RESOREX, a procedure for calculating resonance group cross-sections

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RESOREX, A Procedure for Calculating Resonance Group Cross-Sections

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Abstract

The procedure RESOREX which calculates Resonance Region Group X-sections is described. The procedure uses resonance integrals tabulated as a function of effective NR-scattering cross-section and physical temperature. These resonance integrals are generated on punched cards by the RESAB programme system described in Risö Report No. 234. The effective NR-scattering cross-section is derived from an equivalence principle corresponding to cylinder, square and hexagonal geometries. Correction for a cladding region containing heavy (WR) nuclides is used.

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Abstract to

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1. Introduction

The programme block RESOREX calculates the resonance region X-section in a simple rod cell for the fertile nuclide ^{238}U and the fissile nuclides ^{235}U and ^{239}Pu.

Roughly speaking the programme performs for each energy group an interpolation in a two-entrance table of resonance integrals pertaining to the energy group, nuclide and reaction type (absorption or fission). One entrance is the physical (effective) temperature T of the fuel and the other is the effective NR-scattering cross-section S per absorber nuclide. These tables are produced by the RESAB PROGRAMME SYSTEM (1), (2) in form of a library on punched cards.

The method used in RESOREX rests on the assumption that the resonance integrals in a fuel rod may be calculated sufficiently accurate from resonance integrals of homogeneous media containing one NR-scatterer by help of a suitable equivalence principle. This assumption has been amply tested in (1), but will nevertheless be further tested in the present multigroup version.

2. The Equivalence Principle

The group resonance integral of a nuclide inside a fuel rod is expressed as $RI_g(S,T)$, where index g stands for group number.

S is the effective NR-scattering cross-section per absorber atom and is calculated from the following formula

$$S = \frac{a(1-\alpha)}{\bar{l}\,N_{abs}} \qquad (2.1)$$

$\bar{l} = 2R_f$ is the mean chord of the fuel pin, N_{abs} is the number density of the resonance absorber and a is calculated from the Bell factor, bf, and the Dancoff factor, dc, by the formula

$$a = bf\,\frac{dc}{dc + a(1-dc)} \qquad (2.2)$$

according to the Nordheim approximation.

3. The Bell Factor

The bell factor, bf, is taken as geometry dependent according to formula (4.7) in (1).

$$bf = 1 + \frac{0.16 \cdot x^{1.27}}{x^{1.27} + 0.48\left(1 - \left(\frac{x}{10}\right)^{2}\right)\delta} \tag{3.1}$$

$$x = \frac{1}{\bar{l}\, N_{abs}(5 + \sigma_s)}$$

$$\delta = \begin{cases} 1 & \text{for } x < 10 \\ 0 & \text{for } x \geq 10 \end{cases} \qquad \sigma_s = \begin{cases} 0 & \text{for metal} \\ 7.6 & \text{for dioxide} \end{cases} \tag{3.2}$$

4. Dancoff Factor

The Dancoff correction may be calculated both assuming a cylindrical, square and hexagonal cell.

First macroscopic potential scattering cross sections has to be calculated for the three regions in the cell, fuel, cladding and moderator.

The fuel may apart from the heavy nuclides contain O and C. The cladding region may contain Al, Zr, Fe, Cr and Ni, and the moderator region H, D, C and O.

In case that cylinder geometry is specified in the input the collision matrix is calculated for the three pin cell regions assuming black fuel ($\Sigma_f = 10^5$) and the Dancoff factor is expressed as

$$dc = (V_m \Sigma_m P_{fm} + V_c \Sigma_c P_{fc}) \frac{2}{R_f} \tag{4.1}$$

The indices f, c and m indicates fuel, cladding and moderator respectively. V stands for volume, Σ for macroscopic cross-section and R for outer radius of region.

P_{fm} and P_{fc} are matrix elements corresponding to probabilities of collision in the fuel of neutrons started uniformly and isotropically in moderator and cladding respectively.

In the case that square or hexagonal, lattice geometry is input specified a Dancoff factor, dc', is first calculated neglecting the cladding - that is to say the cladding has been displaced by moderator - using the approximation of Sauer (4) for a square or hexagonal cell according to the following formulas

$$\mathrm{tau} = \left(\sqrt{\frac{\pi}{4} \left(1 + \frac{V_m}{V_f}\right)} - 1 \right) \frac{V_f}{V_m}$$

$$+ \begin{cases} 0.08 & \text{for square lattice} \\ 0.12 & \text{for hexagonal lattice} \end{cases} \qquad (4.2)$$

$$dc' = 1 + \frac{\exp\left[-\mathrm{tau}\, \frac{\Sigma_m 4V_m}{2\pi R_f}\right]}{1 + (1-\mathrm{tau})\, \frac{\Sigma_m 4V_m}{2\pi R_f}} \qquad (4.3)$$

In order to introduce the cladding region, which cannot be done directly in Sauer's approximation, two Dancoff factors dc_1 and dc_2 are calculated in the equivalent cylinder cell.

dc_1 is calculated exactly as in the cylindrical case and dc_2 is obtained by the same procedure with Σ_c put equal to Σ_m.

For the final Dancoff factor the following formula is employed:

$$dc = dc' \frac{dc_1}{dc_2} \qquad (4.4)$$

5. The Cladding Correction

The manner in which the cladding has been introduced so far is only correct as long as the cladding atoms may be considered as NR-scatterers.

Askew has indicated in (3) a treatment of cladding containing infinitely heavy atoms - the WR formalism. In appendix I a derivation is given of an approximate correction factor, $(1-\alpha)$, by which the effective NR-scattering cross-section in this case should be multiplied.

α is calculated in the following way:

$$\alpha = \frac{P_{cf}}{P_{cf}+P_{mf}} \, \frac{R_f}{R_f+R_c} \qquad (5.1)$$

In the cylindrical case the quantities P_{fc} and P_{fm} are the ones already used in (4.1). In the square and hexagonal cases the corrsponding quantities from the calculation of dc_1 is taken.

It has been found convenient in RESOREX to use the correction $(1-\alpha)$ universally since the cladding correction is most important for heavy nuclide containing cladding materials, and since the only cladding material containing lighter nuclide is aluminium for which α is insignificant because of its low cross-section.

To illustrate and justify this procedure table 6.16 from (1) is reproduced below.

Table 5.1.

The influence of cladding on the ^{238}U-oxide resonance integral from 0.5-3500 eV

		Resonance integral, barns		
Cladding material		"H_2O"	Al	SS 348
SDP, het., exact coll. prob. three regions	NR	14.60	13.89	14.76
	NON NR		11.14	11.33
Link ALFA	NR	14.75	14.07	14.90
equival. principle	NON NR		11.22	11.78
Bell factor	NON NR + $(1-\alpha)$corr.		11.18	11.34

The results obtained with SDP may be considered exact in the present context. The difference between NR and NON-NR consists in that in the former case, the integrals from the individual resonances are just added, whereas in the latter case the gradual depletion of neutrons is taken into account.

It is seen that in the realistic NON-NR case there is considerable disagreement, some 4%, between the exact result and the result based on the equivalence principle for cladding containing heavy nuclide (SS 348).

In the last line results are shown not given in the original table and obtained with the (1-α) correction introduced above. It is seen that a considerable improvement is obtained for SS 348 whereas the effect on Al cladding is small although still a slight improvement on an already satisfactory result.

6. The RESOREX LIBRARY

Resonance integrals for absorption in ^{238}U, ^{235}U and ^{239}Pu and fission in the last two nuclides are produced in the following way by use of the RESAB PROGRAMME SYSTEM.

From 1.8550 eV to 3354.6 eV the SDP procedure which solves the slowing down equation numerically has been applied to a standard homogeneous mixture containing 0.015 ^{235}U atom and 0.0025 ^{239}Pu atom per ^{238}U atom, and two ^{16}O-atoms per heavy atom.

Furthermore a NR-scattering cross-section, S, per ^{238}U atom is introduced.

The slowing down equation is solved by SDP utilizing cross-sections taken from a library tape and resonance integrals for absorption and fission in the appropriate energy intervals are calculated. To the ^{238}U resonance integrals is added the p-wave contribution calculated from statistical data by analytical NR method in the LINK ALFA part of the programme system. From 3354,6 eV and upward only ^{238}U absorption integrals are calculated using analytical methods both for s- and p-wave contribution.

The library tape contains ^{235}U and ^{239}Pu cross-sections taken from the UKNDF library and ^{238}U cross-sections generated from resonance parameters contained in the RESAB Resonance Parameter Library. Library tapes for temperatures 300, 861 and 1200°K have been produced so far, but it should be mentioned that only the temperature dependence of ^{238}U is taken into account, because no other than 300°K values exist in the UKNDF so far. Fortunately the Doppler broadening of the fissile nuclides is not considered very important at least in a thermal reactor.

The resonance integrals obtained in this way are printed out on punched cards having the following format.

One card containing library number (equivalent to job number used in RESAB), day, month, year and number of energy regions below 3354.6 eV.

One card containing atomic mass and NR-cross-section per absorber atom for ^{238}U.

A number of cards containing group absorption - resonance integrals for ^{238}U starting at the highest energy.

One card containing a -1 to indicate no fission.

One card containing atomic mass and NR scattering cross-section per absorber atom for ^{235}U. (The NR scattering cross-sections for ^{235}U and ^{239}U are calculated in RESAB from the ^{238}U cross-section taking the relative concentrations into consideration, but they are not used by RESOREX as will be explained later.)

A number of cards containing group absorption resonance integrals for ^{235}U.

A number of cards containing group fission resonance integrals for ^{235}U.

A similar sequence of cards for ^{239}U starting with atomic mass and NR cross-section.

One card containing library number (must be the same all way through!), day, month, year, and number of energy groups above 3354.6 eV.

One card containing atomic mass and NR scattering cross-section (must be the same as above) for ^{238}U.

A number of cards containing group absorption resonance integrals for ^{238}U above 3354.6 starting at the highest energy.

One card containing a -1 to indicate no fission.

In the library these cards are repeated with increasing NR scattering cross-section per ^{238}U atom, all calculated at the same temperature. The resulting bunch of cards is preceded by a card containing the temperature used.

A similar bunch with the same sequence of NR scattering values calculated at a higher temperature follows.

In front of the whole library is put a card containing the number of groups below 3354.6 eV, the number of groups above 3354.6 eV and the number of different values of NR scattering cross-section per ^{238}U atom, followed by a card containing the lethargy widths of the energy groups starting with the highest energy.

In order to use RESOREX the information contained in the library is by the procedure INLIB read into 5 three-dimensional arrays of which the first index runs over the number (two) of temperatures, the second index runs over the number of NR scattering values and the last runs over the number of energy groups. The array containing the ^{238}U group resonance integrals runs over the total number of energy groups, the array containing ^{235}U and

^{239}Pu absorption and fission information runs only over the number of energy groups below 3354.6 eV.

The INLIB procedure has to be declared the block where RESOREX is used and the same has to be the case with the 5 three-dimensional arrays.

7. Group- and NR-Scattering Cross-Section Structure

The group structure is to a certain extent arbitrary as long as the number of groups with specified ^{238}U resonance integrals is greater or equal to the number of groups with specified ^{235}U and ^{239}Pu resonance integrals. The present library contains ^{238}U resonance integrals corresponding to the group structure of the 22 groups from group number 20 to group number 41 used in the 76-group set on the SIGMA MASTER TAPE, and ^{235}U and ^{239}Pu resonance integrals of the 14 groups from group 28 to group 41.

The partition at 3354.6 is determined by this group structure and the fact that the RESAB library tape contain only information up to 3500 eV at which point the UKNDF switches over to smooth cross sections, indicating that at this point resonance information is either lacking or of no importance or both. This is not strictly correct for ^{238}U anyhow (see (1) fig. 3.2). The lowest energy 1.8550 eV is of course also determined by the 76-group set.

The sequence of the NR scattering cross-section values is also arbitrary as long as it contains increasing values. In order to cover practical requirements with reasonable accuracy the following sequence has been chosen:

$$4,\ 9,\ 16,\ 25,\ 36,\ 64,\ 100,\ 225,\ 400 \qquad (7.1)$$

The temperatures available in the present state of the RESOREX LIBRARY are 300, 861 and 1200°K.

8. Interpolation Procedure

The programme calculates the value S 8, which is the S-value calculated by (2.1) for ^{238}U.

Since the resonance integral is roughly linearly dependent on the square root of S 8, this quantity is used to interpolate linearly in the sequence

2, 3, 4, 5, 6, 8, 10, 15, 20 (8. 1)

which represents the square roots of (7. 1).

The interpolation procedure is constructed in such a way that a linear extrapolation takes place if the S 8 value falls outside the sequence (7. 1).

The same interpolation procedure is also used for ^{235}U and ^{239}Pu. Two quantities S 5 and S 9 are calculated as

$$S\ 5 = S\ 8 \cdot 0.015\ \frac{N38}{N35}$$

$$S\ 9 = S\ 8 \cdot 0.0025\ \frac{N38}{N39}$$

N38, N35 and N39 is the concentration in the fuel of ^{238}U, ^{235}U and ^{239}U of the actual problem and 0.015 and 0.0025 reflect the relative concentration assumed in the RESAB calculation.

The square root of S 5 and S 9 is used to interpolate in the sequence (8. 1). Also in this case extrapolation will automatically take place if S 5 or S 9 falls outside (8. 1).

A set of interpolations takes place for each of the two temperatures contained in the library. Since the resonance integral is also roughly linearly dependent on the square root of the physical temperature T, sqrt(T) is used to interpolate between the square root of the two library temperatures. In case T falls outside the range of these two values linear extrapolation will take place.

9. Resonance Overlap Correction

The resonance integrals obtained in this way are already corrected for resonance overlap between the different heavy nuclides. This overlap corresponds to the standard relative concentration chosen in the RESAB library calculation. Remembering that this calculation gives the correct overlap effect, it is seen that in this way it is possible to work with small corrections in the vicinity of these concentrations that are close to concentrations met in many practical problems.

The final correction takes place using the formalism developed in (3) and (1). In order to use this formalism properly it is necessary first to correct back to zero relative concentration. As the verification of the usefulness of the formalism as shown in (1) is valid for the resonance integral over a larger energy interval, the correction is obtained by adding up the resonance integrals of the lowest energy groups up to a certain group number which is left open as a parameter. From the resulting resonance integrals RIA8, RIA5, RIF5, RIA9, RIF9, and the total lethargy width U of the groups concerned the following correction may be calculated according to (1):

$$\frac{1}{1 - \frac{(RIA5 + RIF5)\cdot 0.015 + (RIA9 + RIF9)\cdot 0.0025}{2\,U\,S\,8}} \qquad (9.1)$$

$$\frac{1}{1 - \frac{RIA8 + 0.0025(RIA9 + RIF9)}{U\,S\,8}} \qquad (9.2)$$

$$\frac{1}{1 - \frac{RIA8 + 0.015(RIA5 + RIF5)}{U\,S\,8}} \qquad (9.3)$$

The factor (9.1) corrects the resonance integrals of ^{238}U, (9.2) those of ^{235}U and (9.3) those of ^{239}Pu from the standard relative concentration back to zero concentration of ^{235}U and ^{239}Pu.

This correction is of course only applied to the low energy groups involved.

It has been found convenient to do this correction once and for all in INLIB so that the interpolation takes place in a table of resonance integrals already corrected back to zero ^{238}U and ^{239}Pu concentrations.

After the interpolation a similar summing up of the low-energy group resonance integrals take place yielding new values of RIA8, RIA5, RIF5, RIA9, RIF9, and the following correction factors are introduced.

$$1 - \frac{(RIA5 + RIF5)\,N35 + (RIA9 + RIF9)\,N39}{2U\,N38\,S8} \qquad (9.4)$$

$$1 - \frac{RIA8 + (RIA9 + RIF9)\ N39}{U\ N38\ S8} \tag{9.5}$$

$$1 - \frac{RIA8 + (RIA5 + RIF5)\ N35}{U\ N38\ S8} \tag{9.6}$$

correcting from zero to the actual concentrations of ^{235}U and ^{239}Pu. It is easily seen that if these corresponds to the standard relative concentration the resulting correction factors of subsequent use of (9. 1-3) and (9. 4-6) will all be unity.

10. Effective Resonance Reaction Cross-Sections

As recommended in (1) the effective group cross-sections for a given resonance reaction is obtained by dividing the corresponding resonance integral by the integrated group flux expressed by

$$\bar{\Phi}_g = \Delta u - \frac{RIA38_g + N35(RIA35_g + RIF35_g) + N39(RIA39_g + RIF39_g)}{N38\ S8} \tag{10.1}$$

In this way effective group cross-sections suitable for a fuel region in a subsequent pin cell calculation is generated.

If group cross sections for a homogenized pin cell are wanted the resonance integrals should be divided by the following integrated group flux

$$\bar{\Phi}_g = \Delta u - \frac{V_f}{V_c} \times \text{(second term in (10.1))} \tag{10.2}$$

11. Mean Logarithmic Decrement and Group Escape Probability

The total slowing down power of the pin cell is calculated as

$$SD = \sum_{i=1,\,j=1}^{3,\,N_i} \Sigma_i^j\ \xi_i^j\ V_i \tag{11.1}$$

where Σ_i^j and ξ_i^j are the macroscopic potential scattering cross section and the mean logarithmic decrement of the j-th nuclide in the i-th region. V_i is the volume of the i-th region.

The mean logarithmic decrement for the cell is calculated as

$$\xi_{cell} = SD / \left(\sum_{i=1,j=1}^{3,N_i} \Sigma_i^j V_i \right) \tag{11.2}$$

The group escape probability P_g is calculated as

$$P_g = \exp(-V_f(N38\ RIA38_g + N35(RIA35_g + RIF35_g) + N39(RIA39_g + RIF39_g)) / SD) \tag{11.3}$$

A selfscattering cross-section, $SIGS38_g$, and a cross-section $SIG138_g$ for the scattering to group g + 1 is calculated in RESOREX in the following way:

$$SIGS138_g = \xi_{38}\ \sigma_{S38}(P_g + 1)/2 \tag{11.4}$$

$$SIGS38_g = \sigma_{S38} - SIGS138_g \tag{11.5}$$

Formula (11.4) assumes that ξ_{38} is small compared with ΔU_g. σ_{S38} = 10.64 b is the potential scattering cross-section of ^{238}U and ξ_{38} = 0.088 is the corresponding mean logarithmic decrement.

These two rather rough estimates are good enough to supersede the values calculated by SIGMA that are very far off because of lacking selfshielding of the scattering resonances. The same set of values may also be used for ^{235}U and ^{239}Pu instead of the SIGMA values that suffer from a similar weakness.

12. Incorporation of the INLIB and RESOREX Procedures

When INLIB and RESOREX are incorporated in a programme a number of variables and data should be established.

In the block in which INLIB is called the following integers must be declared and have values assigned in accordance with the library.

REG: number of resonance groups for ^{238}U
(REG = 22 in the present library)
REG1: number of resonance groups for ^{235}U and ^{239}Pu
(REG1 = 14 in the present library)
NSEX: number of NR scattering values in the library
(NSEX = 9 in the present library)
SEC: number of overlap groups
(SEC = 8 is recommended, but the value of SEC is not critical)
LINO: library number
LINO = 1000 in the present library)

In the same block the following arrays should be declared:

```
TB [1:2] , EX [1:NSEX], DELU [1:REG] ,
RI8 [1:2, 1:NSEX, 1:REG]
RIA5, RIF5, RIA9, RIF9 [1:2, 1:NSEX, 1:REG1 ]
```

The procedure call of INLIB takes the following form:

```
INLIB(REG, REG1, NSEX, SEC, LINO, TB, EX, DELU,
      RI8, RIA5, RIF5, RIA9, RIF9, UD)
```

UD is a label that should be established somewhere in the programme and to which the INLIB jumps if the specification in the procedure head are not in agreement with the library. The latter is read as a part of the ordinary data of the programme and should be ready immediately when INLIB is called.

The variables in the procedure head could as such be given any name. However, EX, DELU, TB, RI8, RIA5, RIF5, RIA9, and RIF9 are used in RESOREX and only known under these names. Consequently RESOREX may only be called inside a block in which these names have been established and have been assigned values by a call of INLIB.

The procedure call of RESOREX looks in the following way:

```
RESOREX(GI, NSEX, SEC, FU, REG, REG1, RF, RC, RM,
        N38, N35, N39m ALC, ZRC, FEC, NIC, CRC,
        HM, DM, CM, OM, SIGA38, SIGS38, SIGS138,
        SIGA35, SIGS35, SIGA39, SIGF39, P, CI, T)
```

The variables NSEX, SEC, REG, and REG1 should be identical with the variables carrying the same names in INLIB.

The following integers should be declared and assigned values:

GI: geometry factor
(GI = 1 cylinder cell, GI = 2 square cell and GI $>$ 2 hexagonal cell)
FU: fuel composition factor
(FU = 1 oxide fuel, FU = 0 metal fuel. With the present library only oxide is permitted)

The following reals should be declared and assigned values:

RF: radius of fuel pin
RC: outer radius of cladding
RM: outer radius of moderator for GI = 1, otherwise lattice pitch
N38: atomic density $\times 10^{-24}$ of ^{238}U in fuel pin
N35: atomic density $\times 10^{-24}$ of ^{235}U in fuel pin
N39: atomic density $\times 10^{-24}$ of ^{239}U in fuel pin
ALC: atomic density $\times 10^{-24}$ of Al in cladding
ZRC: atomic density $\times 10^{-24}$ of Zr in cladding
FEC: atomic density $\times 10^{-24}$ of Fe in cladding
NIC: atomic density $\times 10^{-24}$ of Ni in cladding
CRC: atomic density $\times 10^{-24}$ of Cr in cladding
HM: atomic density $\times 10^{-24}$ of H in moderator
DM: atomic density $\times 10^{-24}$ of D in moderator
CM: atomic density $\times 10^{-24}$ of C in moderator
OM: atomic density $\times 10^{-24}$ of O in moderator
T: the physical temperature

The following real arrays should be declared before the call of RESOREX:

SIGS38, SIGS138, P [1:REG]
SIGA38 [1:2, 1:REG]
SIGA35, SIGF35, SIGA39, SIGF39 [1:2, 1:REG1]

After the call they will contain the following results from the procedure:

SIGS38: group self-scattering cross-section for ^{238}U (11.5)
SIGS138: group cross-section for scattering to next group for ^{238}U (11.4)
P: group escape probability (11.3)
SIGA38: group absorption cross-section for ^{238}U

SIGA35 and SIGF39: group absorption and fission cross-section for ^{235}U .

SIGA39 and SIGF39: group absorption and fission cross section for ^{239}Pu

In the two-dimensional arrays SIGA38, SIGA35, SIGF35, SIGA39, and SIGF39 the values with first index equal to one are rod averages (group flux by (10.1)), the values with first index equal to two cell averages (group flux by (10.2)).

Finally the real CI should also be declared before calling RESOREX and contains the cell average mean logarithmic decrement by formula (11.2).

13. Verifications

In order to be able to use group cross sections produced by RESOREX with confidence the reliability of the following procedures should be checked

1. Overlap correction
2. Temperature interpolation
3. NR-scatterer interpolation
4. Dancoff correction
5. SAUERS approximation for square cells
6. Cladding correction.

All checks have been made relative to results from RESAB, which is the only relevant check since RESOREX results are based on tables produced by RESAB. Checks with experiments or other calculation systems should be performed directly with RESAB.

Most of the checking was performed on a YANKEE fuel pin cell with a fuel composition corresponding to 4000 MWD/t burn up. The dimensions and the composition of the fuel pin cell is the following:

Fuel radius	0.3734 cm
Cladding outer radius	0.4318 cm
Pitch (square)	1.0719 cm
Equivalent cylinder radius	0.6047 cm

Number densities × 10^{-24}

Fuel	Cladding	Moderator
^{238}U: 2.186 10^{-2}	Fe: 5.75 10^{-2}	^{1}H: 5.155 10^{2}
^{235}U: 6.857 10^{-4}	Cr: 1.54 10^{-2}	^{16}O: 2.578 10^{-2}
^{239}Pu: 5.406 10^{-5}	Ni: 9.04 10^{-3}	
^{16}O: 4.544 10^{-2}		

RESOREX calculation with varying number of overlap groups were calculated in cylinder geometry and compared with RESAB results. Direct comparison of the group cross sections gives a complicated picture, which is difficult to overlook since the agreement varies from group to group and from reaction type to reaction type. A better and more stable comparison is obtained by calculating the total reaction rate under a suitable flux condition, e. g. the fuel flux in the RESAB output.

The resulting reaction rates are given in table 13. 1 below.

Table 13. 1

Total reaction integral in barn for the 14 lowest groups

	ABS 38	ABS 35	FISS 35	ABS 39	FISS 39
RESAB	15. 83	76. 34	128. 87	106. 58	150. 90
RESOREX number of overlap groups					
0	15. 92	72. 07	122. 8	107. 4	152. 1
7	15. 79	75. 05	127. 4	105. 3	149. 1
9	15. 78	75. 45	128. 1	105. 2	149. 0
13	15. 80	75. 28	128. 3	105. 7	149. 7

It is seen that the exact choice of overlap groups is not critical. 9 overlap groups have been chosen for the remaining tests. The corresponding maximum deviation on any single group cross section is 5%.

To give a realistic impression of the influence of varying concentrations of ^{235}U and ^{239}U calculation have been carried out for the same

YANKEE fuel pin for a number of different burn-ups starting with zero and continuing to 40000 MWD/t.

In fig. 13.1 the deviation in percent between RESAB and RESOREX total reaction rates in the 14 lowest groups is shown.

It is seen that at small burnup values corresponding to equilibrium Xe and equilibrium Sm the deviation for ^{239}Pu is quite large which is a result of the low concentration which brings the S value far outside the range of the library tables. The resulting error in cross section is, however, unimportant at the very low ^{239}Pu concentrations in question.

It is also seen that RESOREX systematically underestimate the total reaction rate except for the ^{239}Pu at burnup above 15000 MWD/t.

The deviation is quite small for ^{238}U, which should be so since the equivalence principle used has mainly been developed with this isotope in view. The greater deviation for ^{235}U and ^{239}Pu is probably partially caused by the shortcomings of the overlap approximation used, partially by the equivalence principle which is less well suited for the low concentration of these isotopes.

The monotonous variation of the ^{239}Pu makes it probable that the NR-interpolation does not have any significant effect since this effect would otherwise cause fluctuations to appear over the large range of Pu concentrations (from $3.0_{10^{-7}}$ to $2.05_{10^{-4}}$).

The effect of temperature interpolation was examined by comparing the results of two RESOREX calculations with a physical temperature of 869°K. One of the calculations used a library with 300°K and 861°K tables, the other calculation 300°K and 1200°K tables.

The greatest deviation between group cross sections in these two cases was less than 1%.

Similar results were obtained with two calculations with a physical temperature of 1200°K, which shows that extrapolation quite far above the upper temperature in the library is possible.

Finally, to examine the numbers 4, 5 and 6 on the list over approximations a number of different modifications of the YANKEE fuel pin cell was calculated as shown in table 13.2.

The second and the third case in table 13.2 shows that the Dancoff factors calculated by RESAB and RESOREX are identical and furthermore that the S8 values agree as they should when there is no cladding correction. The difference of 0.18 in mean between the sets of ABS 38 values is then the true difference between the use of the equivalence principle of

Table 13.2

	ABS 38 b.		Dancoff factor		S 8	
	RESAB	RESOREX	RESAB	RESOREX	RESAB	RESOREX
Cylinder cell with normal cladding	15.85	15.78	-	0.6359	-	38.89
Cylinder cell with vacuum for cladding	15.55	15.72	0.5711	0.5714	37.84	37.87
Cylinder cell with two regions	15.72	15.91	0.5883	0.5882	39.10	39.07
Square cell with two regions	15.48	15.72	0.5657	0.5707	37.40	37.81
Square cell with normal cladding	(15.59)	15.70*	-	0.6180	-	37.70

*Obtained with flux from RESAB square two-region case.

RESOREX and the exact calculation of RESAB.

Turning to the square two-region case we see that the difference on ABS 38 increases from 0.18 to 0.24. This extra difference of 0.06 ~ 4 o/oo is caused by the 1% difference in the Dancoff factors reflecting the effect of Sauers approximation used in RESOREX as compared to the exact Carlvik procedure used in RESAB.

Unfortunately it is not possible to solve three-region problem with square cell boundary in RESAB. A RESAB result is nevertheless given in parenthesis. It has been deduced from the difference between case one and case three, which difference has been added to the result from case four.

The great difference between the RESOREX results in case 1 and 3 is quite out of proportion to the slight change in S 8 and has the opposite trend of the RESAB results. A closer examination shows that this phenomenon is caused by a shift in the RESAB flux spectrum which is used to calculate ABS 38.

This by the way makes the ABS 38 value with the asterisk in case five doubtful. It should probably be reduced so that it came close to the value in the parenthesis.

The very good agreement between RESAB and RESOREX in case 1 thus seems to be a result of the character of the cladding which is indeed very thick and dense for the YANKEE pin.

Less good agreement should consequently be expected for pin cell with less cladding.

To illustrate this, calculations have been made on a fuel pin cell from BROWNS FERRY with the following composition and density.

Fuel radius	0.6228 cm
Cladding outer radius	0.7150 cm
Equivalent cyl. radius	1.063 cm

Number densities $\times 10^{-24}$

Fuel	Cladding	
^{238}U: 2.20 10^{-2}	^{40}Zr: 3.814 10^{-2}	^{1}H: 3.222 10^{-2}
^{235}U: 4.988 10^{-4}		^{16}O: 1.611 10^{-2}

A comparison between these results and the YANKEE results is given in table 13.3.

Table 13.3

	ABS 38		Cladding
	RESAB	RESOREX	Correction $(1-\alpha)$
YANKEE	15.83	15.78	8.56 10^{-2}
BROWNS FERRY	13.26	13.45	3.31 10^{-2}
YANKEE TWO REG (no cladding)	15.72	15.91	(1.5 10^{-4})

The cladding correction is given to indicate the importance of the cladding. The BROWNS FERRY and the no cladding case gives practically the same deviation of 1.5%.

Going back to table 13.2 it is seen that this error is of the same magnitude as the change caused by going from cylinder to square geometry, whereas the error from Sauers approximation is only a fourth hereof.

The resonance absorption of fissile nuclides being closer to saturation is less susceptible to the presence of the cladding. Consequently the error on the total absorption will not be significantly different for the fissile nuclides in the three cases.

References

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(3) I. R. Askew, Calculation of Resonance Captures in Few-Group Approximation. AEEW-R 489 (1966).

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Appendix I

In order to show the relationship between the Dancoff correction, the cladding correction and the Nordheim approximation, let us consider the following two coupled slowing down equations, the left sides of which give the total number of collisions per energy interval respectively in the fuel- and cladding region

$$V_f \Sigma_f \Phi_f = P_{ff}\, V_f \int_E^{E/\alpha_f} \Phi_f \Sigma_f^s \frac{dE'}{(1-\alpha_f)E'} + P_{fc}\, V_c \int_E^{E/\alpha_c} \Phi_c \Sigma_c^s \frac{dE'}{(1-\alpha_c)E'} + $$
$$+ P_{fm}\, V_m \int_E^{E/\alpha_m} \Phi_m \Sigma_m^s \frac{dE'}{(1-\alpha_m)E'} \qquad \text{(AI. 1)}$$

$$V_c \Sigma_c^s \Phi_c = P_{cf}\, V_f \int_E^{E/\alpha_f} \Phi_f \Sigma_f^s \frac{dE'}{(1-\alpha_f)E'} + P_{cc}\, V_c \int_E^{E/\alpha_c} \Phi_c \Sigma_c^s \frac{dE'}{(1-\alpha_c)E'} + $$
$$+ P_{cm}\, V_m \int_E^{E/\alpha_m} \Phi_m \Sigma_m^s \frac{dE'}{(1-\alpha_m)E'} \qquad \text{(AI. 2)}$$

The two equations can be derived under the assumption of flat flux in each of the regions, fuel, cladding and moderator indicated by the indices f, c and m.

No absorption takes place in the cladding or moderator and cross sections Σ_c^s and Σ_m^s - identical with the potential scattering cross-sections - are assumed independent of energy, whereas the fuel cross-sections Σ_f and Σ_f^s and the fluxes Φ_f, Φ_c and Φ_m are functions of energy.

When the reciprocity relations $P_{fm} V_m \Sigma_m^s = P_{nf} V_f \Sigma_f^s$ and $P_{fc} V_c \Sigma_c^s = P_{cf} V_f \Sigma_f^s$ are used (AI. 1) may be rewritten as

$$\Phi_f = P_{ff} \frac{1}{\Sigma_f(E)} \int_E^{E/\alpha_f} \Phi_f \Sigma_f^s \frac{dE'}{(1-\alpha_f)E'} + \frac{P_{cf}}{\Sigma_c^s} \int_E^{E/\alpha_c} \Phi_c \Sigma_c^s \frac{dE'}{(1-\alpha_c)E'} + $$
$$+ \frac{P_{mf}}{\Sigma_m^s} \int_E^{E/\alpha_m} \Phi_m \Sigma_c^s \frac{dE'}{(1-\alpha_m)E'} \qquad \text{(AI. 3)}$$

When the NR-approximation is applied to a region we have

$$\int_{E}^{E/\alpha_i} \Phi_i \Sigma_i^s(E') \frac{dE'}{(1-\alpha_i)E'} \simeq \Sigma_i^p / E$$

where Σ_i^p is the potential scattering cross-section of the region.

When the WR approximation is applied we have

$$\int_{E}^{E/\alpha_i} \Phi_i \Sigma_i^s(E') \frac{dE'}{(1-\alpha_i)E'} \simeq \Phi(E)\, \Sigma_i^s(E)$$

The distinction between Σ_i^p and $\Sigma_i^s(E)$ is unnecessary in the moderator and cladding regions.

IF NR approximation is applied to all three regions we get from (AI. 3)

$$\Phi_f'(E) = \left[\frac{\Sigma_f^p}{\Sigma_f(E)} P_{ff} + P_{cf} + P_{mf} \right] / E$$

$$= \left[\frac{\Sigma_f^p}{\Sigma_f(E)} P_{ff} + 1 - P_{ff} \right] / E = \left[1 - P_{ff} \frac{\Sigma_f(E) - \Sigma_f^p}{\Sigma_f(E)} \right] / E \qquad \text{(AI. 4)}$$

When the WR approximation is used on the fuel and the NR approximation on the cladding and moderator regions we get from (AI. 3)

$$\Phi_f(E) = [P_{cf} + P_{mf}]/E + \frac{\Sigma_s(E) + \Sigma_f^p}{\Sigma_{f(E)}} \Phi_f(E)$$

$$\Phi_f(E) = \frac{1 - P_{ff}}{1 - P_{ff} \dfrac{\Sigma_s(E) + \Sigma_f^p}{\Sigma_f}} \frac{1}{E} \qquad \text{(AI. 5)}$$

$\Sigma_s(E)$ is the resonance scattering cross-section of the fuel atoms.

In case that the fuel contains light nuclides that can be treated as NR scatterers we have to distinguish between the potential scattering cross-section of the fuel, Σ_o and the remaining potential scattering cross-section $\Sigma_f^p - \Sigma_o$.

In this case (AI. 5) is changed into

$$\Phi_f(E) = \frac{1 - P_{ff} + \frac{\Sigma_f^p - \Sigma_o}{\Sigma_f(E)} P_{ff}}{1 - P_{ff} \frac{\Sigma_s(E) + \Sigma_o}{\Sigma_f(E)}} \qquad \text{(AI. 6)}$$

When both fuel atoms and cladding atoms are treated in the WR-approximation and the remaining atoms are treated in the NR approximation we get from (AI. 2) and (AI. 3)

$$\Phi_c(E) = P_{fc} \frac{\Sigma_s(E) + \Sigma_o}{\Sigma_f(E)} + P_{cc} \Phi_c(E) + \frac{P_{mc}}{E} \qquad \text{(AI. 7)}$$

$$\Phi_f(E) = P_{ff} \frac{\Sigma_s(E) + \Sigma_f^p}{\Sigma_f(E)} \Phi_f(E) + F_{cf} \Phi_c(E) + \frac{P_{mf}}{E} \qquad \text{(AI. 8)}$$

Eliminating $\Phi_c(E)$ we get

$$\Phi_f(E) = \frac{1 - \left(P_{ff} - \frac{P_{cf} P_{fc}}{1 - P_{cc}} \right)}{1 - \left(P_{ff} - \frac{P_{cf} P_{fc}}{1 - P_{cc}} \right) \frac{\Sigma_s(E) + \Sigma_o}{\Sigma_f(E)}} \frac{1}{E} \qquad \text{(AI. 9)}$$

If we introduce

$$P'_{ff} = P_{ff} - \frac{P_{cf} P_{fc}}{1 - P_{cc}} \qquad \text{(AI. 10)}$$

a formula quite analogue to (AI. 5) is obtained

$$\Phi_f(E) = \frac{1 - P'_{ff}}{1 - P'_{ff} \frac{\Sigma_s(E) + \Sigma_f^p}{\Sigma_f(E)}} \frac{1}{E} \qquad \text{(AI. 11)}$$

If again a NR scatterer is introduced in the fuel (AI. 10) takes the form

$$\Phi_f(E) = \frac{(1 - P'_{ff}) + \frac{\Sigma_f^p - \Sigma_o}{\Sigma_f(E)} P'_{ff}}{1 - P'_{ff} \frac{\Sigma_s(E) + \Sigma_o}{\Sigma_f}} \qquad \text{(AI. 12)}$$

in complete analogy with (AI. 6).

In order to calculate P'_{ff} we write

$$P_{cf} = (1 - P_{ff})\, G_c \qquad \text{(AI. 13)}$$

$$P_{fc} = (1 - P_{cc})\, G_f \qquad \text{(AI. 14)}$$

G_c is the probability that neutrons escaping from the fuel will collide in the cladding and G_f the probability that neutrons escaping from the cladding will collide in the fuel.

For G_c we take the energy independent expression

$$G_c = \frac{P_{cf}}{P_{cf} + P_{mf}} \qquad \text{(AI. 15)}$$

obtained during the calculation of the Dancoff factor, dc, corresponding to black fuel.

G_f is approximated by the likewise energy independent expression

$$G_f = \frac{R_f}{R_f + R_c} \qquad \text{(AI. 16)}$$

When these approximations are introduced into (AI. 10) we get

$$P'_{ff} = P_{ff} + (1 - P_{ff}) \times \alpha \qquad \alpha = G_f\, G_c \qquad \text{(AI. 17)}$$

In the equivalence principle based on Nordheim's formalism in connection with a rational approximation with a Bell factor bf we have

$$P_{ff} = \frac{\bar{l}\, \Sigma_f(E)}{\bar{l}\, \Sigma_f(E) + a} \quad ; \quad a = \frac{bf \cdot dc}{dc + a(1 - dc)} \qquad \text{(AI. 18)}$$

where dc is the black fuel Dancoff factor.

From (AI. 17) we get

$$P'_{ff} = \frac{\bar{l}\, \Sigma_f(E) + \alpha}{\bar{l}\, \Sigma_f(E) + a} \qquad \text{(AI. 19)}$$

and

$$\Phi_f(E) = \frac{1}{E} \; \frac{a(1-\alpha) + \dfrac{\Sigma_f^p - \Sigma_o}{\Sigma_f(E)} \left(\bar{l}\,\Sigma_f(E) + a\alpha\right)}{\bar{l}\,\Sigma_f(E) + a - \dfrac{\Sigma_s(E) + \Sigma_o}{\Sigma_f(E)} \left(l\,\Sigma_f(E) + a\alpha\right)}$$

$$= \frac{1}{E} \; \frac{a(1-\alpha) + (\Sigma_f^p - \Sigma_o)\left(\bar{l} + \dfrac{a\alpha}{\Sigma_f(E)}\right)}{\Sigma_a(E)\left(\bar{l} + \dfrac{a\alpha}{\Sigma_f(E)}\right) + a(1-\alpha) + (\Sigma_f^p - \Sigma_o)\left(\bar{l} + \dfrac{a\alpha}{\Sigma_f(E)}\right)}$$

The resonance integral becomes in this approximation

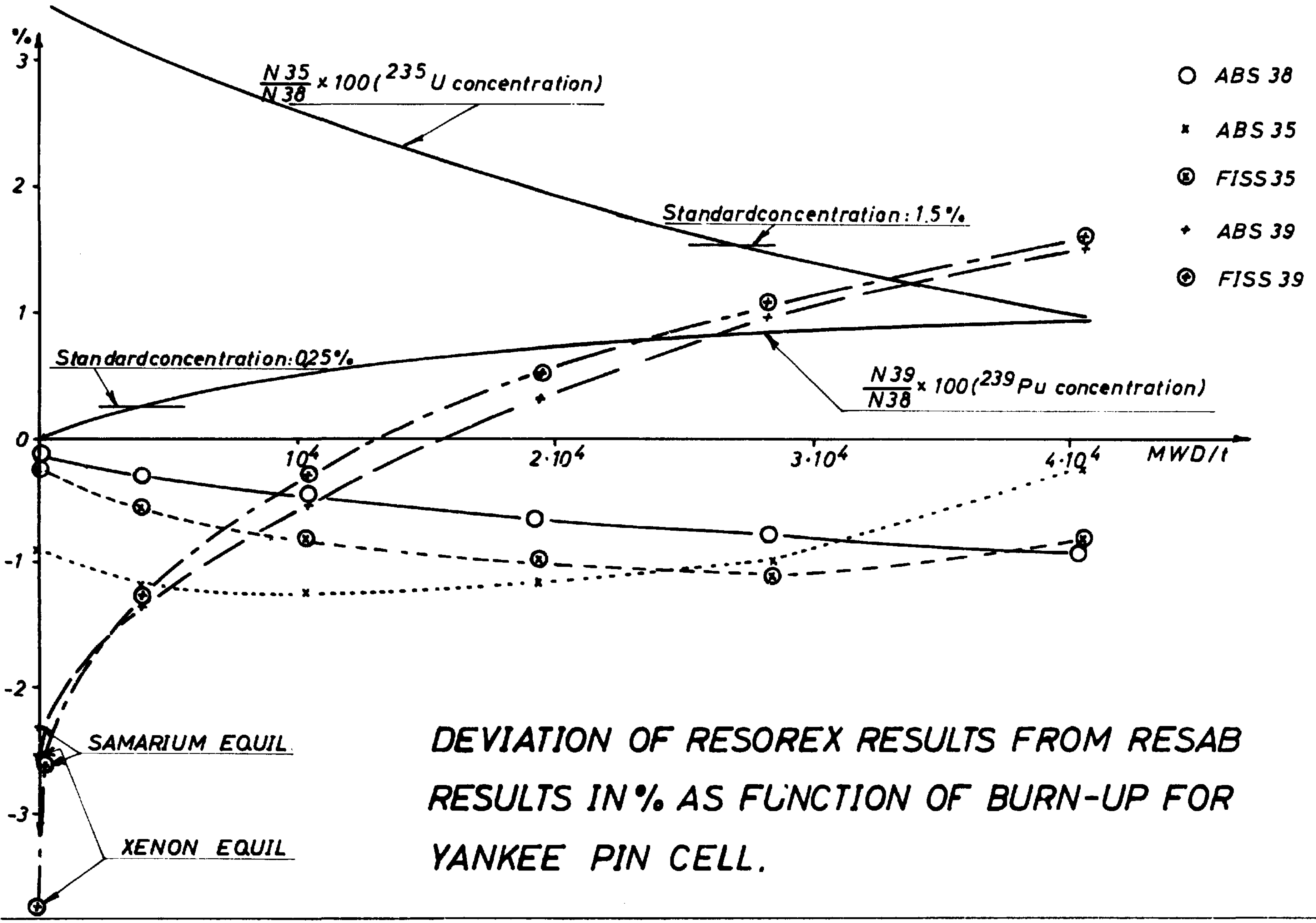
$$RI = \int \Phi_f(E)\,\sigma_a(E)\,dE \simeq \int \frac{\sigma_a(E)\,\left(a(1-\alpha) + (\Sigma_f^p - \Sigma_o)\,\bar{l}\right)}{\Sigma_a(E)\,\bar{l} + a(1-\alpha) + (\Sigma_f^p - \Sigma_o)\,\bar{l}} \; \frac{dE}{E}$$

$$= \int \frac{dE}{E} \; \frac{\sigma_a(E)}{1 + \dfrac{\sigma_a(E)}{\dfrac{S}{4N_{abs}\,V_f}\,a(1-\alpha) + \Sigma_f^p - \Sigma_o}} =$$

$$= RI_{WR}\left(\frac{S}{4N_{abs}\,V_f}\,a(1-\alpha)\right) \qquad \text{(AI. 20)}$$

It is seen that in the WR approximation the influence of cladding takes the form of a correction factor $(1-\alpha)$ on the effective NR scattering cross-section $S = \dfrac{S}{4N_{abs}\,V_f}\,a$.

As the main contribution to RI comes from the low-energy resonances in relation to which the cladding atoms of the most common cladding materials, stainless steel and zircaloy, may be considered as WR scatterers, the correction factor $(1-\alpha)$ may conveniently be used on the resonance integral of all the energy groups.



DEVIATION OF RESOREX RESULTS FROM RESAB RESULTS IN % AS FUNCTION OF BURN-UP FOR YANKEE PIN CELL.