

CALCULATION OF TEMPERATURE REACTIVITY COEFFICIENTS IN KRITZ-2 CRITICAL EXPERIMENTS USING WIMS

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ABSTRACT

The WIMS code is an extremely flexible package of deterministic and Monte Carlo methods which can be used to model any thermal reactor type. WIMS has been used to analyse the KRITZ-2 critical series of experiments, concentrating on the isothermal temperature coefficients, and the results of this study are used to assess the accuracy of approximations used at each stage of a reactor design calculation and also the quality of the nuclear data library.

It is shown that isothermal temperature coefficients calculated by the Monte Carlo approach employing a fine group library are well predicted for both UO₂ and MOX lattices; design route calculations employing a broad group nuclear data library, resonance shielding by equivalent dilution and a diffusion theory calculation gave values which were significantly more discrepant from experiment.

1. INTRODUCTION

Temperature reactivity coefficients are a major reactor safety parameter and it is clearly important that they are accurately predicted by codes employed in reactor analysis. The traditional method for performing core design calculations is to employ a two step approach:

Firstly, so-called lattice calculations are executed to generate cross sections averaged over each fuel assembly. These cross sections are tabulated against reactor operating conditions, known as dependencies, for example temperature, coolant density, dissolved boron etc. Secondly, a core calculation is performed, using a library of cross sections from the lattice code, in a coupled neutronics and thermal hydraulics calculation. Obviously, the accuracy of the prediction of temperature coefficients is heavily dependent on the accuracy of the lattice calculations. A large number of lattice calculations is required in order to build a library with suitable range of dependencies, so in order to obtain a rapid calculation, various approximations may be made, for example:

- Restriction to two dimensions.
- Use of a broad energy group cross section library.
- Further reduction of the number of energy groups by use of a spectrum condensation calculation.
- Representation of resonance shielding by equivalent dilution.
- Use of transport corrected cross sections.
- Use of pincell homogenised data (in diffusion or S_N calculations).

The WIMS code¹⁻² is an extremely flexible package of deterministic and Monte Carlo methods which can be used to model any thermal reactor type. WIMS has been used to analyse the KRITZ-2 series of experiments, and the results of this study may be used to assess the accuracy of approximations used in design calculations and the quality of the nuclear data library.

The features that are studied in this analysis are:

- Nuclear data derived from JEF2.2 in point and multi-group formats.
- Pu^{239} data derived from ENDF/B-VI.
- Flux solution by Monte Carlo or the method of characteristics.
- Resonance shielding treatment by equivalent dilution or by the subgroup method.
- Spectrum calculation by multicell collision probabilities.
- Transport corrected cross sections (P_0 or P_1 data).
- Diffusion theory calculations.

2. KRITZ-2 EXPERIMENTS

The KRITZ-2 series of experiments were performed by Studsvik in Nykoping, Sweden, in the early 1970s³⁻⁴. Each core comprised a lattice of light water moderated pins on a square pitch, surrounded by a light water reflector. The cores were controlled to criticality using a combination of water height and dissolved boron. The experiments analysed were performed at nominal temperatures of 20°C and 245°C. Three lattices were studied: Experiment 2:1, comprising 1.86% enrichment UO₂ pins on a 1.485 cm pitch; Experiment 2:13, comprising 1.86% enrichment UO₂ pins on a 1.635 cm pitch; Experiment 2:19, consisting of MOX rods containing 1.5% PuO₂ on a 1.8cm pitch. Axial buckling measurements at both hot and cold conditions and a core specification are available from the experimental campaign. As these are critical experiments the experimental value of k-effective can be taken to be unity and the isothermal temperature coefficient (ITC), defined as:

$$\frac{\Delta\left(\frac{1}{k}\right)}{\Delta T},$$

is zero for each experiment.

3. MODELLING METHODS

The KRITZ cores were calculated using Monte Carlo methods employing broad and fine group libraries (MONK in WIMS8 and the stand-alone code MONK8), characteristics transport theory (CACTUS in WIMS8), and diffusion theory (GOG in LWRWIMS).

The fine group nuclear data library was employed with MONK8, and broad group nuclear data libraries for the other codes. The standard fine group library for MONK8, known as DICE, is only available at present at a temperature of 293.16K. In order to analyse these experiments a special library at an elevated temperature was created. Among the temperatures for which $S(\alpha,\beta)$ data for H in H₂O are given in JEF2.2, the nearest to the 'hot' values used in the KRITZ experiments is 523.6 K. A DICE library at this temperature was generated for H (in H₂O), B¹⁰, B¹¹, O¹⁶, Zr, U²³⁴, U²³⁵, U²³⁸, Pu²³⁹, Pu²⁴⁰, Pu²⁴¹, Pu²⁴² and Am²⁴¹. The broad group calculations used the WIMS 1996 library¹. Although this library exists in different formats for WIMS8 and LWRWIMS the nuclear data is identical.

In the broad group calculations the resonance shielding was treated in two ways. The NOVICE subgroup method, where the subgroup weight is related to the probability of entering a particular subgroup, was used with MONK. The equivalence approach, based on adjusting the value of the background scatterer according to the problem geometry, was used in MONK, CACTUS and LWRWIMS calculations. The equivalence model used two pin types (core centre and core edge).

The equivalence theory calculations were performed with both P₀ and P₁ scattering data. The use of P₀ data with the subgroup method has not yet been implemented, so scattering in the subgroup method was

restricted to P_1 . The scattering treatment in DICE can be considered to be a close approximation to the JEF2.2 evaluated nuclear data, and is based on representing angular distributions using ranges of scattering angle cosine of equal probability.

The situations modelled by the fine group Monte Carlo methods differed slightly from the experimental specification, because the temperatures of the DICE libraries do not correspond exactly to the experimental values, and because the set of nuclides is restricted. The results were corrected for these effects by setting up two LWRWIMS calculations, one identical to the MONK model and the second a faithful representation of the experimental specification. A correction term was calculated, equal to the difference in k-effective between the two LWRWIMS calculations, and this was applied to the MONK8 k-effective value.

Calculations using the method of characteristics (CACTUS) for the flux calculation were executed in a condensed group structure. The model to generate the condensing flux was a multicell calculation employing the same geometry as the equivalence resonance treatment. The standard PWR condensing vector (8.0×10^5 , 9.1×10^3 , 4.0, 0.625, 0.14, 0.0eV) was used. It is not possible to condense the subgroup cross sections, so the condensed group calculations were restricted to equivalence theory. A method of modelling axial leakage has recently been included in CACTUS, but, since this has not been fully verified, the leakage was incorporated in a homogeneous calculation; the CACTUS flux solution is used to smear the problem, and then the homogeneous criticality problem is solved. The solution method is based on the B_N equations; both B_0 and B_1 were employed in this analysis.

A sufficiently large sample of neutrons was tracked to give a standard deviation of approximately 0.0002 in each case.

All of the calculations were performed in two dimensions, using the experimental axial bucklings to represent leakage in the third dimension. These calculations are sensitive to the moderator to fuel ratio, and so for accurate calculations thermal expansion effects must be considered. This effect was quantified by performing two sets of calculations at the elevated temperature. In the first set of calculations only the water was allowed to expand; in the second set, account was taken of thermal expansion of the whole lattice. The effect of the spacer wires, stated in Reference 3 to be small, was neglected.

The following set of calculations was executed:

- a. A fine group Monte Carlo model. This is taken to be the reference solution for the subsequent calculations .
- b. Using identical geometry, the Monte Carlo calculations were repeated using broad (172 and 69) group nuclear data libraries. The resonance shielding was modelled using the subgroup method, where the subgroup weight is related to the probability of entering a particular subgroup. These calculations employed P_1 scattering data.
- c. The Monte Carlo calculations in [b] were repeated using an equivalence theory approach to resonance shielding, based on adjusting the value of the background scatterer, according to the problem geometry. Shielded cross sections were derived for two pin types (core centre and core edge).
- d. The calculations in [c] were repeated using P_0 scattering data, employing the standard transport correction.
- e. Diffusion theory calculations were performed using the same cross section set as in [d].
- f. For cores 2:13 and 2:19, Monte Carlo calculations were run in the 6 group structure used in UK PWR design calculations. In the library group structure the data was identical to that used in [e]. This was then reduced to 6 groups using a condensing spectrum from a flux solution calculated by the method of multicell collision probabilities.
- g. A characteristics calculation (CACTUS) employing the same 6 group cross sections as in [f] was executed for core 2:19.
- h. The effect of using ENDF/B-VI Pu^{239} data in the analysis of core 2:19 was studied.

4. RESULTS

Hot and cold eigenvalues and difference in isothermal temperature coefficients (ITC) with respect to experiment are presented in Table I, Table II and Table III for cores 2:1, 2:13 and 2:19 respectively. The definition of isothermal temperature coefficient is

$$ITC = \frac{\frac{1}{k_{cold}} - \frac{1}{k_{hot}}}{T_{hot} - T_{cold}} \times 10^5.$$

The uncertainties (σ) quoted are the statistical uncertainties from the Monte Carlo calculations.

The cold k-effective values are well predicted by the best estimate calculation, i.e. fine group Monte Carlo. A small underprediction of around 300pcm is observed, this is consistent with other validation studies of JEF2.2⁵. The fine group Monte Carlo calculations give values of ITC which are slightly underpredicted with respect to experiment (0.3-1.0 pcm/ $^{\circ}\text{C}$) .

The cold k-effective values calculated by the broad group Monte Carlo calculations agree closely with the reference results for the UO₂ cores; a small overprediction of 300 pcm is noted for the MOX core. This gives confidence in the ability of broad group libraries to accurately predict water moderated UO₂ systems. The ITC for the broad group Monte Carlo calculations agree well with the reference for the UO₂ cores; there is some underprediction for MOX.

The difference between 172 group and 69 group calculations was negligible for the UO₂ cores and small for the MOX core. This confirms the AEAT design route recommendation that a 172 group library is required for MOX to represent the Pu thermal resonances.

Using P₀ rather than P₁ scattering has a significant effect on the eigenvalue, but a rather small effect on the ITC. The importance of employing P₁ scattering in the analysis of high leakage systems is emphasised.

A large change in ITC was noted when changing from subgroup to equivalence resonance shielding for UO₂ core 2:13; a corresponding change was not noted for the MOX core. A detailed reaction rate edit should be performed to investigate this further.

A significant change in k-effective was observed when the group structure was reduced from 69 to 6 groups. This indicates that a finer condensed group structure is required to accurately model this high leakage situation.

The ITC values generated from diffusion theory calculations are significantly more discrepant than the reference results. This indicates that a transport solution is required to accurately calculate the core reflector interface.

Employing Pu²³⁹ data derived from ENDF/B-VI, rather than JEF2.2 does not produce a change that is statistically significant.

The CACTUS results give similar trends to the MONK results, indicating that it is a similar treatment.

5. CONCLUSIONS

Analysis of the KRITZ-2 series of experiments employing a fine group Monte Carlo calculation gives good agreement with experiment on both the k-effective at ambient temperature and isothermal temperature coefficients. Similar results are obtained using broad group libraries in 172 and 69 groups, giving confidence in the use of these libraries for reactor analysis. Employing a diffusion calculation yields values of ITC which are significantly more discrepant. This emphasises the importance of using a transport calculation, e.g. the CACTUS module in WIMS, for situations like this with a large amount of leakage.

REFERENCES

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TABLES

Table I k-effective Values and Isothermal Temperature Coefficients for Core 2:1

				Cold		Hot (no expansion)				Hot (expansion)			
Method	Resonance shielding	Scattering	Groups	k-eff	σ	k-eff	σ	ITC (mN/°C)	σ	k-eff	σ	ITC (mN/°C)	σ
MONK8	DICE	-	13193	0.9965	0.0002					0.9942	0.0002	-1.02	0.12
MONK	Subgroup	P ₁	172	0.9966	0.0002	0.9926	0.0003	-1.77	0.16	0.9953	0.0003	-0.57	0.16
MONK	Subgroup	P ₁	69	0.9965	0.0002	0.9925	0.0002	-1.77	0.12	0.9947	0.0003	-0.80	0.16
MONK	Equivalence	P ₁	69	0.9959	0.0002	0.9903	0.0002	-2.49	0.12	0.9934	0.0002	-1.11	0.12
LWRWIMS GOG	Equivalence	P ₀	69	0.9936		0.9887		-2.18		0.9887		-2.18	

Table II k-effective Values and Isothermal Temperature Coefficients for Core 2:13

				Cold		Hot (no expansion)				Hot (expansion)			
Method	Resonance shielding	Scattering	Groups	k-eff	σ	k-eff	σ	ITC (mN/°C)	σ	k-eff	σ	ITC (mN/°C)	σ
MONK8	DICE	-	13193	0.9970	0.0002					0.9964	0.0002	-0.27	0.13
MONK	Subgroup	P ₁	172	0.9978	0.0002	0.9969	0.0002	-0.41	0.13	0.9975	0.0002	-0.14	0.13
MONK	Subgroup	P ₁	69	0.9979	0.0002	0.9963	0.0002	-0.73	0.13	0.9976	0.0002	-0.14	0.13
MONK	Subgroup	P ₁	69	0.9969	0.0002	0.9954	0.0002	-0.68	0.13	0.9964	0.0002	-0.23	0.13
MONK	Equivalence	P ₁	69	1.0006	0.0002	1.0002	0.0002	-0.18	0.13	0.9944	0.0002	-2.82	0.13
MONK	Equivalence	P ₀	69	0.9966	0.0002	0.9964	0.0002	-0.09	0.13	0.9906	0.0002	-2.75	0.13
MONK	Equivalence	P ₁	6	1.0041	0.0002	1.0014	0.0002	-1.22	0.13	0.9993	0.0002	-2.17	0.13
MONK	Equivalence	P ₀	6	0.9950	0.0002	0.9908	0.0002	-1.93	0.13	0.9890	0.0002	-2.76	0.13
LWRWIMS	Equivalence	P ₀	69	0.9970						0.9929		-1.88	

Table III k-effective Values and Isothermal Temperature Coefficients for Core 2:19

Method	Resonance shielding	Scattering	Groups	Cold		Hot (no expansion)				Hot (expansion)			
				k-eff	σ	k-eff	σ	ITC (mN/°C)	σ	k-eff	σ	ITC (mN/°C)	σ
MONK8	DICE	-	13193	0.9964	0.0002					0.9942	0.0002	-1.03	0.13
MONK	Subgroup	P ₁	172	0.9996	0.0003	0.9958	0.0003	-1.78	0.20	0.9967	0.0003	-1.36	0.20
MONK	Subgroup	P ₁	69	0.9997	0.0003	0.9954	0.0003	-2.01	0.20	0.9956	0.0003	-1.92	0.20
MONK ¹	Subgroup	P ₁	69	1.0005	0.0003					0.9965	0.0003	-1.87	0.20
MONK	Equivalence	P ₁	69	0.9984	0.0003	0.9934	0.0003	-2.35	0.20	0.9938	0.0003	-2.16	0.20
MONK	Equivalence	P ₀	69	0.9912	0.0003					0.9875	0.0003	-1.76	0.20
MONK	Equivalence	P ₁	6	1.0071	0.0003	1.0007	0.0002			1.0001	0.0003	-3.24	0.20
MONK	Equivalence	P ₀	6	0.9943	0.0002	0.9873	0.0002	-3.32	0.13	0.9878	0.0002	-3.08	0.13
LWRWIMS	Equivalence	P ₀	69	1.0009						0.9924		-3.98	
CACTUS	Equivalence	P ₁	6	0.9949		0.9888		-2.89		0.9884		-3.08	
CACTUS	Equivalence	P ₀	6	0.9904		0.9858		-2.19		0.9854		-2.39	

1. Pu²³⁹ data from ENDF/B-VI