JEF/DOC-634

Subj: updated results for JEZEBEL

the PSI results for the JEZEBEL criticality as presented
in the PHYSOR paper are firstly given. The revised values, arising
with the same methodology, but a fission spectrum for Pu239 generated
with the same weighting function from (MF,MT)=(6,18) and (5,455),
instead of (6,19), (6,20), (6,21), (6,38) and (5,455), follow.

In particular the new results, showing a k-eff increase of 126 pcm,
appear to confirm the conclusions recently derived
from similar light water reactor studies (Mattes, Bernat), and are
globally more close to the experimental values, since the fission source
becomes harder.

1. Balance tables for JEZEBEL (P2-S32) WITH THE OLD (INCORRECT) FISSION SPECTRUM FOR PU-239, CALCULATED FROM MT=19, 20, 21, 38, 455.

Total Fission Rate	0.3174
Total Capture Rate	0.0158
Total (n,2n) Rate	0.0008
Total Leakage Rate	0.6676

k-eff 0.996548

ABSORPTION

Group (Lower boundary in MeV)	
1 (2.2313 MeV)	0.0995
2 (0.49787 MeV)	0.1640
3	0.0696

LEAKAGE

Group (Lower boundary in MeV)	
1 (2.2313 MeV)	0.2098
2 (0.49787 MeV)	0.3256
3	0.1323

RATIO OF LEAKAGE TO ABSORPTION

Group (Lower boundary in MeV)	
1 (2.2313 MeV)	2.109
2 (0.49787 MeV)	1.985
3	1.901

RATIO OF GROUP 2 TO GROUP 1 ABSORPTION

1.648

RATIO OF GROUP 3 ABSORPTION TO (GROUP 1 + GROUP 2) ABSORPTION

0.264

REACTION RATE RATIOS:

	C	C/E
F49/F25	1.42561	0.98454
F28/F25	0.20159	0.94333
F37/F25	0.91346	0.94954

C197/F25	0.08098	0.97569

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2. Balance tables for JEZEBEL (P2-S32) WITH THE NEW (CORRECT) FISSION SPECTRUM FOR PU-239, CALCULATED FROM MT=18, 455.

Total Fission Rate	0.3174
Total Capture Rate	0.0152
Total (n,2n) Rate	0.0007
Total Leakage Rate	0.6681

k-eff 0.997804

ABSORPTION

Group (Lower boundary in MeV)	
1 (2.2313 MeV)	0.1034
2 (0.49787 MeV)	0.1634
3	0.0659

LEAKAGE

Group (Lower boundary in MeV)	
1 (2.2313 MeV)	0.2184
2 (0.49787 MeV)	0.3242
3	0.1255

RATIO OF LEAKAGE TO ABSORPTION

Group (Lower boundary in MeV)	
1 (2.2313 MeV)	2.112
2 (0.49787 MeV)	1.984
3	1.904

RATIO OF GROUP 2 TO GROUP 1 ABSORPTION

1.580

RATIO OF GROUP 3 ABSORPTION TO (GROUP 1 + GROUP 2) ABSORPTION

0.247

CENTRAL REACTION RATE RATIOS:

	C	C/E
F49/F25	1.43277	0.98948
F28/F25	0.20909	0.97843
F37/F25	0.93203	0.96885
C197/F25	0.07875	0.94880
C23/F25	1.52170	0.96432

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Titel: **Investigations for the CIRANO Benchmarks ZONA-2A, ZONA-2A3, ZONA-2B Using Deterministic Methods**

Ersetzt
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Autoren/
Autorinnen
S. Pelloni
Labor für Reaktorphysik und Systemtechnik

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Abstract

The described investigations aim at explaining the different trends in k_{eff} predictions made at PSI/EPFL, using deterministic and Monte Carlo codes and JEF-2.2 data, for simplified models of the CIRANO experiments ZONA-2A, ZONA-2A3 and ZONA-2B. The computed k_{eff} exhibits consistent, increasing trends from ZONA-2A, ZONA-2A3 to ZONA-2B, i.e. for the configurations containing more sodium/steel pins. However, assuming that the Monte Carlo calculations are more accurate, the relative k_{eff} increase predicted by the deterministic method is too high. Although no final statements can be drawn from the parametric study described in this technical note, it appears that these differences can be primarily attributed to the different neutron slowing down treatment in the reflector regions consisting of sodium/steel pins.

Verteiler

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1 Introduction

This work aims at consolidating the PSI deterministic methods for routine calculations of advanced, plutonium burning fast systems. Starting point for the following investigations were the different k_{eff} predictions made at PSI/EPFL [1] using deterministic (MICROX-2/TWODANT) [2, 3] and Monte Carlo (MCNP-4A) [4] codes for calculating simplified, homogeneous models of CIRANO experiments ZONA-2A, ZONA-2A3 and ZONA-2B defined by R. Jacqmin [5]. The inner core regions of the CIRANO configurations consist of UO_2/PuO_2 rodlets, with about 27 % Pu-enrichment, and Na rodlets in a square matrix of alternating fuel and sodium rodlets. The inner core in ZONA-2A is radially surrounded by a relatively smaller outer core having slightly different Pu-enrichment (24.9 %). The core region is axially and radially surrounded by a blanket consisting of natural UO_2 and Na rodlets. This breeding region is surrounded by a sodium/steel reflector region. The shield region, finally, is represented by a solid mass of stainless steel. ZONA-2A3 is obtained from this reference configuration by replacing the radial blanket region by sodium/steel pins. ZONA-2B is produced from ZONA-2A3 by replacing also the axial blanket region with sodium/steel pins.

Table 1 shows that the computed k_{eff} exhibits a consistent, increasing trend for the configurations containing more sodium/steel pins. However, assuming that the Monte Carlo calculation is more accurate, the relative k_{eff} increase is too high if the deterministic method is used.

Benchmark	MICROX-2/ TWODANT	MCNP-4A
ZONA-2A	1.00260	0.99884±0.00039
ZONA-2A3	1.00926	1.00319±0.00036
ZONA-2B	1.01574	1.00735±0.00039

Table 1: Reference k_{eff} Values Obtained Using Consistently JEF-2.2 Data

In this parametric study, k_{eff} changes induced by the use of different options were calculated using the deterministic approach in an attempt to explain these differences.

2 The Deterministic Reference Solution

The deterministic results displayed in Table 1 were obtained as follows:

2.1 Generation of Pointwise and Fine Group Cross Sections

Pointwise cross sections and P_0-P_4 fine group cross sections in 92 neutron groups between 14.9 MeV and 2.38 eV (the MICROX-2 energy structure [2]) were generated for room temperature. In this processing, NJOY (Edition 89.62, in which some common sizes were increased) was used with some modifications. These were in RECONR for the p-wave capture in structural materials, in UNRESR for shielding the whole unresolved energy range, and in GROUPR for shielding the inelastic scattering cross sections.

The following methodology was used in GROUPR for generating the required fine group cross sections, by distinguishing between three classes of nuclides:

1. **For the most important resonance and moderator nuclides, i.e. for ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{56}Fe, ^{52}Cr, ^{58}Ni, ^{60}Ni, ^{16}O and ^{23}Na**, a method which is based on the B_N approximation for large systems [6] (**"B_N method"**) has been used: Appropriate (regionwise) input weighting functions were used to produce suitably shielded microscopic cross sections **for the core, blanket and stainless steel/sodium regions.** For averaging the cross sections in energy, these continuous functions of energy were 1/E, divided by the (L+1)-th power of the macroscopic total cross section of the region to which the nuclide belongs. The index "L" refers to the L-th Legendre component of the cross sections. The required regionwise macroscopic, energy dependent total cross sections to compute the weighting functions were generated with the new code RES, an undocumented modification of the interface code MICROR [7]. These cross sections, and therefore the weighting functions, were produced for 20002 discrete energy points: For consistency with NJOY, the point with the highest energy was chosen at 20 MeV, 20000 points equally spaced in velocity were defined in the arbitrarily selected energy range between 10 MeV and 100 eV, and the lowest energy point was 10^{-5} eV. The continuous functions arose from these 20002 energy-weighting function pairs by means of a two point "log-log" scheme.

   The basic idea for using these weighting functions is that in an infinite, homogeneous medium, the leakage term of the Boltzmann equation disappears and the flux becomes proportional to the inverse of the total cross section, the proportionality factor, the source term, being a smooth function of energy. The "B_N method" can be used in connection with any cell code which is coupled to NJOY. It is precise, except that the weighting functions are not direction-dependent, the smooth part (1/E) is not absolutely correct above the resolved range, no escape probabilities are calculated to account for the finite size of the region, and the unresolved energy range cannot be completely shielded due to the approximations in UNRESR [6].

2. For the remaining, less important structural materials and heavy nuclides in these and other regions, the standard Bondarenko method has been used. The built-in weighting function option IWT=7, corresponding to a smooth fast reactor spectrum, was used to produce σ_0-dependent cross section tables. The P_L cross sections arose from the use of this spectrum divided by the (L+1)-th power of $(\sigma_0+\sigma_{tot})$ for selected σ_0-values, where σ_{tot} is the microscopic total cross section of the nuclide.

   These cross sections were carefully checked with an independent methodology: For various absorbing nuclides the σ_0-dependent values below 8 keV were in excellent agreement with the values obtained from pointwise resonance calculations (see Section 2.2) for mixtures of the absorbing nuclide in an infinite medium consisting of an almost non-absorbing moderator nuclide (deuterium) with appropriate atom number densities corresponding to the selected σ_0-values.

3. Cross sections for light nuclides were also generated with the Bondarenko method in a similar way, but only for infinite dilution (σ_0 equal to 10^{10}).

As far as actinides are concerned, fine group data for the prompt neutron yield ν, the fission cross section and the fission spectrum χ, were generated for individual fissionable nuclides from the basic data available for the total fission reaction (MT=18). For ^{239}Pu, the basic data used was that for the more detailed partial chain fission reactions (MT=19, 20, and 21).

2.2 Cell Calculations

Libraries in the specific formats GARTAPE and FDTAPE were produced from these pointwise and groupwise data using the interface code MICROR (Edition 2, in which some common sizes were as well increased) [7] for later use in the cell code MICROX-2. The FDTAPE library consists of the computed σ_0-dependent, P_0-P_3 data in the 92 fine group structure; the GARTAPE library consists of

additional data between 8 keV and 2 eV for use in pointwise resonance calculations (the cross sections are given in 24362 energy points equally spaced in lethargy).

Cell calculations were performed with the code MICROX-2 (Ed. 14/694a). In the core regions, they were performed in the fundamental mode spectrum. The global fission spectra used were expressed as linear combinations of the fission spectra available on the fine group library (FDTAPE) for the individual fissionable nuclides, the weighting coefficients in the linear combinations being equal to the fractions of the total neutron production rates for each nuclide computed in the fundamental mode spectrum. This determination resulted in an iterative procedure. In the blanket, stainless steel/sodium and shielding regions, the cell calculations solved fixed-source problems for infinite media, in which the energy-dependent source was proportional to the computed fission spectrum in the core.

MICROX-2 was used to generate microscopic, and macroscopic cross sections and fission spectra for use in the reactor calculations. The (inconsistent) diagonal transport correction was systematically used to generate these P_0-P_2 cross sections in 33 energy broad groups defined by a constant lethargy width of 0.5 and an energy boundary at 10 MeV.

The broad group cross sections in the energy range of elastic scattering below 8 keV were generated from the cross sections available on the pointwise data library (GARTAPE). The pointwise fluxes required for collapsing these cross sections in energy were obtained from a resonance calculation in which an appropriate neutron source was used. The upper energy boundary for the slowing down calculation was 8 keV and the source was calculated using the fine group cross sections and fission spectra available on the fine group library (FDTAPE).

The broad group cross sections in the energy range of elastic and inelastic scattering above 8 keV were derived from the fine group cross sections available on the FDTAPE library. For the nuclides treated with the Bondarenko method (see Section 2.1), the σ_0-dependent fine group cross sections above 8 keV had to be interpolated first. The required energy-dependent σ_0 was calculated using the background cross section method and the interpolation procedure used was a two point "semi-log" scheme [2].

2.3 Reactor Calculations

The resulting broad group cross sections (in 33 neutron groups) were used in two-dimensional transport calculations performed with the TWODANT code (Ed. 9/94), using cylindrical models for the CIRANO configurations, and P_2S_{-8} approximations. S_{-N} is a recommended option for cylindrical geometries, which turns out to be more precise than S_N. In the transport calculations, each radial and axial mesh had the size of about 1 cm in the core, blanket, and stainless steel/sodium regions, and of about 5 cm in the outer shielding regions.

3 New Investigations

All k_{eff} changes are expressed relative to the reference deterministic values summarized in Table 1 (see previous section).

3.1 Refined "B_N Method" and Fission Spectra

3.1.1 "B_N Method"

The use of the "B_N method" in connection with more energy points (50002 instead of 20002) resulted in minor k_{eff} variations (a few pcm) for all the configurations analyzed.

The use of the "B_N method" for also treating less important structural material nuclides in the outer shielding regions resulted also in similar minor k_{eff} variations.

3.1.2 Bondarenko Method and Use of Different Fission Spectra

Table 2, first column, summarizes the k_{eff} changes resulting from the use of a standard methodology for fast reactor calculations, in which in the energy range above 8 keV, the Bondarenko method (see Section 2.1) has been systematically applied instead of the "B_N method" for all nuclides everywhere in the reactor. Because the use of the Bondarenko method also leads to different fission spectra for the individual actinides (different weighting function for the fission matrices), Table 2, second column, includes the k_{eff} changes induced by the use of different fission data for ^{239}Pu. In this case, prompt neutron yield, fission cross section and fission spectrum were processed from MT=18 and not from MT=19, 20, and 21 (see Section 2.1).

Benchmark	Bondarenko Method (IWT=7)	MT=18 for ^{239}Pu
ZONA-2A	+478	+51
ZONA-2A3	+396	+68
ZONA-2B	+208	+80

Table 2: k_{eff} Changes (pcm) Resulting from the Use of the Bondarenko Method for All Nuclides, and from the Use of MT=18 for ^{239}Pu

Table 2, first column, shows that the k_{eff} values obtained using the Bondarenko method are too high. Additional calculations have also demonstrated that similar k_{eff} changes (i.e. the same too high k_{eff}'s) result if this method is used only for the nuclides in the sodium/steel reflector and blanket regions. Consistently, almost no k_{eff} changes were observed if the Bondarenko method is employed only for the nuclides in the fuel or/and remaining regions. This indicates a strong sensitivity of the computed k_{eff} to the macroscopic cross sections for the blanket and reflector regions.

3.1.3 More Precise Slowing Down Treatment in the Reflector

In order to investigate this effect further, a series of MICROX-2 calculations were performed for generating additional reflector cross sections in which various upper energy boundaries were used for the pointwise resonance calculation. The upper energy boundaries ranged from 450 keV to the standard upper energy boundary of 8 keV. Above the chosen upper energy boundary and for the full reactor calculations, the same methodology as described in Section 2 was used. The required pointwise data library (GARTAPE) consisted of cross sections between 450 keV and 2 eV given in 21409 energy points equally spaced in lethargy ($\Delta u=5.76 \times 10^{-4}$). The pointwise resonance treatment in the MICROX-2 code assumes isotropic scattering in the center of mass system and elastic scattering only. Therefore, the resonance part of the cell calculations is exact for the infinite sodium/steel reflector region because, in the absence of fuel, the threshold energy for inelastic scattering (459 keV, corresponding to that for sodium), is higher than 450 keV, and the elastic scattering process is almost isotropic in the center of mass system for energies smaller than about 0.5 MeV.

The substantial k_{eff} changes outlined in Table 3 were found to be relatively insensitive to the position and/or an increased density of the energy points used in the resonance calculation. As indicated in this table, the k_{eff} changes obtained using the **most accurate slowing down treatment in the reflector region**, i.e. **resulting from a resonance calculation with the maximum possible upper**

Upper Energy for Slowing Down Calculations (keV)	ZONA-2A3	ZONA-2B
100	-321	-609
200	-503	-967
400	-723	-1393
450	-740	-1426

Table 3: k_{eff} Changes (pcm) Resulting from the Use of Different Reflector Cross Sections

energy boundary (450 keV), are almost asymptotic, because a smaller number of "important" resonances are available at higher energies. The increasing trend exibited by k_{eff} for the configurations containing more sodium/steel pins disappears, which is consistent with the results obtained with other deterministic methods [1], but not necessarily correct considering that the definition of the homogeneous benchmarks has a certain dependence on calculations. In addition, the MICROX-2/TWODANT based k_{eff} values seem to agree with the Monte Carlo results when the upper energy boundary for the pointwise resonance calculation is chosen at about 100 keV. This clearly results from certain compensating effects, and needs further investigation.

3.2 Sources in Non-Fissionable Zones

The use of different neutron sources in the regions surrounding the core (see Section 2.1) and that of an energy- and region-independent buckling for making a simple attempt to simulate the non-infinite sizes of these regions resulted in a maximum k_{eff} variation of only 10 pcm.

3.3 Anisotropy

The use of P_0-P_3 cross sections and refined meshes in the reactor calculation resulted in a minor k_{eff} decrease of maximum 13 pcm.

The use of S_{-16} instead of S_{-8} resulted in a minor effect of 4 pcm.

k_{eff} changes were also determined for the case that the anisotropic component of inelastic scattering, which is neglected in MICROX-2 [2], is accounted for. For each configuration, these effects were approximated by determining the k_{eff} difference resulting from two additional reactor calculations. The first calculation systematically used fission spectra and unmodified P_0-P_2 fine group cross sections (in 92 groups) obtained using MICROX-2. The second calculation employed the same isotropic data, but the anisotropic cross sections were generated with a different cell code (TRANSX (Ed. 2) [8]), which accounts for the anisotropic component of inelastic scattering. The additional data required for use in TRANSX has been generated in the special format MATXS with the NJOY module MATXSR [6]. The reason for having used the fine group cross sections is that no buckling search option is available in TRANSX.

The resulting k_{eff} changes are summarized in Table 4.

Benchmark	k_{eff} Change (pcm)
ZONA-2A	-50
ZONA-2A3	-90
ZONA-2B	-130

Table 4: k_{eff} Changes (pcm) Resulting from the Inclusion of Anisotropic Inelastic Scattering

3.4 σ_0-Interpolation versus Pointwise Method

This section is aimed at confirming that a precise method for shielding resonance cross sections in energy (see Section 3.1.3) is required for non fissionable, undermoderated zones with large amounts of structural materials.

As a representative example, the total cross section of ^{56}Fe was computed for an infinite stainless steel/sodium region in fine group 55 using different methodologies. Fine group 55 has been chosen because its energy boundaries, 31.8278 and 24.7875 keV, cover important overlapping elastic scattering resonances of structural materials.

- If the Bondarenko method is used in connection with TRANSX, which employs in this particular case a fourth order Lagrangian scheme of $\log(\sigma)$ versus $\log(\sigma_0)$, in which the σ_0- values are 1, 20, 50, 100, and 1000 barns, the calculated cross section is 11.10 barns for a computed background cross section of 4.72 barns (the cross section ranges from about 25 barns for σ_0 equal to 1000 to about 5 barns for σ_0 equal to 1 barn).
- If the Bondarenko method is used in connection with MICROX-2, which employs a two point "semi-log" scheme in which in this particular case the σ_0-values are 1 and 50 barns, the computed cross section is 11.86 barns for the same background cross section of 4.72 barns.
- If the "B_N method" is used, the computed cross section is 8.69 barns.
- If MICROX-2 is used to perform an exact pointwise resonance calculation with the upper energy boundary at 450 keV, the computed cross section is 8.84 barns.

Thus, the ^{56}Fe cross section in fine group 55 obtained with the "B_N method" (8.69 barns) is close to the theoretically best value (8.84 barns), whereas the cross sections generated with the Bondarenko method (probably in connection with a too coarse σ_0-grid) deviate significantly by about 30 %.

4 Conclusions

This parametric study has aimed at explaining the different k_{eff} predictions made at PSI/EPFL, using deterministic and Monte Carlo codes and consistently JEF-2.2 data, for simplified models of the CIRANO experiments ZONA-2A, ZONA-2A3 and ZONA-2B. The computed k_{eff} exhibited a consistent, increasing trend from ZONA-2A, ZONA-2A3 to ZONA-2B, i.e. for the configurations containing more sodium/steel pins. However, assuming that the Monte Carlo calculation is more accurate, the relative k_{eff} increase predicted by the deterministic method was too high.

Using the deterministic approach, we made, in the framework of a parametric study, an attempt to find the explanation for these differences, by varying important neutronics parameters. Self-shielding effects, the treatment of neutron slowing down, fission as a function of incident neutron energy, as well as anisotropic scattering, were investigated. Particular emphasis was given to the non fissionable zones consisting of stainless steel and sodium.

It appears that these differences can be primarily attributed to the different neutron slowing down treatment in the reflector region consisting of sodium/steel pins (see Table 3) and, to a lesser extent, to missing anisotropic inelastic scattering if the deterministic approach is used (see Table 4).

Because the pointwise resonance treatment in the cell code MICROX-2 code assumes isotropic scattering in the center of mass system and elastic scattering only, the most accurate cross sections for the infinite sodium/steel reflector region could be generated by performing a detailed pointwise resonance calculation in which the maximum possible upper energy boundary (450 keV) was chosen. This calculation is exact because, in the absence of fuel, the threshold energy for inelastic scattering (459 keV, corresponding to that for sodium), is higher than 450 keV and the elastic scattering process is almost isotropic in the center of mass system for energies smaller than about 0.5 MeV.

If this exact neutron slowing treatment is performed, the increasing trend exibited by k_{eff} for the configurations containing more sodium/steel pins disappears, which is consistent with the results obtained with other deterministic methods [1], but not necessarily correct considering that the definition of the homogeneous benchmarks has a certain dependence on calculations. In any case, based on the experience gained in this work, the following strategy is recommended for k_{eff} calculations based on the MICROX-2/TWODANT combination:

- For the core regions, cell calculations should be performed in the fundamental mode spectrum, using the fission source as described in Section 2.2. The use of the Bondarenko method is sufficiently accurate for energies larger than 8 keV. A pointwise resonance calculation is needed with the standard upper energy boundary at 8 keV.

- For the (infinite) shield regions a similar treatment can be applied, except that an external, energy-dependent neutron source should be used. The source is proportional to the computed fission spectrum in the main core region.

- Cell calculations for the (infinite) blanket regions should be performed using the same external neutron source as in the shield region. Fine group data obtained using the "B_N method" is required for energies larger than 8 keV (see Section 2.1), whereas a pointwise resonance calculation is needed with the upper energy boundary at 8 keV.

- Cell calculations for the (infinite) stainless steel/sodium reflector regions should be performed in a similar way as for the blanket regions, except that the upper energy boundary for the pointwise resonance calculation, i.e. the lower boundary for the use of the "B_N method", should be 450 keV. The pointwise calculation is to be performed on an energy grid equally spaced in lethargy with a lethargy width of about 0.0005.

- The reactor calculations should be performed using P_2 (modified) and S_8 approximations.

However, there are still two open problems:

Firstly, the MICROX-2/TWODANT based k_{eff} values seem to agree with the Monte Carlo results (see Table 1) when the upper energy boundary for the pointwise resonance calculation is chosen at about 100 keV. This clearly results from certain compensating effects, and needs further investigation.

Secondly, when comparing with preliminary experimental results, the computed fission rate traverses still show the same increasing discrepancy in the reflector regions, particularly for the fissile isotopes more sensitive to the lower part of the energy spectrum, as pointed out in reference [1].

Therefore, further research work should be considered. Firstly, the implementation into the "B_N method" of the methodology proposed by Segev [9] , which consists of a more accurate analytical representation of the solution to the asymptotic slowing down equations of fast neutrons for both fuel and non-fuel regions. Secondly, the macrocell treatment, as available in the cell code ECCO [10], could be additionally implemented, such that the resulting use of appropriate escape probabilities would account for the leakage term in the Boltzmann equation (non-infinite sizes of the non-fuel cells).

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