SOLVERB, and the SNXEDT formatted edit cross section library originated in the previous ONEDANT transport calculation.

If TRAMIX generates the GOXS library, this procedure is looped to determine a problem oriented space dependent fission spectrum and to correct the removal cross section using the accurate B_1 spectrum from SOLVERB.

In WIMS-D, the hexagonal geometry was accounted for in the resonance calculation (a special

card "REGULAR 1,6" had to be added to the input stream), and leakage calculations were performed solving the B_1 equations (iteratively in the case of a buckling search for TRX-3 and TRX-4) on the basis of the two library moderator isotopes (i.e. hydrogen and oxygen) with P_1 scatterring matrices. The use of special options for computing diffusion coefficients such as Benoist or Ariadne proccdures (streaming corrections) did not affect the results presented in this report. All needed capture rates were calculated as the difference between absorption and fission, increased by (n,2n). Since WIMS-D does not compute explicitely the (n,2n) rates, these (small in magnitude) were taken over from the TRAMIX calculations with MAT70, which is a reasonable compromise, since the group structure and the data basis are the same.

In each referenced infinite lattice transport calculation (with ONEDANT or WIMS-D) the cell was subdivided into 20 meshes (15 of them in the fuel). Increasing the number of meshes did not affect the results presented in the next section. All computations were performed using either " inflow" transport corrected P_0 cross sections (WIMS-D), or (uncorrected) P_1 cross sections (TRAMIX and MICROX-2), or P_1 "inflow" transport corrected cross sections (BOXER), and S_4 approximation.

More precisely, in the whole report, results from AARE spectrum calculations with ONEDANT are alternatively referred to BOXER, TRAMIX, or MICROX-2 when the multigroup cross section library GOXS (used latter in ONEDANT and SOLVERB) is originally from BOXER, TRAMIX, or from MICROX-2 respectively.

5 RESULTS AND DISCUSSION

5.1 Results

In Tables 2, 3, 4, and 5 calculated (C) eigenvalues (k_{eff}, except for TRX-3 and TRX-4, and k_∞), reaction rate ratios (ϱ^{28}, δ^{25}, δ^{28}, C^*), and migration areas (M^2), as well as calculated/experimental (C/E) ratios for eigenvalues (k_{eff}, except for TRX-3 and TRX-4) and reaction rate ratios (ϱ^{28}, δ^{25}, δ^{28}, and C^* except for the BAPL experiments where no measurement was reported) are summarized for calculations performed using WIMS-D, BOXER, TRAMIX, and MICROX-2 with the related JEF-1 based data libraries. In Table 6 already published values [4] are reported for the sake of comparison. Briefly, the methodology used in those calculations (which is similar to that presented in the previous sections) based on NJOY for the preparation of JEF-1 multigroup cross sections. A very detailed calculation (in up to about 9000 energy subgroups, in terms of the narrow resonance approximation) of spectral weighted group-constants, critical parameters, and lattice cell reaction rate ratios has been performed using the IKE-RSYST/CGM program system. Then, the effective multiplication factor k_{eff} and the required reaction rate ratios of the different experiments have been calculated using the one-dimensional discrete-ordinates transport code ANISN with a 30 to 60 group collapsed library, and the B_N theory was employed for leakage calculations [4].

Experiment	TRX-1		TRX-2		TRX-3		TRX-4	
Values	C	C/E	C	C/E	C	C/E	C	C/E
k_∞	1.1788	/	1.1635	/	1.0691	/	1.0191	/
k_{eff}	0.9950	0.995	0.9951	0.995	1.	1.	1.	1.
ϱ^{28}	1.3623	1.032	0.8530	1.019	3.0357	1.002	0.4959	1.031
δ^{25}	0.0974	0.987	0.0597	0.972	0.2342	1.014	0.0345	0.964
δ^{28}	0.0995	1.051	0.0705	1.018	0.1746	1.045	0.0497	1.031
C^*	0.8017	1.006	0.6499	1.004	1.2484	0.995	0.5292	0.999
M^2 (cm^2)	32.4	/	30.9	/	36.9	/	30.2	/

Experiment	BAPL-1		BAPL-2		BAPL-3	
Values	C	C/E	C	C/E	C	C/E
k_∞	1.1398	/	1.1422	/	1.1311	/
k_{eff}	0.9989	0.999	0.9991	0.999	0.9997	1.000
ϱ^{28}	1.4284	1.028	1.1889	1.062	0.9308	1.027
δ^{25}	0.0820	0.976	0.0669	0.983	0.0514	0.989
δ^{28}	0.0773	0.991	0.0665	0.950	0.0545	0.956
C^*	0.8190	/	0.7453	/	0.6645	/
M^2 (cm^2)	43.3	/	40.4	/	38.4	/

Table 2: Calculated (C) and calculated/experimental (C/E) eigenvalues, reaction rate ratios, and calculated migration areas (M^2) from cell calculations of TRX and BAPL experiments performed using WIMS-D and the WIMSJEF data library

Experiment	TRX-1		TRX-2		TRX-3		TRX-4	
Values	C	C/E	C	C/E	C	C/E	C	C/E
k_∞	1.1821	/	1.1672	/	1.0689	/	1.0232	/
k_{eff}	0.9983	0.998	0.9989	0.999	1.	1.	1.	1.
ϱ^{28}	1.3501	1.023	0.8396	1.003	3.0751	1.015	0.4853	1.009
δ^{25}	0.1001	1.014	0.0613	0.999	0.2400	1.039	0.0354	0.988
δ^{28}	0.0994	1.051	0.0703	1.015	0.1759	1.053	0.0495	1.026
C^*	0.7982	1.002	0.6426	0.993	1.2550	1.000	0.5288	0.996
M^2 (cm^2)	32.3	/	30.8	/	36.8	/	30.2	/

Experiment	BAPL-1		BAPL-2		BAPL-3	
Values	C	C/E	C	C/E	C	C/E
k_∞	1.1461	/	1.1504	/	1.1367	/
k_{eff}	1.0047	1.005	1.0049	1.005	1.0052	1.005
ϱ^{28}	1.3987	1.006	1.1597	1.035	0.9066	1.001
δ^{25}	0.0844	1.004	0.0667	0.995	0.0527	1.014
δ^{28}	0.0776	0.995	0.0666	0.952	0.0545	0.956
C^*	0.8090	/	0.7364	/	0.6574	/
M^2 (cm^2)	43.2	/	40.8	/	38.2	/

Table 3: Calculated (C) and calculated/experimental (C/E) eigenvalues, reaction rate ratios, and calculated migration areas (M^2) from cell calculations of TRX and BAPL experiments performed using BOXER and the BOXLIB data library

Experiment	TRX-1		TRX-2		TRX-3		TRX-4	
Values	C	C/E	C	C/E	C	C/E	C	C/E
k_∞	1.1737	/	1.1609	/	1.0584	/	1.0202	/
k_{eff}	0.9935	0.994	0.9956	0.996	1.	1.	1.	1.
ϱ^{28}	1.3804	1.046	0.8630	1.031	3.1057	1.025	0.4998	1.039
δ^{25}	0.0999	1.012	0.0612	0.997	0.2395	1.037	0.0353	0.985
δ^{28}	0.0959	1.014	0.0680	0.981	0.1692	1.013	0.0480	0.996
C^*	0.8077	1.013	0.6497	1.009	1.2653	1.008	0.5329	1.004
M^2 (cm^2)	31.8	/	30.4	/	36.2	/	30.0	/

Experiment	BAPL-1		BAPL-2		BAPL-3	
Values	C	C/E	C	C/E	C	C/E
k_∞	1.1372	/	1.1424	/	1.1296	/
k_{eff}	0.9991	0.999	1.0000	1.000	1.0008	1.001
ϱ^{28}	1.4378	1.034	1.1952	1.067	0.9368	1.034
δ^{25}	0.0841	1.001	0.0685	1.007	0.0526	1.011
δ^{28}	0.0746	0.957	0.0641	0.916	0.0525	0.922
C^*	0.8210	/	0.7472	/	0.6664	/
M^2 (cm^2)	42.4	/	40.2	/	37.6	/

Table 4: Calculated (C) and calculated/experimental (C/E) eigenvalues, reaction rate ratios, and calculated migration areas (M^2) from cell calculations of TRX and BAPL experiments performed using TRAMIX and the MAT70 data library

Experiment	TRX-1		TRX-2		TRX-3		TRX-4	
Values	C	C/E	C	C/E	C	C/E	C	C/E
k_∞	1.1755	/	1.1633	/	1.0552	/	1.0239	/
k_{eff}	0.9920	0.992	0.9946	0.995	1.	1.	1.	1.
ϱ^{28}	1.3956	1.057	0.8743	1.045	3.1935	1.054	0.5071	1.054
δ^{25}	0.1016	1.029	0.0621	1.012	0.2435	1.054	0.0357	0.998
δ^{28}	0.0987	1.044	0.0698	1.008	0.1728	1.035	0.0491	1.018
C^*	0.8110	1.018	0.6525	0.995	1.2873	1.026	0.5347	1.015
M^2 (cm^2)	32.5	/	31.0	/	36.4	/	30.2	/

Experiment	BAPL-1		BAPL-2		BAPL-3	
Values	C	C/E	C	C/E	C	C/E
k_∞	1.1365	/	1.1423	/	1.1307	/
k_{eff}	0.9942	0.994	0.9953	0.995	0.9974	0.997
ϱ^{28}	1.4627	1.052	1.2149	1.085	0.9517	1.050
δ^{25}	0.0857	1.020	0.0698	1.027	0.0535	1.029
δ^{28}	0.0770	0.987	0.0662	0.946	0.0541	0.950
C^*	0.8276	/	0.7524	/	0.6705	/
M^2 (cm^2)	43.9	/	41.7	/	39.1	/

Table 5: Calculated (C) and calculated/experimental (C/E) eigenvalues, reaction rate ratios, and calculated migration areas (M^2) from cell calculations of TRX and BAPL experiments performed using MICROX-2 and the GARTAPE, FDTAPE and GGTAPE data libraries

Experiment	TRX-1		TRX-2		TRX-3		TRX-4	
Values	C	C/E	C	C/E	C	C/E	C	C/E
k_{eff}	0.9960	0.996	0.9973	0.997	1.0010	1.001	0.9979	0.998
ϱ^{28}	1.3569	1.028	0.8374	1.000	3.013	1.006	0.476	0.990
δ^{25}	0.0992	1.005	0.0608	0.990	0.236	1.022	0.0344	0.961
δ^{28}	0.1001	1.058	0.0714	1.030	0.1725	1.033	0.0473	0.981
C^*	0.7984	1.002	0.6393	0.988	1.2402	0.988	0.5244	0.988

Experiment	BAPL-1		BAPL-2		BAPL-3	
Values	C	C/E	C	C/E	C	C/E
k_{eff}	1.0001	1.000	0.9999	1.000	0.9988	0.999
ϱ^{28}	1.4196	1.022	1.1771	1.051	0.9201	1.016
δ^{25}	0.0841	1.000	0.0685	1.007	0.0526	1.012
δ^{28}	0.0775	0.994	0.0668	0.954	0.0549	0.963
C^*	0.8130	/	0.7393	/	0.6591	/

Table 6: Previously published calculated (C) and calculated/experimental (C/E) eigenvalues and reaction rate ratios from reactor calculations of TRX and BAPL experiments performed using RSYST/CGM and JEF-1 data in 30 to 60 groups

From these tables following considerations are deduced.

Eigenvalues k_{eff} are well predicted within less than 6 mk by all code systems (except TRX-1 in the case of TRAMIX and MICROX-2, in which the discrepancy is of the order of 7 mk and 8 mk respectively). For TRX-1, the calculation of ϱ^{28} overpredicts the experimental value, so that k_{eff} for TRX-1 is not so accurate as for TRX-2. For each experiment, the eigenvalues k_{eff} from BOXER are up to 10 mk (1 mk = 0.001) larger than those from MICROX-2, whereas WIMS-D and TRAMIX are close within 1.5 mk and lie inbetween. As far as consistency is concerned the computed eigenvalues k_{eff} of the BAPL experiments are systematically higher (by a maximum of 7 mk in the case of TRX-1 in connection with BOXER) than those of TRX. This is consistent with previous studies [1], [4] (see as well Table 6), where similar analyses of the same experiments were made. The computed k_{eff} increases smoothly with increasing moderator to fuel ratio, if the same code system is used. The magnitude of the increase is code dependent. Particularly, the multiplication factor k_{eff} of TRX-2 is slightly larger than that of TRX-1. The same trend (except for the RSYST calculations) can be observed in the BAPL experiments.

Migration areas for each of the cells agree well in all code systems within 4% or less (4% discrepancy arises between TRAMIX and MICROX-2 in the case of BAPL-3). A good agreement in migration areas may be expected due to the similar treatment of leakage in all code systems.

As far as the single reaction rate ratios are concerned, these are mostly predicted well either within or not too far from the experimental uncertainty (compare with Table 1). The results tend to reproduce previously published values (compare with Table 6, and with [1], [4]).

More specifically, the computed ϱ^{28} is systematically either within the experimental error (in the upper part of the experimental uncertainty), or too high (by up to 6σ in MICROX-2 in BAPL-1, compare with Table 1). We may speculate that the general and large code independent overprediction of ϱ^{28} in BAPL-2 (by up to 9σ in MICROX-2) is due to an underestimate of the experimental error. Similar trends were already observed in previous work (see [1], and Table 6).

Globally, the computed δ^{25} reproduces well the measurement, except for TRX-3, where all code systems overpredict it (by up to 3σ in MICROX-2, compare with Table 1). This is consistent with previous studies [1] and with Table 6. δ^{25} decreases smoothly in all methods with increasing moderator to fuel ratio in the case of TRX experiments.

The computed δ^{28} is generally predicted well within the experimental uncertainty. Except TRAMIX, the TRX-1 values are slightly overestimated (by up to 1σ in the RSYST calculations). δ^{28} is underestimated in TRAMIX by up to 1.5σ in BAPL-2 and BAPL-3.

C^* is computed accurately by most code systems, of course in the case of TRX experiments (see Table 1).

Globally it is found that the prediction of experimental values on the basis of JEF-1 is at least as accurate as with ENDF/B-V, which confirms previous studies [4].

5.2 Parameter study

In the following analysis we study the influence of various modifications to the computational model presented in the last section (including a full two lattice reactor model for TRX-3 and TRX-4) on the results displayed in Tables 2, 3, 4, and 5. Main conclusions from these investigations are that

all presented results are representative enough for those from more sophisticated models. Individual effects tend to compensate each other.

5.2.1 Different zone approach

The results are found to be almost independent on the number of zones considered (of at least 2) when processing the multigroup self-shielded cross section GOXS library and when performing the infinite lattice transport calculation with ONEDANT. This was shown by a set of TRAMIX calculations with smeared gap, aluminum clad, and moderator cross sections, or with smeared gap and clad, or with smeared clad and moderator respectively. This proves the reliability of the BOXER (and WIMS-D) and MICROX-2 three and two zones models.

5.2.2 Alternative treatment of leakage

The alternative use of the diffusion approach in the leakage calculation leads to an increase of the computed k_{eff} of about 2 mk and to a corresponding decrease of ϱ^{28} of about 0.5% in both the TRX and BAPL experiments. All other reaction rate ratios and the migration area M^2 remain almost unchanged.

5.2.3 Use of a finer group structure in TRAMIX

The use of MAT193 instead of MAT70 in the TRAMIX calculations results in about 2 mk decrease of k_{eff}, in about 0.5% increase of ϱ^{28}, all other reaction rate ratios and M^2 remaining almost unchanged. Therefore, the results from TRAMIX tend to reproduce those from MICROX-2, if the same group structure is used (compare Table 3 with Table 4).

5.2.4 Use of a more detailed cell model

For the calculation of each experiment (except TRX-4), the combined use of transport corrections in TRAMIX (or in MICROX-2) (consistent P_1 in the case of TRAMIX, inflow in the case of MICROX-2), of higher degree of scattering approximation (up to P_3 in MICROX-2, and in TRAMIX in connection with MAT193), of higher order of angular approximation in ONEDANT (up to S_{16}), resulted in a maximum change of k_{eff} of 2 mk and in a corresponding change of about 0.5% of ϱ^{28}, when defining the same consistent meshing. The migration area varied within a range of about 1%, and all other reaction rate ratios remained almost unchanged. In the case of TRX-4 the change of k_∞ was found to be larger (increase of about 5 mk), due to the high flux disadvantage factors between fuel and moderator coming from the huge moderator to fuel volume ratio (about 9). However, the reaction rate ratios varied in a similar way as in the remaining experiments, due to compensating effects in the buckling search.

5.2.5 Use of problem oriented fission spectrum and elastic removal correction in TRAMIX

In the TRAMIX calculations of each experiment, if the MAT70 library weighting function is used for generating the fission spectrum, and if no elastic correction is applied to the library removal cross section, the computed k_{eff} increases slightly by about 1 mk, and ϱ^{28} decreases by about 0.2%, all other reaction rate ratios and M^2 remaining almost unchanged. The elastic removal correction and the convergence on the fission spectrum in TRAMIX described in previous sections may not be required

for the analysis of TRX and BAPL experiments, and in general for any type of LWR. This is because the library spectrum is soft and very close to the real spectrum [14]. Such considerations cannot be applied in the case of intermediate spectra [25].

5.2.6 More accurate buckling treatment

In addition to the leakage calculation with SOLVERB, the limited size of the reactor (described with the experimental buckling) can be accounted for (in MICROX-2 and WIMS-D) in the preparation of self-shielded multigroup cross sections (so that the space dependence of the flux within the cell is correct when collapsing and homogenizing the cross sections), and in the transport calculation with ONEDANT (finite white cell calculation). We performed a series of MICROX-2 calculations, in which the buckling was either specified (in the case of TRX-1, TRX-2, BAPL-1, BAPL-2, BAPL-3) or searched for (in the case of TRX-3 and TRX-4) in each of the computational steps described in previous sections. The results were almost identical with those presented in Tables 2, 3, 4, and 5 (maximum change of k_{eff} of about 0.5 mk in the case of TRX-4, where the spectrum is strongly space dependent). We may conclude that the infinite lattice white boundary condition cell approach described in previous section is suitable for LWR calculations.

5.2.7 Dancoff factors

In order to estimate the importance of a correct Dancoff factor in the analysis of LWR systems, we neglected the hexagonal geometry in the resonance calculations with MICROX-2 and with WIMS-D, assuming a cylindrical cell.

The use of the Dancoff factor for a cylindrical cell in MICROX-2 (which is about 5% lower than for the hexagonal cell, for the same moderator cross section) results in a maximum k_{eff} decrease of 2 mk, and in a corresponding increase of ϱ^{28} of 0.5% in the case of Dancoff factors higher than 0.1 (such as in TRX-1, TRX-2, and in the BAPL experiments). All other reaction rate ratios and M^2 remain almost unchanged.

The corresponding results from WIMS-D cylindrical cell calculations are summarized in Table 7. The computed eigenvalues k_{eff} decrease by about 2 mk in the case of "intermediate" lattices (i.e. in those for which the ratio between pin rod radius and pitch is neither too large nor too small, such as in TRX-1, TRX-2, and in the BAPL experiments), because in the cylindrical model the Dancoff factor is underestimated. Correspondingly ϱ^{28} increases by about 1%, C^* increases by about 0.5%, and all other reaction rate ratios remain almost unchanged. M^2 increases by up to 2% in the BAPL experiments. For overmoderated systems such as TRX-4 the geometry of the system is not any longer important, and the results remain almost identical.

Experiment	TRX-1		TRX-2		TRX-3		TRX-4	
Values	C	C/E	C	C/E	C	C/E	C	C/E
k_∞	1.1767	/	1.1624	/	1.0655	/	1.0187	/
k_{eff}	0.9933	0.993	0.9942	0.994	1.	1.	1.	1.
ϱ^{28}	1.3755	1.042	0.8593	1.027	3.0695	1.013	0.4984	1.036
δ^{25}	0.0974	0.987	0.0597	0.973	0.2344	1.015	0.0345	0.964
δ^{28}	0.0997	1.053	0.0706	1.019	0.1749	1.048	0.0497	1.031
C^*	0.8062	1.012	0.6521	1.008	1.2586	1.003	0.5301	0.998
M^2 (cm^2)	32.4	/	30.9	/	36.8	/	30.1	/

Experiment	BAPL-1		BAPL-2		BAPL-3	
Values	C	C/E	C	C/E	C	C/E
k_∞	1.1404	/	1.1422	/	1.1295	/
k_{eff}	0.9967	0.997	0.9973	0.997	0.9984	0.998
ϱ^{28}	1.4451	1.040	1.2025	1.074	0.9404	1.038
δ^{25}	0.0821	0.980	0.0670	0.985	0.0515	0.980
δ^{28}	0.0775	0.991	0.0666	0.952	0.0546	0.958
C^*	0.8245	/	0.7499	/	0.6677	/
M^2 (cm^2)	44.2	/	41.0	/	38.4	/

Table 7: Calculated (C) and calculated/experimental (C/E) eigenvalues, reaction rate ratios, and calculated migration areas (M^2) from cell calculations of TRX and BAPL experiments (cylindrized) performed using WIMS-D and the WIMSJEF data library

5.2.8 Full reactor model

Finally, a full reactor calculation was made for the TRX-3 and TRX-4 experiments using the AARE system and the two cell model [13]. Multigroup self-shielded cross sections on the basis of MAT70 were prepared with TRAMIX, and homogenized cross sections were obtained for each cell using ONEDANT, SOLVERB and the same procedure as explained in Section 4. Latter on, the full reactor was computed using a one-dimensional model with a (small) transverse direction experimental buckling for the axial leakage [13]. The resulting eigenvalues k_{eff} were found to be 1.0013 for TRX-3 and 1.0006 for TRX-4 respectively, which is in good agreement with previously published values (see

Table 6). All reaction rate ratios were found to agree well within 0.5% (less than the experimental uncertainty) with those presented in Table 4.

6 CONCLUSIONS

The present analyses dealt with the neutronics of LWR metallic uranium (TRX) and uranium oxide (BAPL) lattices carried out using different code systems (applied to the same cell model), on the basis of the JEF-1 evaluation. The results from the calculations were compared with experiment and with previously published values.

It is shown that with the JEF-1 evaluation eigenvalues are generally well predicted within 8 mk (1 mk = 0.001) or less by all PSI code (systems) utilized (WIMS-D, BOXER, and the AARE modules TRAMIX and MICROX-2 in connection with ONEDANT), and that all methods give mostly reasonable and globally consistent results (within or not too far from the experimental uncertainty) for the measured reaction rate ratios. Using JEF-1 data, a better or at least a comparable consistency is achieved compared to previously published results obtained using ENDF/B-IV or ENDF/B-V [4]. The relatively poor estimate of single reaction rate ratios (such as ϱ^{28} in BAPL-2 and δ^{25} in TRX-3) appears to be systematic and is indicative for an underestimate of the experimental error.

Acknowledgments

The authors would like to acknowledge Mr. P. Vontobel and Dr. J. Stepanek for valuable discussions during the execution of this work.

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